Lec 1 and 2

Stefen - Boltzmann Law : $P = \sigma T^4$ $\sigma = 5.67 \times 10^{-8}\ W/m^2K^4$

$\bar{E} = \frac{\int_0^\infty E e^{-\beta E} dE}{\int_0^\infty e^{-\beta E} dE} = k_B T$ $N(k)\,dk = \frac{1}{8} \cdot 2 \times \frac{4\pi k^2 dk}{(\pi/L)^3} = \frac{V k^2 dk}{\pi^2}$ $k = \frac{2\pi}{\lambda} = \frac{2\pi\nu}{c}$ $dk = \frac{2\pi}{c} d\nu$

$N(k)\,dk = \frac{Vk^2 dk}{\pi^2}$

$\frac{E}{V} = \frac{\int \bar{E}\, N(k)\, dk}{V} = k_B T \int \frac{k^2 dk}{\pi^2} = k_B T \cdot \int \frac{8\pi \nu^2 d\nu}{c^3}$.

$= \int_0^\infty \rho_E(\nu)\, d\nu$ 不对

$\Rightarrow \rho_E(\nu) =$ 错

$\sum_{n=0}^{\infty}$

$Z = 1 + e^{-\beta h\nu} + e^{-\beta 2h\nu} + \cdots e^{-\infty}$

$q = e^{-\beta h\nu}$

$qZ = e^{-\beta h\nu} + \cdots e^{-\infty}$

$(1-q)Z = 1 \Rightarrow Z = \frac{1}{1-e^{-\beta h\nu}}$

$\bar{E} = \frac{\sum_{n=0}^{\infty} nh\nu\, e^{-\beta n h\nu}}{\sum_{n=0}^{\infty} e^{-\beta n h\nu}} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$

$= -(1-e^{-\beta h\nu}) \cdot \frac{-e^{-\beta h\nu} \cdot h\nu}{(1-e^{-\beta h\nu})^2}$

$= \frac{e^{-\beta h\nu}\, h\nu}{1-e^{-\beta h\nu}} = \frac{h\nu}{e^{\beta h\nu}-1} = \frac{h\nu}{e^{\frac{h\nu}{k_B T}}-1}$

$N(k)\,dk = \frac{V\, 8\pi \nu^2}{c^3} d\nu$

$\frac{E}{V} = \int \frac{\bar{E} \cdot N(k) \cdot d(k)}{V} = \int \frac{8\pi h \nu^3\, d\nu}{(e^{\frac{h\nu}{k_B T}} - 1)c^2}$ $\Rightarrow \rho_E(\nu) = \frac{8\pi h}{c^3} \cdot \frac{\nu^3}{e^{\frac{h\nu}{k_BT}} - 1} = \begin{cases} k_B T \dfrac{8\pi \nu^2}{c^3} & \dfrac{h\nu}{k_B T} \ll 1 \quad \text{低频或高温} \\ \dfrac{8\pi h}{c^3} \cdot \dfrac{\nu^2}{e^{\frac{h\nu}{k_BT}}} & \dfrac{h\nu}{k_B T} \gg 1 \quad \text{高频或低温} \end{cases}$

$h\nu = KE_e + h\nu_0$

$E_{nf} - E_{ni} = -13.6\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$|\vec{r} \times \vec{p}| = n\hbar$

$p_e = \frac{h}{\lambda}$

Lec 3 and 4

QM $\rightarrow$ classical $n \rightarrow \infty$ or $\hbar \rightarrow 0$

$\hat{p} = -i\hbar\frac{\partial}{\partial x}$ $\hat{E} = i\hbar\frac{\partial}{\partial t}$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + V\phi = i\hbar\frac{\partial\phi}{\partial t}$$

$$\int_D |\psi(x,t)|^2 dx = 1 \quad \rightarrow P(x,t) = \psi^*\psi$$

$$\Rightarrow \frac{\partial\phi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\phi}{\partial x^2} + \frac{V}{i\hbar}\phi$$

use this

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\psi(x,t)|^2 dx = 0$$

$$\langle\hat{x}\rangle = \int_{-\infty}^{+\infty}\psi^* x \psi \, dx$$

$$\langle\hat{p}\rangle = \int_{-\infty}^{+\infty}\psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi \, dx$$

if $\psi(x,t) = \frac{1}{\sqrt{L}} \cdot e^{i(p_0x - E_0t)/\hbar}$

$$\langle\hat{p}\rangle = p_0 \cdot \int_{-\infty}^{+\infty}|\psi|^2 dx$$

Ehrenfest's theorm

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m} = \langle\hat{v}\rangle$$

$$\frac{d\langle\hat{p}\rangle}{dt} = \langle -\frac{\partial V}{\partial x}\rangle$$

Lec 5

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

$$\int_{-\infty}^{+\infty}\phi_i^*\phi_i = 1$$

$$\psi(x,t) = \phi(x)e^{-i\frac{Et}{\hbar}}$$

$$\int \phi_2^*\hat{H}\phi_1 - \phi_1\hat{H}\phi_2^* = (E_1 - E_2)\int\phi_1\phi_2^* = 0$$

if $E_1 \neq E_2 \Rightarrow \int_{-\infty}^{+\infty}\phi_1\phi_2^* = 0$

$$\psi(x,t_0) = \sum_i c_i\phi_i(x) \qquad c_i = \int_{-\infty}^{+\infty}\phi_i^*\psi(x,t_0)\,dx$$

$$\int|\psi|^2 = \sum_{j=1}^{\infty}\sum_{i=1}^{\infty}c_j^*c_i\int\phi_j^*\phi_i\,dx = \sum_j\sum_i c_j^*c_i\delta_{ji} = \sum_i|c_i|^2 = 1$$

$$\psi(x,t) = \sum_i c_i\phi_i(x)e^{-i\frac{E_it}{\hbar}}$$

$$\hat{H}\phi_i = E_i\phi_i$$

Lec 6

Infinite S-W $\quad V(x) = \begin{cases} 0 & |x| < \frac{a}{2} \\ \infty & \text{other} \end{cases} \quad E > 0$

$$-\frac{\hbar^2}{2m}\phi'' = E\phi \Rightarrow \phi'' = -\frac{2mE}{\hbar^2}\phi = -k^2\phi$$

$\phi = A\sin kx + B\cos kx$

boundary condition

$\phi(-\frac{a}{2}) = -A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0 \quad ①$

$\phi(\frac{a}{2}) = A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0 \quad ②$

$① + ② \quad 2B\cos\frac{ka}{2} = 0 \Rightarrow \frac{k_n a}{2} = \frac{n\pi}{2} \Rightarrow k_n = \frac{n\pi}{a} \quad n = 1,3,5$

$① - ② \quad -2A\sin\frac{ka}{2} = 0 \Rightarrow k_n = \frac{n\pi}{a} \quad n = 2,4,6$

$\int_{-\infty}^{+\infty}\phi^2 = 1 \Rightarrow B^2\int_{-\frac{a}{2}}^{\frac{a}{2}}\cos^2\frac{n\pi x}{a}\,dx = 1 \Rightarrow B^2\cdot\frac{a}{2} = 1 \Rightarrow B = A = \sqrt{\frac{2}{a}}$

$$\phi_n = \begin{cases} \sqrt{\frac{2}{a}}\cos k_n x & k_n = \frac{n\pi}{a} \quad n = 1,3,5 \\ \sqrt{\frac{2}{a}}\sin k_n x & k_n = \frac{n\pi}{a} \quad n = 2,4,6 \end{cases}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a} = \frac{n^2\pi^2\hbar^2}{2ma^2}\phi_n$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} = \frac{n^2\pi^2\hbar^2}{2ma^2}\phi_n$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Lec 7. HO

$$\left[\frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}\right]\phi = E\phi$$

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{dx^2} + \frac{m\omega^2\hat{x}^2}{2}\right]\phi = E\phi$$

$\hat{\xi} = \frac{\hat{x}}{b}$ $\quad b = \sqrt{\frac{\hbar}{m\omega}}$ $\quad \hat{p} = \frac{1}{i}\frac{d}{d\xi}$ $\qquad [\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} - \hat{A}[\hat{B}, \hat{C}]$

$\frac{\hbar\omega}{2}(\hat{p}_\xi^2 + \hat{\xi}^2)\phi(\xi) = E\phi(\xi) \Rightarrow \frac{\hbar\omega}{2}[-\frac{d^2}{d\xi^2} + \xi^2]\phi(x) = E\phi(x)$

The following are properties of the ascending and descending operators

$\hat{a}_+ = \frac{1}{\sqrt{2}}(-i\hat{p}_\xi + \hat{\xi}) = \frac{1}{\sqrt{2}}(-\frac{d}{d\xi} + \xi)$

$\hat{a}_- = \frac{1}{\sqrt{2}}(+i\hat{p}_\xi + \hat{\xi}) = \frac{1}{\sqrt{2}}(\frac{d}{d\xi} + \xi)$

