积分公式. $\int_{-\infty}^{\infty}exp[ix^2]dx=\sqrt{\pi}exp[i\pi/4]$(Fresnel 积分公式); $\int_{-\infty}^{\infty}dxexp[-\alpha x^2+\beta x]=\sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty}x^n exp[-ax^2]dx=\frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty}xexp[-\frac{1}{2}ax^2+bx]dx=\frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty}x^2exp[-\frac{1}{2}ax^2+bx]dx=\frac{1}{a}(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty}x^{2n}exp[-\frac{1}{2}ax^2]dx=\frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(广义 Guass 积分式); $\int_0^{+\infty}x^{2n+1}exp[-ax^2]dx=\frac{n!}{2a^{n+1}}$; $(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[-\frac{i}{\hbar}\vec{p}'\cdot\vec{r}](p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})exp[\frac{i}{\hbar}\vec{p}\cdot\vec{r}]d\tau=(p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}]d\tau=(p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})\delta(\vec{p}-\vec{p}')$

基础知识 1.$\lambda=h/p,E=hc/\lambda,\lambda=h/\sqrt{2mE}$; 2.$\hat{p}=-i\hbar\frac{\partial}{\partial x},\hat{x}=i\hbar\frac{\partial}{\partial p}$; 3. 简并度 (求有序对数量)e.g.(无限高势垒立方)$E=\frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2)$, 求 (n_x,n_y,n_z) 对数 (1/3/3/3/1/6...); 4. 玻尔半径 $a_0=\frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$; 5. 量子数关系:$n=1,2,3...;l=0,1,2...n-1;m_l=0,\pm1,\pm2...\pm l;m_s=\pm\frac{1}{2}$; 6. 磁矩与哈密顿量:$\hat{H}_B=-\gamma\cdot\vec{B}\cdot\vec{S}(\vec{S}:Spin)$; 7.$s=1(triplet)\left|11\right\rangle=uu,\left|10\right\rangle=\frac{1}{\sqrt{2}}(ud+du),\left|1-1\right\rangle=dd;s=0(singlet)\left|00\right\rangle=\frac{1}{\sqrt{2}}(ud-du)$ 8.$\oint p_k\mathrm{d}q_k=n_kh,n_k=1,2,3\ldots$(**Bohr-Sommerfiled 条件**)e.g.$(V(x)=\frac{mw^2x^2}{2})\oint p\mathrm{d}x=2\int_{-a}^{a}\mathrm{d}x\sqrt{2m(E-\frac{1}{2}mw^2x^2)}$; 转动惯量为 $I,L\cdot 2\pi=nh,L=n\hbar,E=\frac{L^2}{2I}=\frac{n^2\hbar^2}{2I}$

已知 $\psi(x,0)$，求 $\psi(x,t)$1. 一维自由传播子 $G(x,x';t,t')=\sqrt{\frac{m}{2\pi\hbar it}}exp[\frac{im}{2\hbar}\frac{(x-x')^2}{t-t'}]$,e.g.$\psi(x,0)=\delta(x),\psi(x,t)=\int_{-\infty}^{\infty}dx'G(x,x';t,t')\psi(x,0)=\frac{1}{(2\pi\hbar)^{1/2}}exp[i(p_0x-\frac{p_0^2t}{2m})/\hbar]$;2. 不含时 $\hat{H}$. 解基函数 $\psi_n(x)$, 展开 $\psi(x,0)=\sum_{n=1}^{+\infty}c_n\psi_n(x),c_m=\int\psi_m^*\psi(x,0)dx,\psi(x,t)=\sum_{n=1}^{+\infty}c_n\psi_n(x)exp[-iE_nt/\hbar]$

已知 V(x,y) 求简并度分离变量法.$E=E_x+E_y$, 拆分方程.e.g.$V(x,y)=\frac{1}{2}\mu\omega^2(x^2+y^2),\therefore\ \psi(x,y)=X(x)Y(y),(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial y^2}+\frac{1}{2}\mu\omega^2y^2)Y=E_yY,(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\mu\omega^2x^2)X=E_xX=(E-E_y)X,E_y=(n_y+\frac{1}{2})\hbar\omega,E_x=(n_x+\frac{1}{2})\hbar\omega,E=E_x+E_y=\hbar\omega(n+1)$ 所以简并度为 $(n+\frac{1}{2})$

