$\boxed{k=\frac{p}{\hbar},\ \omega=\frac{E}{\hbar}}$

$\lambda=\frac{h}{p}$, $\nu=\frac{E}{h}$

$(\hbar=\frac{h}{2\pi}, k=\frac{2\pi}{\lambda})$

联系粒子性&波动性

$p=\frac{E}{c}=\frac{h}{\lambda}, E=h\nu$

自由粒子波函数：

$\vec{p}$，能量守恒 $\Rightarrow \omega, k$ 不变

$\psi(\vec{r},t)=Ae^{-i(\omega t-\vec{k}\cdot\vec{r})}$

$=Ae^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{r})}$

正则方程：$\dot{p}=-\frac{\partial H}{\partial q}, \dot{q}=\frac{\partial H}{\partial p}$ 坐标

干涉效应：

$|\psi|^2=|c_1\psi_1|^2+|c_2\psi_2|^2+$ 干涉项

$\psi=e^{i\varphi_1}(|c_1|\psi_1+|c_2|e^{i(\varphi_2-\varphi_1)}\psi_2)$

实体的相位在观测中反映

(位置空间不，动量空间可以)

归一化与δ函数：(+动量本征)

$\psi_p=\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$

$\delta(x)=\frac{1}{2\pi}\int_\infty e^{ikx}dx$

$$\begin{cases}\psi(\vec{r},t)=\int_\infty c(\vec{p},t)\psi_{\vec{p}}(\vec{r})\,d^3\vec{p}\\ \quad=\frac{1}{(\sqrt{2\pi\hbar})^3}\int_\infty c(\vec{p},t)e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\,d^3\vec{p}\\ c(\vec{p},t)=\int_\infty \psi_{\vec{p}}^*(\vec{r})\psi(\vec{r},t)\,d^3\vec{r}\\ \quad=\left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3\int_\infty \psi(\vec{r},t)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\,d\vec{r}^3\end{cases}$$

$\int_\infty \psi_{p'}^*(\vec{r})\cdot\psi_p(\vec{r})=\delta(\vec{p}-\vec{p}')$

$\int_0^\infty e^{-x}\cdot x^2dx=2$

$\int e^{-x}x\,dx=1$

$\int_\infty e^{\frac{i}{\hbar}(p_x-p_x')x}dx=2\pi\delta\left(\frac{p_x-p_x'}{\hbar}\right)=2\pi\hbar\,\delta(p_x-p_x')$

几率流密度：

$\frac{\partial w}{\partial t}+\nabla\cdot\vec{J}=0\quad(w=|\psi|^2)$

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

电流密度：$\vec{J}_e=e\cdot\vec{J}$

全空间积分即全空间几率守恒

故若 $w(0)=\int|\psi(\vec{r},0)|^2d\tau=1$

一开始归一化，后续一直归一 $w(t)=1$

薛定谔

$i\hbar\frac{\partial}{\partial t}\psi=\left(\frac{\hat{p}^2}{2m}+U\right)\psi$

(含时定量的方程)

一维方势阱：

$\frac{d^2\psi}{dx^2}+\underbrace{\frac{2\mu(E-U)}{\hbar^2}}_{k^2}\psi=0$

$[0,a]\to\psi=\begin{cases}\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\\0\end{cases}$

利用边界条件.

$E=\frac{k^2\hbar^2}{2\mu}\ (k=\frac{n\pi}{a})$

三维无限深方势阱

$\psi_{n,m,l}(x,y,z)=\sqrt{\frac{8}{abc}}\sin\frac{n\pi}{a}x\sin\frac{m\pi}{b}y\sin\frac{l\pi}{c}z$

$E_{n,m,l}=\frac{\pi^2\hbar^2}{2\mu}\left[\left(\frac{n}{a}\right)^2+\left(\frac{m}{b}\right)^2+\left(\frac{l}{c}\right)^2\right]$

平行极板：

$\psi(x,y,z)=e^{ik_xx}e^{ik_yy}\sin(k_zz)$

$k_x^2+k_y^2+k_z^2=1\quad k_z=\frac{n\pi}{a}$

一维谐振子

$\psi_n(x)=N_nH_n(\alpha x)e^{-\frac{1}{2}\alpha^2x^2}$

$(\alpha=\sqrt{\frac{\mu\omega}{\hbar}}, \xi=\alpha x)$

$N_n=\sqrt{\frac{\alpha}{\sqrt{\pi}2^n\cdot n!}}$

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

$\langle H_0=1, H_1(\xi)=2\xi, H_2(\xi)=4\xi^2-2\rangle$

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

基：$E_0=\frac{1}{2}\hbar\omega$, $\psi_0(x)=\left(\frac{\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}}e^{-\frac{\alpha^2x^2}{2}}$

一：$E_1=\frac{3}{2}\hbar\omega$, $\psi_1(x)=\left(\frac{2\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}}\alpha x e^{-\frac{1}{2}\alpha^2x^2}$

二：$E_2=\frac{5}{2}\hbar\omega$, $\psi_2(x)=\left(\frac{\alpha}{2\sqrt{\pi}}\right)^{\frac{1}{2}}(2\alpha^2x^2-1)e^{-\frac{1}{2}\alpha^2x^2}$

