$|nlm\rangle$, $E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2}$. 简并度 $2n^2$

① 精细结构 (fine structure)

i) 相对论修正

$$T=\frac{p^2}{2m} \Longrightarrow T=\sqrt{p^2c^2+m^2c^4}-mc^2 \approx \frac{p^2}{2m}-\frac{p^4}{8m^3c^2}$$

对束缚态电子 $(p \ll mc)$

用 $\{\hat{l}^2, \hat{l}_z\}$ 来对角 $\hat{H}_0$, $\hat{V}$.

因为 $[\hat{p}^4, \hat{l}^2]=0$ $[\hat{p}^4, \hat{l}_z]=0 \Longrightarrow |n,l,m\rangle$

$$E_r = \langle nlm| -\frac{\hat{p}^4}{8m^3c^2}|nlm\rangle$$

$$= -\frac{E_n^2}{2mc^2}\left(\frac{4n}{l+\frac{1}{2}}-3\right) \quad \text{(相对论一阶修正)}$$

而 $\frac{E_n}{2mc^2} \sim 10^{-5}$.

因此 $E_r \sim 10^{-5} E_n$.

ii) 自旋-轨道耦合.

$$\hat{H}_{so} = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2}\frac{1}{c^2r^3}\hat{S}\cdot\hat{L}$$

$[\hat{H}_{so}, \hat{L}^2] = [\hat{H}_{so}, \hat{S}^2]=0$

但 $[\hat{H}_{so}, \hat{l}_z] \neq 0$, $[\hat{H}_{so}, \hat{S}_z] \neq 0$.

而 $\hat{J} = \hat{L}+\hat{S}$

$[\hat{H}_{so}, \hat{J}^2]=0$ $[\hat{H}_{so}, \hat{J}_z]=0$

$\Rightarrow$ 选择 $\{|nlsjm_j\rangle\}$ 耦合表象

$$E_{so} = \frac{E_n^2}{mc^2}\left\{\frac{n[j(j+1)-l(l+1)-\frac{3}{4}]}{l(l+\frac{1}{2})(l+1)}\right\}$$

精细结构

$$E_{nj} = E_n + \frac{E_n^2}{2mc^2}\left(3-\frac{4n}{j+\frac{1}{2}}\right)$$

$$= -13.6\,eV \times \left[1+\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\right]$$ 其中 $\alpha = \frac{e^2}{4\pi\varepsilon\hbar c} \sim \frac{1}{137}$

② Zeeman 效应.

③ 超精细结构

核自旋与电子轨道/自旋的相互作用

$$\hat{H}_{hf} = \bar{A}\frac{1}{r^3}\left[3(\hat{\vec{I}}\cdot\vec{e}_r)(\hat{\vec{S}}\cdot\vec{e}_r)-\hat{\vec{I}}\cdot\hat{\vec{S}}\right]+\frac{8\pi}{3}\bar{A}\hat{\vec{I}}\cdot\hat{\vec{S}}\delta(\vec{r})$$
$$+B(r)\hat{\vec{I}}\cdot\hat{\vec{L}}$$

$$\sim \boxed{\ }\ \hat{\vec{I}}\cdot\hat{\vec{J}}$$

$$\hat{\vec{F}} = \hat{\vec{I}}+\hat{\vec{J}} = \hat{\vec{I}}+\hat{\vec{L}}+\hat{\vec{S}} \quad |F, m_F\rangle$$

$$l=0 \quad \hat{H}_{hf} = A\hat{\vec{I}}\cdot\hat{\vec{S}}$$

$$[\hat{F}_z, \hat{H}_{hf}] = [\hat{F}^2, \hat{H}_{hf}] = 0 \Rightarrow |n\,l\,s\,j\,I\,F\,m_F\rangle$$

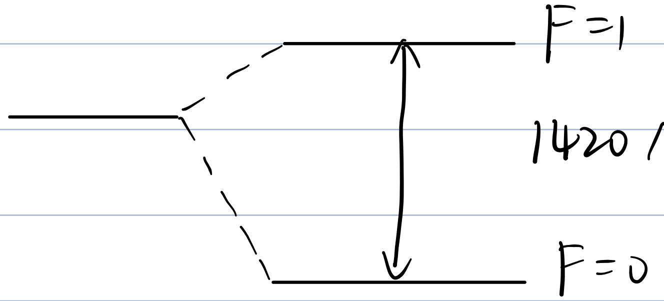
如 $l=0,\ S=\frac{1}{2}\quad I=\frac{1}{2}$

$\Rightarrow J=\frac{1}{2},\ I=\frac{1}{2}. \Rightarrow F=0, 1.$

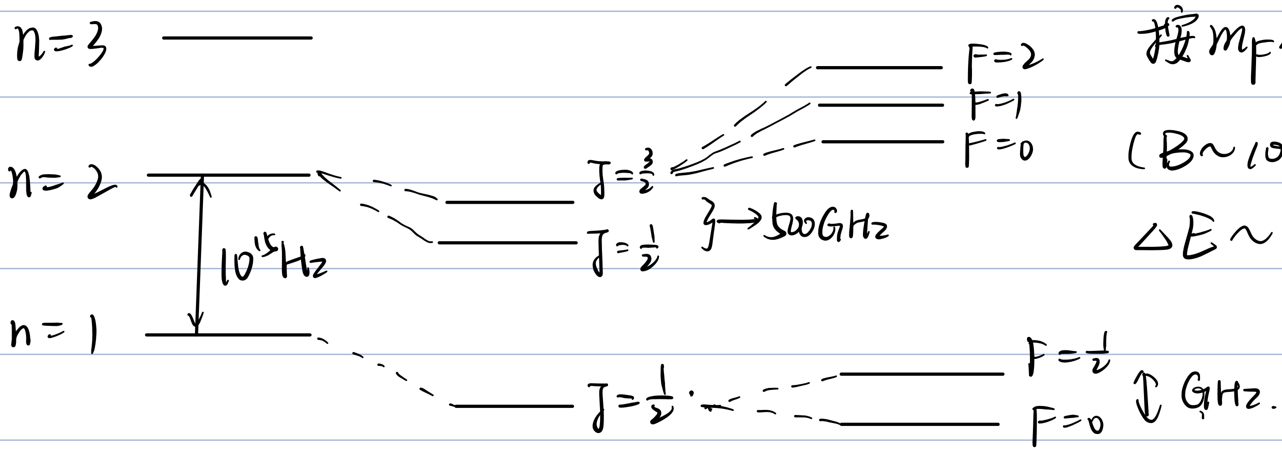
$F=0.\ m_F=0 \qquad F=1.\ m_F=-1, 0, 1.$

$$E_{hf}^{(1)} = \langle F\,m_F|A\hat{\vec{I}}\cdot\hat{\vec{S}}|F\,m_F\rangle$$
$$= \langle F\,m_F|\frac{1}{2}A[F(F+1)-I(I+1)-S(S+1)]\hbar^2|F\,m_F\rangle$$
$$= A\hbar^2\begin{cases}\frac{1}{4}, & 三重态, F=1\\ -\frac{3}{4}, & 单态\quad F=0\end{cases}$$

氢原子基态



总体图像 以Na原子为例



加 $\vec{B}$ 之后

按 m_F 分裂.

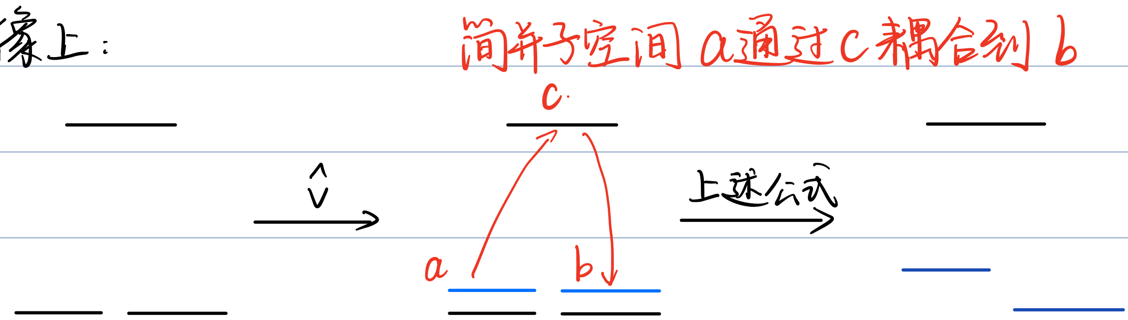
(B~100 G)

ΔE~100MHz.

注：如 $\hat{V}$ 不能消除简并，则需联立入的一次项与二次项，(不考)

得到：
$$\sum_{\mu}\left[\sum_{n\neq m}\frac{V_{m\nu,n}V_{n,m\mu}}{E_m^{(0)}-E_n^{(0)}}-E_m^{(2)}\delta_{\mu,\nu}\right]C_{m\mu}^{(0)}=0$$

图像上：



eg:
$$\left(\begin{array}{cc|c} E_1 & 0 & a\\ 0 & E_1 & b\\ \hline a^* & b^* & E_2\end{array}\right)\xrightarrow{\text{代上述公式}}\begin{pmatrix}\dfrac{|a|^2}{E_1-E_2} & \dfrac{ab^*}{E_1-E_2}\\[2ex] \dfrac{a^*b}{E_1-E_2} & \dfrac{|b|^2}{E_1-E_2}\end{pmatrix}$$

例：自旋 $\frac{1}{2}$ 的三维各向同性谐振子处于基态，求在微扰 $\hat{V} = \lambda \hat{\sigma}_x \hat{y}^2$ 作用下的基态能量，精确到 λ 的二阶小量.