含时波函数求势能代入薛定谔方程即可.$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x,t)\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}$

已知 $\psi(x)$ 求 E 可能值与 P(E)$\psi(x)=\sum c_n\psi_n(x),c_n=\int\psi_n^*\psi(x)dx(\psi_n$ 应归一化)

概率流对定态 S.E., 有 $\frac{\partial\psi}{\partial t}=\frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}-\frac{i}{\hbar}V\psi,\frac{\partial\psi^*}{\partial t}=-\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial z^2}+\frac{i}{\hbar}V^*\psi^*,\therefore\ (whenV^*=V)\frac{\partial}{\partial t}|\psi|^2=\frac{i\hbar}{2m}(\psi^*\frac{\partial^2}{\partial x^2}-\frac{\partial^2\psi^*}{\partial x^2})=\frac{\partial}{\partial x}[\frac{i\hbar}{2m}(\psi^*\frac{\partial\psi}{\partial x}-\frac{\partial\psi^*}{\partial x}\psi)]$

一维散射 0. 基础结论 (一维无限深: 宽为 a,$\psi_n=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a},E_n=\frac{n^2h^2}{8ma^2}$)1. 方法 (1) 按势能分段求解基函数 (2) 待定系数法 (基函数的线性组合)(3) 求解条件 $\psi_1(a)=\psi_2(a),\psi_1'(a)=\psi_2'(a)$(4);$\lim_{x\longrightarrow\infty}\psi(x)=0$;(5) 节点 (e.g. 无限深势阱的壁处为 0) 分偶宇称态 $\psi(-x)=\psi(x)$ 和奇宇称态 $\psi(-x)=-\psi(x)$ 来讨论;2. 方势垒穿透 (0,V_0,0):$\psi(x)=exp[ikx]+Rexp[-ikx](x\leq 0);Sexp[ikx](x\geq a);Aexp[\kappa x]+Bexp[-\kappa x](k=\sqrt{2mE}/\hbar,\kappa=\sqrt{2m(V_0-E)}/\hbar).|S|^2=\frac{4k^2\kappa^2}{(k^2+\kappa^2\sinh^2\kappa a+4k^2\kappa^2)}=[1+\frac{1}{E/V_0(1-E/V_0)}\sinh^2\kappa a]^{-1},|R|^2=\frac{(k^2+\kappa^2)\sinh^2\kappa a}{(k^2+\kappa^2)^2\sinh^2\kappa a+4k^2\kappa^2}$3.$\delta$ 势垒/势阱 $(V(x)=\gamma\delta(x))\psi(x)=exp[ikx]+Rexp[-ikx](x\leq 0);Sexp[ikx](x\geq 0)$, 跃变条件 $\psi'(0^+)-\psi'(0^-)=\frac{2\mu\gamma}{\hbar^2}\psi_0.S=\frac{1}{1+i\mu\gamma/\hbar^2k},R=-\frac{i\mu\gamma}{\hbar^2k}/(1+\frac{i\mu\gamma}{\hbar^2k})(V(x)=-\gamma\delta(x))$, 跃变条件 $\psi'(0^+)-\psi'(0^-)=-\frac{2\mu\gamma}{\hbar^2}\psi_0,\beta=\sqrt{-2\mu E}/\hbar,\psi(x)=\frac{1}{\sqrt{L}}exp[-|x|/L](\sqrt{\beta}=1/\sqrt{L},L=1/\beta=\frac{\hbar^2}{\mu\gamma})$(只有偶宇称态)

