1. Cauchy – Schwartz $\|\psi\|\|\varphi\| \geq |(\psi,\varphi)|$

2. 厄密阵 $A=(A^*)^T=A^\dagger$ $\lambda\in\mathbb{R}$, $\langle a_i|a_j\rangle=\delta_{ij}$ 一定可对角

3. 酉阵 $U^\dagger U = U U^\dagger = I$ $|\lambda_i|=1$ 行/列向量正交归一 $\psi^2 \sim e^{i\gamma}\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix}$

4. 表象基变换 $U=\sum_r |b^{(r)}\rangle\langle a^{(r)}|$ e.g Hadamard $U=|x+\rangle\langle z+|+|x-\rangle\langle x-| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$

5. 投影算子 ① $\Pi_i=\Pi_i^\dagger$ ② $\Pi_i\Pi_j=\delta_{ij}\Pi_i$ ③ $\Pi_i^2=\Pi_i$ ④ $\lambda=1$ or 0 ⑤ $\sum_i\Pi_i=I$

子空间投影 $\Pi^S=\sum_{j=1}^{n}|a_{ij}\rangle\langle a_{ij}|$ 子空间S上基向量

6. $[A,B]=0 \Rightarrow$ 共同本征态

7. 密度算子 ρ ① $Tr(\rho)=1$ ② $\rho=\rho^\dagger$ ③ 半正定

8. $\vec{n}=(\sin\theta\cos\varphi\quad \sin\theta\sin\varphi\quad \cos\theta) \longrightarrow \sigma_n$ $|n+\rangle=\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\varphi}\end{pmatrix}$ $|n-\rangle=\begin{pmatrix}-\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2}e^{i\varphi}\end{pmatrix}$

$|n\pm\rangle\langle n\pm| = \frac{1\pm\sigma_n}{2}$

9. $\rho=\frac{I+\vec{r}\cdot\vec{\sigma}}{2}$ $r_i=Tr(\rho\sigma_i)$

$\begin{cases} A=a_0 I + a_i\sigma_i \\ a_i=\frac{1}{2}Tr(A\sigma_i)\end{cases}$

10. $Tr(\rho_1\rho_2)=\frac{1}{2}+\frac{1}{2}\vec{r_1}\cdot\vec{r_2}$

11. $(A,B)=Tr(A^\dagger B)$

12. $U(z,\varphi)=e^{-i\frac{\varphi}{2}\sigma_z}$ 绕z转φ角

13. $e^{A}Be^{-A}=B+[A,B]+\frac{1}{2!}[A,[A,B]]+\cdots$

14. $[A,[A,B]]=[B,[A,B]]=0 \Rightarrow e^{A+B}=e^{A}e^{B}e^{-\frac{1}{2}[A,B]}$

15. $\begin{cases} i\hbar\frac{d|\psi(t)\rangle}{dt}=H|\psi(t)\rangle \\ i\hbar\frac{d\rho(t)}{dt}=[H,\rho(t)]\end{cases}$ $U(t)=\begin{cases} ① \frac{\partial H}{\partial t}=0 \Rightarrow e^{-iHt/\hbar} \\ ② [H(t_1),H(t_2)]=0 \Rightarrow U=e^{-\frac{i}{\hbar}\int_0^t H(t')dt'}\end{cases}$

16. $\frac{d}{dt}\langle A\rangle(t)=\frac{1}{i\hbar}\langle[A,H]\rangle+\langle\frac{\partial A}{\partial t}\rangle$

17. $H\sim a\sigma_z+b\sigma_x\sim\sigma_n$

18. $U(t)=e^{-i\frac{\omega_0 t}{2}\sigma_z} \Rightarrow \sigma_x(t)=\sigma_x\cos\omega_0 t-\sigma_y\sin\omega_0 t$.

19. 总相 $\gamma=\arg\langle\psi(t_0)|\psi(t)\rangle$ 动力学相 $\gamma_d=-i\int_0^t\langle\psi(t)|\dot{\psi}(t)\rangle dt$

$\langle\psi|\dot{\psi}\rangle=0 \Rightarrow$ 平行输运(有且仅有一条) 几何相 $\longrightarrow$ 立体角一半

20. Bell 测量 $\begin{cases}|\Psi\pm\rangle=\frac{1}{\sqrt{2}}(|01\rangle\pm|10\rangle)\\ |\Phi\pm\rangle=\frac{1}{\sqrt{2}}(|00\rangle\pm|11\rangle)\end{cases}$ 最大纠缠态

21. 不相容: $|\langle\psi|\varphi\rangle|\in(0,1)$ $|\langle\psi|\varphi\rangle|=\frac{1}{\sqrt{N}} \longrightarrow$ 互补

22. 2体泡利基: $I\otimes I$ $I\otimes\sigma_i$ $\sigma_i\otimes I$ $\sigma_i\otimes\sigma_j$

