

# Outlines of Quantum Physics

- 1 Wave-Particle Duality
- 2 The Schrödinger Equation
- 3 The Hydrogen Atom
- 4 Theorems of Quantum Mechanics
  - Hermitian Operator
  - Properties of Hermitian Operator
  - The Postulates of Quantum Mechanics
  - Commutator and Uncertainty Principle
  - Representation
  - Electron Spin
  - Exchange of Identical Particles
  - Two-State System

# 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 $\hat{O}^\dagger$

## ④ 厄米算符: $\hat{O}^\dagger = \hat{O}$

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## • Linear Operator

$$\forall \Psi_1, \Psi_2, \forall c_1, c_2 \in \mathbb{C}$$

$$\text{if } \hat{O}(c_1\Psi_1 + c_2\Psi_2) =$$

$$c_1\hat{O}\Psi_1 + c_2\hat{O}\Psi_2$$

then, Linear Operator  $\hat{O}$

## • 例: $\hat{p} = -i\hbar\nabla, \int dx, \Delta, \dots$

## • 量子力学中所有刻画力学量的算符都应该是线性算符。

← 满足态叠加原理的要求

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## • 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 $\forall \psi, \varphi$

$$(\psi, \hat{A}\varphi) = (\psi, \hat{B}\varphi),$$

$$\text{then } \hat{A} = \hat{B}$$

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•  $\hat{O}^+ = \tilde{O}^*$ :

$$\forall \psi, \varphi$$

$$(\psi, \hat{O}^+\varphi) = (\hat{O}\psi, \varphi)$$

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- Hermitian Operator, if  $\forall \psi, \varphi$   
 $(\psi, \hat{O}\varphi) = (\hat{O}\psi, \varphi)$ ,  
 $\hat{O}$  is Hermitian.

# 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

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# 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)。

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- 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  $x \rightarrow \hat{x}$ ,  $p_x \rightarrow -i\hbar \frac{\partial}{\partial x}$  对应产生)
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可构造  $\{\varphi_m\}$ ；  $\hat{F}\varphi_m = f_m\varphi_m$ ；  $(\varphi_m, \varphi_n) = \delta_{mn}$ ；  
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“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

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- 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  $\Psi$  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

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# 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:  $\{|k\rangle\}$ ,
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# 对易式 Commutator

$$\begin{aligned}
 [A, B] &\equiv AB - BA & [A, A] &= 0 & [A, \text{const}] &= 0 \\
 [A, B] &= -[B, A] \\
 [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}
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# 例子, 基本对易关系

$$[x, p_x] = i\hbar;$$

$$[x, p_y] = 0;$$

$$[x, y] = 0$$

$$[L_x, y] = i\hbar z;$$

$$[L_x, z] = -i\hbar y;$$

$$[L_x, x] = 0$$

$$[L_x, p_y] = i\hbar p_z;$$

$$[L_x, p_z] = -i\hbar p_y;$$

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$$[L_x, L_y] = i\hbar L_z;$$

$$[L_x, L_z] = -i\hbar L_y;$$

$$[x_\alpha, p_\beta] = i\hbar \delta_{\alpha\beta}$$

$$[L_\alpha, x_\beta] = \sum_\gamma \epsilon_{\alpha\beta\gamma} i\hbar x_\gamma$$

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$$[L_\alpha, L_\beta] = \sum_\gamma \epsilon_{\alpha\beta\gamma} i\hbar L_\gamma$$

$$[L^2, L_\alpha] = 0$$

$$L_\pm = L_x \pm iL_y$$

$$[L_z, L_\pm] = \pm \hbar L_\pm$$



# 对易子与测不准关系

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

⇒ 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。

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

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）。

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# 共同本征态

若  $[\hat{A}, \hat{B}] = 0$ ,  
 则**存在**完备函数集  $\{\varphi_i\}$ ,  
 $\varphi_i$  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  $[\hat{A}, \hat{B}] = 0$ ,  $\hat{A}|\lambda\rangle = a_\lambda|\lambda\rangle$ ,  $\hat{A}|j\rangle = a_j|j\rangle$ ,  $a_\lambda \neq a_j$   
 then  $\langle \lambda | \hat{B} | j \rangle = 0$