解：态：$|n_x\, n_y\, n_z \uparrow\rangle \quad |n_x\, n_y\, n_z \downarrow\rangle$

$$E_{n_x n_y n_z} = (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega.$$

基态简并度为 2：

	$\|000\uparrow\rangle$	$\|000\downarrow\rangle$
$\langle 000\uparrow\|$	$\frac{3}{2}\hbar\omega$	
$\langle 000\downarrow\|$		$\frac{3}{2}\hbar\omega$

$$\hat{y} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_y + \hat{a}_y^+) \qquad \hat{y}^2 = \frac{\hbar}{2m\omega}\left[2\hat{a}_y^+\hat{a}_y + 1 + \hat{a}_y^2 + (\hat{a}_y^+)^2\right]$$

但注意到 $\langle 020|\hat{a}_y^{+2}|000\rangle = \sqrt{2}$

$$\langle 000|\hat{a}_y^2|020\rangle = \sqrt{2}.$$

因此 $\hat{V}$ 会将 $|020\rangle$ 耦合到 $|000\rangle$

	$\|000\uparrow\rangle$	$\|000\downarrow\rangle$	$\|020\uparrow\rangle$	$\|020\downarrow\rangle$
$\langle 000\uparrow\|$	$\frac{3}{2}\hbar\omega$	$\frac{\hbar}{2m\omega}\lambda$	0	$\frac{\sqrt{2}\hbar}{2m\omega}\lambda$
$\langle 000\downarrow\|$	$\frac{\hbar}{2m\omega}\lambda$	$\frac{3}{2}\hbar\omega$	$\frac{\sqrt{2}\hbar}{2m\omega}\lambda$	0
$\langle 020\uparrow\|$	0	$\frac{\sqrt{2}\hbar}{2m\omega}\lambda$	$\frac{7}{2}\hbar\omega$	$\frac{5}{2}\frac{\hbar}{m\omega}\lambda$
$\langle 020\downarrow\|$	$\frac{\sqrt{2}\hbar}{2m\omega}\lambda$	0	$\frac{5}{2}\frac{\hbar}{m\omega}\lambda$	$\frac{7}{2}\hbar\omega$

注意到 $\langle\uparrow|\hat{\sigma}_x|\uparrow\rangle = 0 \quad \langle\uparrow|\hat{\sigma}_x|\downarrow\rangle = 1$

一阶简并微扰

$$\frac{3}{2}\hbar\omega \pm \frac{\hbar}{2m\omega}\lambda \qquad |\psi_\pm^{(0)}\rangle = \frac{\sqrt{2}}{2}(|000\uparrow\rangle \pm |000\downarrow\rangle)$$

二阶非简并微扰

$$E_\pm^{(2)} = \frac{|\langle 020\uparrow|\hat{V}|\psi_\pm^{(0)}\rangle|^2}{\frac{3}{2}\hbar\omega - \frac{7}{2}\hbar\omega} + \frac{|\langle 020\downarrow|\hat{V}|\psi_\pm^{(0)}\rangle|^2}{\frac{3}{2}\hbar\omega - \frac{7}{2}\hbar\omega}$$

$$E_{\pm}^{(2)} = \frac{2\left|\frac{\sqrt{2}}{2}\frac{\sqrt{2}}{2}\frac{\hbar}{m\omega}\lambda\right|^2}{\frac{3}{2}\hbar\omega - \frac{7}{2}\hbar\omega} = -\frac{\hbar\lambda^2}{4m^2\omega^3}$$

$$E \approx \frac{3}{2}\hbar\omega \pm \frac{\hbar}{2m\omega}\lambda - \frac{\hbar\lambda^2}{4m^2\omega^3}$$

2. 变分法

对于给定 $\hat{H}$，和任一态 $|\psi\rangle$，均有如下关系：

$\langle\psi|\hat{H}|\psi\rangle \geqslant E_{gs}$ （$\hat{H}$ 的基态能量）

这给我们猜测 E_{gs} 提供了方向.

我们选取 $|\psi(\alpha_n)\rangle$ 与对应的 $E(\alpha_n) = \dfrac{\langle\psi(\alpha_n)|\hat{H}|\psi(\alpha_n)\rangle}{\langle\psi(\alpha_n)|\psi(\alpha_n)\rangle}$

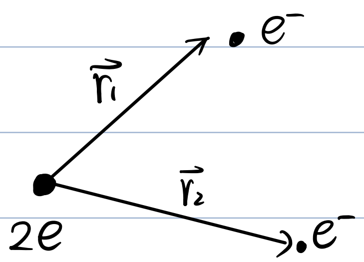
α_n：变分参数.

由 $\dfrac{\partial E(\alpha_n)}{\partial \alpha_n} = 0$，求得 $\{\alpha_n\}$ 与 $E(\alpha_n)$

最重要的是去猜 $|\psi(\alpha_n)\rangle$ 与 $E(\alpha_n)$ 的形式！

（eg：BCS 波函数）

例：He 原子的基态能量.



$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)$$

由于电子的屏蔽效应，类比氢原子基态波函数 $\frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$.

我们写下

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a}$$

Z：等效电荷.

（变分参数）

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{Z}{r_1}+\frac{Z}{r_1}\right)}_{\hat{H}_0} + \underbrace{\frac{e^2}{4\pi\varepsilon_0}\left(\frac{Z-2}{r}+\frac{Z-2}{r}\right)}_{\hat{H}_1} + \underbrace{\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}}_{\hat{V}}$$

则 $\langle \hat{H}_0\rangle_\psi = 2Z^2E_1$，其中 $E_1 = \frac{e^2}{4\pi\varepsilon_0 a} = -13.6\,\text{eV}$.

$$\langle \hat{H}_1\rangle_\psi = 2(Z-2)\frac{e^2}{4\pi\varepsilon_0}\left\langle\frac{1}{r}\right\rangle = 2(Z-2)\frac{e^2}{4\pi\varepsilon_0}\frac{Z}{a}.$$

$$\langle \hat{V}\rangle_\psi = -\frac{5}{4}ZE_1$$

$$\Rightarrow \langle \hat{H}\rangle_\psi = (-2Z^2+\frac{27}{4}Z)E_1$$

$\Downarrow$ 求最小值

$$Z = \frac{27}{16} \approx 1.69 \Rightarrow \langle\hat{H}\rangle \approx -77.5\,\text{eV}$$

(实验上测得为 $-78.795\,\text{eV}$)

3. 含时微扰

a. 迭代形式

$$\hat{H} = \hat{H}_0 + \hat{V}(t).$$

假定 $\hat{H}_0$ 的本征态与本征值为 $\{|\psi_n\rangle\}$ 与 $\{E_n\}$.

$$|\psi(t)\rangle = \sum_n C_n(t)|\psi_n\rangle,$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = [\hat{H}_0+\hat{V}(t)]|\psi(t)\rangle \qquad \langle\psi_m|\hat{V}(t)|\psi_n\rangle$$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}C_m(t) = E_m C_m(t) + \sum_n V_{mn}(t)C_n(t)$$

变换 $\tilde{C}_m(t) = e^{iE_mt/\hbar}C_m(t)$

$$i\hbar\frac{\partial}{\partial t}\tilde{C}_m(t) = -E_m\tilde{C}_m(t) + e^{iE_mt/\hbar}\,i\hbar\frac{\partial}{\partial t}C_m(t)$$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}\tilde{C}_m(t) = \sum_n V_{mn}e^{i(E_m-E_n)t/\hbar}\tilde{C}_n(t)$$

$$= \sum_n V_{mn}e^{i\omega_{mn}t}\tilde{C}_n(t) \qquad \omega_{mn} = \frac{E_m-E_n}{\hbar}$$

$$i\hbar\frac{\partial}{\partial t}\Big(\ \Big)=\Big(\quad \Big) \rightarrow E_m\delta_{mn}+V_{mn}(t)$$

迭代微扰

i) $t=0$ 时的初态为零级近似

ii) 零级近似代入方程

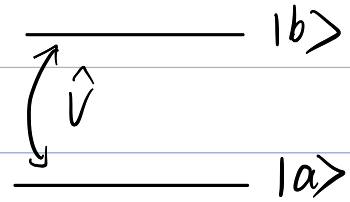
$$i\hbar\frac{\partial}{\partial t}\tilde{C}_m(t)=\sum_n V_{mn}(t)e^{i\omega_{mn}t}\tilde{C}_n$$

的右边得到一级修正。

⋮

iii) 把 $(n-1)$ 级近似修正代入方程右边 $\Rightarrow$ n 级修正。

例：二能级系统。



$$i\hbar\frac{\partial}{\partial t}\tilde{C}_a=V_{aa}\tilde{C}_a+V_{ab}e^{i\omega_{ab}t}\tilde{C}_b$$

$$i\hbar\frac{\partial}{\partial t}\tilde{C}_b=V_{bb}\tilde{C}_b+V_{ba}e^{i\omega_{ba}t}\tilde{C}_a$$

