

δ势	线性	谐振子	库仑κ= Ze ²
μ = ħ = γ = 1	μ = ħ = F = 1	μ = ħ = ω = 1	μ = ħ = κ = 1
能量[E]	μγ ² /ħ ² (ħ ² F ² /μ) ^{1/3}	ħω	μκ ² /ħ ²
长度[L]	ħ ² /μγ (ħ ² /μF) ^{1/3}	√ħ/μω	ħ ² /μκ
时间[T]	ħ ³ /μγ ² (ħμ/F ²) ^{1/3}	1/ω	ħ ³ /μκ ²
速度[v]	γ/ħ (ħF/μ ²) ^{1/3}	√ħω/μ	κ/ħ
动量[p]	μγ/ħ (ħμF) ^{1/3}	√ħμω	μκ/ħ

1. 数学速查

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

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

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

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

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

$$+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}u_\phi$$

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

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

定义 1.1 (连带 Legendre 多项式):

$$(1-\xi^2)\frac{\mathrm{d}^2P}{\mathrm{d}\xi^2}-2\xi\frac{\mathrm{d}P}{\mathrm{d}\xi}$$

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

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

定理 1.2 (连带 Legendre 多项式的正交性):

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

定义 1.3 (Legendre 多项式):

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

定理 1.4 (Legendre 多项式的正交性):

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

定理 1.5 (厄米多项式的正交性):

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

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):

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

定义 1.8 (合流超几何函数):

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

where $\alpha_k=\alpha(\alpha+1)\dots(\alpha+k-1)$

$$\gamma_k=\gamma(\gamma+1)\dots(\gamma+k-1)$$

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 δ(x), 那么

$$\delta(\vec{r})=\delta(x)\delta(y)\delta(z)$$

$$=\frac{1}{r^2\sin\theta}\delta(r)\delta(\theta)\delta(\phi)$$

$$=\frac{1}{\rho}\delta(\rho)\delta(\phi)\delta(z)$$

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):

$$\frac{z}{r}Y_{lm}=\cos\theta Y_{lm}$$

$$=a_{lm}Y_{l+1,m}+a_{l-1,m}Y_{l-1,m}$$

$$=e^{+i\phi}\sin\theta Y_{lm}$$

$$\frac{x+iy}{r}Y_{lm}=e^{+i\phi}\sin\theta Y_{lm}$$

$$=b_{l-1,-(m+1)}Y_{l-1,m+1}-b_{lm}Y_{l+1,m}$$

$$=e^{-i\phi}\sin\theta Y_{lm}$$

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

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

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):

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

$$D=\begin{pmatrix}\lambda_1&&\\&\dots&\\&&\lambda_n\end{pmatrix},P=(v_1\;\dots\;v_n)$$

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

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

2. 算符

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

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

$$\vec{p}_r=\frac{1}{2}(\hat{r}\cdot\vec{p}+\vec{p}\cdot\hat{r})$$

$$=-i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)$$

$$=-\hbar^2\frac{1}{r^2}\frac{\partial^2}{\partial r^2}r^2\frac{\partial}{\partial r}$$

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

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

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

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

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

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

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):

$$H=\frac{p^2}{2\mu}+V(r)$$

$$=\frac{p_r^2}{2\mu}+\frac{\vec{l}^2}{2\mu r^2}+V(r)$$

$$=-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\vec{l}^2}{2\mu r^2}+V(r)$$

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 χ(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

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

能量本征值为

$$E_N=\left(N+\frac{3}{2}\right)\hbar\omega$$

$$N=2n_r+l$$

$$n_r,l=0,1,2,\dots$$

简并度为

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

径向本征函数为

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

$$r^le^{-a^2r^2/2}F\left(-n_r,l+\frac{3}{2},a^2r^2\right)$$

如果在直角坐标系中求解,这两套本征态通过么正变换联系起来

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

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

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

$$E_n=-\frac{\mu e^4}{2\hbar^2}\frac{1}{n^2}=-\frac{e^2}{2a}\frac{1}{n^2}$$

$$n=n_r+l+1$$

$$n_r=0,1,2,\dots$$

径向本征函数为

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

$$e^{-\xi/2}\xi^lF(-n_r,2l+2,\xi)$$

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

$$\vec{j}=\frac{ie\hbar}{2\mu}(\psi^*\nabla\psi-\psi\nabla\psi^*)$$

$$=-\frac{e\hbar m}{\mu}\frac{1}{r\sin\theta}|\psi_{nlm}|^2\hat{e}_\phi$$

总的磁矩为

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

$$=-\frac{e\hbar m}{2\mu c}\hat{z}$$

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): $\vec{l}=\vec{r}\times\vec{p}$