表象变换 1. 傅里叶变换.$-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\psi(x)=E\psi(x),\frac{p^2}{2\mu}\varphi(p)+V(i\hbar\frac{\partial}{\partial p})\varphi(p)=E\varphi(p)$(3D:$\frac{\boldsymbol{p}^2}{2\mu}\phi(\boldsymbol{p})+V(i\hbar\nabla_p)\phi(\boldsymbol{p})=E\phi(\boldsymbol{p}),or\frac{p^2}{2m}\phi(p)+\int_{-\infty}^{\infty}V(pp')\phi(p')dp'=E\phi(p)(V_{pp'}=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dxV(x)e^{i(p-p')x/\hbar})$);$\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\varphi(p,t)exp[ipt]dp;\varphi(p,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\psi(x,t)exp[-ipx]dx$;2. 表象变换理论 $\hat{F}\psi=\lambda\psi,\hat{F}'\phi=\hat{S}^{-1}\hat{F}\hat{S}\hat{S}^{-1}\psi=\hat{S}^{-1}\hat{F}\psi=\lambda\hat{S}^{-1}\psi=\lambda\phi,tr(\hat{F}')=tr(\hat{S}^{-1}\hat{F}\hat{S})=tr(\hat{F}\hat{S}\hat{S}^{-1})=tr\hat{F}$

厄密多项式 1.定义$H_n(x)=(-1)^nexp[x^2]\frac{d^n}{dx^n}exp[-x^2]$,e.g.$H_0=1,H_1=2x,H_2=4x^2-2,H_3=8x^3-12x,H_4=16x^4-48x^2+12,H_5=32x^5-160x^3+120x$;2. 谐振子 $\psi_n(x)=\sqrt{\frac{\alpha}{2^nn!\sqrt{\pi}}}exp[-\alpha^2x^2/2]H_n(\alpha x),\alpha=\frac{\mu\omega}{\hbar}$(思路: 换元简化方程, 极限值猜测形式为 $\psi(\xi)=H(\xi)exp[-\xi^2/2]$, 级数解法.)

对易运算 1.定义$[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}([\hat{A},\hat{B}]=0,\hat{A}\hat{B}\left|\psi\right\rangle=\hat{B}\hat{A}\left|\psi\right\rangle)$;2.展开式$[\hat{A}\hat{B},\hat{C}]=\hat{A}\hat{B}\hat{C}-\hat{C}\hat{A}\hat{B}=(\hat{A}\hat{B}\hat{C}-\hat{A}\hat{C}\hat{B})+(\hat{A}\hat{C}\hat{B}-\hat{C}\hat{A}\hat{B})=\hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B},[\hat{A},\hat{B}\hat{C}]=\hat{B}[\hat{A},\hat{C}]+[\hat{A},\hat{B}]\hat{C}$

对易关系 笛卡尔下:$[\hat{x}_i,\hat{x}_j]=0$, $[\hat{p}_i,\hat{p}_j]=0$, $[\hat{x}_i,\hat{p}_j]=i\hbar\delta_{ij}$; $[\hat{L}_i,\hat{x}_j]=i\hbar\epsilon_{ijk}\hat{x}_k$ $(\epsilon_{ijk}=1,if$(i,j,k)$(even);-1,if$(i,j,k)$(odd);0,others)$, $[\hat{L}_i,\hat{p}_j]=i\hbar\epsilon_{ijk}\hat{p}_k$, $[\hat{L}_i,\hat{L}_j]=i\hbar\epsilon_{ijk}\hat{L}_k$ $(\hat{L}\times\hat{L}=i\hbar\hat{L})$, $[\hat{L}_i,\hat{F}]=0,\hat{F}$(any scalar), $[\hat{L}_i,\hat{F}]=i\hbar\epsilon_{ijk}\hat{F}_k,\hat{F}$(any vector), $[\hat{L}^2,\hat{L}_i]=0$, $[\hat{L},\hat{p}^2]=0$, $[\hat{L}^2,\hat{p}^2]=0$, $[\hat{L}_i,\hat{p}^2]=0$, $[\hat{L},\hat{r}^2]=0$, $[\hat{L}_i,\hat{r}^2]=0$, $[\hat{L},\hat{U}(r)]=[\hat{L}^2,\hat{U}(r)]=0(\hat{U}(r)$,any radial), $[\hat{S}_i,\hat{S}_j]=i\hbar\epsilon_{ijk}\hat{S}_k$ (anti-reciprocal : $\hat{S}_i\hat{S}_j+\hat{S}_j\hat{S}_i=0$); $[S^2,S_z]=0$;$[\hat{f},\hat{p}_i]=i\hbar\frac{\partial f}{\partial x_i}$

