	δ势	线性	谐振子	库仑$\kappa = Ze^2$
	$\mu = \hbar = \gamma = 1$	$\mu = \hbar = F = 1$	$\mu = \hbar = \omega = 1$	$\mu = \hbar = \kappa = 1$
能量$[E]$	$\mu\gamma^2/\hbar^2$	$(\hbar^2 F^2/\mu)^{1/3}$	$\hbar\omega$	$\mu\kappa^2/\hbar^2$
长度$[L]$	$\hbar^2/\mu\gamma$	$(\hbar^2/\mu F)^{1/3}$	$\sqrt{\hbar/\mu\omega}$	$\hbar^2/\mu\kappa$
时间$[T]$	$\hbar^3/\mu\gamma^2$	$(\hbar\mu/F^2)^{1/3}$	$1/\omega$	$\hbar^3/\mu\kappa^2$
速度$[v]$	$\gamma/\hbar$	$(\hbar F/\mu^2)^{1/3}$	$\sqrt{\hbar\omega/\mu}$	$\kappa/\hbar$
动量$[p]$	$\mu\gamma/\hbar$	$(\hbar\mu F)^{1/3}$	$\sqrt{\hbar\mu\omega}$	$\mu\kappa/\hbar$

1. 数学速查

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

$$\sum_{i=1}^{3} \varepsilon_{ijk}\varepsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

$$\left(\vec{A} \times \vec{B}\right)_k = \sum_{ij} \varepsilon_{kij} A_i B_j$$

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \frac{1}{r}\hat{\theta}\frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta}\hat{\phi}\frac{\partial}{\partial \phi}$$

$$\nabla \cdot \vec{u} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 u_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta u_\theta) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}u_\phi$$

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

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

定义 *1.1* (**连带 Legendre 多项式**):

$$(1-\xi^2)\frac{\mathrm{d}^2 P}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}P}{\mathrm{d}\xi} + \left(l(l+1) - \frac{m^2}{1-\xi^2}\right)P = 0$$

$$P_l^m(x) = \frac{1}{2^l l!}(1-x^2)^{\frac{m^2}{2}}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}(x^2-1)^l$$

定理 *1.2* (**连带 Legendre 多项式的正交性**):

$$\int_{-1}^{1} P_k^m(\xi)P_l^m(\xi)\,\mathrm{d}\xi = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{kl}$$

定义 *1.3* (**Legendre 多项式**):

$$P_l(x) = \frac{1}{2^l l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2-1)^2$$

定理 *1.4* (**Legendre 多项式的正交性**):

$$\int_{-1}^{1} P_k(x)P_l(x)\,\mathrm{d}x = \frac{2}{2l+1}\delta_{kl}$$

定理 *1.5* (**厄米多项式的正交性**):

$$\int_{-\infty}^{+\infty} H_m(\xi)H_n(\xi)e^{-\xi^2}\,\mathrm{d}\xi = \sqrt{\pi}2^n n!\delta_{mn}$$

定理 *1.6* (**厄米多项式的递推关系**):

$$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2nH_{n-1}(\xi) = 0$$

定义 *1.7* (**合流超几何微分方程**):

$$z\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + (\gamma - z)\frac{\mathrm{d}y}{\mathrm{d}z} - \alpha y = 0$$

定义 *1.8* (**合流超几何函数**):

$$F(\alpha, \gamma, z) = \sum_{k=0}^{\infty}\frac{\alpha_k}{\gamma_k}\frac{z^k}{k!}$$

$$\text{where } \alpha_k = \alpha(\alpha+1)...(\alpha+k-1)$$
$$\gamma_k = \gamma(\gamma+1)...(\gamma+k-1)$$

定理 *1.9* (**δ函数的性质**):

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,\mathrm{d}k$$

$$x\delta(x) = 0$$

$$\delta(f(x)) = \sum_i \frac{\delta(x-x_i)}{|f'(x_i)|}$$

定义 *1.10* (**三维δ函数**): 假设已定义一维 Dirac 函数$\delta(x)$,那么

$$\begin{aligned}\delta(\vec{r}) &= \delta(x)\delta(y)\delta(z) \\ &= \frac{1}{r^2\sin\theta}\delta(r)\delta(\theta)\delta(\phi) \\ &= \frac{1}{\rho}\delta(\rho)\delta(\phi)\delta(z)\end{aligned}$$