可以看到由于 V_{ab}. V_{ba} 的存在，$|a\rangle$ $|b\rangle$ 产生了耦合。

设 $\tilde{C}_a(0)=1$，$\tilde{C}_b(0)=0$ $\Rightarrow$ 零级修正。

一级修正。

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\tilde{C}_a^{(1)}=V_{aa} \\ i\hbar\frac{\partial}{\partial t}\tilde{C}_b^{(1)}=V_{ba}e^{i\omega_{ba}t}\end{cases}\Rightarrow\begin{cases}\tilde{C}_a^{(1)}=-\frac{i}{\hbar}\int_0^t V_{aa}(t')dt' \\ \tilde{C}_b^{(1)}=-\frac{i}{\hbar}\int_0^t V_{ba}(t')e^{i\omega_{ba}t'}dt'\end{cases}$$

考试要求到一级

二级修正.

$$i\hbar\frac{\partial}{\partial t}\tilde{C}_a^{(2)} = V_{aa}\underbrace{\left(-\frac{i}{\hbar}\right)\int_0^t V_{aa}(t')dt'}_{\hookrightarrow \tilde{C}_a^{(1)}} + V_{ab}\,e^{i\omega_{ab}t}\underbrace{\left(-\frac{i}{\hbar}\right)\int_0^t V_{ba}(t')\,e^{i\omega_{ba}t'}dt'}_{\hookrightarrow \tilde{C}_b^{(1)}}$$

$$\Rightarrow \tilde{C}_a^{(2)} = \left(-\frac{i}{\hbar}\right)^2\int_0^t V_{aa}(t'')\int_0^{t''}V_{aa}(t')\,dt'dt''$$
$$+\left(-\frac{i}{\hbar}\right)^2\int_0^t e^{i\omega_{ab}t}\,V_{ab}(t'')\int_0^{t''}V_{ba}(t')\,e^{i\omega_{ab}t'}\,dt'dt''$$

精确到一级修正.

$$\tilde{C}_a \simeq 1-\left(\frac{i}{\hbar}\right)\int_0^t V_{aa}(t')\,dt'$$

$$\tilde{C}_b \simeq \left(-\frac{i}{\hbar}\right)\int_0^t V_{ba}(t')\,e^{i\omega_{ba}t'}\,dt'$$

可以得到: $|\tilde{C}_a|^2+|\tilde{C}_b|^2 = 1+O(V^2)$

另一种讨论:

定义 $d_a = e^{\frac{i}{\hbar}\int_0^t V_{aa}(t')dt'}\,\tilde{C}_a$

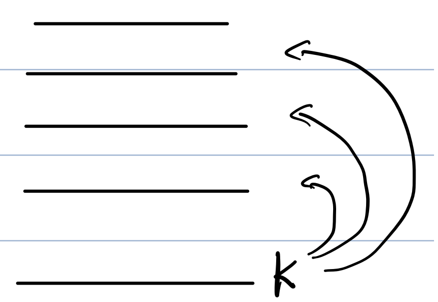
$d_b = e^{\frac{i}{\hbar}\int_0^t V_{bb}(t')dt'}\,\tilde{C}_b$

$$\Rightarrow \begin{cases} i\hbar\frac{\partial}{\partial t}d_a = e^{i\varphi}V_{ab}\,e^{i\omega_{ab}t}d_b \\ i\hbar\frac{\partial}{\partial t}d_b = e^{-i\varphi}V_{ba}\,e^{i\omega_{ba}t}d_b \end{cases}$$

其中 $\varphi = \frac{1}{\hbar}\int_0^t [V_{aa}(t')-V_{bb}(t')]\,dt'$

(详细见 Griffith).

b. 跃迁



$$i\hbar\frac{\partial}{\partial t}\tilde{C}_m = \sum_n V_{mn}\tilde{C}_n\,e^{i\omega_{mn}t}$$

设初态为某K态,零级波函数为 $\tilde{C}_n = \delta_{nk}$

一级含时微扰

$$i\hbar\frac{\partial}{\partial t}\tilde{C}_m^{(1)} = V_{mk}\,e^{i\omega_{mk}t}$$

$$\Rightarrow C_m^{(1)} = -\frac{i}{\hbar}\int_0^t V_{mk}(t')\,e^{i\omega_{mk}t'}\,dt'$$

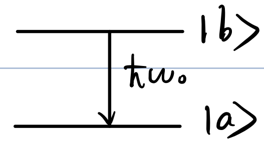
$$\Rightarrow \boxed{\tilde{C}_m \simeq \delta_{mk}-\frac{i}{\hbar}\int_0^t V_{mk}(t')\,e^{i\omega_{mk}t'}\,dt'}$$

对 $m\neq k$ 的态 跃迁概率

$$P_{k\to m}(t) = \frac{1}{\hbar^2}\left|\int_0^t V_{mk}(t')\, e^{i\omega_{mk}(t')} dt'\right|^2$$ ☆☆ 记下

例：光场与二能级原子的耦合.

$$V(t) = V(\vec r)\,(e^{i\omega t}+e^{-i\omega t})$$



$E_b - E_a = \hbar\omega_0$

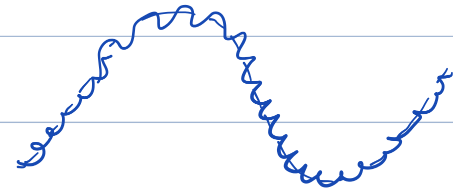
i) $\langle a|V(\vec r)|b\rangle = V_{ab}$

$V_{aa} = V_{bb} = 0$ （光场不对自己耦合；$V(\vec r)$ 为 r 的一次项，使 $\int \psi_a^* r\, \psi_a d^3\vec r = 0$ ）

初态为 $|a\rangle$

$$\tilde C_b(t) = -\frac{i}{\hbar}\int_0^t V_{ba}(e^{i\omega t'}+e^{-i\omega t'})\,e^{i\omega_0 t'}dt$$

$$= -\frac{V_{ba}}{\hbar}\left[\underbrace{\frac{e^{i(\omega_0+\omega)t}-1}{\omega_0+\omega}}_{\text{贡献很小}} + \underbrace{\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}}_{\text{主体}}\right]$$



$$P_{a\to b}(t) = |\tilde C_b(t)|^2$$

我们认为 $V_{ab}, |\omega_0-\omega| \ll \omega_0, \omega, \omega_0+\omega$

$\frac{e^{i(\omega_0+\omega)t}}{\omega_0+\omega}$ 振荡快，对平均值的贡献近似为0，我们可以忽略.

$$\tilde C_b(t) \approx -\frac{V_{ab}}{\hbar}\,\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}$$

$$= -\frac{V_{ab}}{\hbar}\, e^{i(\omega_0-\omega)t/2}\,\frac{1}{\omega_0-\omega}\cdot 2i\sin\frac{\omega_0-\omega}{2}t$$

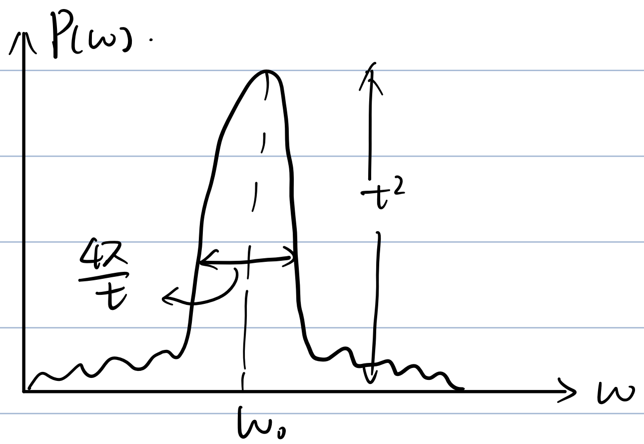
则 $$P_{a\to b}(t) = \frac{4|V_{ab}|^2}{\hbar^2}\,\frac{\sin^2(\frac{\omega_0-\omega}{2}t)}{(\omega_0-\omega)^2}$$

利用 $\lim\limits_{\alpha\to\infty}\frac{\sin^2\alpha x}{\alpha x^2} = \pi\delta(x)$ $\quad \delta[\alpha(x-x')] = \frac{1}{\alpha}\delta(x-x')$

则 $$\lim_{t\to\infty}\frac{\sin^2(\frac{\omega_0-\omega}{2}t)}{(\omega_0-\omega)^2} = \frac{\pi}{4}t\,\delta\left(\frac{\omega_0-\omega_0}{2}\right)$$

$$\Longrightarrow P_{a\to b}(t) \xlongequal{t\to\infty} \frac{2\pi}{\hbar^2}t\,|V_{ba}|^2\,\delta(\omega_0-\omega)$$

在固定 t，ω_0 的情况下

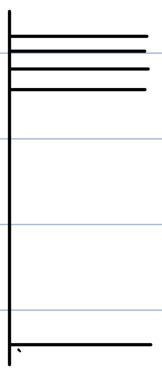


我们也可以注意到 ω 较小时原子也可能到高能级，这是由于 $\Delta E \Delta t \sim \hbar$，即短时间内可以"不满足能量守恒"

注：$t \to \infty \Longrightarrow \frac{1}{|V_{ab}|} \gg t \gg \frac{1}{\omega_0-\omega}$（即应用此理论有条件）

单位时间跃迁速率：

$$W_{a\to b} = \frac{2\pi}{\hbar^2}|V_{ba}|^2\delta(\omega_0-\omega)$$



很多密集的高能态
认为是连续的

基态

能态密度

$$\lim_{t\to\infty}\sum_b P_{a\to b} = \int dE\,\rho(E)\frac{2\pi}{\hbar}|V_{ab}|^2\delta(E-E_0)\,t$$

$$= \rho(E_0)\frac{2\pi}{\hbar}|V_{ab}|^2 t.$$

Fermi's Golden Rule.