$\rho=\frac{1}{4}[I\otimes I+\vec{r}\cdot\vec{\sigma}\otimes I+I\otimes\vec{\sigma}\cdot\vec{s}+\sum_{m,n}t_{mn}\sigma_m\otimes\sigma_n]$

23. $e^{-i\tau\sigma_z\otimes\sigma_z}=I\otimes I\cos\tau-i\sigma_z\otimes\sigma_z\sin\tau$

24. 仪器初态 eg. $\sigma_z\otimes\sigma_y \longrightarrow$ $|0\rangle$ 测 $\langle\sigma_x\rangle$ $|x+\rangle$ 测 $\langle\sigma_z\rangle$ $|y+\rangle$ × 三个量互补

25. Kraus 算子 $K_\mu=\langle\mu|U|\varphi\rangle$ (M基矢, M初态) $\sum_\mu K_\mu^\dagger K_\mu=I$

要求初态为直积态 $\rho^Q(t)=\sum_\mu K_\mu(t)\rho^Q(0)K_\mu^\dagger(t)$

一般情况 $\rho^Q(t)=Tr_M[U(t)\rho(0)U^\dagger(t)]$ $p_\mu=Tr(\underbrace{K_\mu^\dagger K_\mu}_{E_\mu}\psi)$ 多对一

① 半正定 $\sum_\mu E_\mu=I$

26. $\frac{I}{2}\equiv\frac{1}{4}(\rho+\sigma_x\rho\sigma_x+\sigma_y\rho\sigma_y+\sigma_z\rho\sigma_z)$

27. 仪测量 $E_1=c|\psi_2^\perp\rangle\langle\psi_2^\perp|$, $E_2=c|\psi_1^\perp\rangle\langle\psi_1^\perp|$ $E_3=I-E_1-E_2$

$p^{failure}=Tr(E_3\rho)$ $\min=|\langle\psi_1|\psi_2\rangle|$

$$\begin{cases} [R_i, f] = i\hbar \frac{\partial f}{\partial P_i} \\ [P_i, f] = -i\hbar \frac{\partial f}{\partial R_i} \end{cases}$$

$$U^{-1} f(A) U = f(U^{-1} A U)$$

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

循环置换

$$\begin{cases} U|\psi_k\rangle = u_k |\psi_k\rangle \\ |\psi_k\rangle\langle\psi_k| = \frac{1}{n}\sum_{l=1}^{n} \left(\frac{U}{u_k}\right)^l \end{cases}$$

$$\begin{cases} \varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, \psi(x) e^{-ipx/\hbar} \\ \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp\, \varphi(p) e^{ipx/\hbar} \end{cases}$$

$$\begin{cases} e^{-iq_l P} Q e^{-iq_l P} = Q - q_l \mathbb{1} \\ e^{ip_k Q} P e^{-ip_k Q} = P - p_k \mathbb{1} \\ [Q, P] = i\mathbb{1} \end{cases}$$

$$\begin{cases} \delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(x-x_0)} dk \\ \delta(ax) = \frac{1}{|a|} \delta(x) \end{cases}$$

S-G实验

$$e^{-iL(t)\sigma_z \otimes P} = \begin{pmatrix} e^{-iL(t)P} & \\ & e^{iL(t)P} \end{pmatrix}$$

$$I_{ij} = \int_{-\infty}^{+\infty} \varphi_i(P_z, t)\varphi_j^*(P_z, t)\, dP_z$$

$$\varphi_i = \varphi\left(P_z - (-1)^i g t\right)$$

$$H = -g\sigma_z \otimes z \qquad \rho^{spin}(t) = \begin{pmatrix} |c_0|^2 & c_0 c_1^* I_{01}(t) \\ c_0^* c_1 I_{10}(t) & |c_1|^2 \end{pmatrix}$$

$$H = v(t)\sigma_z \otimes P \qquad \begin{cases} \eta = \alpha\varphi(q-L)|0\rangle + \beta\varphi(q+L)|1\rangle \\ L = \int_0^t v(\tau) d\tau \end{cases} \qquad \rho^{spin}(t) = \int dq\, |\eta\rangle\langle\eta|$$

$$\mathrm{prob}(\alpha) = \int_{a_1}^{a_2} dq \left[|\alpha|^2 |\varphi(q-L)|^2 + |\beta|^2 |\varphi(q+L)|^2 \right]$$