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# 谐振子的代数解法, $a, a^+$ 算符

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

$$[x, p] = i$$

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

$$[a, a^+] = 1,$$

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

$$N = a^+ a$$

$$N|n\rangle = n|n\rangle,$$

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

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

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

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# 角动量的定义

## 定义

如果算符  $\hat{J}$  满足:

$$[J_x, J_y] = i\hbar J_z$$

$$[J_y, J_z] = i\hbar J_x$$

$$[J_z, J_x] = i\hbar J_y$$

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：

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$$[J_z, J_x] = i\hbar J_y$$

$$[J^2, J_\alpha] = 0$$

$$J_\pm = J_x \pm iJ_y$$

$$[J_z, J_\pm] = \pm\hbar J_\pm$$

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

$$J_+ J_- - J_- J_+ = 2\hbar J_z$$

$$J_+ J_- + J_- J_+ = 2(J^2 - J_z^2)$$

仅由这些对易关系可证明：

证明

$$J^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle$$

$$J_z |jm\rangle = m\hbar |jm\rangle$$

$$J_\pm |jm\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)} |jm \pm 1\rangle$$

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$$

$$m = -j, -j+1, \dots, j-1, j$$

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# 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)

$$|\psi\rangle = \sum_k |k\rangle \langle k|\psi\rangle$$

$$= \sum_k c_k |k\rangle$$

$$c_k = \langle k|\psi\rangle$$

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



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一个波函数与一个列向量  
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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。  
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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,

$$\hat{F}|\psi\rangle = |\phi\rangle$$

$$|\psi\rangle = \sum_k a_k |k\rangle$$

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$$\sum_k b_k |k\rangle = \hat{F} \sum_k a_k |k\rangle = \sum_k a_k \hat{F}|k\rangle$$

$$\Rightarrow \forall m,$$

$$\langle m | \sum_k b_k |k\rangle = \langle m | \sum_k a_k \hat{F}|k\rangle$$

$$\because \langle m | k \rangle = \delta_{mk}$$

$$\therefore b_m = \sum_k a_k \langle m | \hat{F} | k \rangle = \sum_k F_{mk} a_k$$

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

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# 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  $\{|jm\rangle\}$  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:

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

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

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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？

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 $F_{mn} = \langle m|F|n\rangle$ ;  $|\Psi\rangle = \sum_k a_k |k\rangle$
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# 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 \\
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 &= -\mu_B\vec{L}/\hbar \\
 \mu_{\ell z} &= -m_\ell\mu_B
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玻尔磁子 Bohr magneton

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

Magnet in a  $B$  field:

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# Magnetic Moment of a Circulating Flow of Charge

$$\vec{\mu}_\ell = I\vec{A}$$

$$I = -e/T = -e\omega/2\pi$$

$$\vec{\mu}_\ell = -e\vec{r} \times \vec{v}/2$$

$$= -\frac{e}{2m_e}\vec{L}$$

$$= -\mu_B\vec{L}/\hbar$$

$$\mu_{\ell z} = -m_\ell\mu_B$$

## 玻尔磁子 Bohr magneton

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

## Magnet in a $B$ field:

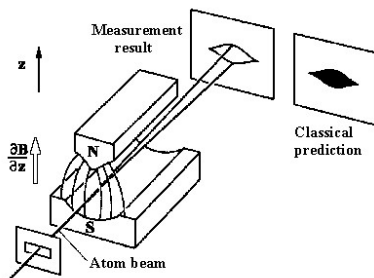
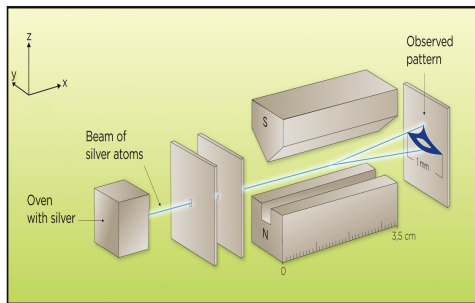
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# Stern-Gerlach experiment



1922, Otto Stern<sub>NP1943</sub> (1888-1969) & Walther Gerlach (1889-1979), University of Frankfurt



$$\vec{F} = -\nabla U = -\nabla(-\vec{\mu} \cdot \vec{B}),$$

$$F_z = \mu_z \frac{\partial B_z}{\partial z}$$



# Electron Spin

## Hypothesis of Electron Spin

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- 1928 P.A.M.Dirac: Electron has a spin in relativistic Quantum Mechanics.
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## Magnetic moment of electron spin

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

$$g_s \approx 2.0023... \quad (\text{Note. } g_l = 1)$$

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

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# Exchange of Identical Particles



Identical Particles: must be indistinguishable!