以上所有为考试内容.

ii) 上述问题的严格解（Rabi振荡）

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} C_a \\ C_b \end{pmatrix} = \begin{pmatrix} E_a & V_{ab}(e^{i\omega t}+e^{-i\omega t}) \\ V_{ab}^*(e^{i\omega t}+e^{-i\omega t}) & E_b \end{pmatrix}\begin{pmatrix} C_a \\ C_b \end{pmatrix}$$

定义 $\tilde{C}_a = C_a e^{i\left(\frac{E_a+E_b}{2\hbar}-\frac{\omega}{2}\right)t}$ $\quad \tilde{C}_b = C_b e^{i\left(\frac{E_a+E_b}{2\hbar}+\frac{\omega}{2}\right)t}$

$$\Rightarrow\ i\frac{\partial}{\partial t}\begin{pmatrix}\tilde{C}_a\\ \tilde{C}_b\end{pmatrix}=\begin{pmatrix}\frac{\delta}{2} & \frac{V_{ab}}{\hbar}(1+e^{-2i\omega t})\\ \frac{V_{ab}^*}{\hbar}(1+e^{2i\omega t}) & -\frac{\delta}{2}\end{pmatrix}\begin{pmatrix}\tilde{C}_a\\ \tilde{C}_b\end{pmatrix}$$

$\delta=\omega-\omega_0 \quad \omega_0=(E_b-E_a)/\hbar$

(失谐)

仍然使用全波近似，将矩阵中的 $e^{2i\omega t}$ 忽略.

之后利用 Pauli 矩阵展开 $\hat{V}$

$$\hat{V}=\frac{\delta}{2}\sigma_z+\mathrm{Re}\left(\frac{V_{ab}}{\hbar}\right)\sigma_x-\mathrm{Im}\left(\frac{V_{ab}}{\hbar}\right)\sigma_y$$

$$\Rightarrow\ \begin{pmatrix}\tilde{C}_a(t)\\ \tilde{C}_b(t)\end{pmatrix}=e^{-i\hat{V}t}\begin{pmatrix}\tilde{C}_a(0)\\ \tilde{C}_b(0)\end{pmatrix}$$

而 $e^{-i\varphi\hat{\vec{\sigma}}\cdot\vec{n}}=\cos\varphi\,\hat{I}-(\hat{\vec{\sigma}}\cdot\vec{n})\sin\varphi$ 注意此处 $\vec{n}$ 要归一

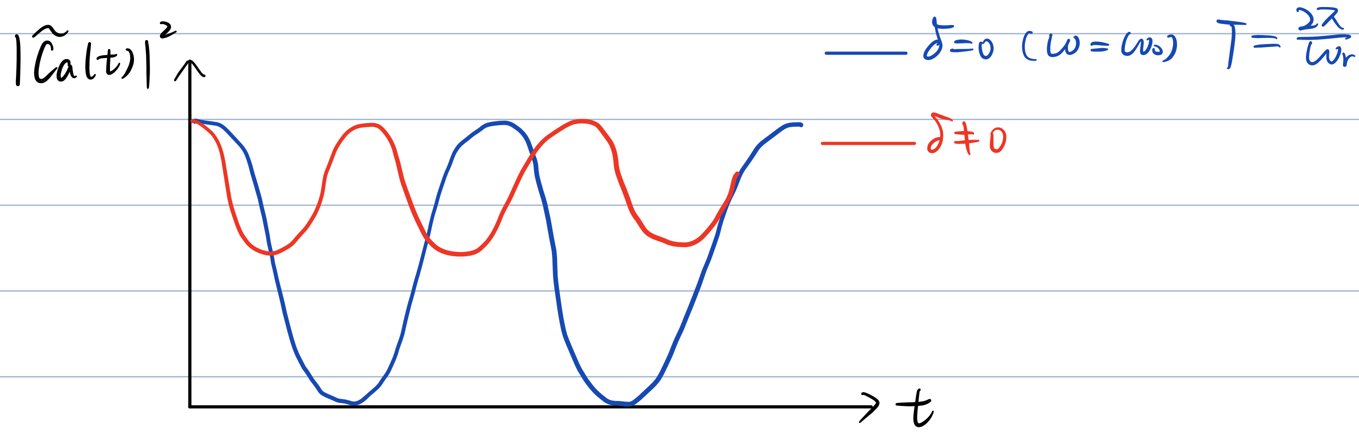
得到

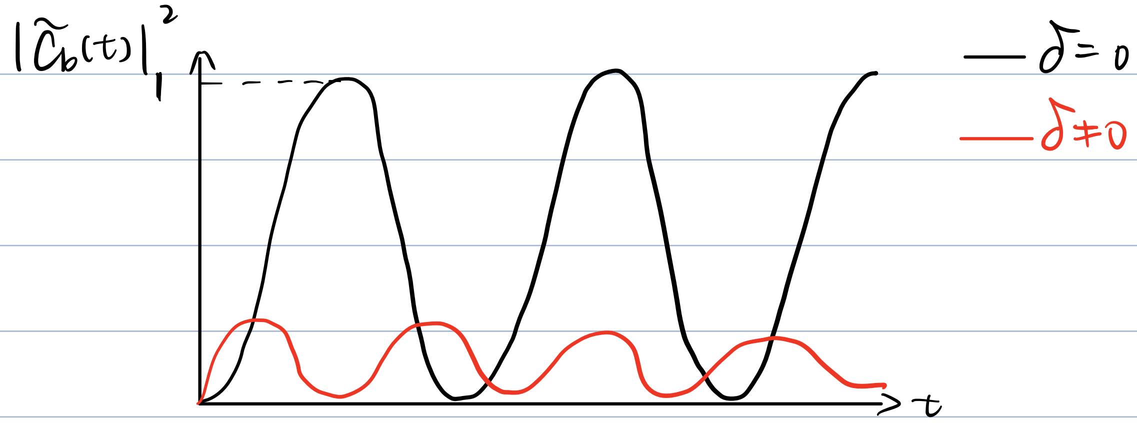
$$\begin{pmatrix}\tilde{C}_a(t)\\ \tilde{C}_b(t)\end{pmatrix}=\begin{bmatrix}\cos\frac{\omega_r t}{2}+i\frac{\delta}{\omega_r}\sin\frac{\omega_r t}{2} & -i\frac{2V_{ab}}{\hbar\omega_r}\sin\frac{\omega_r t}{2}\\ -i\frac{2V_{ab}^*}{\hbar\omega_r}\sin\frac{\omega_r t}{2} & \cos\frac{\omega_r t}{2}-i\frac{\delta}{\omega_r}\sin\frac{\omega_r t}{2}\end{bmatrix}\begin{pmatrix}\tilde{C}_a(0)\\ \tilde{C}_b(0)\end{pmatrix}$$

$$\omega_r=\sqrt{\delta^2+\frac{4|V_{ab}|^2}{\hbar^2}}$$

如 $\tilde{C}_a(0)=1$, 则

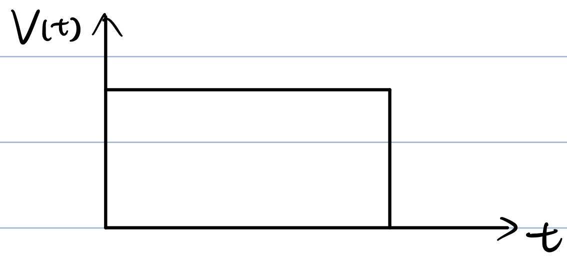
$$\tilde{C}_a(t)=\cos\frac{\omega_r t}{2}+i\frac{\delta}{\omega_r}\sin\frac{\omega_r t}{2}$$





C. 含时问题的特例

① 常微扰



初态 $|n\rangle \Rightarrow$ 末态 $|m\rangle$

一阶修正

$$\tilde{C}_m^{(1)}(t) = -\frac{i}{\hbar}\int_0^t V_{mn}\, e^{i\omega_{mn}t'} dt'$$