谐振子

$$[a, a^+] = \mathbb{1} \qquad [N, a] = -a \qquad [N, a^+] = a^+$$

$$H|n\rangle = \hbar\omega(n+\tfrac{1}{2})|n\rangle \qquad a|n\rangle = \sqrt{n}|n-1\rangle \qquad a^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$\begin{cases} x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^+) \\ p = i\sqrt{\frac{m\hbar\omega}{2}}(a^+ - a) \end{cases} \qquad \begin{cases} a(t) = a(0)e^{-i\omega t} \\ a^+(t) = a^+(0)e^{i\omega t} \end{cases} \qquad \begin{cases} x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \\ p(t) = -m\omega x(0)\sin\omega t + p(0)\cos\omega t \end{cases}$$

$$|n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|0\rangle = \sqrt{\frac{\beta}{\sqrt{\pi}\, 2^n n!}} \underbrace{H_n(\beta x)}_{\text{Hermite 多项式}} e^{-\frac{1}{2}\beta^2 x^2}$$

$$\begin{cases} \langle x | 0 \rangle = \frac{\sqrt{\beta}}{\sqrt[4]{\pi}} e^{-\frac{1}{2}\beta^2 x^2} \\ \beta = \sqrt{\frac{m\omega}{\hbar}} \end{cases}$$

$$\Delta x \Delta p = (n+\tfrac{1}{2})\hbar \qquad \text{宇称 } (-1)^n$$

相干态

$$\begin{cases} \langle\psi|a|\psi\rangle = \alpha \\ \langle\psi|a^+ a|\psi\rangle = |\alpha|^2 \end{cases} \xleftarrow{\text{2者等价}} a|\alpha\rangle = \alpha|\alpha\rangle$$

$$|\alpha(t)\rangle = e^{-\frac{i\omega t}{2}} |\alpha_0 e^{-i\omega t}\rangle$$

$$|\alpha\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle \quad \text{H表象} \quad f(n) = e^{-\frac{|\alpha|^2}{2}} \frac{\alpha^n}{\sqrt{n!}}$$

$$\begin{cases} \langle x\rangle(t) = \sqrt{\tfrac{2}{\beta}}\, \mathrm{Re}[\alpha_0 e^{-i\omega t}] \\ \langle p\rangle(t) = \sqrt{2}\hbar\beta\, \mathrm{Im}[\alpha_0 e^{-i\omega t}] \end{cases}$$

$$\begin{cases} D(\alpha) = e^{\alpha a^+ - \alpha^* a} = e^{\frac{i}{\hbar}(p_0 X - x_0 P)} \\ \quad = e^{-\frac{|\alpha|^2}{2}} e^{\alpha a^+} e^{\alpha^* a} \\ |\alpha\rangle = D(\alpha)|0\rangle \end{cases}$$

$$\int |\alpha\rangle\langle\alpha| d\alpha = \pi\mathbb{1}$$

$$\psi_\alpha(x) = e^{\frac{\alpha^{*2} - \alpha^2}{4}} e^{\frac{i}{\hbar}\langle P\rangle_\alpha x} \psi_0(x - \langle X\rangle_\alpha)$$

角动量

时空变换
$$\begin{cases} \text{本征值不变} & a_j' = a_j \\ \text{观测结果几率不变} & |c_j'| = |c_j| \end{cases}$$

$|\langle\psi'|\varphi'\rangle| = |\langle\psi|\varphi\rangle| \Rightarrow U$ 反酉 or 酉

向量算子
$$\begin{cases} [V_i, J_j] = i\varepsilon_{ijk}\hbar V_k \\ [J_i, V_j] = i\varepsilon_{ijk}\hbar V_k \\ [J^2, J_n] = 0 \\ [\vec{L}, p^2] = [\vec{L}, x^2] = 0 \end{cases}$$

标量算子
$$\begin{cases} [L^2, \vec{R}] = [L^2, \vec{S}] = 0 \\ [J_z, J_\pm] = \pm\hbar J_\pm \\ [J_+, J_-] = 2\hbar J_z \end{cases}$$

旋转
$$\begin{cases} U(n,\theta) = e^{-\frac{i}{\hbar}\vec{n}\cdot\vec{J}\theta} \\ \vec{R}' = \vec{R} - \delta\theta\, \vec{n}\times\vec{R} \quad \text{顺时针转动} \quad [J_n, \vec{R}] = -i\hbar\vec{n}\times\vec{R} \\ U(n,2\pi)|j,m\rangle = (-1)^{2j}|j,m\rangle \end{cases}$$

$$L^2 = R^2p^2 - (\vec{R}\cdot\vec{p})^2 + i\hbar\vec{R}\cdot\vec{p}$$

升降算子 $J_\pm = J_x \pm iJ_y$ $\qquad L_i = \dfrac{i\varepsilon_{ijk}(a_j a_k^\dagger - a_j^\dagger a_k)}{2}$ (指标不求和)

$$J_\pm|j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\,|j,m\pm1\rangle$$

$$\begin{cases} \langle x'|L_\pm|\alpha\rangle = -i\hbar e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\varphi}\right)\langle x'|\alpha\rangle \\ \langle x'|L_x|\alpha\rangle = -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\langle x'|\alpha\rangle \\ \langle x'|L_y|\alpha\rangle = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)\langle x'|\alpha\rangle \\ \langle x'|L_z|\alpha\rangle = -i\hbar\frac{\partial}{\partial\varphi}\langle x'|\alpha\rangle \end{cases}$$