定义 *1.11* (**球谐函数**):

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

$$Y_{00} = \frac{1}{\sqrt{4\pi}}, Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{2\pm1} = \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta e^{\pm i\phi}$$

$$Y_{2\pm2} = \frac{1}{2}\sqrt{\frac{15}{8\pi}}\sin^2\theta e^{\pm 2i\phi}$$

定理 *1.12* (**球谐函数的完备性**): 平方可积的球谐函数形成了一个希尔伯特空间

$$\iint Y_{l'm'}Y_{lm}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \delta_{ll'}\delta_{mm'}$$

$$\sum_{l=0}^{+\infty}\sum_{m=-l}^{+l} Y_{lm}(\theta, \phi)Y_{l'm'}^*(\theta', \phi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\phi-\phi')$$

定理 *1.13* (**球谐函数的递推性质**):

$$\begin{aligned}\frac{z}{r}Y_{lm} &= \cos\theta Y_{lm} \\ &= a_{lm}Y_{l+1,m} + a_{l-1,m}Y_{l-1,m}\end{aligned}$$

$$\begin{aligned}\frac{x+iy}{r}Y_{lm} &= e^{+i\phi}\sin\theta Y_{lm} \\ &= b_{l-1,-(m+1)}Y_{l-1,m+1} - b_{lm}Y_{l+1,m+1}\end{aligned}$$

$$\begin{aligned}\frac{x-iy}{r}Y_{lm} &= e^{-i\phi}\sin\theta Y_{lm} \\ &= -b_{l-1,m-1}Y_{l-1,m-1} + b_{l,-m}Y_{l+1,m-1}\end{aligned}$$

$$a_{lm} = \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}}$$

$$b_{lm} = \frac{\sqrt{(l+m+1)(l+m+2)}}{(2l+1)(2l+3)}$$

定理 *1.14* (**傅里叶变换**):

$$f(x) = \frac{1}{\sqrt{2\pi}}\int e^{ikx}g(k)\,\mathrm{d}k$$

$$g(k) = \frac{1}{\sqrt{2\pi}}\int e^{-ikx}f(x)\,\mathrm{d}x$$

定理 *1.15* (**正交对角化**):

$$A = PDP^{-1}$$

$$D = \begin{pmatrix}\lambda_1 & & \\ & ... & \\ & & \lambda_n\end{pmatrix}, P = \begin{pmatrix}v_1 & ... & v_n\end{pmatrix}$$

$$\int_{-\infty}^{+\infty} e^{-a^2x^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{|a|}$$

$$\int_0^{+\infty} r^n e^{-r/a}\,\mathrm{d}r = n!a^{n+1}$$

2. 算符

$$\vec{p} = -i\hbar\nabla$$

$$\vec{p}^2 = -\hbar^2\nabla\cdot\nabla$$

$$\begin{aligned}\vec{p}_r &= \frac{1}{2}(\hat{r}\cdot\vec{p} + \vec{p}\cdot\hat{r}) \\ &= -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \\ &= -\hbar^2\frac{1}{r^2}\frac{\partial^2}{\partial r^2}r^2\frac{\partial}{\partial r}\end{aligned}$$

$$\vec{p}^2 = \frac{1}{r^2}\vec{l}^2 + \vec{p}_r^2$$

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

$$[l_\alpha, x_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar x_\gamma$$

$$[l_\alpha, p_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar p_\gamma$$

$$[l_\alpha, l_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar l_\gamma$$

$$[\vec{r}, H] = \frac{i\hbar}{m}\vec{p}$$

公设 *2.1* (**Schödinger Equation**):

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

3. 中心力场

定理 *3.1* (**中心力场中运动粒子的哈密顿量**):

$$\begin{aligned}H &= \frac{p^2}{2\mu} + V(r) \\ &= \frac{p_r^2}{2\mu} + \frac{\vec{l}^2}{2\mu r^2} + V(r) \\ &= -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\vec{l}^2}{2\mu r^2} + V(r)\end{aligned}$$