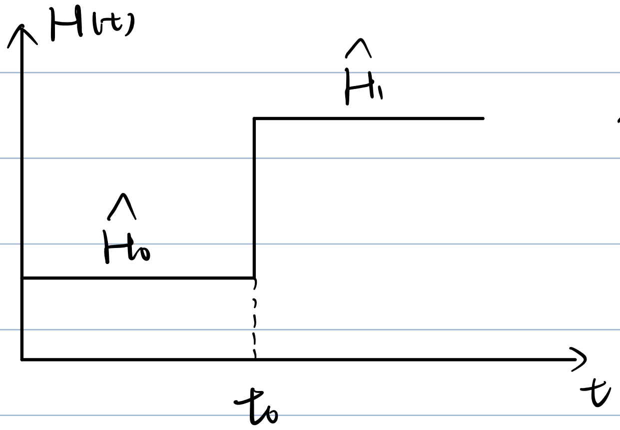
$$\lim_{t\to\infty} P_{n\to m}(t) = \lim_{t\to\infty} \frac{|V_{mn}|}{\hbar^2}\frac{|e^{i\omega_{mn}t}-1|^2}{\omega_{mn}^2}$$

$$= \frac{2\pi}{\hbar^2}|V_{mn}|^2 t\,\delta(\omega_m-\omega_n)$$

$$\omega_{n\to m} = \frac{2\pi}{\hbar}|V_{mn}|^2\delta(E_m-E_n)$$

(只有两能级能量足够近才可以跃迁)

② 突变近似



假设在 t_0 时刻 $\hat{H}$ 突变，$|\psi(t_0)\rangle$ 近似不变

$$\hat{H}_0|\psi_n\rangle = E_n|\psi_n\rangle$$

$$\hat{H}_1|\varphi_\alpha\rangle = E_\alpha|\varphi_\alpha\rangle$$

$t=0$ $\quad |\psi\rangle = \sum_n C_n|\psi_n\rangle$

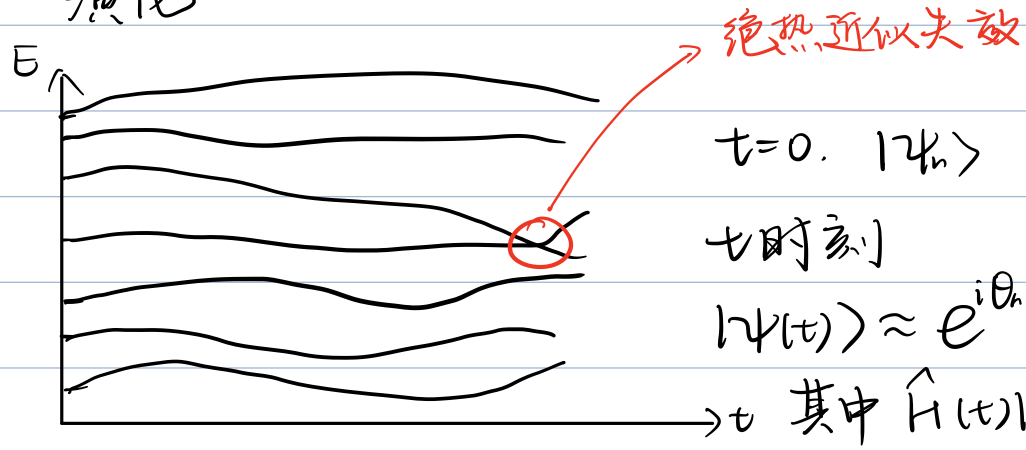
则 $t<t_0$. $|\psi\rangle = \sum_n C_n e^{-iE_nt/\hbar}|\psi_n\rangle$

$t=t_0$ $|\psi\rangle = \sum_n C_n e^{-iE_nt_0/\hbar}|\psi_n\rangle$

$t>t_0$ $|\psi\rangle = \sum_n C_n e^{-iE_nt_0/\hbar}\sum_\alpha\langle\varphi_\alpha|\psi_n\rangle e^{-iE_\alpha(t-t_0)/\hbar}|\varphi_\alpha\rangle$

③ 绝热近似

$\hat{H}(t)$ 缓变，则初始本征态 绝热跟随当前 $\hat{H}(t)$ 的本征态演化



$t=0$. $|\psi_n\rangle$ $\hat{H}_0(0)|\psi_n\rangle = E_n(0)|\psi_n\rangle$

t 时刻

$|\psi(t)\rangle \approx e^{i\theta_n(t)}e^{i\gamma_n(t)}|\psi_n(t)\rangle$

其中 $\hat{H}(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle$

$\theta_n = -\frac{1}{\hbar}\int_0^t E_n(t')dt'$ 动力学相位

$\gamma_n = i\int_0^t \langle\psi_n(t')|\frac{\partial}{\partial t'}|\psi_n(t')\rangle dt'$ 几何相位

第九章 主题讨论

1. 对称性与守恒量

对称操作 $\longleftrightarrow$ 对称算符 $\hat{Q}$

$|\psi\rangle \longrightarrow |\psi'\rangle = \hat{Q}|\psi\rangle$

$\hat{A} \longrightarrow \hat{A}' = \hat{Q}\hat{A}\hat{Q}^{-1}$

$\hat{Q}$ 为线性算符 且 $\hat{Q}^+\hat{Q} = \hat{Q}\hat{Q}^+ = \hat{I}$ (幺正)

如果算符在 $\hat{Q}$ 的作用下不变，则其具有相应的对称性.

$\hat{H} \xrightarrow{\hat{Q}} \hat{H}' = \hat{Q}\hat{H}\hat{Q}^+ = \hat{H} \Rightarrow [\hat{H},\hat{Q}] = 0$.

$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

$\Rightarrow i\hbar\frac{\partial}{\partial t}(\hat{Q}|\psi\rangle) = \hat{Q}\hat{H}\hat{Q}^{-1}\hat{Q}|\psi\rangle = \hat{H}(\hat{Q}|\psi\rangle)$

即 $\hat{Q}|\psi\rangle$, $|\psi\rangle$ 均为 $\hat{H}$ 的本征态，且有相同本征值.

若 $\hat{Q}|\psi_n\rangle \sim e^{i\varphi}|\psi_n\rangle$: $|\psi_n\rangle$ 也具有与 $\hat{H}$ 相同的对称性

若 $\hat{Q}|\psi_n\rangle \neq e^{i\varphi}|\psi_n\rangle$: $|\psi_n\rangle$ 对称性自发破缺.

说明 $\hat{Q}|\psi_n\rangle$, $|\psi_n\rangle$ 构成 $\hat{H}$ 的一个简并子空间.

连续变换与守恒量.

$\hat{Q} = \hat{I} + i\varepsilon\hat{F} + O(\varepsilon^2)$　　$(\varepsilon > 0;\ \varepsilon \ll 1)$

$\hat{Q}\hat{Q}^{+} = \hat{I} \Rightarrow (\hat{I} + i\varepsilon\hat{F})(\hat{I} - i\varepsilon\hat{F}^{+}) = \hat{I} + i\varepsilon(\hat{F} - \hat{F}^{+}) + O(\varepsilon^2)$

$\Rightarrow \hat{F} = \hat{F}^{+}$ ($\hat{Q}$ 的生成元)

若 $[\hat{H}, \hat{Q}] = 0 \Rightarrow [\hat{H}, \hat{F}] = 0 \Rightarrow \hat{F}$ 守恒.

例：空间平移不变性对应动量守恒.

定义 $\hat{D}(a)\psi(x) = \psi(x-a)$

平移不变性要求 $[\hat{D}(a), \hat{H}] = 0$.

考察无穷小平移.

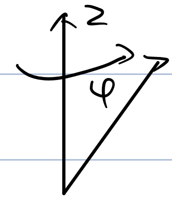
$\hat{D}(\varepsilon)\psi(x) = \psi(x-\varepsilon) \approx \psi(x) - \varepsilon\frac{\partial\psi}{\partial x}$

$= (1 - i\frac{\varepsilon}{\hbar}\hat{p})\psi(x)$.　$(\hat{p} = -i\hbar\frac{\partial}{\partial x})$

$[\hat{D}, \hat{H}] = 0 \Rightarrow [\hat{p}, \hat{H}] = 0$. 动量守恒.

$\hat{D}(a) = \lim_{N\to\infty}\left(1 - i(\frac{a}{N})\frac{1}{\hbar}\hat{p}\right)^N = e^{-\frac{i\hat{p}a}{\hbar}}$

例：转动不变对应角动量守恒.



$$\hat{R}_z(\alpha)\psi(\varphi)=\psi(\varphi-\alpha)$$

转动不变 $[\hat{R}_z,\hat{H}]=0$.

$$\hat{l}_z\to -i\hbar\frac{\partial}{\partial\varphi}$$

$$\hat{R}_z(\varepsilon)\psi(\varphi)=\psi(\varphi-\alpha)=\left(1-i\frac{\varepsilon}{\hbar}\hat{l}_z\right)\psi(\varphi)$$

注：对称变换只能是幺正或反幺正的

连续变换均为幺正变换

体系有守恒量 $\Longrightarrow$ 体系有对称性

$\not\Longleftarrow$

C. 全同粒子与交换对称

$\hat{P}_{ij}$：粒子交换算符

$$\hat{P}_{ij}\psi(q_1,q_2\ldots q_i\ldots q_j\ldots q_n)=\psi(q_1.q_2\ldots q_j\ldots q_i\ldots q_n)$$

若 $\hat{H}$ 描述全同粒子体系，则 $[\hat{P}_{ij},\hat{H}]=0$，有共同本征态

$$\hat{P}_{ij}\psi=\lambda\psi\Longrightarrow\hat{P}_{ij}^2\psi=\lambda^2\psi\Rightarrow\lambda^2=1\Rightarrow\lambda=\pm1$$

$\lambda=1$：交换对称 ψ^S

$\lambda=-1$：交换反对称 ψ^A.