偶、奇、偶. ……

方势垒：

$$\begin{cases}Ae^{ikx}+Be^{-ikx}\\Fe^{\alpha x}+Ge^{-\alpha x}\\Ce^{ikx}\end{cases}$$

$\begin{cases}\psi''+k^2\psi=0 & (k=\frac{\sqrt{2\mu E}}{\hbar})\ 外\\ \psi''-\alpha^2\psi=0 & (\alpha=\frac{\sqrt{2\mu(U_0-E)}}{\hbar})\ 内\end{cases}$

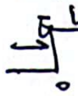
$R=\frac{|B|^2}{|A|^2}=\frac{(k^2+\alpha^2)^2\mathrm{sh}^2(\alpha a)}{(k^2+\alpha^2)^2\mathrm{sh}^2(\alpha a)+4k^2\alpha^2}$

$D=\frac{|C|^2}{|A|^2}=\frac{4k^2\alpha^2}{(k^2+\alpha^2)^2\mathrm{sh}^2(\alpha a)+4k^2\alpha^2}$

。定态下所有一维散射均有 $R+D=1$

$\Rightarrow\frac{\partial\rho}{\partial t}+\frac{\partial J}{\partial x}=0$. 定态 $\frac{\partial\rho}{\partial t}=0$

半无限高势垒



$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & (x>0)\\ De^{-\alpha x} & (x<0)\end{cases}$

$(\alpha=\frac{\sqrt{2\mu(U_0-E)}}{\hbar})$

$\psi(x),\psi'(x)$ 衔接 $\Rightarrow D=\frac{2k^2-2i\alpha k}{k^2+\alpha^2}A$

$B=\frac{k^2-\alpha^2-2i\alpha k}{k^2+\alpha^2}A$

注：$x>0$ 时，

$J=|A|^2v-|B|^2v+\frac{i\hbar}{2\mu}[\underbrace{AB^*e^{2ikx}(ik)}+\underline{BA^*(-ik)e^{-2ikx}}-c.c.]$

$(v=\frac{\hbar k}{\mu})$

$=|A|^2v-|B|^2v$

厄米：$\int\psi^*\hat{F}\phi\,d\tau=\int\phi(\hat{F}\psi)^*d\tau$

力学量厄米算符本征值均 ∈ ℝ.

证明：$\lambda\int\psi^*\psi\,dx=\lambda^*\int\psi^*\psi\,d\tau$

厄米共轭

$\hat{L}_z=-i\hbar(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x})$

$\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi}$

$\hat{L}^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$

$\hat{L}=-i\hbar(\vec{e}_\varphi\frac{\partial}{\partial\theta}-\vec{e}_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi})$

$\hat{L}_z\psi_m=\lambda\psi_m$, $\psi_m=\frac{1}{\sqrt{2\pi}}e^{im\varphi}$

$\hat{L}^2Y=\lambda\hbar^2Y$, $\lambda=l(l+1)$

$Y_{lm}(\theta,\varphi)=N_{lm}P_l^{|m|}(\cos\theta)e^{im\varphi}$.

$N_{lm}=(-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}$

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

相反：$Y_{lm}(x,y,z)(-1)^l=Y_{lm}(-x,-y,-z)$

共轭：$Y_{lm}^*(\theta,\varphi)=(-1)^mY_{l,-m}(\theta,\varphi)$

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

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

(Y_{00} $\hat{L}_x=Y_{00}\hat{L}_y=Y_{00}\hat{L}_z$ 无方向)

(Y_{10}, $Y_{1,\pm1}$ 有方向性)

$\nabla=\hat{e}_r\frac{\partial}{\partial r}+\hat{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}+\hat{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}$

$\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$

$\vec{L}=\vec{r}\times\vec{p}=-i\hbar r\hat{e}_r\times\nabla$

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

$R_{nl}(r)=\frac{N_{nl}\rho^{l+1}e^{-\frac{\rho}{2}}V_{nl}(\rho)}{r}$ 偶

$(d\Omega=\sin\theta d\theta d\varphi)$ $\int|\psi|^2r^2d\Omega$ 径向

$(d\Omega=\frac{ds}{r^2})$ $\int|\psi|^2r^2dr$ 角向

径向：$w(r)=R_{nl}^2(r)r^2dr$

角向：$|Y_{lm}(\theta,\varphi)|^2d\Omega$

推导过程：

$H=\frac{p_r^2}{2\mu}+\frac{p^2}{2\mu}+U$

$\hat{T}=-\frac{\hbar^2}{2\mu}\nabla^2=-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})+\frac{1}{2\mu r^2}\hat{L}^2$

电子

$\hat{p}=\mu\dot{\vec{r}}$, $\mu=\frac{m_em_N}{m_e+m_N}$

$E_n=-\frac{m_e}{2\hbar^2n^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2$

电流密度

$\vec{J}_e=J_{e\varphi}\hat{\varphi}=-\frac{e\hbar m}{\mu r\sin\theta}|\psi_{nlm}|^2$

($m\neq0$ 有磁矩)

氢原子基态为球对称.