$\hat{a}_-\hat{a}_+ = \frac{1}{2}[\hat{p}_\xi^2 + \hat{\xi}^2 - i[\hat{\xi}, \hat{p}_\xi]]$ $\quad [\hat{\xi}, \hat{p}_\xi] = i$ $\qquad \hat{a}_-\hat{a}_+ = \frac{1}{2}[\hat{p}_\xi^2 + \hat{\xi}^2 + 1] \Rightarrow \hat{H} = \hbar\omega[\hat{a}_-\hat{a}_+ - \frac{1}{2}]$

$\hat{a}_+\hat{a}_- = \frac{1}{2}[\hat{p}_\xi^2 + \hat{\xi}^2 + i[\hat{\xi}, \hat{p}_\xi]]$ $\qquad \hat{a}_+\hat{a}_- = \frac{1}{2}[\hat{p}_\xi^2 + \hat{\xi}^2 - 1] \Rightarrow \hat{H} = \hbar\omega[\hat{a}_+\hat{a}_- + \frac{1}{2}]$

$[\hat{a}_-, \hat{a}_+] = 1$ $\qquad \hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_- = 1$ $\qquad \Rightarrow [\hat{a}_-, \hat{a}_+] = 1$

$\hat{H} = \hbar\omega[\hat{a}_-\hat{a}_+ - \frac{1}{2}]$

$\hat{H} = \hbar\omega[\hat{a}_+\hat{a}_- + \frac{1}{2}]$

$[\hat{H}, \hat{a}_+] = \hbar\omega[\hat{a}_+\hat{a}_-, \hat{a}_+] = \hbar\omega\hat{a}_+ \Rightarrow \hat{H}\hat{a}_+ - \hat{a}_+\hat{H} = \hbar\omega\hat{a}_+$ $\qquad \hat{a}_-\hat{a}_+\hat{c}_p - \hat{c}_p\hat{a}_-\hat{c}_p$

$\cancel{(\hat{H} - \frac{1}{2}\hbar\omega)\hat{a}_+ = \hat{a}_+(\hat{H} - \frac{1}{2}\hbar\omega)} + \hbar\omega\hat{a}_+$

$\Rightarrow \hat{H}\hat{a}_+ = \hat{a}_+\hat{H} + \hbar\omega\hat{a}_+$

$\hat{H}\hat{a}_+\phi = \hat{a}_+\hat{H}\phi + \hbar\omega\hat{a}\phi$

$\hat{H}(\hat{a}_+\phi) = (E + \hbar\omega)(\hat{a}_+\phi)$

$$[\hat{H}, \hat{a}_-] = \hbar\omega[\hat{a}_-\hat{a}_+, \hat{a}_-] = \hbar\omega\left([\hat{a}_-,\hat{a}_-]\hat{a}_+ + \hat{a}_-[\hat{a}_+,\hat{a}_-]\right) = -\hbar\omega\hat{a}_-$$

$$\hat{H}\hat{a}_- = \hat{a}_-\hat{H} - \hbar\omega\hat{a}_-$$

$$\Rightarrow \hat{H}(\hat{a}_-\phi) = \hat{a}_-(\hat{H}\phi) - \hbar\omega\hat{a}_-\phi \Rightarrow \hat{H}(\hat{a}_-\phi) = (E-\hbar\omega)\hat{a}_-\phi$$

$$\hat{a}_-\phi_0(x) = 0 \Rightarrow \frac{1}{\sqrt{2}}\left(\frac{d}{d\xi}+\xi\right)\phi_0(\xi) = 0 \Rightarrow y'+\xi y=0 \Rightarrow \phi_0(\xi) = Ae^{-\frac{\xi^2}{2}}$$

$\xi = \frac{x}{b}$

$$1 = \int_{-\infty}^{+\infty} A^2 e^{-\xi^2}dx = A^2\int_{-\infty}^{+\infty} e^{-\frac{x^2}{b^2}}dx = A^2\sqrt{\pi b^2} \Rightarrow A = \left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}} \Rightarrow \phi_0(x) = \left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}} e^{-\frac{x^2}{2b^2}}$$

$$\hat{H}\phi_0 = \frac{\hbar\omega}{2}[\hat{p}_\xi^2 + \hat{\xi}^2]\phi_0(x) = \frac{\hbar\omega}{2}\left[-\frac{d^2}{d\xi^2}+\xi^2\right]\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}} = \frac{\hbar\omega}{2}\phi_0(\xi) \Rightarrow E_0 = \frac{\hbar\omega}{2}$$

$$\phi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\phi_0 \qquad \phi_0 = \left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}} \qquad E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$\phi_1 = \sqrt{2}\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}\xi e^{-\frac{\xi^2}{2}}$$

try $\phi_1 = \frac{1}{\sqrt{1}}\boxed{\frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi}+\xi\right)}\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}}$

$$= \frac{1}{\sqrt{1}}\frac{1}{\sqrt{2}}2\xi\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}} = \frac{1}{\sqrt{1}}\cdot\sqrt{2}\cdot\frac{x}{b}\cdot\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}}$$

$$-\frac{d}{d\xi}\phi_0 = \phi_0(-\xi)$$

对的

$$\phi_2 = \frac{1}{\sqrt{2}}\cdot(\hat{a}_+)\phi_1$$

$$= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi}+\xi\right)\phi_1 \qquad \phi_2 = \frac{1}{\sqrt{2}}\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}}(2\xi^2-1)$$

$$= \frac{1}{2}\left[-\sqrt{2}\left(\frac{1}{\pi b^2}\right)^{\frac{1}{4}}\left(e^{-\frac{\xi^2}{2}}-2\xi^2e^{-\frac{\xi^2}{2}}\right)\right]$$

$\hat{a}_+ = \frac{1}{\sqrt{2}}(-i\hat{p}_\xi + \xi)$. $\quad \hat{a}_+^* = \hat{a}_-$

$\hat{a}_+\hat{a}_- \phi_m^* = m\phi_m$

$\hat{a}_+\hat{a}_- \phi_m = m\phi_m$

$\hat{a}_- = \frac{1}{\sqrt{2}}(i\hat{p}_\xi + \xi)$

$(AB)^* = B^* A^*$

$\hat{H} = \hbar\omega(\hat{a}_+\hat{a}_- + \frac{1}{2}) \Rightarrow \hat{a}_+\hat{a}_- = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$ $\quad \hat{a}_+\hat{a}_-\phi_n = \left(\frac{\hbar\omega(n+\frac{1}{2})}{\hbar\omega} - \frac{1}{2}\right)\phi_n = n\phi_n$

$$\int_{-\infty}^{+\infty} \phi_m^* \hat{a}_+\hat{a}_- \phi_n \, dx = \int_{-\infty}^{+\infty} (\hat{a}_-\phi_m)^* (\hat{a}_-\phi_n)\, dx = \int_{-\infty}^{+\infty} (\hat{a}_+\hat{a}_-\phi_m)^* \phi_n \, dx = m\int \phi_m^* \phi_n \, dx$$

$$\parallel$$

$$n\int_{-\infty}^{+\infty} \phi_m^* \phi_n \, dx$$

$$\Rightarrow (m-n)\int_{-\infty}^{+\infty} \phi_m^* \phi_n \, dx = 0 \qquad \int_{-\infty}^{+\infty} \phi_i^* \phi_j \, dx = \delta_{ij}$$

$[\hat{a}_-, \hat{a}_+] = 1 \qquad [\hat{a}_-, \hat{a}_-] = 0 \qquad [\hat{a}_+, \hat{a}_+] = 0$

$\hat{a}_-\phi_0 = 0 \qquad \hat{H} = \hbar\omega[\hat{a}_-\hat{a}_+ - \frac{1}{2}] = \hbar\omega[\hat{a}_+\hat{a}_- + \frac{1}{2}]$

$\phi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n \phi_0 \qquad E_n = (n+\frac{1}{2})\hbar\omega$

Lec 8. The same as Lec.7

$\boxed{\text{Lec. 9. Free particle}}$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} = E\phi(x) \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\frac{d^2\phi(x)}{dx^2} = -k^2\phi(x)$$

$$\phi(x) = Ae^{ikx} + Be^{-ikx} = Ae^{ikx}$$

$$\psi(x,t) = Ae^{(ikx - i\frac{Et}{\hbar})} + Be^{(-ikx - i\frac{Et}{\hbar})}$$

k runs over positive / negative Continuous

$$\psi(x,t) = Ae^{(ikx - i\frac{Et}{\hbar})} = Ae^{i(kx - \frac{\hbar k^2}{2m}t)}$$

$$kx - \frac{\hbar k^2}{2m}t = k(x+\Delta x) - \frac{\hbar k^2}{2m}(t+\Delta t)$$

change some Δx, change some Δt, phase not change, so that's the phase velocity

$$k\Delta x - \frac{\hbar k^2}{2m}\Delta t = 0 \Rightarrow \frac{\Delta x}{\Delta t} = \frac{\hbar k}{2m}$$