定理 *3.2* (**中心力场中能量本征方程**): 一般将势函数分离变量为

$$\Psi(r, \theta, \phi) = R(r)Y_{lm}(\theta, \phi)$$

令$\chi(r) = rR(r)$,有

$$\chi_l'' + \left(\frac{2\mu}{\hbar^2}(E - V) - \frac{l(l+1)}{r^2}\right)\chi_l = 0$$

3.1. 三维各向同性谐振子

$$V(r) = \frac{1}{2}\mu\omega^2 r^2$$

能量本征值为

$$E_N = \left(N + \frac{3}{2}\right)\hbar\omega$$
$$N = 2n_r + l$$
$$n_r, l = 0, 1, 2, ...$$

简并度为

$$f_N = \frac{1}{2}(N+1)(N+2)$$

径向本征函数为

$$R_{n_r l}(r) = a^{l+3/2}\sqrt{\frac{2^{l+2-n_r}(2l+2n_r+1)!!}{\sqrt{\pi}n_r!((2l+1)!!)^2}}\, r^l e^{-a^2r^2/2}F\left(-n_r, l+\frac{3}{2}, a^2r^2\right)$$

如果在直角坐标系中求解,这两套本征态通过幺正变换联系起来

$$\varphi_{01m} = \sum_{n_x n_y n_z}\psi_{n_x n_y n_z}\int\psi_{n_x n_y n_z}^*\varphi_{01m}\,\mathrm{d}\tau$$

$$\begin{pmatrix}\varphi_{011} \\ \varphi_{01-1} \\ \varphi_{010}\end{pmatrix} = \begin{pmatrix}-\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\psi_{100} \\ \psi_{010} \\ \psi_{001}\end{pmatrix}$$

3.2. 氢原子

化为单体问题后有

$$V(r) = -\frac{e^2}{r}$$

定义 *3.2.1* (**Bohr 半径**): $a = \frac{\hbar^2}{\mu e^2}$

能量本征值为

$$E_n = -\frac{\mu e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{e^2}{2a}\frac{1}{n^2}$$
$$n = n_r + l + 1$$
$$n_r = 0, 1, 2, ...$$

径向本征函数为

$$R_{nl}(r) = \frac{2}{a^{3/2}n^2(2l+1)!}\sqrt{\frac{(n+1)!}{(n-l-1)!}}\, e^{-\xi/2}\xi^l F(-n_r, 2l+2, \xi)$$

$$\text{where } \xi = \frac{2r}{na}$$

$$R_{10} = \frac{2}{a^{3/2}}e^{-r/a}$$

$$R_{20} = \frac{1}{\sqrt{2}a^{3/2}}\left(1 - \frac{r}{2a}\right)e^{-r/2a}$$

$$R_{21} = \frac{1}{2\sqrt{6}a^{3/2}}\frac{r}{a}e^{-r/2a}$$

$$R_{30} = \frac{2}{3\sqrt{3}a^{3/2}}\left(1 - \frac{2r}{3a} + \frac{2}{27}\frac{r^2}{a^2}\right)e^{-r/3a}$$

本征函数为

$$\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \phi)$$

简并度为

$$f_n = \sum_{l=0}^{n-1}(2l+1) = n^2$$

统计意义上,电子的电流密度(绕 z 轴的环电流密度)为

$$\begin{aligned}\vec{j} &= \frac{ie\hbar}{2\mu}(\psi^*\nabla\psi - \psi\nabla\psi^*) \\ &= -\frac{e\hbar m}{\mu}\frac{1}{r\sin\theta}|\psi_{nlm}|^2\hat{e}_\phi\end{aligned}$$

总的磁矩为

$$\begin{aligned}\overrightarrow{M} &= -\frac{e\hbar m}{2\mu c}\hat{z}\int|\psi_{nlm}|^2\,\mathrm{d}\tau \\ &= -\frac{e\hbar m}{2\mu c}\hat{z}\end{aligned}$$

定义 *3.2.2* (**Bohr 磁子**):

$$\mu_B = \frac{e\hbar}{2\mu c}$$

定义 *3.2.3* (**Larmor 频率**):

$$\omega_L = \frac{eB}{2\mu c}$$

类氢离子(He^+, Li^{++}, ...)需将核电荷数$+e$换成$+Ze$,约化质量换成相应的μ

$$E_n = -\frac{\mu e^4}{2\hbar^2}\frac{Z^2}{n^2} = -\frac{e^2}{2a}\frac{Z^2}{n^2}$$