若干定理 1.Ehrenfest Theorem$\frac{d}{dt}\langle A\rangle=\frac{1}{i\hbar}\langle[A,H]\rangle+\langle\frac{\partial A}{\partial t}\rangle(Proof.\frac{d}{dt}\langle A\rangle=\frac{d}{dt}\int\psi^*A\psi dx)=\int(\frac{\partial\psi^*}{\partial t})A\psi dx+\int\psi^*(\frac{\partial A}{\partial t})\psi dx+\int\psi^*A(\frac{\partial\psi}{\partial t})dx=\int(\frac{\partial\psi^*}{\partial t})A\psi dx+\langle\frac{\partial A}{\partial t}\rangle+\int\psi^*A(\frac{\partial\psi}{\partial t})dx,\because\ H\psi=i\hbar\frac{\partial\psi}{\partial t},(H\psi)^*=-i\hbar\frac{\partial\psi^*}{\partial t},(H\psi)^*=\psi^*H^*=\psi^*H,\therefore=\frac{1}{i\hbar}\int\psi^*(AH-HA)\psi dx+\langle\frac{\partial A}{\partial t}\rangle=\frac{1}{i\hbar}\langle[A,H]\rangle+\langle\frac{\partial A}{\partial t}\rangle$e.g.(1)$\langle x\rangle:H(x,p,t)=\frac{p^2}{2m}+V(x,t),\frac{d}{dt}\langle x\rangle=\frac{1}{i\hbar}\langle[x,H]\rangle+\langle\frac{\partial x}{\partial t}\rangle=\frac{1}{i\hbar}\langle[x,H]\rangle=\frac{1}{i2m\hbar}\langle[x,p^2]\rangle=\frac{1}{i2m\hbar}\langle xpp-ppx\rangle,\because\ xpp-ppx=i2\hbar p,\therefore\ \frac{d}{dt}\langle x\rangle=\frac{1}{m}\langle p\rangle=\langle v\rangle$;(2)$\langle p\rangle:\frac{d}{dt}\langle p\rangle=\frac{1}{i\hbar}\langle[p,H]\rangle+\langle\frac{\partial p}{\partial t}\rangle,\because p=\frac{\hbar}{i}\frac{\partial}{\partial x}\longrightarrow[p,p^2]=0,\therefore\ \frac{d}{dt}\langle p\rangle=\frac{1}{i\hbar}\langle[p,V]\rangle=\int\psi^*V\frac{\partial}{\partial x}\psi dx-\int\psi^*\frac{\partial}{\partial x}(V\psi)dx=\langle-\frac{\partial}{\partial x}V\rangle$;2.Virial Theorem(位力定理)$\frac{d}{dt}\langle xp\rangle=2\langle T\rangle-\langle x\frac{dV}{dx}\rangle(Proof.\frac{d}{dt}\langle xp\rangle=\frac{i}{\hbar}\langle[H,xp]\rangle;[H,xp]=[H,x]p+x[H,p];[H,x]=-\frac{i\hbar p}{m};[H,p]=i\hbar\frac{\partial V}{\partial x},\frac{d}{dt}\langle xp\rangle=\frac{i}{\hbar}[-\frac{i\hbar}{m}\langle p^2\rangle+i\hbar\langle x\frac{\partial V}{\partial x}\rangle]=2\langle\frac{p^2}{2m}\rangle-\langle x\frac{\partial V}{\partial x}\rangle=2\langle T\rangle-\langle x\frac{\partial V}{\partial x}\rangle)$

矩阵元 A 第 i 行第 j 列元素 $A_{ij}=\langle i|\hat{A}|j\rangle=\int u_i^*(a)\hat{A}u_j(a)da$,a 为表象所用变量 (动量表象就是 p, 位置表象就是 x)