$k \begin{cases} \text{positive} \rightarrow \text{move to the right} \\ \text{negative} \rightarrow \text{left} \end{cases}$

V_{phase} x

$$\lambda = \frac{2\pi}{|k|} \qquad p = \frac{h}{a} = \hbar k$$

Curiosities

①

$$|V|_{quantum} = \frac{\hbar k}{2m} = \frac{\hbar}{2m}\cdot\frac{\sqrt{2mE}}{\hbar} = \sqrt{\frac{E}{2m}}$$

classical

$$|V|_{classical} = \sqrt{\frac{2E}{m}}$$

② $\int_{-\infty}^{+\infty} \psi^*(x,t)\,\psi(x,t)\,dx = A^2 \int_{-\infty}^{+\infty} dx \to \infty$

① $\frac{1}{\sqrt{2\pi a}} e^{ikx}$

② boundary periodic ③

$k = \frac{n}{a}$

$[-\pi a, \pi a]$

$\phi_k(x) = \frac{1}{\sqrt{2\pi a}} e^{ikx}$

boundary condition

$\frac{1}{\sqrt{2\pi a}} e^{ikx}\Big|_{x=-\pi a} = \frac{1}{\sqrt{2\pi a}} e^{ikx}\Big|_{x=\pi a} \Rightarrow e^{i2\pi ka} = 1 \quad \begin{cases} \cos 2\pi ka = 1 \Rightarrow 2\pi ka = 2n\pi \\ \sin 2\pi ka = 0 \end{cases}$

$k = \frac{n}{a}, (n = \dots -2, -1, 0, 1, 2 \dots)$

normalized

$\int_{-\pi a}^{\pi a} \phi_n^*(x)\,\phi_n(x) = \frac{1}{2\pi a}\int_{-\pi a}^{\pi a} dx = 1$

orthonormal

$\int_{-\pi a}^{\pi a} \phi_n^*(x)\,\phi_m(x) = \frac{1}{2\pi a}\int_{-\pi a}^{\pi a} e^{ix(\frac{m-n}{a})}\,dx = \frac{1}{2\pi a}\cdot\frac{a}{n-m}\left[\sin\left(\frac{n-m}{a}\right) \times \Big|_{-\pi a}^{\pi a}\right] = 0$

$\cos\left(\frac{n-m}{a}\right)x$ unless $n=m$

$\phi_n(x) = \frac{1}{\sqrt{2\pi a}} e^{ik_n x}, \quad k_n = \frac{n}{a}, \quad n = \dots -2, -1, 0, 1, 2 \dots$

According prime directive

$$\psi(x,t)=\sum_n \frac{1}{\sqrt{2\pi a}} e^{ik_n x} e^{-i\frac{E_n t}{\hbar}} \cdot \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi a}} e^{-ik_n y}\psi(y,0)\,dy$$

$$\Delta k = k_{n+1}-k_n = \frac{n+1}{a}-\frac{n}{a}=\frac{\Delta n}{a} \qquad \Delta n=1$$

$$\sum_n = \sum_n \Delta n = \sum a\Delta k \Rightarrow a\int_{-\infty}^{+\infty} dk$$

$$\psi(x,t)=\int_{-\infty}^{+\infty} dk \frac{1}{\sqrt{2\pi}} e^{ikx} e^{-i\frac{E(k)t}{\hbar}} \int dy \frac{1}{\sqrt{2\pi}} e^{-iky}\psi(y,0)$$

$$= \int_{-\infty}^{+\infty} dk \frac{1}{\sqrt{2\pi}} e^{ikx} e^{-i\frac{E(k)t}{\hbar}} a(k) \qquad E(k)=\frac{\hbar^2k^2}{2m}$$

$$\psi(x,0)=\int_{-\infty}^{+\infty} a(k)\,\phi(k,x)\,dk \qquad a(k)=\int_{-\infty}^{+\infty} \phi^*(k,y)\,\psi(y,0)\,dy$$

integral for each k. Σ

solve Questions

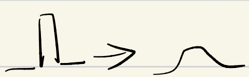
$$\psi(x,t)=\int_{-\infty}^{+\infty} a(k)\,\phi(k,x)\,e^{-i\frac{E(k)t}{\hbar}}\,dk$$

$$\phi(k,x)=\frac{1}{\sqrt{2\pi}}e^{ikx}, \quad E(k)=\frac{\hbar^2k^2}{2m}$$

Continuous Fourier transforms, which we use to expand wave packets on a finite interval.

First issue solved

e.g. $\psi(x,0)=\begin{cases}\frac{1}{\sqrt{2a}} & a\in[-a,a]\\ 0 & |x|>a\end{cases}$ → expand



free particle, use $\phi_n=\frac{1}{\sqrt{2\pi}}e^{ikx}$

so $a(k)=\int_{-\infty}^{+\infty}\frac{1}{\sqrt{2\pi}}e^{-ikx}\psi(x,0)\,dx = \frac{1}{\sqrt{\pi a}}\frac{\sin ka}{k}$

$\psi(x,t)=\int_{-\infty}^{+\infty} a(k)\phi(k,x)e^{-i\frac{E(k)t}{\hbar}}\,dk$

$$a_k=\int_{-a}^{a}\frac{1}{\sqrt{2\pi}}e^{ikx}\frac{1}{\sqrt{2a}}\,dx = \frac{1}{2\sqrt{\pi a}}\frac{1}{k}\sin(kx)\Big|_{-a}^{a} = \frac{1}{\sqrt{\pi a}}\frac{\sin ka}{k}$$

$$\psi(x,t)=\int_{-\infty}^{+\infty} a_k\,\phi(k,x)\,e^{-i\frac{E(k)t}{\hbar}}\,dk=\int_{-\infty}^{+\infty}\frac{1}{\sqrt{\pi a}}\frac{\sin ka}{k}\frac{1}{\sqrt{2\pi}}e^{ikx}e^{i\frac{\hbar k^2}{2m}t}\,dk$$

for the second issue

$e^{ikx} e^{i\frac{E(k)t}{\hbar}}$

$e^{i(kx - \frac{E(k)t}{\hbar})}$

$\frac{E(k)}{\hbar} = \omega(k) = \frac{\hbar k^2}{2m}$

$\frac{p^2}{2m} = \hbar$

$p = \sqrt{2mE}$

$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \phi(k)\, e^{i(kx - \omega(k)t)}$$

$$\omega = \frac{\hbar k^2}{2m}$$

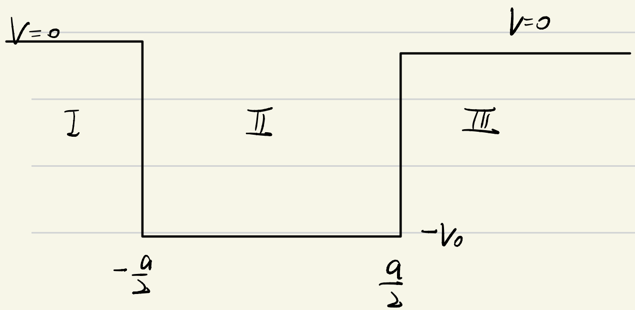
$$v_{phase} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{\hbar}{2m}\cdot\frac{\sqrt{2mE}}{\hbar} = \sqrt{\frac{E}{2m}}$$

$$v_{phase} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \sqrt{\frac{2mE}{4m^2}} = \sqrt{\frac{E}{2m}}$$

$$v_{group} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \sqrt{\frac{2E}{m}}$$

$$v_{group} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{\hbar}{m}\cdot\frac{\sqrt{2mE}}{\hbar} = \sqrt{\frac{2E}{m}}$$ → match classical

Lec. 10 Finite Square Well



I、III

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = -|E|\phi \Rightarrow \phi'' = k^2\phi \Rightarrow \phi = Ae^{-kx} + Be^{kx}$$

I , $x \to -\infty$, $\phi = 0$ $\Rightarrow \phi_I = Be^{kx}$ $x < -\frac{a}{2}$ $\phi_I'(x) = Bke^{kx}$

III , $x \to +\infty$, $\phi = 0$ $\Rightarrow \phi_{III} = Ae^{-kx}$ $x > \frac{a}{2}$ $\phi_{III}'(x) = -Ake^{-kx}$

II $\frac{-\hbar^2}{2m}\phi'' + -V_0\phi = -|E|\phi \Rightarrow \phi'' = -\frac{2m(V_0-|E|)}{\hbar^2}\phi = -k^2\phi$

$\phi_{II} = C\cos kx + D\sin kx$ $-\frac{a}{2} < x < \frac{a}{2}$

even-parity solution $\phi_{II}(x) = C\cos kx$ $-\frac{a}{2} < x < \frac{a}{2}$ $\phi_{II}'(x) = -Ck\sin kx$

boundary $\phi_I = \phi_{II}\Big|_{-\frac{a}{2}} \Rightarrow Be^{-\frac{ka}{2}} = C\cos\frac{ka}{2}$ $\Rightarrow B = Ce^{\frac{ka}{2}}\cdot\cos\frac{ka}{2}$ ①