$j=1$
$$\begin{cases} J_+ = \hbar \begin{array}{c} \begin{array}{ccc} m=1 & 0 & -1 \end{array} \\ \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \end{array} \\ J_- = \hbar\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ J_x = \frac{\hbar}{2}\begin{pmatrix} & \sqrt{2} & \\ \sqrt{2} & & \sqrt{2} \\ & \sqrt{2} & \end{pmatrix} \\ J_- = \frac{\hbar}{2}\begin{pmatrix} & -\sqrt{2}i & \\ \sqrt{2}i & & -\sqrt{2}i \\ & \sqrt{2}i & \end{pmatrix} \end{cases}$$

$$D^{(j)}_{m'm} = \langle j,m'|U(\alpha,\beta,\gamma)|j,m\rangle = e^{-i(\alpha m' + \gamma m)}d^{(j)}_{m'm}(\beta)$$
$$Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}}\,D^{(l)}_{m,0}(\varphi,\theta,0)\}^*$$

角动量相加 $J_i = \sum J_i$

$|j_1,j_2;m_1,m_2\rangle$

$|j_1,j_2;j,m\rangle$

$$\begin{cases} [J^2, J^{A2}] = 0 \\ [J, J^{A2}] = 0 \\ [J_z, J_z^A] = 0 \end{cases} \qquad [J^2, J_z^A] \neq 0$$

$$J^2 = (J^A)^2 + (J^B)^2 + 2J_z^A J_z^B + J_+^A J_-^B + J_-^A J_+^B$$
$$\Rightarrow 2\vec{S_1}\cdot\vec{S_2} = 2S_{1z}S_{2z} + S_{1+}S_{2-} + S_{1-}S_{2+}$$

$$|l+\tfrac{1}{2},m\rangle = \frac{1}{\sqrt{2l+1}}\begin{pmatrix} \sqrt{l+m+\frac{1}{2}} \\ \sqrt{l-m+\frac{1}{2}} \end{pmatrix} \begin{array}{l} |m-\frac{1}{2},\frac{1}{2}\rangle \\ |m+\frac{1}{2},-\frac{1}{2}\rangle \end{array}$$

$$|l-\tfrac{1}{2},m\rangle = \frac{1}{\sqrt{2l+1}}\begin{pmatrix} -\sqrt{l-m+\frac{1}{2}} \\ \sqrt{l+m+\frac{1}{2}} \end{pmatrix} \begin{array}{l} |m-\frac{1}{2},\frac{1}{2}\rangle \\ |m+\frac{1}{2},-\frac{1}{2}\rangle \end{array}$$

标量算子 $[A, J_n] = 0 \Rightarrow \mathcal{H}_j$ 中 $A \propto \mathbb{I}$

向量算子 $\vec{V} = \dfrac{\langle\vec{J}\cdot\vec{V}\rangle}{\langle J^2\rangle_j}\vec{J}$ $\qquad \vec{V}\propto\vec{J}$ $\qquad \vec{R}\ \ \vec{P}\ \ \vec{J}$

全同粒子
$$\begin{cases} S_{12} = \frac{1}{2}(1 + P_{12}) & \text{对称化算子} \\ A_{12} = \frac{1}{2}(1 - P_{12}) & \text{反对称化算子} \end{cases}$$

波函数连续；$V(r)$有限 $\longrightarrow \psi''$有限 $\rightarrow \psi'$连续

$V(\vec{r}) = V(x) + V(y) + V(z) \longrightarrow$ 分离变量求解　e.g. $\begin{cases} E_{n_x,n_y,n_z} = (n+\frac{3}{2})\hbar\omega \\ n = n_x+n_y+n_z \end{cases}$

$V(\vec{r}) = V(r) \longrightarrow$ 球坐标分离变量

$$\begin{cases} \nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} \\ \nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{(r\sin\theta)^2}\frac{\partial^2}{\partial\varphi^2} \\ \quad = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{1}{r^2}\frac{L^2}{\hbar^2} = -\frac{1}{\hbar^2}(p_r^2 + \frac{L^2}{r^2}) \\ \vec{L} = \vec{R}\times\vec{P} = -i\hbar(\hat{\varphi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}) \\ P_r = -i\hbar(\hat{R}\cdot\nabla + \frac{1}{r}) = -i\hbar(\frac{\partial}{\partial r} + \frac{1}{r}) \\ \frac{P^2}{2m} = \frac{P_r^2}{2m} + \frac{L^2}{2mr^2} \end{cases}$$