$\Rightarrow\psi_{100}$ 球对称，ψ_{200} 球对称

ψ_{21m} 不球对称

$\psi_{100}=\sqrt{\frac{1}{\pi a^3}}e^{-\frac{r}{a}}$

$\psi_{nlm}(-\vec{r})=(-1)^l\psi_{nlm}(\vec{r})$

$R_{10}(r)=\sqrt{\frac{4}{a^3}}e^{-\frac{r}{a}}$

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

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

不确定性关系：

$[\hat F,\hat G]=i\hat C$

$\Rightarrow \overline{(\Delta F)^2}\cdot\overline{(\Delta G)^2}\geq\frac{\overline{C}^2}{4}$

若 $\hat F,\hat G$ 厄米，则 $C\in\mathbb{R}$.

对易关系

$[\hat x,\hat p]=i\hbar$

$[\hat x,\hat H]=i\hbar\frac{\hat p}{\mu}$

$[\hat p_i,\hat p_j]=0$

$[\hat L_x,\hat L_y]=i\hbar\hat L_z$

$[\hat L^2,\hat L]=0$

$[\hat S_x,\hat S_y]=i\hbar\hat S_z$

$[\hat\sigma_x,\hat\sigma_y]=2i\hat\sigma_z$

$[\hat S^2,\hat S_x]=[\hat S^2,\hat S_y]=[\hat S^2,\hat S_z]=0$

守恒量：

$$\frac{d}{dt}\overline{F}=\frac{1}{i\hbar}\overline{[\hat F,\hat H]}$$

海森堡绘景用此得力学量随时间变化

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

$\langle\psi(0)|U^\dagger F U|\psi(0)\rangle$

$|\psi(t)\rangle=U|\psi(0)\rangle$，$F_H=U^\dagger(t)FU(t)$

时间演化因子：

$U=e^{-i\frac{Ht}{\hbar}}$

$[U,H]=0$

$$H=\frac{\hbar\omega}{2}\Big(\underbrace{\frac{p^2}{m\hbar\omega}}_{p'^2}+\underbrace{\frac{m\omega^2x^2}{\hbar\omega}}_{x'^2}\Big)$$

$$\begin{cases}a=\frac{1}{\sqrt2}(\hat x'+i\hat p')\\ a^\dagger=\frac{1}{\sqrt2}(\hat x'-i\hat p')\end{cases}$$

$[x',p']=i$

$p'=\frac{i}{\sqrt2}(a^\dagger-a)$

$H=\hbar\omega(\hat a^\dagger\hat a+\frac12)=\hbar\omega(\hat N+\frac12)$

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

$H=\frac{\hbar\omega}{2}[(x'-ip')(x'+ip')+1]$

零阶：$a|\psi_0\rangle=0$ 基态方程

升降 $\begin{cases}a|n\rangle=\sqrt n|n-1\rangle\\ a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle\end{cases}$

能量表象下：

$x_{mn}=\sqrt{\frac{\hbar}{2m\omega}}(\sqrt n\,\delta_{m,n-1}+\sqrt{n+1}\,\delta_{m,n-1})$

$=\sqrt{\frac{\hbar}{2m\omega}}(\langle m|\hat a|n\rangle+\langle m|\hat a^\dagger|n\rangle)$

$p_{mn}=\langle m|\hat p|n\rangle=i\sqrt{\frac{m\hbar\omega}{2}}(\langle m|\hat a^\dagger|n\rangle-\langle m|\hat a|n\rangle)$

$=i\sqrt{\frac{m\hbar\omega}{2}}(\sqrt{n+1}\,\delta_{m,n+1}-\sqrt n\,\delta_{m,n-1})$

$\vec M_s=-\frac{e}{mc}\vec S$，$M_L=-\frac{e}{2mc}\vec L$

$U=-M\cdot B$

$S_x=\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$ | $\frac{1}{\sqrt2}\begin{pmatrix}1\\1\end{pmatrix},\frac{1}{\sqrt2}\begin{pmatrix}1\\-1\end{pmatrix}$

$S_y=\frac{\hbar}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$ | $\frac{1}{\sqrt2}\begin{pmatrix}1\\i\end{pmatrix},\frac{1}{\sqrt2}\begin{pmatrix}1\\-i\end{pmatrix}$

$S_z=\frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ | $\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}$

旋量波函数（增加了自旋的…）

$\psi(\vec r,t)=\psi_1(\vec r,t)\begin{pmatrix}1\\0\end{pmatrix}+\psi_2(\vec r,t)\begin{pmatrix}0\\1\end{pmatrix}$

$\overline{G}=\int\psi^\dagger\hat G\psi\,d\tau$

$\hat G\to\begin{pmatrix}G_{11}&G_{12}\\G_{21}&G_{22}\end{pmatrix}$

$\vec J=\vec L+\vec S$

给定 l 时：

$\begin{cases}l>0,\ j=l-\frac12 \text{ 或 } j=l+\frac12\\ l=0,\ j=l+\frac12=\frac12 \text{ 一值}\end{cases}$

$l=0$ 时 $J^2=\frac34\hbar^2$ $(j=\frac12)$