$\phi_I' = \phi_{II}'\Big|_{-\frac{a}{2}} \Rightarrow Bke^{-\frac{ka}{2}} = Ck\sin\frac{ka}{2}$ $\Rightarrow$ $k\tan\frac{ka}{2} = k$ ③

$\phi_{III} = \phi_{II}\Big|_{\frac{a}{2}} \Rightarrow Ae^{-\frac{ka}{2}} = C\cos\frac{ka}{2} \Rightarrow A = Ce^{\frac{ka}{2}}\cos\frac{ka}{2}$ ②

$\phi_{III}' = \phi_{II}'\Big|_{\frac{a}{2}} \Rightarrow -Ake^{-\frac{ka}{2}} = -Ck\sin\frac{ka}{2}$

$$\begin{cases} \phi_I = Ce^{\frac{ka}{2}}\cos(\frac{ka}{2})\cdot e^{kx} & x < -\frac{a}{2} \\ \phi_{II} = C\cos kx & -\frac{a}{2} < x < \frac{a}{2} \\ \phi_{III} = Ce^{\frac{ka}{2}}\cos(\frac{ka}{2})\cdot e^{-kx} & x > \frac{a}{2} \end{cases}$$

& $k\tan\frac{ka}{2} = k$

we need C、D、E

Similarly

odd-parity solution

$$\begin{cases} \phi_I = -De^{\frac{ka}{2}} \sin\frac{ka}{2} \cdot e^{\kappa x} \\ \phi_{II} = D\sin kx \\ \phi_{III} = De^{\frac{ka}{2}} \sin(\frac{ka}{2})\, e^{-\kappa x} \end{cases}$$

$$\& \quad k\cot\frac{ka}{2} = -\kappa$$

$$\tan z = \sqrt{(\frac{z_0}{z})^2 - 1}$$

$$z_0 \Rightarrow z \Rightarrow |E|$$

$$\begin{cases} k\tan\frac{ka}{2} = \kappa \\ k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \end{cases}$$

$$k = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar}$$

$$\kappa = \frac{\sqrt{2m|E|}}{\hbar}$$

$$\Rightarrow \frac{ka}{2} \cdot \tan\frac{ka}{2} = \frac{\kappa a}{2} \Rightarrow z\tan z = \frac{\kappa a}{2}$$

$$\Rightarrow (\frac{ka}{2})^2 + (\frac{\kappa a}{2})^2 = (\frac{a}{2}\frac{\sqrt{2mV_0}}{\hbar})^2 \Rightarrow z_0^2 - z^2 = (\frac{\kappa a}{2})^2$$

$$\frac{z_0}{\frac{a}{2}} = \frac{\sqrt{2mV_0}}{\hbar}$$

$$z\tan z = \sqrt{z_0^2 - z^2} \Rightarrow \tan z = \sqrt{(\frac{z_0}{z})^2 - 1}$$

$$|E| \sim 0 \Leftrightarrow \kappa \sim 0 \Leftrightarrow z \sim 0 \Leftrightarrow z_0 - z = 0 \Leftrightarrow \tan z_0 = 0 \Rightarrow z_0 = n\frac{\pi}{2} \qquad n = 0, 2, 4 \cdots$$

E 接近顶端时

$\square$ 内模式 Max

$$(\frac{a}{2} \cdot \frac{\sqrt{2mV_0}}{\hbar})^2 = (\frac{n\pi}{2})^2 \Rightarrow \frac{a^2}{4} \cdot \frac{2mV_0}{\hbar^2} = \frac{n^2\pi^2}{4} \Rightarrow a^2 V_0 = \frac{n^2\pi^2\hbar^2}{2m}$$

$\frac{(n+2)^2\pi^2\hbar^2}{2m} > a^2V_0 > \frac{n^2\pi^2\hbar^2}{2m}$ have $\frac{n}{2}+1$ even bound states

$n = 0, 2, 4 \cdots$

odd

$\cot z \sim \cot z_0 = 0$ $\quad z_0 = n\frac{\pi}{2}$ $\quad n = 1, 3, 5 \cdots$

$\frac{(n+2)^2 \pi^2 \hbar^2}{2m} > a^2 V_0 > \frac{n^2\pi^2\hbar^2}{2m}$, $n = 1, 3, 5 \cdots$, $\frac{n+1}{2}$ odd bound state

How many

together

$n+1$??? yes?

$\frac{(n+1)^2\pi^2\hbar^2}{2m} > a^2 V_0 > \frac{n^2\pi^2\hbar^2}{2m}$ $\quad n = 0, 1, 2, \cdots$, have $n+1$ bound states

$(n+1)\frac{\pi}{2} > z_0 > n\cdot\frac{\pi}{2}$ (equivalent condition)

eigenvalue function

Inf → S-W

$V_0 \to \infty \Leftrightarrow z_0 \to \infty \Rightarrow$ try to contain all solution

$\tan z = \tan\frac{ka}{2} = \frac{1}{z}\sqrt{z_0^2 - z^2} \to \infty$ $\qquad \frac{k_n a}{2} = \frac{n\pi}{2}$ $\quad n = 1, 3, 5, \cdots$

$-\cot z = -\cot\frac{ka}{2} = \frac{1}{z}\sqrt{z_0^2 - z^2} \to \infty$ $\qquad \frac{k_n a}{2} = \frac{n\pi}{2}$ $\quad n = 2, 4, 6 \cdots$

$\Rightarrow k_n a = n\pi$ $\quad n = 1, 2, 3 \cdots$ $\qquad E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

$z = \frac{ka}{2} = \frac{a}{2}\frac{\sqrt{2m(V_0 - |E|)}}{\hbar}$

$z_0 = \frac{a}{2}\frac{\sqrt{2mV_0}}{\hbar}$

$z = z_0\sqrt{1 - \frac{|E|}{V_0}}$

e.g. $z_0 = \frac{\pi}{20}$ $\qquad z_0 = \frac{a}{2}\cdot\frac{\sqrt{2mV_0}}{\hbar} \Rightarrow V_0 = \frac{4\hbar^2 z_0^2}{2ma^2} = \frac{4\hbar^2}{2ma^2}\left(\frac{\pi}{20}\right)^2$ step 1

$k = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar} < \frac{\sqrt{2mV_0}}{\hbar} = \frac{z_0}{\frac{a}{2}} = \frac{\pi}{10a}$

$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \Rightarrow z = \text{Ans}$ step 2 $\qquad \frac{2\hbar^2}{ma^2} = V_0\cdot\left(\frac{20}{\pi}\right)^2$

$\frac{ka}{2} = \sqrt{z_0^2 - z^2} = \text{Ans}$ step 3

$\lambda = \frac{2\pi}{k} > 20a$

$k = \frac{\sqrt{2m|E|}}{\hbar} \Rightarrow |E| = \frac{(k\hbar)^2}{2m} = \left(\frac{ka}{2}\right)^2\cdot\frac{2\hbar^2}{ma^2}$ step 4

Lec. 11 Delta function

$$\delta(x) = \lim_{a \to 0} \frac{1}{|a|\sqrt{\pi}} e^{-\frac{x^2}{a^2}}$$

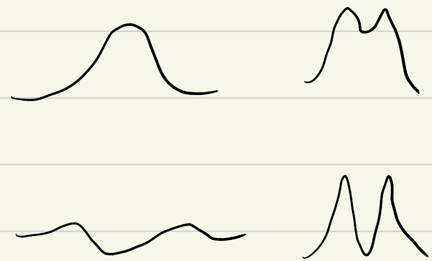
$$\int_{-\infty}^{+\infty} \delta(x) = 1$$

$$\int_{-\infty}^{+\infty} f(x)\,\delta(x) = 0 \qquad \int_{-\infty}^{+\infty} f(x)\,\delta(x-a) = f(a)$$

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

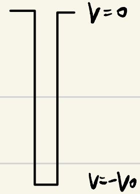
$$V_\delta(x) = -a V_0\, \delta(x) = -\alpha\, \delta(x)$$

$f(x)$ $F(k)$



Δx $\Delta k \to \infty$ accurate

Lec. 12 A narrow infinite well



E 必 <0 $\because$ V_0 太深了

$V_\delta(x) = -a V_0 \delta(x)$

$\frac{ka}{2}\tan\frac{ka}{2} = \frac{\kappa a}{2}$ $\quad \frac{ka}{2} = \frac{a}{2}\cdot\frac{\sqrt{2m(V_0+E)}}{\hbar}$

$a\to\infty \Rightarrow \frac{ka}{2}\to\infty$ $\quad \frac{\kappa a}{2} = \frac{a}{2}\frac{\sqrt{2m|E|}}{\hbar}$