Non-classical, Absolutely Quantum!

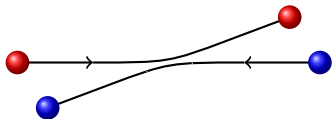
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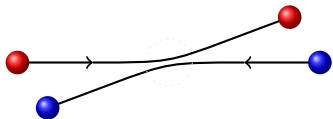
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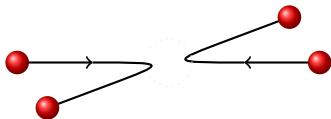
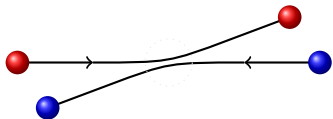
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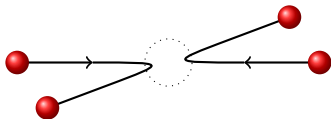
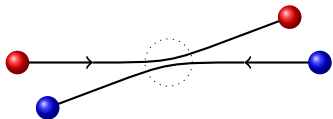
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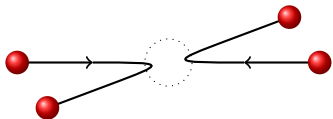
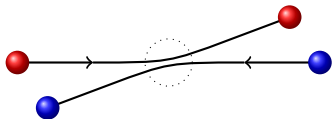
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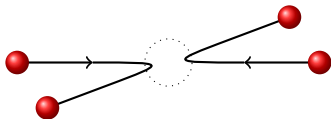
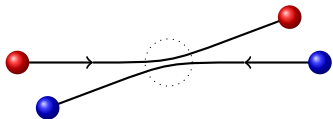
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## Ground State of Helium

- spacial function:  $1s(1)1s(2)$   
 $\mathbf{P}_{12}[1s(1)1s(2)] = [1s(1)1s(2)]$ , symmetric
- spin function:  $\alpha(1)\alpha(2)$ ,  $\alpha(1)\beta(2)$ ,  $\beta(1)\alpha(2)$ ,  $\beta(1)\beta(2)$   
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- 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  $\Psi$  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  $\Psi$  must be anti-symmetric:

- $(1s2s)^3 S_1$ , spacial: anti-symmetric & spin: symmetric:

$$\psi(1,2)_1 = [1s(1)2s(2) - 2s(1)1s(2)]\alpha(1)\alpha(2)/\sqrt{2}$$

$$\psi(1,2)_2 = [1s(1)2s(2) - 2s(1)1s(2)]\beta(1)\beta(2)/\sqrt{2}$$

$$\psi(1,2)_3 = [1s(1)2s(2) - 2s(1)1s(2)][\alpha(1)\beta(2) + \beta(1)\alpha(2)]/2$$

- $(1s2s)^1 S_0$ , spacial: symmetric & spin: anti-symmetric:

$$\psi(1,2)_4 = [1s(1)2s(2) + 2s(1)1s(2)][\alpha(1)\beta(2) - \beta(1)\alpha(2)]/2$$

$$E(^3S_1) < E(^1S_0)$$

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# Ground State of Atomic Lithium, Pauli Exclusion Principle

## Ground State of The Lithium Atom

- Spatial: could it be possible to have 3 electrons all in  $1s$ ?  
 $[1s(1)1s(2)1s(3)]$

$$P_{ij}[1s(1)1s(2)1s(3)] = [1s(1)1s(2)1s(3)], \text{ symmetric}$$

- Spin:  $\alpha(1)\alpha(2)\alpha(3)$ ,  $\alpha(1)\beta(2)\alpha(3)$ ,  $\dots$

Make it symmetric or anti-symmetric for  $P_{12}$ ,  $P_{13}$  &  $P_{23}$

Symmetric:

- ①  $\alpha\alpha\alpha$
- ②  $\beta\beta\beta$
- ③  $[\alpha\alpha\beta + \alpha\beta\alpha + \beta\alpha\alpha]/\sqrt{3}$
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Anti-symmetric: none

- Impossible to construct an anti-symmetric  $\Psi$ !