升降算符-谐振子 1. 构造 $V(x)=\frac{1}{2}mw^2x^2,\hat{H}=\frac{\hat{p}^2+m^2w^2\hat{x}^2}{2m},\hat{a}_\pm=\frac{mw\hat{x}\mp i\hat{p}}{\sqrt{2mw\hbar}}$;2. 运算性质:(1)$H(\hat{a}_+\psi)=(E+\hbar\omega)(\hat{a}_+\psi);H(\hat{a}_-\psi)=(E-\hbar\omega)(\hat{a}_-\psi)$;(2)$\hat{a}_+\psi_n=\sqrt{n+1}\psi_{n+1};\hat{a}_-\psi_n=\sqrt{n}\psi_{n-1}$;(3)$[\hat{H},\hat{a}_\pm]=\frac{1}{2m\sqrt{2mw\hbar}}[\hat{p}^2+m^2w^2\hat{x}^2,mw\hat{x}\mp i\hat{p}]=\frac{1}{2m\sqrt{2mw\hbar}}([\hat{p}^2,mw\hat{x}]\mp[\hat{p}^2,i\hat{p}]+[m^2w^2\hat{x}^2,mw\hat{x}]\pm[m^2w^2\hat{x}^2,i\hat{p}]),\because\ [\hat{p}^2,mw\hat{x}]=mw(\hat{p}[\hat{p},\hat{x}]+[\hat{p},\hat{x}]\hat{p})=-2imw\hbar\hat{p},[m^2w^2\hat{x}^2,i\hat{p}]=im^2w^2[\hat{x}^2,\hat{p}]=im^2w^2(\hat{x}[\hat{x},\hat{p}]+[\hat{x},\hat{p}]\hat{x})=-2m^2w^2\hbar\hat{x},[\hat{p}^2,i\hat{p}]=$

$[m^2w^2\hat{x}^2, mw\hat{x}] = 0; [\hat{p}, \hat{x}] = -i\hbar \therefore [\hat{H}, \hat{a}_\pm] = \frac{-2imw\hbar\hat{p} \pm 2m^2w^2\hbar\hat{x}}{2m\sqrt{2mw\hbar}} = \pm\frac{w\hbar(mw\hat{x} \mp i\hat{p})}{2m\sqrt{2mw\hbar}} = \pm w\hbar\hat{a}_\pm (4)\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0\{PS.\psi_0 = (\frac{m\omega}{\pi\hbar})^{1/4}exp[-\frac{m\omega}{2\hbar}x^2]\}$3. 计算期望值.$\hat{a}_\pm = \frac{1}{2\hbar m\omega}(\mp i\hat{p} + m\omega x) \implies x = \frac{\sqrt{2\hbar m\omega}}{2m\omega}(\hat{a}_+ + \hat{a}_-), p = \frac{1}{2i}\sqrt{2\hbar m\omega}(\hat{a}_- - \hat{a}_+); x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-), p = i\sqrt{\frac{\hbar\omega m}{2}}(\hat{a}_+ - \hat{a}_-); x^2 = \frac{\hbar}{2m\omega}(\hat{a}_+^2 + \hat{a}_-^2 + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+), p^2 = -\frac{m\hbar\omega}{2}(\hat{a}_+^2 + \hat{a}_-^2 - \hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+); \langle\frac{1}{2}m\omega^2x^2\rangle = \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\int\psi_n^*(\hat{a}_+^2 + \hat{a}_-^2 + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+)\psi_n dx = \frac{\hbar\omega}{4}[n + (n+1)] = \frac{\hbar\omega}{n+\frac{1}{2}}; \langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\int\psi_n^*(\hat{a}_+ + \hat{a}_-)\psi_n dx = 0; \langle p\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\int\psi_n^*(\hat{a}_+ - \hat{a}_-)\psi_n dx = 0; \langle x^2\rangle = \frac{\hbar\omega}{2}(n+\frac{1}{2})\frac{2}{m\omega^2} = \frac{\hbar}{m\omega}(n+\frac{1}{2}); \langle p^2\rangle = -\frac{m\hbar\omega}{2}\int\psi_n^*(\hat{a}_+^2 + \hat{a}_-^2 - \hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+)\psi_n dx; -\frac{m\hbar\omega}{2}[-n-(1+n)] = m\omega\hbar(n+\frac{1}{2}); \langle T\rangle = \frac{p^2}{2m} = \frac{\hbar\omega}{2}(n+\frac{1}{2})$