例：两粒子体系

$$\hat{H}=\hat{h}_1(q_1,p_1)+\hat{h}_2(q_2,p_2)$$ （忽略相互作用）

已知 $\hat{h}_i\varphi_{p_i}(q_i)=\varepsilon_{p_i}\varphi_{p_i}(q_i)$ （即单粒子本征问题已知）

$$\hat{H}\varphi_{p_1}(q_1)\varphi_{p_2}(q_2)=(\varepsilon_{p_1}+\varepsilon_{p_2})\varphi_{p_1}(q_1)\varphi_{p_2}(q_2)$$

注意到 $[\hat{P}_{12}, \hat{H}] = 0$

$\Rightarrow \varphi_{p_1}(q_1)\varphi_{p_2}(q_2)$ 与 $\varphi_{p_1}(q_2)\varphi_{p_2}(q_1)$ 简并.

交换对称 (自旋为整数, 玻色子)

$$\psi^{S}_{p_1p_2}(q_1 q_2) = \frac{\sqrt{2}}{2}[\varphi_{p_1}(q_1)\varphi_{p_2}(q_2) + \varphi_{p_1}(q_2)\varphi_{p_2}(q_1)]$$

交换反对称 (自旋为半整数, 费米子)

$$\psi^{A}_{p_1p_2}(q_1 q_2) = \frac{\sqrt{2}}{2}\begin{vmatrix} \varphi_{p_1}(q_1) & \varphi_{p_1}(q_2) \\ \varphi_{p_2}(q_1) & \varphi_{p_2}(q_2) \end{vmatrix}$$

$$= \frac{\sqrt{2}}{2}[\varphi_{p_1}(q_1)\varphi_{p_2}(q_2) - \varphi_{p_1}(q_2)\varphi_{p_2}(q_1)]$$

例: 交换相互作用

直积态 $|a\rangle_1 |b\rangle_2$, a, b 标记内态 (自旋, 能级等)

对称 $\frac{\sqrt{2}}{2}(|a\rangle_1|b\rangle_2 + |b\rangle_1|a\rangle_2)$

反对称 $\frac{\sqrt{2}}{2}(|a\rangle_1|b\rangle_2 - |b\rangle_1|a\rangle_2)$

求 $\langle(\hat{x}_1-\hat{x}_2)^2\rangle$ $\hat{x}_1\ \hat{x}_2$: 位置坐标算符.

直积态: $_1\langle a|\,_2\langle b|\,(\hat{x}_1^2+\hat{x}_2^2-2\hat{x}_1\hat{x}_2)\,|a\rangle_1|b\rangle_2$

$= {}_1\langle a|\hat{x}_1^2|a\rangle_1 + {}_2\langle b|\hat{x}_2^2|b\rangle_2 - 2\,{}_1\langle a|\hat{x}_1|a\rangle_1 \oplus {}_2\langle b|\hat{x}_2|b\rangle_2$

$= \langle\hat{x}_1^2\rangle_a + \langle\hat{x}_2^2\rangle_b - 2\langle\hat{x}_1\rangle_a\langle\hat{x}_2\rangle_b$.

对称 & 反对称

① ② ③

$\frac{1}{2}(\,{}_1\langle a|\,{}_2\langle b| \pm {}_1\langle b|\,{}_2\langle a|)(\hat{x}_1^2+\hat{x}_2^2-2\hat{x}_1\hat{x}_2)|(|a\rangle_1|b\rangle_2 \pm |b\rangle_1|a\rangle_2)$

$= \frac{1}{2}(\langle\hat{x}_1^2\rangle_a + \langle\hat{x}_1^2\rangle_b \pm 0 \pm 0)$ ··· ①

$\langle\hat{x}_1\rangle_{ab} = \langle a|\hat{x}_1|b\rangle$

$+\frac{1}{2}(\langle\hat{x}_1^2\rangle_a + \langle\hat{x}_2\rangle_b)$ ··· ②

$+\frac{1}{2}\{-2\langle\hat{x}_1\rangle_a\langle\hat{x}_2\rangle_b - 2\langle\hat{x}_1\rangle_b\langle\hat{x}_2\rangle_a \mp 2\langle\hat{x}_1\rangle_{ab}\langle\hat{x}_2\rangle_{ba} \mp 2\langle\hat{x}_1\rangle_{ba}\langle\hat{x}_2\rangle_{ab}\}$

$$= \langle \hat{x}_1^2\rangle_a + \langle \hat{x}_2^2\rangle_b - 2\langle \hat{x}_1\rangle_a \langle \hat{x}_2\rangle_b \mp 2|\langle \hat{x}\rangle_{ab}|^2$$

（设 $\langle \hat{x}_1\rangle_a = \langle \hat{x}_2\rangle_a$，$\langle \hat{x}_1\rangle_{ab} = \langle \hat{x}_2\rangle_{ab}$）

即对称与反对称会影响粒子之间的间距.

2. 电磁场中带电粒子的 Schrödiger 方程.

ψ 的规范对称性.

$\psi \longrightarrow e^{i\varphi}\psi$（相同的运动，相同的状态）

但若 $\varphi = \varphi(\vec{r})$，我们仍有上述结论.

为保持 $\psi'(\vec{r}) = e^{iq\chi(\vec{r})/\hbar c}\psi(\vec{r})$

规范不变的 Schrödiger 方程为

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}(\hat{\vec{p}} - \frac{q}{c}\hat{\vec{A}})^2\psi + q\varphi\psi$$

其中 $\vec{A} \to \vec{A}' = \vec{A} + \nabla\chi(\vec{r})$

$\varphi \to \varphi' = \varphi - \frac{1}{c}\frac{\partial \chi(\vec{r})}{\partial t}$

则 $\vec{B} = \nabla\times\vec{A}$ $\quad\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t} - \nabla\varphi$ 在规范变化下不变.

例：Landun 能级

三维电子气在 $\hat{z}$ 方向均匀磁场下的能谱.

选规范. $A_x = -By \quad A_y = A_z = 0 \quad \varphi = 0 \quad (\nabla\times\vec{A} = \vec{B})$

$$\hat{H} = \frac{1}{2m}[(\hat{p}_x - \frac{e}{c}By)^2 + \hat{p}_y^2 + \hat{p}_z^2]$$

对于给定 p_z 或 k_z，有

$$H_{xy} = \frac{\hat{p}_y^2}{2m} + \frac{e^2B^2}{2mc^2}(y - \frac{c\hat{p}_x}{eB})^2$$

对于给定 p_x，$H_{x\text{-}y}$ 为一维谐振子，$\omega_c = \frac{eB}{mc}$.

$E=(n+\frac{1}{2})\hbar\omega_c,\quad n=0,1,2\cdots$

（由于 P_x 有无限的取值，则对每一个n，有无穷简并）

例：正常 Zeeman 效应、

$A_x=-\frac{1}{2}By\qquad A_y=\frac{1}{2}Bx\qquad A_z=0$

$$H=\frac{1}{2m}\left[(\hat{P}_x-\frac{eB}{2c}y)^2+(\hat{P}_y+\frac{eB}{2c}x)^2+\hat{P}_z^2\right]+V(\vec{r})$$

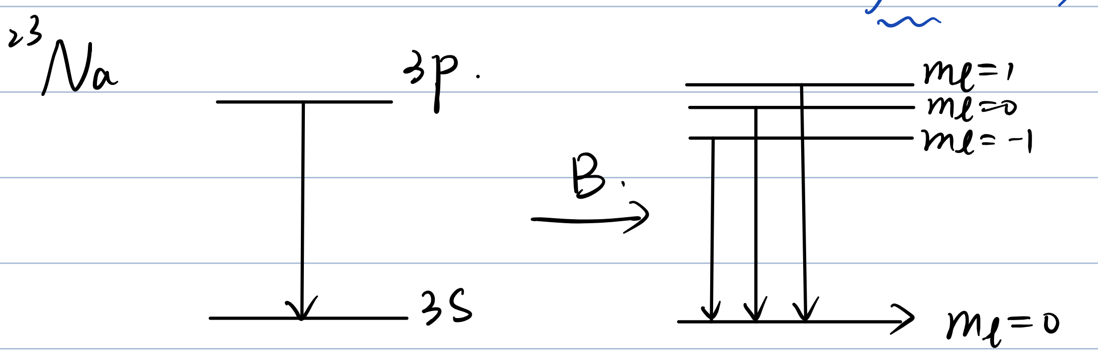
$$=\frac{\hat{P}^2}{2m}+V(\vec{r})+\frac{eB}{2mc}\underbrace{(\hat{x}\hat{P}_y-\hat{y}\hat{P}_x)}_{\hat{l}_z}+\frac{e^2B^2}{8mc^2}(\hat{x}^2+\hat{y}^2)$$

由于 $\frac{B^2\text{项}}{B\text{项}}\approx\frac{e^2B^2}{4c}\langle x^2+y^2\rangle\sim10^{-4}$. 忽略 B^2 项.