4. 角动量和自旋

4.1. 角动量

定义 *4.1.1* (**角动量**): $\vec{l} = \vec{r} \times \vec{p}$

$$l_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$l_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$l_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\vec{l} \times \vec{l} = i\hbar\vec{l}$$

$$\begin{aligned}\vec{l}^2 &= l_z^2 + l_y^2 + l_z^2 \\ &= -\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}l_z^2\end{aligned}$$

定义 *4.1.2* (**角动量升降算符**):

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

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

$$\vec{J}^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2$$

$$[J_+, J_-] = 2\hbar J_z, [J_z, J_\pm] = \pm\hbar J_\pm$$

$$[J_x, J_\pm] = \mp\hbar J_z, [J_y, J_\pm] = -\hbar J_z$$

$$\left[\vec{J}^2, J_\pm\right] = 0$$

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

4.2. 自旋

定义 4.2.1 (**Pauli 矩阵**):

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

$$\sigma_\alpha\sigma_\beta = \delta_{\alpha\beta} + i\sum_\gamma \varepsilon_{\alpha\beta\gamma}\sigma_\gamma$$

$$\sigma_\alpha = \sigma_\alpha^\dagger$$

定义 4.2.2 (**磁矩算符**):

$$\vec{\mu} = g\frac{\mu_B}{\hbar}\vec{j}$$

$$\vec{j} = \vec{s}, \vec{l}, g_l = -1, g_s = -2$$

定义 4.2.3 (**磁矩磁场相互作用能**):

$$W = -(\vec{\mu}_l + \vec{\mu}_s)\cdot\vec{B}$$

定义 4.2.4 (**旋量波函数**):

$$\psi(\vec{r}, s_z) = \begin{pmatrix}\psi_1(\vec{r}, +\frac{\hbar}{2})\\ \psi_2(\vec{r}, -\frac{\hbar}{2})\end{pmatrix}$$

在哈密顿量不含自旋或可以表示成与自旋部分之和的时候

$$\psi(\vec{r}, s_z) = \psi(\vec{r})\chi(s_z)$$

$$\alpha = \chi_{+1/2}(s_z) = \begin{pmatrix}1\\ 0\end{pmatrix}$$

$$\beta = \chi_{-1/2}(s_z) = \begin{pmatrix}0\\ 1\end{pmatrix}$$

4.3. 耦合与非耦合表象的基底变换

$$|j_1j_2jm\rangle = \sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} C^{j_1j_2jm}_{j_1m_1j_2m_2}|j_1m_1j_2m_2\rangle$$

$$C^{jm}_{j_1m_1j_2m_2} = \langle j_1m_1j_2m_2|j_1j_2jm\rangle$$

4.4. 电子耦合与非耦合表象变换

$$\Psi_{l,j=l+\frac{1}{2},m_j} = \frac{1}{\sqrt{2j}}\begin{pmatrix}\sqrt{j+m_j}\,Y_{l,m_j-\frac{1}{2}}\\ \sqrt{j-m_j}\,Y_{l,m_j+\frac{1}{2}}\end{pmatrix}$$

$$\Psi_{l,j=l-\frac{1}{2},m_j} = \frac{1}{\sqrt{2j+2}}\begin{pmatrix}-\sqrt{j-m_j+1}\,Y_{l,m_j-\frac{1}{2}}\\ \sqrt{j+m_j+1}\,Y_{l,m_j+\frac{1}{2}}\end{pmatrix}$$

$$Y_{lm_l}\chi_{\frac{1}{2}} = \sqrt{\frac{l+m_l+1}{2l+1}}\Psi_{l,j=l+\frac{1}{2},m_l+\frac{1}{2}} - \sqrt{\frac{l-m_l}{2l+1}}\Psi_{l,j=l-\frac{1}{2},m_l+\frac{1}{2}}$$

$$Y_{lm_l}\chi_{-\frac{1}{2}} = \sqrt{\frac{l-m_l+1}{2l+1}}\Psi_{l,j=l+\frac{1}{2},m_l-\frac{1}{2}} + \sqrt{\frac{l+m_l}{2l+1}}\Psi_{l,j=l-\frac{1}{2},m_l-\frac{1}{2}}$$