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# Wavefunction of a system consisted of identical particles

Total wavefunction 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

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

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(q_1) & \phi_1(q_2) & \cdots & \phi_1(q_N) \\ \phi_2(q_1) & \phi_2(q_2) & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \phi_N(q_1) & \phi_N(q_2) & \cdots & \phi_N(q_N) \end{vmatrix}$$

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# 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  $\Delta \gg h'$ :

$$E \doteq \varepsilon \mp \Delta \left(1 + \frac{1}{2} \frac{h'^2}{\Delta^2}\right)$$

$$E_I \doteq \varepsilon_1 + \frac{h'^2}{2\Delta}$$

$$E_{II} \doteq \varepsilon_2 - \frac{h'^2}{2\Delta}$$

- If  $\Delta \ll h'$ :

$$E \doteq \varepsilon \pm h' \left(1 + \frac{1}{2} \frac{\Delta^2}{h'^2}\right)$$

$$E_I \doteq \varepsilon + h' + \frac{\Delta^2}{2h'}$$

$$E_{II} \doteq \varepsilon - h' - \frac{\Delta^2}{2h'}$$

“Avoid Crossing”



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“Avoid Crossing”





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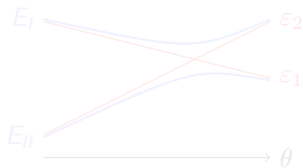
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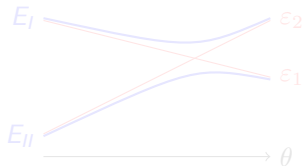
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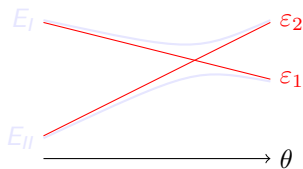
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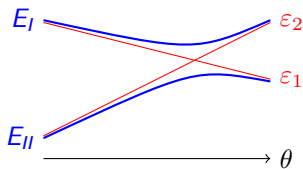
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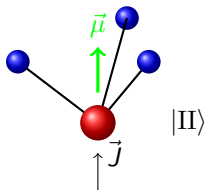
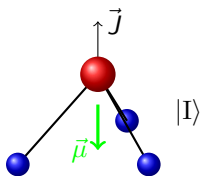
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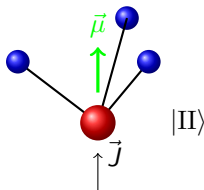
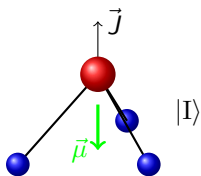
# Double States of the Ammonia Molecule\*



- Base states:  $|I\rangle$  &  $|II\rangle$
- Hamiltonian:  $\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$
- Eigenvalues and eigenfunctions:
  - $E_1 = E_0 - A$
  - $E_2 = E_0 + A$
  - $|1\rangle = \frac{1}{\sqrt{2}}(|I\rangle - |II\rangle)$
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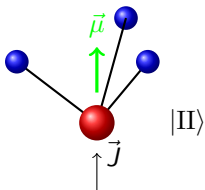
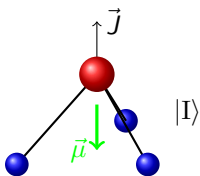
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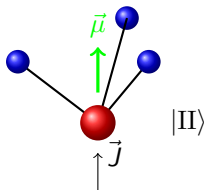
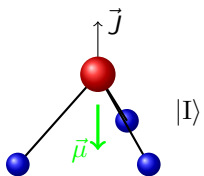
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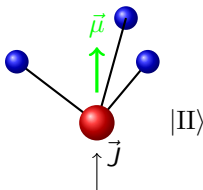
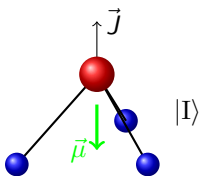
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# Ammonia molecule in a static electric field\*

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

- Hamiltonian (using bases  $|I\rangle$  &  $|\text{II}\rangle$ ):

$$H_{\mathcal{E}} = \begin{pmatrix} E_0 - \mu\mathcal{E} & -A \\ -A & E_0 + \mu\mathcal{E} \end{pmatrix}$$