$\left(\frac{ka}{2}\right)^2 = \frac{\kappa a}{2}$

$\frac{2ma^2V_0(1-\frac{|E|}{V_0})}{4\hbar^2} = \frac{a\sqrt{2m|E|}}{2\hbar}$ $\quad$ small

$\Rightarrow \left(\frac{2ma^2V_0}{4\hbar^2}\cdot\frac{2\hbar}{a}\right)^2 / 2m$

$= \left(\frac{maV_0}{\hbar}\right)^2/2m = \frac{m a^2 V_0^2}{2\hbar^2} = \frac{m\alpha^2}{2\hbar^2} = |E|$

V_0 is large $\quad \kappa \approx \frac{\sqrt{2mV_0}}{\hbar}$ 已有是 constant $\Rightarrow$ 且只有一解 even

So $\phi_L(x) = Ce^{\frac{\kappa a}{2}}\cos\frac{ka}{2}\, e^{\kappa x} = Ce^{\kappa(x+\frac{a}{2})}$

$\cos\frac{ka}{2} \to 1$ $\quad$ even

$\phi(0) = C\cos 0 = C$

$\kappa = \frac{\sqrt{2m\frac{m\alpha^2}{2\hbar^2}}}{\hbar} = \frac{m\alpha}{\hbar}$

$\phi_L' = C\kappa e^{\kappa(x+\frac{a}{2})}$ $\quad \phi_R' = -C\kappa e^{-\kappa(x-\frac{a}{2})}$ when $x > -\frac{a}{2}$ and $\frac{a}{2}$

$\phi_R'(0) - \phi_L'(0) = -2\kappa\phi(0) = -2\cdot\frac{\sqrt{2m|E|}}{\hbar}\phi(0) = -\frac{2m\alpha}{\hbar^2}\phi(0)$

Discontinuous ~~对解方程屁用没有~~，只是边界有用有用，可解出 κ

$\phi_L = Ce^{\kappa x}$ $\quad \phi_R = Ce^{-\kappa x}$ (Without considering derivative $e^{\frac{\kappa a}{2}}$ is constant

再通过 normalizable 解出 $C=\sqrt{\kappa}$

Normalization $\int_{-\infty}^{0}|C|^2e^{2\kappa x}dx + \int_0^{+\infty}|C|^2e^{-2\kappa x}dx$

$= \frac{|C|^2}{2\kappa} + \frac{|C|^2}{+2\kappa} = \frac{|C|^2}{\kappa} = 1 \Rightarrow C = \sqrt{\kappa} = \sqrt{\frac{m\alpha}{\hbar^2}}$

$$\phi(x) = \begin{cases}\sqrt{\kappa}\,e^{\kappa x} & x<0\\ \sqrt{\kappa}\,e^{-\kappa x} & x>0\end{cases}$$

$V_\delta = -\alpha\,\delta(x)$

$|E| = \dfrac{m\alpha^2}{2\hbar^2}$

$k = \dfrac{m\alpha}{\hbar^2}$

$$\phi(x) = \begin{cases} \sqrt{k}\,e^{kx} & x<0 \\ \sqrt{k}\,e^{-kx} & x>0 \end{cases}$$

$a\to0 \quad \frac{ka}{2}\to0 \quad V_0\to0 \quad \frac{|E|}{V_0}\to0$

$\left(\frac{ka}{2}\right)^2 = \frac{ka}{2}$

$\frac{a^2}{4}\,\frac{2mV_0\left(1+\frac{|E|}{V_0}\right)}{\hbar^2} = \frac{a}{2}\,\frac{\sqrt{2m|E|}}{\hbar}$

$\frac{a\,mV_0}{\hbar} = \sqrt{2m|E|}$

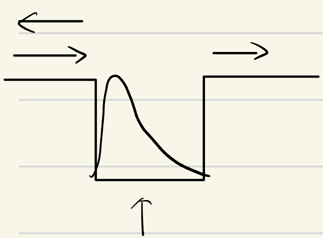
$\frac{a^2m^2V_0^2}{\hbar^2} = 2m|E|$

$\Rightarrow |E| = \frac{m\alpha^2}{2\hbar^2}$

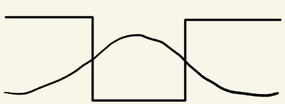
$K = \frac{\sqrt{2m|E|}}{\hbar} = \frac{m\alpha}{\hbar}$

Schrodinger Equation
boundary condition
normalization ϕ
S-E to get E_n

Real Prime Derivative



un symmetric



symmetric

Lec 14. Finite S-W $E>0$

T, R

Lec 15, 16, 17, 18

1. $\sum_i |i\rangle\langle i| = 1$

2. $|\alpha\rangle = \sum_i |i\rangle\langle i|\alpha\rangle = \sum_i |i\rangle a_i$

$= \int |x\rangle\langle x|\alpha\rangle dx = \int |x\rangle \phi_\alpha(x)\, dx$

3. $\langle\alpha|i\rangle = \langle i|\alpha\rangle^*$

4. Hermitian $\hat{Q}$

5. $\langle\alpha|\hat{Q}\alpha\rangle = \langle\hat{Q}^\dagger\alpha|\alpha\rangle = \langle\hat{Q}\alpha|\alpha\rangle$

6. $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ $\quad \langle p'|p\rangle = \delta(p'-p)$

7. $|\alpha\rangle = \int dp\, |p\rangle\langle p|\alpha\rangle = \int dp\, |p\rangle \phi_\alpha(p)$

8. $Q_\alpha = \langle\alpha|\hat{Q}\alpha\rangle = \langle\hat{Q}\alpha|\alpha\rangle = \langle\hat{Q}\alpha\rangle^*|\alpha\rangle = Q_\alpha^*\langle\alpha|\alpha\rangle = Q_\alpha^*$ real ①

9. $\langle\alpha|\hat{Q}\beta\rangle = \langle\hat{Q}\alpha|\beta\rangle$

$(Q_\beta - Q_\alpha^*)\langle\alpha|\beta\rangle = 0$ $\quad Q_\alpha \neq Q_\beta \Rightarrow \langle\alpha|\beta\rangle = 0$ ② eigenfunction orthogonal

$\downarrow$

Q_α

belonging to diff eigenvalues

③ eigenfunction complete: Any state in Hilbert space can be expanded in terms of this basis

10. $\langle \gamma | \alpha + \beta \rangle = \langle \gamma | \alpha \rangle + \langle \gamma | \beta \rangle$

$\langle \beta | a\alpha \rangle = a \langle \beta | \alpha \rangle$

$\langle \alpha | \alpha \rangle \geq 0$

$\langle \alpha | \beta \rangle^* = \langle \beta | \alpha \rangle$

$\langle \alpha + \beta | \gamma \rangle = \langle \gamma | \alpha + \beta \rangle^* = (\langle \gamma | \alpha \rangle + \langle \gamma | \beta \rangle)^* = \langle \alpha | \gamma \rangle + \langle \beta | \gamma \rangle$

$\langle a\alpha | \beta \rangle = a^* \langle \alpha | \beta \rangle$ $\quad \langle \alpha | \hat{T} \hat{U} \beta \rangle^+$ $\quad [\hat{T}\hat{U}]^+ = U^+ T^+$

$T \alpha \rangle^+ = \langle \alpha | T^+$ $\quad = \langle \hat{T}\hat{U}\beta | \alpha \rangle$

$= |\hat{T}\hat{U}\beta\rangle^+ |\alpha\rangle = \langle U\beta | T^+ \alpha \rangle$

$|U\beta\rangle^+$

$\langle \beta | U^+ T^+ | \alpha \rangle$

$\langle \alpha | \beta \rangle^+ = \langle \alpha | \beta \rangle^* = \langle \beta | \alpha \rangle$

$\langle \alpha | \hat{T} | \beta \rangle^+ = \langle \beta | \hat{T}^+ | \alpha \rangle$ $\quad \langle \hat{T}\beta | \alpha \rangle = \langle \beta | T^+ | \alpha \rangle$

$\langle \alpha | \hat{T} \hat{U} | \beta \rangle^+ = \langle \beta | \hat{U}^+ \hat{T}^+ | \alpha \rangle$ $\quad \langle T\beta | \alpha \rangle = \langle \beta | T^+ | \alpha \rangle$

$|T\beta\rangle^+$

$[\hat{T}\hat{U}]^+ = \hat{U}^+ \hat{T}^+$

$[\hat{A}_1 \hat{A}_2 \cdots \hat{A}_n]^+ = \hat{A}_n^+ \cdots \hat{A}_2^+ \hat{A}_1^+$ $\quad \langle \beta | T^+$

$\langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq \langle \frac{1}{2i} [\hat{A}, \hat{B}] \rangle^2$

If $[\hat{A}, \hat{B}]$ commute $\sigma_A^2 \sigma_B^2 = 0$

Lec 19

$$\sigma_A^2 \sigma_B^2 \geq \langle \frac{1}{2i} [\hat{A}, \hat{B}] \rangle^2$$

Lec 20

Commuting Hermitian operators. These operators represent observables that are simultaneously measurable.