$u(r) = rR(r)$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]}_{V_{eff}} u = Eu$$

$$\Rightarrow \begin{cases} \psi(\vec{r}) = ru\, Y_l^m(\theta,\varphi) \\ \int_0^{+\infty}|u(r)|^2 dr = 1, \quad u(r) \xrightarrow{r\to\infty} 0 \\ \text{无量纲化} \quad \frac{1}{\rho^2}\frac{d}{d\rho}(\rho^2\frac{dR}{d\rho}) + [\frac{n}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2}]R = 0 \end{cases}$$

$$\Rightarrow \begin{cases} R(\rho) = \rho^k L(\rho) e^{-\frac{\rho}{2}} \quad (k=l) \\ L(\rho) = L_{n+l}^{2l+1}(\rho) \end{cases}$$

ψ_{100}	$\frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$
ψ_{200}	$\frac{1}{\sqrt{8\pi a_0^3}}(1-\frac{r}{2a_0})e^{-\frac{r}{2a_0}}$
ψ_{211}	$-\frac{1}{8\sqrt{\pi a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\sin\theta e^{i\varphi}$
ψ_{210}	$\frac{1}{4\sqrt{2\pi a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\cos\theta$
ψ_{21-1}	$\frac{1}{8\sqrt{\pi a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\sin\theta e^{-i\varphi}$

$$\begin{cases} \psi_{nlm} = -\sqrt{\frac{4(n-l-1)!}{(na_0)^3 n[(n+l)!]^3}}\rho^l L_{n+l}^{2l+1}(\rho)e^{-\frac{\rho}{2}}Y_l^m(\theta,\varphi) \\ \rho = \frac{2r}{na_0} \\ a_0 = \frac{\hbar^2}{\mu e^2} \end{cases}$$

$$Y_l^m(\theta,\varphi) = \langle\theta,\varphi|l,m\rangle = C e^{im\phi}P_l^m(\cos\theta)$$
$$= (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}e^{im\phi}P_l^{|m|}(\cos\theta)$$

$$\begin{cases} Y(\theta,\varphi+2\pi) = Y(\theta,\varphi) \Rightarrow m\text{为整数} \\ |P_{l,m}(\pm1)| < \infty \Rightarrow l\text{非负整数 且 } l\geq|m| \\ \text{宇称} \quad (-1)^l \end{cases}$$

$$Y_l^m(\theta,\phi) \equiv \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi},$$

$$\langle\hat{n}|l,l\rangle = Y_l^l(\theta,\varphi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}e^{il\varphi}\sin^l\theta$$

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta}} = \sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l(\cos\theta) \qquad P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}Y_l^{m*}(\theta_1,\phi_1)Y_l^m(\theta_2,\phi_2)$$

$$\int Y_l^m(\theta,\varphi)d\Omega = \sqrt{4\pi}\,\delta_{l0}\delta_{m0} \quad (\text{与 } Y_0^0 \text{ 正交性})$$

H原子(2体系统)
$$\begin{cases} H = \frac{P_p^2}{2m_p} + \frac{P_e^2}{2m_e} - \frac{e^2}{|\vec{R}_p - \vec{R}_e|} \\ \vec{P} = \frac{\sum m_i p_i}{\sum m_i} \qquad \vec{P}_c = \sum P_i \qquad \mu = \frac{m_1m_2}{m_1+m_2} \\ H = \frac{P_c^2}{2(\sum m_i)} + \frac{p^2}{2\mu} - \frac{e^2}{|R|} \end{cases}$$

$$\longrightarrow -\frac{\hbar^2}{2\mu}\nabla^2\psi - \frac{e^2}{r}\psi = E\psi$$

z	200	211	210	21-1
200			*	
211				
210	*			
21-1				

非0元 $\begin{cases} m = m' \\ \Delta l = \pm1 \end{cases}$

选择定则　$\langle n'l'm'|[L_z, R_i]|nlm\rangle \Rightarrow$ 非0元　　$\langle n'l'm'|R_i|nlm\rangle$　$m' = m$，$m'-m = \pm1$　　$\Delta m = 0, \pm1$

$\langle n'l'm'|[L^2,[L^2,\vec{R}]]|nlm\rangle \Rightarrow$ 非0元　$\Delta l = \pm1$

$$\psi(\vec{R},t) = \sqrt{\rho(\vec{R},t)}\, e^{\frac{iS(\vec{R},t)}{\hbar}} \Rightarrow j = \frac{\rho \nabla S}{m}$$

$$\begin{cases} H = \frac{p^2}{2m} + V \\ \vec{j}(\vec{r},t) = -\frac{i\hbar}{2m}(\psi^* \nabla\psi - \psi\nabla\psi^*) = \frac{\hbar}{m} Im(\psi^*\nabla\psi) = Re[\psi^* V \psi] \\ V = \frac{p}{m} = -\frac{i\hbar}{m}\nabla \end{cases}$$

$$\begin{cases} H = \frac{(p-qA)^2}{2m} + q\phi = \frac{mV^2}{2} + q\phi \\ \vec{j} = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \psi^* \frac{qA}{m}\psi = Re[\psi^* V\psi] \\ V = \frac{p-qA}{m} \\ [R_j, V_k] = \frac{i\hbar}{m}\delta_{jk} \qquad [V_j, V_k] = \frac{i\hbar q}{m^2}\epsilon_{jkl}B_l \\ \langle m\frac{d\vec{V}}{dt}\rangle = q\langle\vec{E}\rangle + \frac{1}{2}q(\vec{V}\times\vec{B} - \vec{B}\times\vec{V}) \end{cases}$$