定义 4.4.1 (**自旋三重态与单态**): 选择 $\{\vec{S}^2, S_z\}$作为对易自旋力学量完全集

$$\vec{S}^2\chi_{SM_S} = S(S+1)\hbar^2\chi_{SM_S}$$

$$S_z\chi_{SM_S} = M_S\hbar\chi_{SM_S}$$

χ_{SM_S}	S	M_S
$\alpha_1\alpha_2$	1	1
$\frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \beta_1\alpha_2)$	1	0
$\beta_1\beta_2$	1	−1
$\frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \beta_1\alpha_2)$	0	0

$$(\vec{\sigma}_1\cdot\vec{\sigma}_2)^2 = 3 - 2\vec{\sigma}_1\cdot\vec{\sigma}_2$$

5. 定态微扰

$$H = H_0 + W$$

一些情况下,基态无简并,可用非简并微扰论处理基态,简并微扰论处理激发态.

5.1. 非简并微扰论

$$E_n^1 = \langle\psi_n^0|W|\psi_n^0\rangle = W_{nn}$$

$$\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|W|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$$

$$E_n^2 = \langle\psi_n^0|W|\psi_n^1\rangle = \sum_{m\neq n}\frac{|W_{mn}|^2}{E_n^0 - E_m^0}$$

5.2. 简并微扰论

对某能级n

$$|\psi^0\rangle = \sum_{\mu=1}^{f_n} a_\mu|\psi^0_{n\mu}\rangle$$

$$\sum_\mu (W_{\mu'\mu} - E_n^1\delta_{\mu'\mu})a_\mu = 0$$

$$\det(W_{\mu'\mu} - E_n^1\delta_{\mu'\mu}) = 0$$

$$E_n^1 = E_{n\alpha}^1, \alpha = 1, 2, ..., f_n$$

6. 跃迁

对于哈密顿量不含时的体系,通过 Schödinger 方程可求解体系随时间的演化,含时的情况要用含时微扰处理.

6.1. 含时微扰

$$H(t) = H_0 + H'(t)$$

$$\Psi(t) = \sum_n C_{nk}(t)e^{-\frac{i}{\hbar}E_nt}|n\rangle, C_{nk}(0) = \delta_{nk}$$

定理 6.1.1 (**一级 Dirac 近似公式**): 从$t = 0$到t时刻,体系从$|k\rangle$跃迁到$|k'\rangle$的概率幅

$$C_{k'k}(t) = \frac{1}{i\hbar}\int_0^t H'_{k'k}(t)e^{i\omega_{k'k}t}\,\mathrm{d}t$$

$$P_{k'k}(t) = \frac{1}{\hbar^2}\left|\int_0^t H'_{k'k}(t)e^{i\omega_{k'k}t}\,\mathrm{d}t\right|^2$$

$$H'_{k'k}(t) = \langle k'|H'(t)|k\rangle, \omega_{k'k} = \frac{E_{k'} - E_k}{\hbar}$$

6.2. 光的吸收与辐射

$$H = -\vec{D}\cdot\vec{E}$$

7. 矩阵形式

定理 7.1 (**幺正变换**): 对 2 套各自正交归一的基矢,存在幺正算符

$$U = \sum_n |b_n\rangle\langle a_n|$$

使得

$$|b_1\rangle = U|a_1\rangle, ..., |b_n\rangle = U|a_n\rangle$$

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

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

$$\langle p|H|\psi\rangle = \frac{p^2}{2m}\langle p|\psi\rangle + V\left(i\hbar\frac{\partial}{\partial p}\right)\langle p|\psi\rangle$$

8. 势阱的解

8.1. 一维无限深方势阱

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2 \text{ where } n = 1, 2, 3, ...$$

$$\psi_n(x) = \begin{cases}\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) & \text{if } 0 < x < a\\ 0 & \text{elsewhere}\end{cases}$$