Hermitian do not commute. These operators represent observables are not simultaneously observable.

$$\sigma_A \sigma_B \geq \langle \frac{1}{2i} [\hat{A}, \hat{B}] \rangle$$

1. $[\hat{x}, \hat{p}] = i\hbar$ $\quad \sigma_x \sigma_p \geq \frac{\hbar}{2}$

Generalized Ehrenfest theorem: $\frac{d}{dt} \langle \phi | \hat{Q} | \phi \rangle = \frac{i}{\hbar} \langle \phi | [\hat{H}, \hat{Q}] | \phi \rangle + \langle \phi | \underbrace{\frac{\partial \hat{Q}}{\partial t}}_{0?} | \phi \rangle$

$$\sigma_H^2 \sigma_Q^2 \geq \langle \phi | \frac{1}{2i} [\hat{H}, \hat{Q}] | \phi \rangle^2 = [-\frac{\hbar}{2} \frac{d}{dt} \langle \phi | \hat{Q} | \phi \rangle]^2 \Rightarrow \sigma_H \sigma_Q \geq \frac{\hbar}{2} \left| \frac{d}{dt} \langle \phi | \hat{Q} | \phi \rangle \right|$$

2. $\langle H \rangle = E \Rightarrow \sigma_H^2 = \Delta E^2$ $\quad \sigma_Q = \left| \frac{d \langle \phi | \hat{Q} | \phi \rangle}{dt_0} \right| \Delta t_Q \Rightarrow \Delta E \cdot \Delta t_Q \geq \frac{\hbar}{2}$

$$\sqrt{\langle \phi | \hat{H}^2 | \phi \rangle - \langle \phi | \hat{H} | \phi \rangle^2}$$

3. In other cases $\quad \sigma_x = \sqrt{\langle \phi | \hat{x}^2 | \phi \rangle - \langle \phi | \hat{x} | \phi \rangle^2}$

4. e.g. $2p \rightarrow 1s$

photon 10eV

$$\frac{dN(t)}{dt} = -\omega N(t) \qquad N(0) = N_0 \Rightarrow N(t) = N_0 e^{-\omega t}$$

平均寿命

$$t = \frac{\ln 2}{\omega} \Rightarrow N(t) = \frac{N_0}{2}$$

$$t_m = \frac{1}{N_0}\int_0^\infty dt\, t \cdot \left|\frac{dN(t)}{dt}\right| = \frac{1}{\omega}$$

$$N(t_{\frac{1}{2}}) = \frac{N_0}{2} \Rightarrow t_{\frac{1}{2}} = \frac{\ln 2}{\omega} = \ln 2\, t_m$$

$$\Delta E \cdot \Delta t \sim \frac{\hbar}{2} \Rightarrow \Delta E = \frac{\hbar}{2}\frac{1}{\Delta t} = \frac{\hbar}{2 t_m} \approx \frac{\hbar\omega}{2} \sim 2\times 10^{-7}\,eV$$

$$\frac{\Delta E}{E} \sim \frac{2\times 10^{-7}\,eV}{10\,eV} \sim 10^{-8}$$

Lec. 21 3D cube

$$\hat{H}|\psi\rangle = \hat{E}|\psi\rangle$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$\psi(\vec{r},t) \to \phi_n e^{-i\frac{E_n t}{\hbar}} \Rightarrow \text{for each } \phi_n \quad \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\phi_n(\vec{r}) = E_n\phi_n(\vec{r})$$

$$V(x,y,z) = \begin{cases} 0 & \text{if } x,y,z \in [-\frac{a}{2}, \frac{a}{2}] \\ \infty & \text{otherwise} \end{cases}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\phi(x,y,z) = E\,\phi(x,y,z) \qquad \phi_{n_x n_y n_z}(x,y,z) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)$$

$$\frac{1}{\phi_{n_x}}\frac{d^2\phi_{n_x}}{dx^2} + \frac{1}{\phi_{n_y}}\frac{d^2\phi_{n_y}}{dy^2} + \frac{1}{\phi_{n_z}}\frac{d^2\phi_{n_z}}{dz^2} = -\frac{2m}{\hbar^2}E_{n_x,n_y,n_z} \qquad \frac{1}{\phi_{n_x}}\frac{d^2\phi_{n_x}}{dx^2} = -k_{n_x}^2 \qquad \frac{1}{\phi_{n_y}}\frac{d^2\phi_{n_y}}{dy^2} = -k_{n_y}^2 \qquad \frac{1}{\phi_{n_z}}\frac{d^2\phi_{n_z}}{dz^2} = -k_{n_z}^2$$

$$-(k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2) = -\frac{2m}{\hbar^2}E_{n_x,n_y,n_z} \Rightarrow E = \frac{\hbar^2}{2m}(k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2)$$

$\phi_n(\xi) = A\cos k_n\xi + B\sin k_n\xi$

$\phi_n(-\frac{a}{2}) = 0 \Rightarrow A\cos\frac{ka}{2} - B\sin\frac{ka}{2} = 0$

$\phi_n(\frac{a}{2}) = 0 \Rightarrow A\cos\frac{ka}{2} + B\sin\frac{ka}{2} = 0$

① + ②

$2A\cos\frac{k_n a}{2} = 0 \Rightarrow k_n = \frac{n\pi}{a}$ $\quad n = 1, 3, 5$

① − ②

$2B\sin\frac{k_n a}{2} = 0 \Rightarrow k_n = \frac{n\pi}{a}$ $\quad n = 2, 4, 6$

$$\phi_n(\xi) = \begin{cases} \sqrt{\frac{2}{a}}\cos\frac{\pi n\xi}{a} & n = 1, 3, 5 \quad \text{even} \\ \sqrt{\frac{2}{a}}\sin\frac{\pi n\xi}{a} & n = 2, 4, 6 \quad \text{odd} \end{cases} \qquad k_n^2 = \frac{n^2\pi^2}{a^2}$$

$$\Rightarrow \phi_{n_x n_y n_z}(x, y, z) = \phi_{n_x}(x)\,\phi_{n_y}(y)\,\phi_{n_z}(z) \qquad E_{n_x, n_y, n_z} = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$$

properties

① $\int d\vec{r}\, |\phi_{n_x n_y n_z}(x,y,z)|^2 = \left[\int dx\, |\phi_{n_x}(x)|^2\right]\left[\int dy\, |\phi_{n_y}|^2\right]\left[\int dz\, |\phi_{n_z}|^2\right] = 1$

② $\int d\vec{r}\, \phi^*_{n_x' n_y' n_z'}(x,y,z)\, \phi_{n_x, n_y, n_z}(x,y,z) = \left[\int dx\, \phi^*_{n_x'}(x)\, \phi_{n_x}(x)\right]\left[\int dy\, \phi^*_{n_y'}(y)\, \phi_{n_y}(y)\right]\left[\int dz\, \phi^*_{n_z'}(z)\, \phi_{n_z}(z)\right] = \delta_{n_x', n_x}\, \delta_{n_y', n_y}\, \delta_{n_z', n_z}$

③ The solutions provide a complete basis $\Rightarrow$ so we can $|\psi(t)\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi(0)\rangle e^{-i\frac{E_n t}{\hbar}}$

$\psi(\vec{r}, t) = \langle\vec{r}|\psi(t)\rangle = \sum_n \langle\vec{r}|\phi_n\rangle\langle\phi_n|\psi(0)\rangle e^{-i\frac{E_n t}{\hbar}} = \sum_n \phi_n(\vec{r})\langle\phi_n|\psi(0)\rangle e^{-i\frac{E_n t}{\hbar}}$

④ Solutions are no longer unique

⑤ 1D $\phi_n(-x) = (-1)^{n+1}\phi_n(x)$

3D $\phi_{n_x}(-x)\,\phi_{n_y}(-y)\,\phi_{n_z}(-z) = (-1)^{n_x+n_y+n_z+1}\phi_{n_x}(x)\,\phi_{n_y}(y)\,\phi_{n_z}(z)$

Lec. 22 3D Spherical

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

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\phi(\vec{r}) = E\phi(\vec{r}) \qquad \phi(\vec{r}) = R(r)\,Y(\theta,\phi)$$

$$\left\{\left[-\frac{\hbar^2}{2m}\nabla_r^2 + V(r)\right] + \left[-\frac{\hbar^2}{2m}\nabla_{\theta\phi}^2\right]\right\}RY = E\,RY \qquad 同 \times -\frac{2mr^2}{\hbar^2 RY}$$

$$\underbrace{\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)\right]}_{l(l+1)} + \underbrace{\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]}_{-l(l+1)} = 0$$