规范变换 $\begin{cases} \vec{A}' = \vec{A} + \nabla\chi \\ \phi' = \phi - \frac{\partial\chi}{\partial t} \end{cases} \Rightarrow \begin{cases} \psi' = \psi e^{\frac{iq}{\hbar}\chi} \\ \langle\vec{V}\rangle_{\psi'} = \langle\vec{V}\rangle_{\psi} \quad V_i' = V_i \text{ (本征值)} \\ \vec{j}' = \vec{j} \text{ (几率流)} \end{cases}$

$\vec{B} = B\hat{z} \Rightarrow [V_z, V_i] = 0 \Rightarrow H = H_{xy} + H_z = \frac{1}{2}\frac{\hbar qB}{m}(P'^2 + Q'^2) + \frac{mV_z^2}{2}$ (7-5)

$E_n = (n+\frac{1}{2})\frac{\hbar qB}{m} + \frac{1}{2}mV_z^2$

设 $\vec{A} = -yB\hat{x}$ $\quad H = \frac{1}{2m}[(P_x + yqB)^2 + P_y^2 + P_z^2]$ $\quad [H, P_x] = [H, P_z] = 0$

$\Rightarrow$ 设 $\psi = e^{i(k_x x + k_z z)}\varphi(y) \xrightarrow{S\text{方程}}$ 求解 $\varphi(y)$

$\nabla\cdot\vec{A} \Rightarrow \vec{A}\cdot\vec{P} = \vec{P}\cdot\vec{A}$

H本征向量波函数

传播子 $\begin{cases} K(2,1) = \langle\vec{r_2}|U(t_2,t_1)|\vec{r_1}\rangle = \sum_k u_k^*(\vec{r_1})u_k(\vec{r_2})e^{-iE_k(t_2-t_1)/\hbar} \quad (t_2 > t_1) \\ \psi(\vec{r_2},t_2) = \int d^3r_1\, K(2,1)\psi(\vec{r_1},t_1) \end{cases}$

$[i\hbar\frac{\partial}{\partial t} - H]K(2,1) = i\hbar\delta(t_2-t_1)\sum_k u_k^*(\vec{r_1})u_k(\vec{r_2})e^{-iE_k(t_2-t_1)/\hbar}$

对称性 $\quad \pi = \pi^{-1} = \pi^{\dagger} \quad [\pi, \vec{J}] = 0 \quad \{\pi, \vec{R}\} = \{\pi, \vec{P}\} = 0$

$\begin{cases} [A, \pi] = 0 \\ |\alpha\rangle \text{ 非简并} \end{cases} \Rightarrow |\alpha\rangle$ 有确定宇称

$\pi|l, m\rangle = (-1)^{l_1+l_2}$

$\begin{cases} [H, \pi] = 0 \\ |n\rangle \text{ 无简并} \end{cases} \Rightarrow \langle n|D|n\rangle = 0$

偶极矩

反线性算子 $\begin{cases} AC = C^*A \\ \langle\psi|\varphi\rangle = \langle\psi'|\varphi'\rangle^* \end{cases}$

$\Theta^2|\psi\rangle = \pm|\psi\rangle$

$[H, \Theta] = 0 \Rightarrow \begin{cases} |\psi(t)\rangle \\ \Theta|\psi(-t)\rangle \end{cases}$

$V(r) \in \mathbb{R}$

$\Theta\psi(\vec{r},t) = \psi^*(\vec{r},t)$

$\Theta|l,m\rangle = (-1)^m|l,m\rangle$

$\Theta\psi(\vec{p}) = \psi^*(-\vec{p})$

自旋 $\quad \Theta = e^{-i2\pi S_y/\hbar}K$

$\Theta|j,m\rangle = i^{2m}|j,-m\rangle$

微扰论 $|n\rangle \times$ 归一化因子

无t，非简并

(十-I) 一级 $E_n^{(1)} = \langle n^{(0)}|\,V\,|n^{(0)}\rangle = V_{nn}$.

$$|n^{(1)}\rangle = \sum_{m\neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}\,|m^{(0)}\rangle .$$