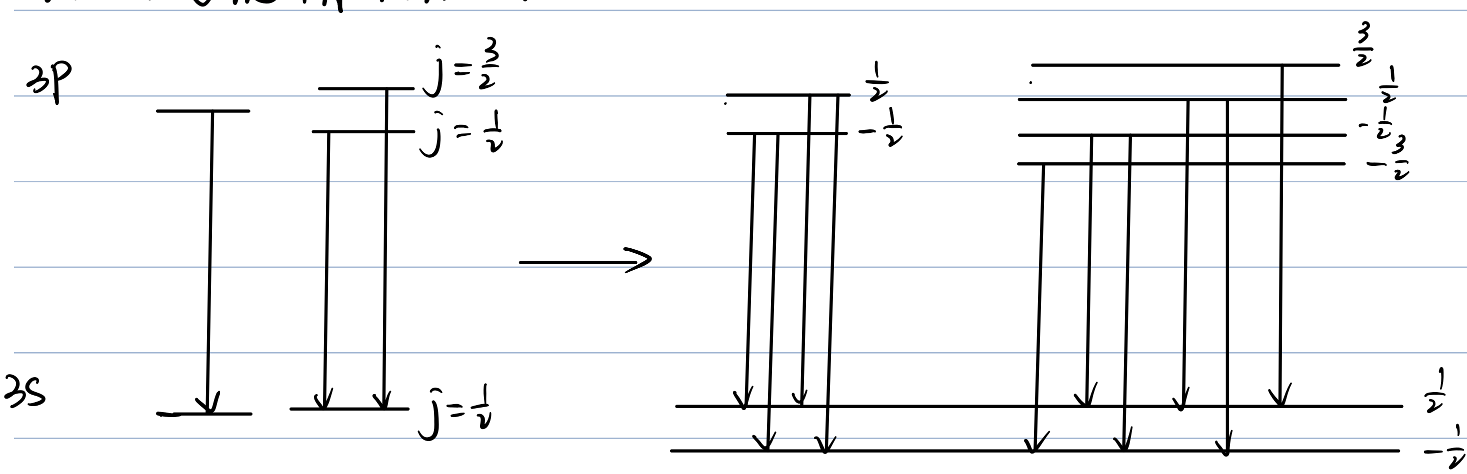
则 $H=\underbrace{\frac{\hat{P}^2}{2m}+V(\vec{r})}_{E_n\,l\,(\psi_{nlm})}+\frac{eB}{2mc}\hat{l}_z$ 解简并

$\Rightarrow E_{nlm}=E_{nl}+\frac{eB}{2mc}m_l\hbar$

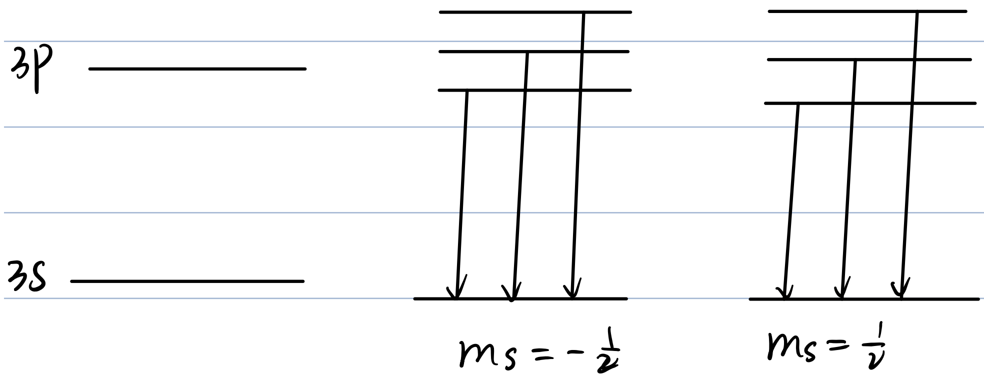
$=m_l\mu_B B\qquad \mu_B=\frac{e\hbar}{2mc}.$



弱场，考虑精细结构



强场 $E = E_{nl} + \frac{eB}{2mc}\hbar(m_l + 2m_s)$



量子信息初步 (John Preskill)

1. 密度矩阵.

a. 对任意 $|\psi\rangle$, 其密度矩阵 $\hat{\rho} = |\psi\rangle\langle\psi|$

$$\hat{A}: \langle\psi|\hat{A}|\psi\rangle = \sum_n \langle\psi|\hat{A}|\psi_n\rangle\langle\psi_n|\psi\rangle$$

$$= \sum_n \langle\psi_n|\underset{\sim\sim\sim\sim\sim}{\psi\rangle\langle\psi|\hat{A}}|\psi_n\rangle$$

$$= \sum_n \langle\psi_n|\hat{\rho}\hat{A}|\psi_n\rangle$$

$$= \mathrm{Tr}(\hat{\rho}\hat{A})$$

例: 二能级体系 (qubit)

$$|\psi\rangle = |\uparrow_x\rangle = \frac{\sqrt{2}}{2}(|\uparrow_z\rangle + |\downarrow_z\rangle)$$

$$\Rightarrow \hat{\rho} = |\psi\rangle\langle\psi|$$

$$= \frac{1}{2}(|\uparrow_z\rangle + |\downarrow_z\rangle)(\langle\uparrow_z| + \langle\downarrow_z|)$$

$$= \frac{1}{2}(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\uparrow_z| + |\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\downarrow_z|)$$

在 $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ 下

非对角元: 相干项

$\hat{\rho}$ 对应的矩阵为 $\rho = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ (纯态)

在 $|\psi\rangle$ 下测 $\hat{S}_z$: $\begin{cases} 50\%, & \uparrow_z \ (\frac{1}{2}\hbar), \text{态塌缩到 } |\uparrow_z\rangle \\ 50\%, & \downarrow_z \ (\frac{1}{2}\hbar), \text{态塌缩到 } |\downarrow_z\rangle \end{cases}$

相比之下 若 $\hat{\rho} = \frac{1}{2}\left(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z| \right)$

$= \frac{1}{2}\hat{I}$ (mixed state)

则对任意方向上的测量，均为50%↑，50%↓.

b. 两个二能级体系

$|\psi_{AB}\rangle = a\,|\uparrow_z\rangle_A|\uparrow_z\rangle_B + b\,|\downarrow_z\rangle_A|\downarrow_z\rangle_B \quad (|a|^2+|b|^2=1)$

对A态测 $\hat{S}_z$ $\begin{cases} |a|^2, & \uparrow_z A \longrightarrow \text{态塌缩为 } |\uparrow_z\rangle_A|\uparrow_z\rangle_B \\ |b|^2, & \downarrow_z A \longrightarrow \cdots\cdots\ |\downarrow_z\rangle_A|\downarrow_z\rangle_B \end{cases}$

如果不关心B的结果，只对$\hat{A}$的$\hat{M}_A$进行测量.

$\langle\psi_{AB}|\,\hat{M}_A\otimes\hat{I}_B\,|\psi_{AB}\rangle$

$= \left(a^*\,{}_A\langle\uparrow_z|\,{}_B\langle\uparrow_z| + b^*\,{}_A\langle\downarrow_z|\,{}_B\langle\downarrow_z|\right)\hat{M}_A\otimes\hat{I}_B$

$\left(a\,|\uparrow_z\rangle_A|\uparrow_z\rangle_B + b\,|\uparrow_z\rangle_A|\uparrow_z\rangle_B\right)$

$= |a|^2\langle\uparrow_z|\hat{M}_A|\uparrow_z\rangle_A + |b|^2\langle\downarrow_z|\hat{M}_A|\downarrow_z\rangle_A$

设 $\{|\varphi_0\rangle, |\varphi_1\rangle\}$ 为A中的基

则上式 $= |a|^2\langle\uparrow_z|\hat{M}_A|\varphi_0\rangle\langle\varphi_0|\uparrow_z\rangle + |a|^2\langle\uparrow_z|\hat{M}_A|\varphi_1\rangle\langle\varphi_1|\uparrow_z\rangle$

$+ |b|^2\langle\downarrow_z|\hat{M}_A|\varphi_0\rangle\langle\varphi_0|\downarrow_z\rangle + |b|^2\langle\downarrow_z|\hat{M}_A|\varphi_1\rangle\langle\varphi_1|\downarrow_z\rangle$

$= \langle\varphi_0|\,|a|^2|\uparrow_z\rangle_A\langle\uparrow_z|\hat{M}_A|\varphi_0\rangle + \langle\varphi_1|\,|a|^2|\uparrow_z\rangle_A\langle\uparrow_z|\hat{M}_A|\varphi_1\rangle$

$+ \langle\varphi_0|\,|b|^2|\downarrow_z\rangle_A\langle\downarrow_z|\hat{M}_A|\varphi_0\rangle + \langle\varphi_1|\,|b|^2|\downarrow_z\rangle_A\langle\downarrow_z|\hat{M}_A|\varphi_1\rangle$

$= \mathrm{Tr}(\hat{\rho}_A\hat{M}_A)$

其中 $\hat{\rho}_A = |a|^2|\uparrow_z\rangle_A\langle\uparrow_z| + |b|^2|\downarrow_z\rangle_A\langle\downarrow_z|$

$\mathrm{Tr}(\hat{\rho}_A) = 1$

$\mathrm{Tr}(\hat{\rho}_A^2) \neq 1$ （$\neq 1$为混态，$=1$为纯态）

混态定义 $\hat{\rho} = \sum_a P_a |\psi_a\rangle\langle\psi_a|$ $\begin{cases} \text{求和多于一项} \to \text{混态} \\ \text{只有一项} \to \text{纯态} \end{cases}$

$\hat{\rho}_A = Tr_B(|\psi_{AB}\rangle\langle\psi_{AB}|)$ （A的约化密度阵）

$= {}_B\langle\uparrow_z|(a|\uparrow_z\rangle_A|\uparrow_z\rangle_B + b|\downarrow_z\rangle_A|\downarrow_z\rangle_B)({}_A\langle\uparrow_z|{}_B\langle\uparrow_z|a^* + {}_A\langle\downarrow_z|{}_B\langle\downarrow_z|b^*)|\uparrow_z\rangle_B$

$+ {}_B\langle\downarrow_z|(\qquad)(\qquad)|\downarrow_z\rangle_B$

$= |a|^2|\uparrow_z\rangle_A\langle\uparrow_z| + |b|^2|\downarrow_z\rangle_A\langle\downarrow_z|$

算出来的 $\hat{\rho}_A$ 的纯态还是混态可以反映 A. B是否纠缠.