Seperate 1st 第一项 $l(l+1)$

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -l(l+1) \qquad Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi) \qquad 同 \times \sin^2\theta$$

$$\underbrace{\left[\frac{1}{\Theta}\sin\theta\frac{d}{d\theta}\sin\theta\frac{d\Theta}{d\theta} + l(l+1)\sin^2\theta\right]}_{m^2} + \underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}}_{-m^2} = 0$$

Seperate 2nd 第一项 m^2

① 角向 $\Phi(\phi)$ 方程

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi \Rightarrow \Phi(\phi) = e^{im\phi} \qquad \Phi(0) = \Phi(2\pi) \Rightarrow e^{im2\pi} = 1 \Rightarrow m\cdot 2\pi = 2k\pi \Rightarrow m = k \text{ (intergar)} \quad (0, \pm1, \pm2 \cdots)$$

$$\sin\theta \frac{d}{d\theta} = \sin\theta \frac{d}{d\cos\theta} \cdot \frac{d\cos\theta}{d\theta} = -(1-\cos^2\theta)\frac{d}{d\cos\theta}$$

$$\left[\frac{1}{\Theta} \sin\theta \frac{d}{d\theta} \sin\theta \frac{d\Theta}{d\theta} + l(l+1)\sin^2\theta\right] = m^2$$

$$\Rightarrow \left[\sin\theta \frac{d}{d\theta} \sin\theta \frac{d}{d\theta} + l(l+1)\sin^2\theta\right]\Theta = m^2\Theta$$

$$\Rightarrow (1-\cos^2\theta)\frac{d}{d\cos\theta}(1-\cos^2\theta)\frac{d}{d\cos\theta} + l(l+1)(1-\cos^2\theta)]\ \Theta = m^2\Theta$$

$$\Rightarrow \left[\frac{d}{d\cos\theta}(1-\cos^2\theta)\frac{d}{d\cos\theta} + \left(l(l+1) - \frac{m^2}{1-\cos^2\theta}\right)\right]\Theta = 0$$

Legendre on the interval $-1 \le \cos\theta \le 1$

$$\Rightarrow \left[(1-\cos^2\theta)\frac{d^2}{d\cos^2\theta} - 2\cos\theta \frac{d}{d\cos\theta} + \left[l(l+1) - \frac{m^2}{1-\cos^2\theta}\right]\right]\Theta(\cos\theta) = 0$$

$l \Rightarrow |m| \le l$ 才有解　　角向 $\Theta(\theta)$ 方程

② $\Rightarrow \Theta(\cos\theta) = A_{lm} P_l^m(\cos\theta)$　　$P_l^m(x) = (-1)^m (1-x^2)^{\frac{m}{2}} \left(\frac{d}{dx}\right)^m P_l(x)$　　$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$

spherical harmonics

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

(a) normalization 归一

$$\int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\phi\, |Y_{lm}(\theta,\phi)|^2 = 1$$

(b) orthonormal

$$\int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\phi\, Y_{l'm'}^*(\theta,\phi)\, Y_{lm}(\theta,\phi) = \delta_{l'l}\delta_{m'm}$$

$l = 0, 1, 2$　　$m = -l, -l+1, \dots, l-1, l$

(c) properties

$$Y_{lm}^*(\theta,\phi) = (-1)^m Y_{l(-m)}(\theta,\phi)$$

Y_{00}　Y_{1m}　Y_{2m}

角度部分解完，应用

$$\vec{L} = \vec{r}\times\vec{p} = \vec{r}\times\frac{\hbar}{i}\nabla \Rightarrow \begin{cases} L_x \\ L_y \\ L_z \end{cases} \Rightarrow \vec{L}^2 = \hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \Rightarrow \hbar^2\cdot r^2\cdot\nabla^2_{\theta\phi}$$

$$\Rightarrow \vec{L}^2 Y_{lm}(\theta,\phi) = \hbar^2 l(l+1) Y_{lm}(\theta,\phi)$$

$$L_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(r) = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+V(r)\right] + \frac{-\hbar^2}{2m}\cdot\frac{\vec{L}^2}{\hbar^2 r^2} = -\frac{\hbar^2}{2m}\left[\nabla_r^2+V(r)\right]+\frac{\vec{L}^2}{2mr^2}$$

$$\hat{H}\phi_{Elm} = E\phi_{Elm} \qquad \hat{\vec{L}}^2\phi_{Elm} = \hbar^2 l(l+1)\phi_{Elm} \qquad \hat{L}_z\phi_{Elm} = m\hbar\phi_{Elm}$$ → label our stationary state solutions.

And $\hat{H}$, $\hat{\vec{L}}^2$, $\hat{L}_z$ are mutually commuting Hermitian operators.

$$\Rightarrow [\hat{H},\hat{\vec{L}}^2]=0 \qquad [\hat{\vec{L}}^2, L_z]=0 \qquad [\hat{H},\hat{L}_z]=0$$

E.g. 3D infinite spherial well

$$V(r) = \begin{cases} 0 & \text{if } r<a \\ \infty & \text{otherwise} \end{cases}$$

$V(r)$ 只影响 $R(r)$ 的解

$$\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-\frac{2mr^2}{\hbar^2}(V(r)-E)\right]R_l = l(l+1)R_l \Rightarrow \left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{2mr^2}{\hbar^2}E\right]R_l = l(l+1)R_l$$ 径向方程

$$R_l(r) = \frac{u_l(r)}{r} \Rightarrow \frac{d}{dr}r^2\frac{d}{dr}\frac{u(r)}{r} = \frac{d}{dr}\cancel{r^2}\frac{u'(r)\cdot r-u(r)}{\cancel{r^2}} = u''(r)\cdot r+u'(r)-u'(r) = r\cdot\frac{d^2u(r)}{dr^2}$$

for $l=0$

$$r\frac{d^2u_l(r)}{dr}+\frac{2mr}{\hbar^2}E\,u(r)=0 \Rightarrow u_l''(r) = -\frac{2mE}{\hbar^2}u_l(r) = -k^2u_l(r) \Rightarrow u(r) = A\sin kr + B\cos kr$$

$$k=\frac{\sqrt{2mE}}{\hbar} \Rightarrow R(r) = A\frac{\sin kr}{r}+B\frac{\cos kr}{r}$$

boundary conditions

$R(0) < \infty \Rightarrow B = 0$ $\qquad k = \frac{n\pi}{a}$

$R(a) = 0 \Rightarrow \frac{\sin ka}{a} = 0 \Rightarrow ka = n\pi \,, \quad n = 1, 2, 3 \cdots \Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2}$

normalization

$$1 = \int_0^a r^2 dr \, |A|^2 \frac{\sin^2 kr}{r^2} = |A|^2 \int_0^a \underbrace{\sin^2 kr}_{\frac{1-\cos 2kr}{2}} \, dr = |A|^2 \frac{1}{2}\Big[a - \frac{\overbrace{\sin 2ka}^{2n\pi}}{2k}\Big] = \frac{a}{2} \cdot |A|^2 \Rightarrow A = \sqrt{\frac{2}{a}}$$

$\Rightarrow l = 0$ so $m = 0$ $\qquad m \in [-l, l]$

So $\phi_{n\, l=0\, m=0}(\vec{r}) = \underbrace{\sqrt{\frac{2}{a}} \cdot \frac{\sin(\frac{n\pi r}{a})}{r}}_{R(r)} \cdot \underbrace{Y_{00}(\theta, \phi)}_{\frac{1}{\sqrt{4\pi}}} = \frac{1}{\sqrt{2\pi a}} \frac{\sin \frac{n\pi r}{a}}{r} \qquad E_{n\, l=0} = \frac{n^2\hbar^2\pi^2}{2ma^2}$

General case

$k^2 = \frac{2mE}{\hbar^2}$

$$\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + k^2r^2\right] R_l(r) = l(l+1) R_l(r)$$

$$R_{nl}(r) = A \underbrace{j_l(kr)}_{\text{spherical Bessel}} + B \underbrace{\eta_l(kr)}_{\text{spherical Neumann}}$$

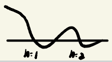
$j_\ell(x) = \frac{x^\ell}{(2\ell+1)!!}$ $\eta_\ell(x) \Rightarrow -\frac{(2\ell-1)!!}{x^{\ell+1}}$ η_ℓ 在 $kr \Rightarrow 0$ 时 $\Rightarrow \infty$ ，舍

$j_0(x) = \frac{\sin x}{x}$ $j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$ $j_{\ell+1}(x) = \frac{2\ell+1}{x} j_\ell(x) - j_{\ell-1}(x)$

$\nearrow$

just we got from

$\ell = 0$

j_ℓ 

$\beta_{n\ell}$ 为 j_ℓ 的第 n 个零点

$j_\ell(ka) = 0 \Rightarrow ka = \beta_{n\ell}$ $n = 1, 2, 3$ $\Rightarrow k = \frac{\beta_{n\ell}}{a} \Rightarrow j_\ell\left(\frac{\beta_{n\ell}}{a} r\right)$