升降算符-角动量 1. 定义 $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$2. 运算性质 $\hat{L}_+\hat{L}_- = (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) = \hat{L}_x^2 + \hat{L}_y^2 - i[\hat{L}_x, \hat{L}_y] = \hat{L}^2 - \hat{L}_z^2, \therefore \hat{L}_+\hat{L}_- |lm\rangle = \hbar^2 l(l+1)|lm\rangle - \hbar^2m^2|lm\rangle + m\hbar^2|lm\rangle = \hbar^2[l(l+1) - m(m+1)]|lm\rangle, \hat{L}_-|lm\rangle = \hbar\sqrt{l(l+1)-m(m-1)}\,|l(m-1)\rangle; \hat{L}_+|lm\rangle = \hbar\sqrt{l(l+1)-m(m+1)}\,|l(m+1)\rangle$

升降算符-(自旋) 角动量 $1.\hat{L}_z$:$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$, 有 $[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm, \hat{L}_z\hat{L}_\pm|\psi\rangle = (c\pm\hbar)|\psi\rangle 2.\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y, [\hat{S}_z, \hat{S}_\pm] = \pm\hbar\hat{S}_\pm$

氢原子波函数-球谐函数 1.SE:$\{-\frac{\hbar^2}{2\mu}(\frac{1}{r^2})[\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\varphi^2}] - V\}\psi = E\psi(\hat{L}^2 = -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \sin\theta^2\frac{\partial^2}{\partial\varphi^2}])$, 分离变量$\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi), \frac{1}{R}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{2mr^2}{\hbar^2}[V(r) - E] = l(l+1), \frac{1}{Y}[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial Y}{\partial\theta}) + \frac{1}{\sin\theta^2}\frac{\partial^2 Y}{\partial\varphi^2}] = -l(l+1)$.Y:$Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi) : \frac{1}{\Theta}[\sin\theta\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta})] + l(l+1)\sin\theta^2 + \frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} = 0; \frac{1}{\Theta}[\sin\theta\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta})] + l(l+1)\sin\theta^2 = m^2, \frac{1}{\Phi}\frac{d^2\Phi}{d\Phi^2} = -m^2, \Phi = e^{-im\varphi}\ \sin\theta\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + [l(l+1)\sin\theta^2 - m^2]\Theta = 0, \Theta(\theta) = AP_l^m(\cos\theta), P_l^m(x) = (1-x^2)^{|m|/2}(\frac{d}{dx})^{|m|}P_l(x), P_l(x) = \frac{1}{2^l l!}(\frac{d}{dx})^l(x^2-1)^l.|m| > l, P_l^m(x) = 0, |m| \le l$

角动量算符, 其本征值与性质 $1.\hat{L}_z : \hat{L}_z\psi(\phi) = -i\hbar\frac{d}{d\phi}\psi(\phi) = l_z\psi(\phi), \psi(\phi) = \psi(\phi+2\pi); l_z = m\hbar, (m = 0, \pm1, \pm2\cdots), \psi(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \langle\psi_m||\psi_n\rangle = \delta_{mn}; \hat{l}_z|\psi_m\rangle = m\hbar\psi_m, \langle\psi_m|\hat{l}_z = \langle\psi_m|m\hbar; [\hat{l}_y, \hat{l}_z] = i\hbar\hat{l}_x, \therefore \langle\hat{l}_z\rangle = \langle\psi_m|\hat{l}_y\hat{l}_z - \hat{l}_z\hat{l}_y|\psi_m\rangle = m\hbar\langle\psi_m|\hat{l}_y - \hat{l}_y|\psi_m\rangle = 0; \langle\hat{l}_x\rangle = \langle\hat{l}_y\rangle = 0; \langle i\hbar\hat{l}_x^2\rangle = \langle i\hbar\hat{l}_y^2\rangle + \langle Y_{lm}|\hat{l}_y\hat{l}_x\hat{l}_z - \hat{l}_z\hat{l}_y\hat{l}_x|Y_{lm}\rangle = \langle i\hbar\hat{l}_y^2\rangle$2. 算符的矩阵表示 (1)$|lm\rangle$ 的 $L_x = \frac{\hbar}{\sqrt{2}}[0,1,0;1,0,1;0,1,0], L_y = \frac{\hbar}{\sqrt{2}}[0,-i,0;i,0,-i;0,i,0]$;3.$\langle L^2\rangle = l(l+1)\hbar^2$4. 角动量不确定性关系 $\sigma_{L_i}\sigma_{L_j} \ge \frac{\hbar}{2}|\langle L_k\rangle|$