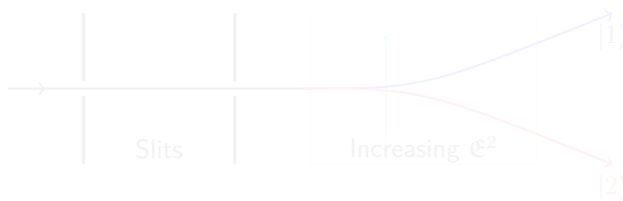
- $E_1 = E_0 - \sqrt{A^2 + \mu^2\mathcal{E}^2}$ ,  $E_2 = E_0 + \sqrt{A^2 + \mu^2\mathcal{E}^2}$

- If the applied field is weak,

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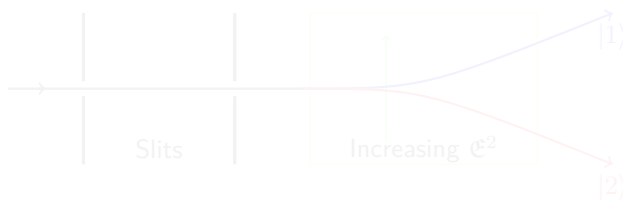
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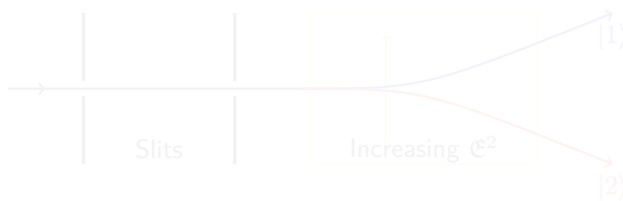
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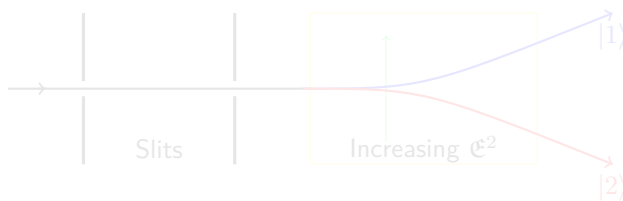
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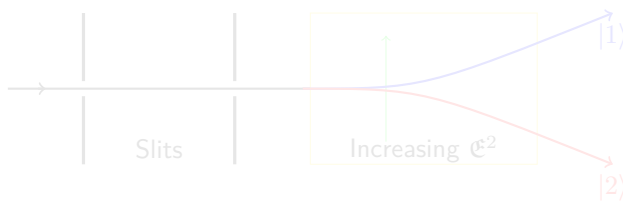
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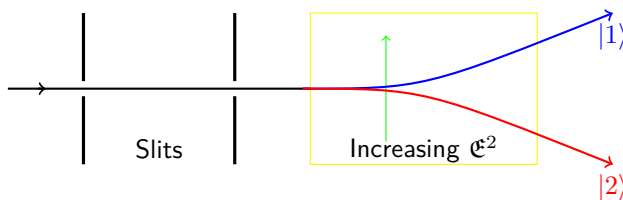
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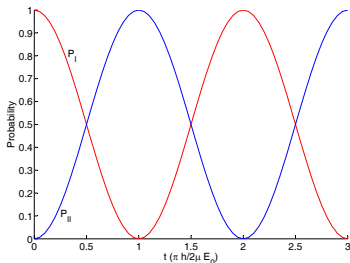
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# If $\hat{F}$ is Hermitian, then $\forall \Psi, \bar{F} \in \mathbb{R}$

Hermitian 算符在任意一个态上的平均值都是实数

 $\forall \Psi$ 

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

 $\implies$ 

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右 =  $(\hat{F}\phi_1, \phi_1) + |c|^2(\hat{F}\phi_2, \phi_2) +$   
 $c(\hat{F}\phi_1, \phi_2) + c^*(\hat{F}\phi_2, \phi_1)$
- $c[(\phi_1, \hat{F}\phi_2) - (\hat{F}\phi_1, \phi_2)] =$   
 $-c^*[(\phi_2, \hat{F}\phi_1) - (\hat{F}\phi_2, \phi_1)]$
- $(\phi_1, \hat{F}\phi_2) - (\hat{F}\phi_1, \phi_2) =$   
 $-(\phi_2, \hat{F}\phi_1) + (\hat{F}\phi_2, \phi_1)$
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- 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;
- $(\phi_1, \hat{F}\phi_1) = (\hat{F}\phi_1, \phi_1);$   
 $(\phi_2, \hat{F}\phi_2) = (\hat{F}\phi_2, \phi_2)$
- $\therefore c$  任意, 取  $c = 1,$
- 取  $c = i$