$\Rightarrow E_{n\ell} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \beta_{n\ell}^2}{2ma^2}$

normalization

$R_{n\ell}(r) = A_{n\ell}\, j_\ell\left(\beta_{n\ell}\frac{r}{a}\right)$

$|A_{n\ell}|^2 \int_0^a r^2 dr \left[j_\ell\left(\beta_{n\ell}\frac{r}{a}\right)\right]^2 = 1$

$\psi_{n\ell m}(r,\theta,\phi) = A_{n\ell}\, j_\ell\left(\beta_{n\ell}\frac{r}{a}\right) \cdot Y_{\ell m}(\theta,\phi)$ $E_{n\ell} = \frac{\hbar^2 \beta_{n\ell}^2}{2ma^2}$

Lec 23 The Hydrogen atom

$$\left[-\frac{\hbar^2}{2m_e}\vec{\nabla}^2_{\vec{r}_e}-\frac{\hbar^2}{2m_p}\vec{\nabla}^2_{\vec{r}_p}+V(|\vec{r}_e-\vec{r}_p|)\right]\phi(\vec{r}_e,\vec{r}_p)=E\phi(\vec{r}_e,\vec{r}_p)$$

$\vec{r}\equiv\vec{r}_e-\vec{r}_p$ $M\vec{R}=m_e\vec{r}_e+m_p\vec{r}_p$ $M=m_e+m_p$

$$\Rightarrow\left[-\frac{\hbar^2}{2\mu}\vec{\nabla}^2_{\vec{r}}-\frac{\hbar^2}{2M}\vec{\nabla}^2_{\vec{R}}+V(\vec{r})\right]\phi(\vec{r},\vec{R})=E\phi(\vec{r},\vec{R})$$

$$\mu=\frac{m_e m_p}{m_e+m_p}$$

approximate $\mu=m_e$ $M\to\infty$

$\times\left(-\frac{\hbar^2}{2mr^2}\right)$

$$\Rightarrow\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-\frac{2mr^2}{\hbar^2}(V(r)-E)\right]R_l=l(l+1)R_l$$

$$V(r)=-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}=\left[-\frac{e^2}{4\pi\varepsilon_0\hbar c}\right]\frac{\hbar c}{r}=-\alpha\frac{\hbar c}{r}=V(r)_{ws}$$

$$\Rightarrow\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\alpha\frac{\hbar c}{r}+\frac{\hbar^2}{2m}\frac{1}{r^2}l(l+1)\right]\frac{u_l}{r}=E\frac{u_l}{r}$$

之前 三维无限深球 $\bigcirc$ ∞ $E>0$

现在 三维有限深球 $\bigcirc$ $E<0$

$\frac{1}{r}\frac{d^2u_l}{dr^2}$ 同 $\times r$

$$k=\frac{\sqrt{-2m_eE}}{\hbar}$$

$$\Rightarrow\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-\alpha\frac{\hbar c}{r}+\frac{\hbar^2}{2m}\frac{1}{r^2}l(l+1)\right]u_l=Eu_l$$

$$\rho=kr=\frac{\sqrt{2m_e|E|}}{\hbar}\cdot r$$

$d\rho=k\,dr\Rightarrow dr=\frac{1}{k}d\rho$

$$\left[-\frac{\hbar^2}{2m}\frac{2m|E|}{\hbar^2}\frac{d^2}{d\rho^2}+\alpha\frac{\sqrt{2m|E|}}{\hbar}\frac{\hbar c}{\rho}+\frac{\hbar^2}{2m}\frac{2m|E|}{\hbar^2}\frac{1}{\rho^2}l(l+1)\right]u_l(\rho)=-|E|u_l(\rho)$$

$$\rho_0=\alpha\sqrt{\frac{2mc^2}{|E|}}$$

$$\Rightarrow\frac{d^2}{d\rho^2}u_l(\rho)=\left[1-\frac{\rho_0}{\rho}+\frac{l(l+1)}{\rho^2}\right]u_l(\rho)$$

$$\rho\to\infty\Rightarrow\frac{d^2u_l(\rho)}{d\rho^2}=u_l(\rho)\Rightarrow\lambda=\pm1\Rightarrow u_l(\rho)=Ae^{-\rho}+\underbrace{Be^{\rho}}_{\rho\to\infty\text{ diverge}}\Rightarrow u_l(\rho)=Ae^{-\rho}$$

$$\rho \to \infty \Rightarrow \frac{d^2 u_l(\rho)}{d\rho^2} = \frac{l(l+1)}{\rho^2} u_l(\rho) \Rightarrow u_l(\rho) \sim C\rho^{l+1} + \underbrace{D\rho^{-l}}_{\rho\to 0 \text{ diverge}} \Rightarrow u_l(\rho) = C\rho^{l+1}$$

$$u_l(\rho) = \rho^{l+1} e^{-\rho} v_l(\rho)$$

plug $u_l(\rho)$ into equation

$$\rho \frac{d^2}{d\rho^2} + 2(l+1-\rho)\frac{d}{d\rho} + \rho_0 - 2(l+1)] v_l(\rho) = 0$$

plug into

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \Rightarrow \frac{dv(\rho)}{d\rho} = \sum_{j=0}^{\infty} c_{j+1}(j+1)\rho^j$$

$$\frac{d^2 v(\rho)}{d\rho^2} = \sum_{j=0} c_{j+1} j(j+1)\rho^{j-1}$$

$$\sum_{j=0}^{\infty} c_{j+1} j(j+1)\rho^j + 2(l+1)c_{j+1}(j+1)\rho^j - 2c_j j\rho^j + (\rho_0 - 2(l+1))c_j\rho^j] = 0$$

$$c_{j+1} j(j+1) + 2(l+1)c_{j+1}(j+1) - 2c_j j + (\rho_0 - 2(l+1))c_j = 0$$

$$\Rightarrow c_{j+1}(j+1)(j+2l+2) - c_j(2j+2l+2-\rho_0) = 0 \Rightarrow c_{j+1} = \left[\frac{2(j+l+1)-\rho_0}{(j+1)(j+2l+2)}\right] c_j$$

large j

$$\Rightarrow c_{j+1} \sim \frac{2}{j+1} c_j \Rightarrow c_{j+1} \sim \frac{2^{j+1}}{(j+1)!} c_0$$

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \sim c_0 \sum_{j=0}^{\infty} \frac{(2\rho)^j}{j!} \sim c_0 e^{2\rho}$$

$u_\ell(\rho) = \rho^{\ell+1} e^{-\rho} v_\ell(\rho) \sim C_0 \rho^{\ell+1} e^{\rho}$ not normalizable diverge

$\Rightarrow \hat{v}(\rho)$ must be truncate $\Downarrow$ 必须有限项

Bound-state Coulomb solutions $C_j = 0 \quad j = 1,2,3$

$$C_{j_{max}+1} = \left[\frac{2(j+\ell+1)-\rho_0}{(j+1)(j+2\ell+2)}\right] C_{j_{max}}$$

$C_{j_{max}}$ is the last nonzero coefficient

$2(j_{max}+\ell+1) = \rho_0 \qquad j_{max} = 0, 1, 2, \cdots$

$n = j_{max} + \ell + 1$

j_{max} runs from 0 onward

$\ell = 0 \Rightarrow n = 1, 2, 3, \cdots \qquad \ell = 1 \Rightarrow n = 2, 3, 4, \cdots \qquad \ell = \ell \Rightarrow n = \ell+1, \ell+2, \cdots$

$$\Rightarrow 2n = \rho_0 = \alpha\sqrt{\frac{2mc^2}{|E|}} \Rightarrow |E_n| = \left(\frac{\alpha}{2n}\right)^2 \cdot 2mc^2 = \frac{\alpha^2 mc^2}{2n^2} = \frac{|E_1|}{n^2} \qquad \frac{\alpha^2 mc^2}{2n^2}$$

degeneracy : number of states with energy E_n : $\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell} = \sum_{\ell=0}^{n-1}(2\ell+1) = n^2$

$r_n = \frac{r}{n}$ $\qquad \frac{\hbar}{\alpha mc}$

$$\rho = kr = \frac{\sqrt{2m|E_n|}}{\hbar} r = \frac{\sqrt{2m|E_1|}}{n\hbar} r = \frac{k_1 r}{n}$$

$n = 1,\ r = a_0,\ \rho = 1$

$$\Rightarrow 1 = k_1 a_0 \Rightarrow a_0 = \sqrt{\frac{\hbar^2}{2m|E_1|}} = \sqrt{\frac{\hbar^2}{2m\frac{\alpha^2 mc^2}{2}}} = \frac{\hbar}{\alpha mc} = \frac{\hbar c}{\alpha m_e c^2} = \frac{137 \times 1973\,\text{eV}\cdot\text{Å}}{511000\,\text{eV}} \sim 0.529\,\text{Å}$$