无t，简并

$$\underbrace{V\sum_{\mu} c_{n,\mu}\,|n^{(0)},\mu\rangle}_{\text{简并子空间}} = E_n^{(1)}\underbrace{\sum_{\nu} c_{n,\nu}\,|n^{(0)},\nu\rangle}_{\text{本征向量}} \qquad \underbrace{E_n = E_n^{(0)} + E_{n,\lambda}^{(1)}}_{\text{本征值}}$$

二级

$$E_n^{(2)} = \sum_{m\neq n} \frac{\langle m^{(0)}|\,V\,|n^{(0)}\rangle\,\langle n^{(0)}|\,V\,|m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} = \sum_{m\neq n}\frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$|n^{(2)}\rangle = \sum_{\ell\neq n}\sum_{m\neq n}\frac{V_{m\ell}V_{\ell n}}{(E_n^{(0)}-E_\ell^{(0)})(E_n^{(0)}-E_m^{(0)})}\,|m^{(0)}\rangle - \sum_{m\neq n}\frac{V_{nn}V_{mn}}{(E_n^{(0)}-E_m^{(0)})^2}\,|m^{(0)}\rangle$$

(十-II). eg

① Stark 效应（m=0 分裂） $H = \frac{p^2}{2m} - \frac{e^2}{R} - e\mathcal{E}z$ 简并微扰

② S-O $(\sim\alpha^2)$ $H = \frac{p^2}{2m} + V(r) + W(r)\,\vec L\cdot\vec S \to \frac{1}{2}(J^2 - L^2 - S^2)$ 对角 简并微扰

不同j 解除简并

③ Zeeman 效应 简并完全解除 简并微扰

$$\begin{cases} \vec A = \frac{1}{2}(\vec B\times\vec R), \quad \vec B = B\hat z \\ H = \frac{p^2}{2m} - \frac{e}{2mc}\vec B\cdot\vec L + \frac{e^2}{8mc^2}(\vec B\times\vec R)^2 + V(R) - \vec\mu\cdot\vec B + W(r)\,\vec L\cdot\vec S \end{cases}$$

1) 无自旋 弱场 $H = H_0 - \frac{eB}{2mc}L_z \to$ 对角

2) 无自旋 强场

3) 自旋 弱场 $H' = \lambda\vec L\cdot\vec S + \mu L_z + \nu S_z \to$ 非对角，考虑矩阵元 $\langle j',m'|S_z|j,m\rangle$

对角

(十-III) ③ 相对论修正 $(\sim\alpha^2)$ $H = mc^2 + H_0 + W_{mv} + H_{S-L} + W_D$

$W_{mv} \propto p^4$，$H_{S-L} \propto \frac{1}{R}\frac{dV}{dR}\vec L\cdot\vec S$，$W_D \to$ 抬升S态，$W_D \propto \nabla^2 V(R)$

$\Rightarrow$ $2S_{\frac12}$ 与 $2P_{\frac12}$ 简并

(十-III-7) 含时微扰 $|\psi(t)\rangle = \sum_n c_n(t)e^{-iE_n^{(0)}t/\hbar}\,|n^{(0)}\rangle$ $\quad i\hbar\frac{\mathrm{d}c_m(t)}{\mathrm{d}t} = \sum_n \langle m^{(0)}|V(t)|n^{(0)}\rangle\, e^{i\omega_{mn}t}c_n(t)$ $\quad \omega_{mn} = \frac{E_m^{(0)} - E_n^{(0)}}{\hbar}$

$V \to \lambda V \Rightarrow c_m^{(0)}(t) = c_m(0)$ $\quad i\hbar\frac{\mathrm{d}c_m^{(1)}}{\mathrm{d}t} = \sum_n \langle m^{(0)}|V(t)|n^{(0)}\rangle\, e^{i\omega_{mn}t}c_n^{(0)}(t)$

① $[0,T]$ 内介入，初态为 $|i\rangle$ $\quad c_i^{(1)}(t) = \frac{1}{i\hbar}\int_0^t V_{ii}(t')\,\mathrm{d}t'$ 对 $|i\rangle$ 相位修正

$c_f^{(1)}(T) = \frac{1}{i\hbar}\int_0^T \langle f|V(t)|i\rangle\, e^{i\omega_{fi}t}\,\mathrm{d}t, \quad f\neq i$ 对 $|n\rangle \neq |i\rangle$ 有模修正

② 常微扰 $V(t) = \theta(t)V$（V 不随时间变化 $[V,H]=0$） $\Rightarrow c_f^{(1)}(t) = \frac{V_{fi}}{E_f - E_i}(1 - e^{i\omega_{fi}t})$

② 简谐微扰 $V(t) = V_0e^{-i\omega t} + V_0^{\dagger}e^{i\omega t}$

近似 $\begin{cases} \text{两峰较远} & t \gg \frac{1}{\omega_{fi}} \approx \frac{1}{\omega} \\ \text{相干项较小} & t \text{ 较大} \end{cases}$