Back

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 =  $(\phi_1, \hat{F}\phi_1) + |c|^2(\phi_2, \hat{F}\phi_2) + c(\phi_1, \hat{F}\phi_2) + c^*(\phi_2, \hat{F}\phi_1)$   
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# Eigenvalues and Eigenfunctions of Hermitian Operators

## 厄米算符的本征值是实数

$$\hat{F}\phi_m = f_m\phi_m, \hat{F} \text{ is Hermitian,}$$

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

## 厄米算符的属于不同本征值的本征函数正交

- $(\phi_n, \hat{F}\phi_m) = (\phi_n, f_m\phi_m) = f_m(\phi_n, \phi_m)$
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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  $[\hat{A}, \hat{B}] = i\hat{C}$ ,  
 $\hat{C}^\dagger = \hat{C}$
- ②  $\forall \Psi, \sqrt{\overline{A^2} \cdot \overline{B^2}} \geq \frac{1}{2} |\overline{C}|$
- ③  $\Delta A = \hat{A} - \bar{A}$ ,  $\Delta B = \hat{B} - \bar{B}$ ,  
 $\sqrt{\overline{\Delta A^2} \cdot \overline{\Delta B^2}} \geq \frac{1}{2} |\overline{C}|$

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

$$\begin{aligned} & ([\hat{A}, \hat{B}])^+ \\ &= (\hat{A}\hat{B} - \hat{B}\hat{A})^+ \\ &= \hat{B}^+ \hat{A}^+ - \hat{A}^+ \hat{B}^+ \\ &= \hat{B}\hat{A} - \hat{A}\hat{B} \\ &= [\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}] \end{aligned}$$

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$\Delta A$ ,  $\Delta B$  are also Hermitian;  
 $[\Delta A, \Delta B] = [\hat{A}, \hat{B}]$   
 前面结论适用!

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

$$I(\xi) = (\xi \hat{A}\Psi + i\hat{B}\Psi, \xi \hat{A}\Psi + i\hat{B}\Psi)$$

$$\forall \xi \in \mathbb{R}, I(\xi) \geq 0$$

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

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

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# 谐振子的因式分解解法

Factorization 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:  $\forall \psi, \bar{N} \geq 0$   
 设  $\{|\alpha\rangle\}$ ,  $N|\alpha\rangle = \alpha|\alpha\rangle$
- 可证:  
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## 无量纲化

- $\begin{cases} a = (x + ip)/\sqrt{2} \\ a^+ = (x - ip)/\sqrt{2} \end{cases}$   
 $\Leftrightarrow \begin{cases} x = (a^+ + a)/\sqrt{2} \\ p = i(a^+ - a)/\sqrt{2} \end{cases}$
- $[x, p] = i \Rightarrow [a, a^+] = 1$
- $H = \{(a^+ + a)^2 - (a^+ - a)^2\}/4$   
 $= \{a^+ a + a a^+ + a^+ a + a a^+\}/4$   
 $= a^+ a + \frac{1}{2}$

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$$\begin{aligned}\bar{N} &= \langle \psi | N | \psi \rangle \\ &= \langle \psi | a^+ a | \psi \rangle \\ &= \langle a \psi | a \psi \rangle \\ &\geq 0\end{aligned}$$

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$$\begin{aligned}
 [N, a] &= [a^+ a, a] = -a \\
 [N, a^+] &= a^+ \\
 [N, a]|\alpha\rangle &= N a|\alpha\rangle - a N|\alpha\rangle \\
 &= N a|\alpha\rangle - \alpha a|\alpha\rangle \\
 &= -a|\alpha\rangle \\
 N a|\alpha\rangle &= (\alpha - 1)a|\alpha\rangle \\
 [N, a^+]|\alpha\rangle &= N a^+|\alpha\rangle - a^+ N|\alpha\rangle \\
 &= N a^+|\alpha\rangle - \alpha a^+|\alpha\rangle \\
 &= a^+|\alpha\rangle \\
 N a^+|\alpha\rangle &= (\alpha + 1)a^+|\alpha\rangle
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## 角动量本征值的代数解法 \*