2. 纠缠的纠缠态

可分离的态： $|\psi_{AB}\rangle = |\varphi_A\rangle\otimes|\chi_B\rangle$ （直积态）

$\hat{\rho}_A = Tr_B(\hat{\rho}_{AB})$

$= \sum_n {}_B\langle\psi_n|(|\varphi_A\rangle\otimes|\chi_B\rangle\langle\varphi_A|\langle\chi_B|)|\psi_n\rangle_B$

$= |\varphi_A\rangle\langle\varphi_A| \otimes \sum_n {}_B\langle\psi_n|\chi_B\rangle\langle\chi_B|\psi_n\rangle_B$

$= |\varphi_A\rangle\langle\varphi_A|$ （纯态）

例： $|\psi_{AB}\rangle = \frac{\sqrt{2}}{2}|\uparrow_z\rangle_A|\uparrow_z\rangle_B + \frac{\sqrt{2}}{2}|\downarrow_z\rangle_A|\downarrow_z\rangle_B$

对 B进行 $\hat{S}_z$ 方向的测量 $\begin{cases} 50\%, \uparrow_z \\ 50\%, \downarrow_z \end{cases}$

考虑对 $\vec{n}$ 方向的测量.

$|\psi_{AB}\rangle = \frac{\sqrt{2}}{2}|\uparrow_z\rangle_A(\underline{\langle\uparrow_n|\uparrow_z\rangle}|\uparrow_n\rangle_B + \underline{\langle\downarrow_n|\uparrow_z\rangle}|\downarrow_n\rangle_B)$

$+ \frac{\sqrt{2}}{2}|\downarrow_z\rangle_A(\underline{\langle\uparrow_n|\downarrow_z\rangle}|\uparrow_n\rangle_B + \underline{\langle\downarrow_n|\downarrow_z\rangle}|\downarrow_n\rangle_B)$

↳ 这四项在A. B中给出相同结果

$$= \frac{\sqrt{2}}{2}\left(\langle\uparrow_n|\uparrow_z\rangle|\uparrow_z\rangle_A + \langle\uparrow_n|\downarrow_z\rangle|\downarrow_z\rangle_A\right)|\uparrow_n\rangle_B$$

$$+ \frac{\sqrt{2}}{2}\left(\langle\downarrow_n|\uparrow_z\rangle|\uparrow_z\rangle_A + \langle\downarrow_n|\downarrow_z\rangle|\downarrow_z\rangle_A\right)|\downarrow_n\rangle_B$$

$$= \frac{\sqrt{2}}{2}\left(|\uparrow_n\rangle_A|\uparrow_n\rangle_B + |\downarrow_n\rangle_A|\downarrow_n\rangle_B\right)$$

A, B强关联！

常见的两体纠缠态 (Bell态)

$$|\phi^+_{AB}\rangle = \frac{\sqrt{2}}{2}\left(|00\rangle_{AB} + |11\rangle_{AB}\right)$$

$$|\phi^-_{AB}\rangle = \frac{\sqrt{2}}{2}\left(|00\rangle_{AB} - |11\rangle_{AB}\right)$$

$$|\psi^+_{AB}\rangle = \frac{\sqrt{2}}{2}\left(|01\rangle_{AB} + |10\rangle_{AB}\right)$$

$$|\psi^-_{AB}\rangle = \frac{\sqrt{2}}{2}\left(|01\rangle_{AB} - |10\rangle_{AB}\right)$$

应用：

① 测量的理解 / 消相干

② 量子密钥分发

$A \longrightarrow B$

i) A把文本变为ASCII码.

ii) 加密.

iii) $A \xrightarrow{key} B$ 纠缠态在这一步起作用.

iv) B 解密.

分发方法.

i) 制备 $\{|\psi^-\rangle\}$ 系综，分发给A和B.

ii) A, B各自随机测量 $\hat{S}_x$ 或 $\hat{S}_y$，几率各为 $\frac{1}{2}$

iii) A, B于公开信道公布其测量过程，但不公布结果

iv) A, B各自丢弃测量不同的结果.

v) 余下的结果：随机，但对A, B而言，结果完全相反. (key)

如何保密？

如果存在E可以与A、B纠缠，

$$|\psi\rangle_{ABE} = |00\rangle_{AB}|e_{00}\rangle_E + |01\rangle_{AB}|e_{01}\rangle_E + |10\rangle_{AB}|e_{10}\rangle_E + |11\rangle_{AB}|e_{11}\rangle_E$$

而 $|\psi^-\rangle$ 为 $\hat{\sigma}_x^A\hat{\sigma}_x^B$ 与 $\hat{\sigma}_z^A\hat{\sigma}_z^B$ 的本征值为 -1 的本征态

i) 由 $\hat{\sigma}_z^A\hat{\sigma}_z^B|\psi^-\rangle = (-1)|\psi^-\rangle$ 可得.

$$|\psi_{ABE}\rangle = |01\rangle_{AB}|e_{01}\rangle_E + |10\rangle|e_{10}\rangle_E.$$

ii) 由 $\hat{\sigma}_x^A\hat{\sigma}_x^B = -1$ 可得.

$$|\psi_{ABE}\rangle = \frac{1}{2}(|0_x0_x\rangle_{AB} + |1_x1_x\rangle_{AB})(|e_{01}\rangle + |e_{10}\rangle) + \frac{1}{2}(|0_x1_x\rangle_{AB} - |1_x0_x\rangle_{AB})(|e_{01}\rangle - |e_{10}\rangle)$$

$$\Rightarrow |\psi_{ABE}\rangle = \frac{\sqrt{2}}{2}(|0_x1_x\rangle_{AB} - |1_x0_x\rangle)|e\rangle = \frac{\sqrt{2}}{2}(|0_z1_z\rangle_{AB} - |1_z0_z\rangle)|e\rangle = \underbrace{|\psi^-\rangle|e\rangle}_{\text{直积态}}$$

即测量完后通过检测是否为 $\hat{\sigma}_z^A\hat{\sigma}_z^B = -1$，$\hat{\sigma}_x^A\hat{\sigma}_x^B = -1$.
来检测是否被窃听.

③量子远程传态

A有一个未知的 qubit. 如何通过经典信道给B.

$$|\psi\rangle = a|\uparrow_n\rangle + b|\downarrow_n\rangle$$

$$|\psi_c\rangle = a|0\rangle + b|1\rangle$$

设 AB 有一对纠缠态 $|\phi^+\rangle_{AB}$

$$|\psi_c\rangle|\phi^+\rangle_{AB} = (a|0\rangle + b|1\rangle)\frac{\sqrt{2}}{2}(|00\rangle_{AB} + |11\rangle_{AB})$$
$$= \frac{\sqrt{2}}{2}(a|000\rangle_{CAB} + a|011\rangle_{CAB} + b|100\rangle_{CAB} + b|111\rangle_{CAB})$$

$$= \frac{1}{2}a(|\phi^+\rangle_{CA} + |\phi^-\rangle_{CA})|0\rangle_B + \frac{1}{2}a(|\psi^+\rangle_{CA} + |\psi^-\rangle_{CA})|1\rangle_B$$

$$+\frac{1}{2}b(|\psi^+\rangle_{CA} - |\psi^-\rangle_{CA})|0\rangle_B + \frac{1}{2}b(|\phi^+\rangle_{CA} - |\phi^-\rangle_{CA})|1\rangle_B$$

$$= \frac{1}{2}\underline{\underline{|\phi^+\rangle_{CA}}}\underbrace{(a|0\rangle_B + b|1\rangle_B)}_{|\psi_B\rangle} + \frac{1}{2}\underline{\underline{|\psi^+\rangle_{CA}}}\underbrace{(a|1\rangle_B + b|0\rangle_B)}_{\hat{\sigma}_x|\psi_B\rangle}$$

投影到CA的

四个Bell态上、 $+\frac{1}{2}\underline{\underline{|\psi^-\rangle_{CA}}}\underbrace{(a|1\rangle_B - b|0\rangle_B)}_{-i\hat{\sigma}_y|\psi_B\rangle} + \frac{1}{2}\underline{\underline{|\phi^-\rangle_{CA}}}\underbrace{(a|0\rangle_B - b|1\rangle_B)}_{\hat{\sigma}_z|\psi_B\rangle}$

对通纠缠的A、B传输C的状态☆.