一级近似 t 不能太大 $t \ll \frac{\hbar}{|\langle f|V_0|i\rangle|} \longrightarrow \hbar|\omega_{fi}| \gg |\langle f|V_0|i\rangle|$

Fermi 规则 $\underset{\text{跃迁速率}}{w_{i\to[f]}} = \frac{2\pi}{\hbar}|\langle E_f = E_i|V|i\rangle|^2\rho(E_f = E_i)$ $\quad (t\to\infty)$

③ Zeeman 效应. $\vec A = \vec A(\vec R, t)$ $\quad \vec A\cdot\vec P$ 形式微扰 $\longrightarrow$ 无自旋弱场

↓偶极近似

简谐微扰 $V_0 \propto P_z$ $(\vec A = A_0\hat z)$ $\xrightarrow[\text{无相干性}]{\text{不同}\,\omega\,\text{之间}}$ $P_{i\to f}(t)$

定理一：

设 $\psi(x)$ 是一维量子力学体系定态 Schrödinger 方程的属于能量本征值 E 一个解，则 $\psi^*(x)$ 也是其属于能量本征值 E 的解.

定理二：

对应于某个确定的能量本征值 E，总可以找到定态 Schrödinger 方程的一组实函数解，使得属于 E 的任何能量本征函数均可表达成这一组实函数解的线性叠加.

定理三：

设势场的势能具有空间反射不变性，即 $V(x) = V(-x)$. 在此情形下，如果 $\psi(x)$ 是定态 Schrödinger 方程属于能量本征值 E 的本征函数，则 $\psi(-x)$ 也是其属于同一能量本征值 E 的本征函数.

定理四：

设 $V(x) = V(-x)$，则定态 Schrödinger 方程的属于某个能量本征值 E 的任一线性独立能量本征函数，无论此能级简并与否，总可以选择为具有确定宇称的波函数.

定理五：

对于阶梯形方位势，

$$V(x) = \begin{cases} V_1, & x < a \\ V_2, & x > a \end{cases}$$

若差值 $(V_1 - V_2)$ 有限，则能量本征函数 $\psi(x)$ 及其一阶空间导数 $\psi'(x)$ 在 x 轴上各处必定是处处连续的.

定理六：

对于一维量子力学体系，若 $\psi_1(x)$ 和 $\psi_2(x)$ 是定态薛定谔方程属于同一能量本征值 E 的两个能量本征函数，则 Wronski 行列式

$$\begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix} = \psi_1\psi_2' - \psi_1'\psi_2$$

是一个与体系位置坐标无关的常数.

定理七：

设某一维量子力学体系在正常 (regular) 势场中运动，即 $V(x)$ 无奇点. 若体系存在束缚态，则其能级必定是不简并的.

定理八：

对于任一处于束缚态的一维量子力学体系而言，其能量本征值不会小于势能的最小值.

Proposition：

一维量子力学体系任一能级 E 的简并度最多为 2，$D(E) \leqslant 2$，即能量本征值 E 最多只存在两个线性独立的本征函数.

$W(\psi_1, \psi_2) = C_{12}$
$W(\psi_1, \psi_3) = C_{13}$

$\tilde{\psi} = C_{13}\psi_2 - C_{12}\psi_3$

Bloch Theorem:

周期势场中粒子的能量本征函数可以取为：

$$\psi(x) = e^{iKx}\Phi_K(x)$$

其中函数 $\Phi_K(x)$ 是周期函数，

$$\Phi_K(x + a) = \Phi_K(x)$$

参数 K 称为 Bloch 波数，它是可以在闭区间 $-\pi/a \leqslant K \leqslant \pi/a$ 上任意选择的.

- Jacobi 恒等式：

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$$

位力定理

$$2\langle\hat{T}\rangle = \langle\vec{r}\cdot\nabla V\rangle$$

$$\hat{T} = \hat{\vec{p}}^2/2m$$

1. 若势场是其位置坐标的 n 次齐次函数，

$$V(c\,x, c\,y, c\,z) = c^n V(x, y, z)$$

式中 c 为一任意常参数，则 $\vec{r}\cdot\nabla V = nV$.

此情形下，Virial 定理简化为：

$$2\langle\hat{T}\rangle = n\langle V\rangle$$

$$\frac{\partial E_n}{\partial\lambda} = \left\langle \psi_n(\lambda) \middle| \frac{\partial\hat{H}(\lambda)}{\partial\lambda} \middle| \psi_n(\lambda) \right\rangle$$

λ为实参数

简并，若 $\begin{cases} [A, H] = [B, H] = 0 \\ [A, B] \neq 0 \end{cases}$ $|\alpha\rangle$ 不平行于 $B|\alpha\rangle$