## Eigenvalues of an Angular Momentum Operator

- $J^2|\lambda m\rangle = \lambda|\lambda m\rangle, \quad J_z|\lambda m\rangle = m|\lambda m\rangle, \quad (\hbar = 1)$
- If  $\lambda' \neq \lambda, \langle \lambda' m' | J_\alpha | \lambda m \rangle = 0 \quad \alpha = x, y, z, \pm$  proof
- $J_\pm(J_\pm|\lambda m\rangle) = (m \pm 1)(J_\pm|\lambda m\rangle),$  "Ladder Operators" proof
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- $\exists \bar{m}, \underline{m}, \quad J_+|\bar{m}\rangle = 0, \quad J_-|\underline{m}\rangle = 0$
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- $\bar{m} = j, \quad \lambda = j(j+1), \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$

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- $J^2 - J_z^2 = J_x^2 + J_y^2, \quad \langle \psi | A^2 | \psi \rangle \geq 0$  proof
- $\exists \bar{m}, \underline{m}, \quad J_+|\bar{m}\rangle = 0, \quad J_-|\underline{m}\rangle = 0$
- $\underline{m} = \bar{m} - n, \quad \underline{m} = -\bar{m}$  proof
- $\bar{m} = j, \quad \lambda = j(j+1), \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$

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## 角动量本征值的代数解法 \*

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

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

在  $\{|\lambda m\rangle\}$  表象中, 所有  $J_\alpha$  的表示 (矩阵), 对  $\lambda$  都是“块”对角化的。

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# 角动量本征值的代数解法 \*

## Ladder Operators

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

$$\because [J_z, J_{\pm}] = \pm J_{\pm} \quad (\hbar = 1)$$

$$\therefore [J_z, J_{\pm}] |\lambda m\rangle = \pm J_{\pm} |\lambda m\rangle$$

$$\Rightarrow (J_z J_{\pm} - J_{\pm} J_z) |\lambda m\rangle = \pm J_{\pm} |\lambda m\rangle$$

$$\Rightarrow J_z J_{\pm} |\lambda m\rangle - m J_{\pm} |\lambda m\rangle = \pm J_{\pm} |\lambda m\rangle$$

$$\Rightarrow J_z (J_{\pm} |\lambda m\rangle) = (m \pm 1) (J_{\pm} |\lambda m\rangle).$$

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## 角动量本征值的代数解法 \*

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

$$[J^2, J_{\pm}] = 0 \Rightarrow J^2 J_{\pm}^k = J_{\pm}^k J^2$$

$$\Rightarrow J^2 J_{\pm}^k |\lambda m\rangle = \lambda J_{\pm}^k |\lambda m\rangle$$

$$J_z J_{\pm} |\lambda m\rangle = (m \pm 1) J_{\pm} |\lambda m\rangle \Rightarrow J_z J_{\pm}^k |\lambda m\rangle = (m \pm k) J_{\pm}^k |\lambda m\rangle$$

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

$$J^2 |m \pm k\rangle = \lambda |m \pm k\rangle$$

$$J_z |m \pm k\rangle = (m \pm k) |m \pm k\rangle$$

$$J_z^2 |m \pm k\rangle = (m \pm k)^2 |m \pm k\rangle$$

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

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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 \*

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

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

$$J_- |\underline{m}\rangle = 0$$

$$J_+ J_- |\underline{m}\rangle = (\lambda - \underline{m}^2 + \underline{m}) |\underline{m}\rangle = 0$$

$$\Rightarrow \lambda = \underline{m}^2 - \underline{m}$$

$$J_+ |\bar{m}\rangle = 0$$

$$J_- J_+ |\bar{m}\rangle = (\lambda - \bar{m}^2 - \bar{m}) |\bar{m}\rangle = 0$$

$$\Rightarrow \lambda = \bar{m}^2 + \bar{m}$$

$$\Rightarrow \underline{m}^2 - \underline{m} = \bar{m}^2 + \bar{m}$$

$$\Rightarrow (\underline{m} + \bar{m})(\bar{m} - \underline{m} + 1) = 0$$

$$\therefore \bar{m} > \underline{m}$$

$$\therefore \underline{m} = -\bar{m}$$

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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