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

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

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

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

$$\vec{l}^2=l_z^2+l_y^2+l_x^2$$

$$=-\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}l_z^2$$

定义 4.1.2 (角动量升降算符):

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

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

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

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

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

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

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

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

$|j_1 j_2 j m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C_{j_1 m_1 j_2 m_2}^{j_1 j_2 j m} |j_1 m_1 j_2 m_2\rangle$
 $E_{j_1 m_1 j_2 m_2}^{j m} = \langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle$
 $E_n^2 = \langle \psi_n^0 | W | \psi_n^0 \rangle = \sum_{m \neq n} \frac{|W_{mn}|^2}{E_n^0 - E_m^0}$

4.4. 电子耦合与非耦合表象变换

$\Psi_{l,j=l+\frac{1}{2},m_j} = \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j} Y_{l,m_j-\frac{1}{2}} \\ \sqrt{j-m_j} Y_{l,m_j+\frac{1}{2}} \end{pmatrix}$
 $\sum_\mu (W_{\mu'\mu} - E_n^1 \delta_{\mu'\mu}) a_\mu = 0$

$\Psi_{l,j=l-\frac{1}{2},m_j} = \frac{1}{\sqrt{2j+2}} \begin{pmatrix} -\sqrt{j-m_j+1} Y_{l,m_j-\frac{1}{2}} \\ \sqrt{j+m_j+1} Y_{l,m_j+\frac{1}{2}} \end{pmatrix}$
 $\det(W_{\mu'\mu} - E_n^1 \delta_{\mu'\mu}) = 0$
 $E_n^1 = E_{n\alpha}^1, \alpha = 1, 2, \dots, f_n$

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

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

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

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

定义 4.4.1 (自旋三重态与单态): 选择 $\{S^2, S_z\}$ 作为对易自旋力学量全集
 $\vec{S}^2 \chi_{SM_S} = S(S+1) \hbar^2 \chi_{SM_S}$
 $S_z \chi_{SM_S} = M_S \hbar \chi_{SM_S}$

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

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

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

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

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

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

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

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

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

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

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

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

6.2. 光的吸收与辐射

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

7. 矩阵形式

定理 7.1 (么正变换): 对 2 套各自正交归一的基矢,存在么正算符

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

使得

$|b_1\rangle = U|a_1\rangle, \dots, |b_n\rangle = U|a_n\rangle \quad \langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x | (a^\dagger)^n | 0 \rangle$

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

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

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

8. 势阱的解

8.1. 一维无限深方势阱

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

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

8.2. 一维谐振子

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

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

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

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

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

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

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

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

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

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

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

$[N, a] = -a$

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

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

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

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

$a|0\rangle = 0$

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

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

$= \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$

$\left(\sqrt{\frac{m\omega}{\hbar}} x + \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx}\right)^n e^{-\frac{m\omega}{2\hbar} x^2}$

9. 守恒量

定理 9.1 (Ehrenfest): 若力学量A不显含时间,有

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

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

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

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 $\{H, l^2, l_z\}$.

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

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

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

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

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):

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

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

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

定义 10.2 (散射边界条件):

$\psi_{sc}(\vec{r}) \xrightarrow{r \rightarrow \infty} f(\theta, \phi) \frac{e^{ikr}}{r}$

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

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

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

如 $V(\vec{r})$ 只与r有关,积掉 θ, ϕ 有

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

定义 10.4 (散射截面): $\sigma(\theta, \phi) = \frac{1}{J_i} \frac{dJ}{d\Omega}$

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