8.2. 一维谐振子

$$V(x) = \frac{1}{2}kx^2$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} + (\lambda - \xi^2)\psi = 0$$

$$\text{where } \omega = \sqrt{\frac{k}{m}}, \lambda = \frac{2E}{\hbar\omega}, \xi = x\sqrt{\frac{m\omega}{\hbar}}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^nn!}}H_n(\xi)e^{-\frac{\xi^2}{2}}$$

$$\text{where } H_n(x) = (-1)^ne^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}e^{-x^2}$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

$$N = a^\dagger a$$

$$[a, a^\dagger] = 1$$

$$H|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$[N, a] = -a$$

$$[N, a^\dagger] = a^\dagger$$

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

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

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

$$a|0\rangle = 0$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\begin{aligned}\langle x|n\rangle &= \frac{1}{\sqrt{n!}}\left\langle x\middle|(a^\dagger)^n\middle|0\right\rangle\\ &= \frac{1}{\sqrt{2^nn!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \sqrt{\frac{\hbar}{m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right)^ne^{-\frac{m\omega}{2\hbar}x^2}\end{aligned}$$

9. 守恒量

定理 9.1 (**Ehrenfest**): 若力学量A不显含时间,有

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

证明: 考虑力学量$A(t)$在任意$|\psi(t)\rangle$上的演化,可得

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

此外A不显含时间,有$\frac{\partial A}{\partial t} = 0$. ■

定理 9.2: 若力学量A不显含时间,且$[A, H] = 0$,则A在任何$|\psi(t)\rangle$下的平均值与概率分布均不变.

例 9.1: 中心力场中的守恒量为$\{H, \vec{l}^2, l_z\}$.

例 9.2: 自由粒子的态可以用$\{p_x, p_y, p_z\}$标记,对应能量的简并度一般是无穷大.

定理 9.3 (**Feynman-Hellmann**): 若系统哈密顿量含有某参数λ,E_n为哈密顿量的本征值,相应归一化本征态(束缚态)为$|\psi_n\rangle$,有

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

定理 9.4 (**位力(virial)**): 处于势场$V(\vec{r})$中的粒子,动能算符在定态上的平均值为

$$\langle T\rangle = \frac{1}{2}\langle\vec{r}\cdot\boldsymbol{\nabla}V\rangle$$

推论 9.4.1: 当势能为坐标的n次齐次函数时,有

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

10. Born 近似法

定理 10.1 (**Lippman-Schwinger 方程**):

$$\begin{aligned}\psi(\vec{r}) &= e^{i\vec{k}\cdot\vec{r}} + \frac{2\mu}{\hbar^2}\int\mathrm{d}^3r'G(\vec{r}, \vec{r}')V(\vec{r}')\psi(\vec{r}')\\ &= \psi_i(\vec{r}) + \psi_{\mathrm{sc}}(\vec{r})\end{aligned}$$

$$G(\vec{r}, \vec{r}') = G(\vec{r} - \vec{r}') = -\frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|}$$

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{\mu}{2\pi\hbar^2}\int\mathrm{d}^3r'\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}V(\vec{r}')\psi(\vec{r}')$$

定义 10.2 (**散射边界条件**):

$$\psi_{\mathrm{sc}}(\vec{r}) \overset{r\to\infty}{\longrightarrow} f(\theta, \phi)\frac{e^{ikr}}{r}$$

定理 10.3 (**Born 近似方法**): 将$\psi(\vec{r}')$用零级近似解$e^{i\vec{k}\cdot\vec{r}'}$代替

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{\mu}{2\pi\hbar^2}\int\mathrm{d}^3r'\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}V(\vec{r}')e^{i\vec{k}\cdot\vec{r}'}$$

$$f(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2}\int\mathrm{d}^3r'e^{-i\vec{q}\cdot\vec{r}'}V(\vec{r}')$$

如$V(\vec{r})$只与r有关,积掉θ, ϕ有

$$f(\theta) = -\frac{2\mu}{\hbar^2q}\int_0^{+\infty}\mathrm{d}r'r'\sin(qr')V(r')$$

$$q = 2k\sin(\theta/2)$$

定义 10.4 (**散射截面**): $\sigma(\theta, \phi) = \frac{1}{j_1}\frac{\mathrm{d}n}{\mathrm{d}\Omega}$

$$\sigma(\theta) = |f(\theta)|^2$$