自旋算符 1. 定义 $\hat{S}_z\Phi_{\frac{1}{2}} = \frac{\hbar}{2}\Phi_{\frac{1}{2}}, \hat{S}_z\Phi_{-\frac{1}{2}} = \frac{\hbar}{2}\Phi_{-\frac{1}{2}}, \therefore \hat{S}_z = \frac{\hbar}{2}diag\{1,-1\}$;2.Puali 算符:$\hat{\vec{S}} = \hbar\hat{\vec{\sigma}}, \hat{\vec{S_i}} = \frac{\hbar}{2}\sigma_i; \vec{S}\times\vec{S} = i\hbar\vec{S}; \hat{S}^2 = \frac{3\hbar^2}{4}diag\{1,1\}, S^2|s,m\rangle = \hbar^2 s(s+1)|s,m\rangle; [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k, \hat{\sigma}_i\hat{\sigma}_j = i\epsilon_{ijk}\hat{\sigma_k}, \sigma_i^2 = 1; S^2 = s(s+1)\hbar^2, S_z = m_s\hbar(m_s = -s, -s+1, ...s-1, s)4.\sigma_x = [0,1;1,0], \sigma_y = [0,-i;i,0]; \sigma_z = [1,0;0,-1]$;

本征旋量 1. 自旋的线性展开 $\chi = [\alpha,\beta]^T, \chi^\dagger\chi = 1, \chi = c_+^{(x)}\chi_+^{(x)} + c_-^{(x)}\chi_-^{(x)}$,2. 求各自旋概率:$\sqrt{P_x(\frac{\hbar}{2})} = c_+^{(x)} = (\chi_+^{(x)})^\dagger\chi, \sqrt{P_x(-\frac{\hbar}{2})} = c_-^{(x)} = (\chi_-^{(x)})^\dagger\chi; \hat{S}_x\chi_\pm^{(x)} = \pm\frac{\hbar}{2}\chi_\pm^{(x)}, \chi_\pm^{(x)} = \frac{1}{\sqrt{2}}[1,\pm1]^T; \hat{S}_y\chi_\pm^{(y)} = \pm\frac{\hbar}{2}\chi_\pm^{(y)}, \chi_\pm^{(y)} = \frac{1}{\sqrt{2}}[1,\mp i]^T$;3. 求自旋期望值:$\langle S_x\rangle = P_x(\frac{\hbar}{2})\frac{\hbar}{2} + P_x(-\frac{\hbar}{2})(-\frac{\hbar}{2}); \langle S_y\rangle = \chi^\dagger\hat{S}_y\chi$

C-G 系数查表 1. 顺展开:$|s,m\rangle = \sum c_{s,s_1,s_2}^{m,m_1,m_2}|s_1,m_1\rangle|s_2,m_2\rangle$.e.g. 对 $s_1 = 2, s_1 = 1$ 的两粒子, 求其 $s = 3, m = 0$ 的组合方式. 找到 2×1 的表格, 找到 $[3,0]^T$ 的一列, 列的左边则是有详细的 (m_1, m_2) 的信息.$|3,0\rangle = \sqrt{\frac{1}{5}}|2,+1\rangle|1,-1\rangle + \sqrt{\frac{3}{5}}|2,0\rangle|1,0\rangle + \sqrt{\frac{1}{5}}|2,-1\rangle|1,+1\rangle$2. 逆展开:$|s_1,m_1\rangle|s_2,m_2\rangle = \sum_s C_{s,s_1,,s_2}^{m,m_1,m_2}|s,m\rangle$. 比如要对 $\frac{3}{2}\times1$ 的 $m_1 = \frac{1}{2}, m_2 = 0$ 状态进行展开, 即有 $|\frac{3}{2},1,\frac{1}{2},0\rangle = \sqrt{\frac{3}{5}}|\frac{5}{2},+\frac{1}{2}\rangle + \sqrt{\frac{1}{15}}|\frac{3}{2},+\frac{1}{2}\rangle + (-1)\sqrt{\frac{1}{3}}|\frac{1}{2},+\frac{1}{2}\rangle$(线性展开时, 取系数应开根, 符号在根号外)

Vocabulary