

To: Felix Temie

Further Quantum Mechanics I

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$$1. \quad \hat{H} = \hat{H}_0 + \delta H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \epsilon\hat{x}^2$$
$$= \frac{\hat{p}^2}{2m} + \left(\frac{1}{2}m\omega^2 + \epsilon\right)\hat{x}^2$$

From our knowledge about simple-harmonic-oscillator,
Ground state:

$$\hat{H}|0\rangle = \frac{\hbar\omega'}{2}|0\rangle \quad \text{where}$$

$$\hbar\omega' = \hbar\omega + \epsilon \quad \frac{1}{2}m\omega'^2 = \frac{1}{2}m\omega^2 + \epsilon$$

$$\omega'^2 = \omega^2 + \frac{2\epsilon}{m}$$

$$\rightarrow \omega' = \sqrt{\omega^2 + \frac{2\epsilon}{m}}$$

$$\therefore \text{Ground state energy } E_0' = \frac{1}{2}\hbar\sqrt{\omega^2 + \frac{2\epsilon}{m}}$$

$$E_0' = \frac{1}{2}\hbar\omega\sqrt{1 + \frac{2\epsilon}{m\omega^2}}$$

$$\Rightarrow \Delta E_0 = E_0' - E_0 = \boxed{\frac{1}{2}\hbar\omega\left(\sqrt{1 + \frac{2\epsilon}{m\omega^2}} - 1\right)}$$

is the exact change in ground state energy level

Expand ΔE_0 gives

$$\Delta E_0 = \frac{1}{2}\hbar\omega \left(1 + \frac{\epsilon}{m\omega^2} - \frac{\epsilon^2}{2m^2\omega^3} + \dots \right)$$

$$\approx \underbrace{\frac{\hbar\epsilon}{2m\omega}}_{\delta E_0^{(1)}} - \underbrace{\frac{\epsilon^2\hbar}{4m^2\omega^3}}_{\delta E_0^{(2)}} + O(\epsilon^3)$$

$$(b) \quad \delta E_0^{(1)} = \langle 0 | \delta \hat{H} | 0 \rangle$$

$$= \epsilon \langle 0 | \hat{x}^2 | 0 \rangle$$

From SHO we know

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) \equiv l (\hat{a}^\dagger + \hat{a})$$

($\hat{a}^\dagger$ = raising operator, $\hat{a}$ = lowering operator).

$$\therefore \delta E_0^{(1)} = \epsilon \langle 0 | \hat{x}^2 | 0 \rangle = \epsilon l^2 \langle 0 | \hat{a}^\dagger \hat{a}^\dagger + \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger + \hat{a} \hat{a} | 0 \rangle$$

$$\hat{a} | 0 \rangle = 0 \Rightarrow \delta E_0^{(1)} = \epsilon l^2 \langle 0 | \hat{a}^\dagger \hat{a}^\dagger + \hat{a} \hat{a}^\dagger | 0 \rangle$$

$$\hat{a} | 0 \rangle = \hat{a} | 1 \rangle = | 1 \rangle$$

$$\Rightarrow \frac{\delta E_0^{(1)}}{\epsilon l^2} = \langle 0 | \hat{a} \hat{a}^\dagger | 0 \rangle + \langle 0 | \hat{a}^\dagger \hat{a} | 0 \rangle$$

$$= \langle 0 | \hat{a} | 1 \rangle + \langle 0 | \hat{a}^\dagger | 1 \rangle$$

$$= \langle 0 | 0 \rangle + \sqrt{2} \langle 0 | 2 \rangle$$

$$= \langle 0 | 0 \rangle = 1$$

$$\therefore \delta E_0^{(1)} = \epsilon l^2 = \boxed{\frac{\epsilon \hbar}{2m\omega}}$$

$$(c) \quad \delta \psi^{(1)} = |\delta \psi_0^{(1)}\rangle = \sum_{m \neq 0} \frac{\langle m | \delta \hat{H} | 0 \rangle}{-(E_m - E_0)} | m \rangle$$

$$\langle m | \delta \hat{H} | 0 \rangle = \epsilon l^2 \langle m | \hat{x}^2 | 0 \rangle$$

$$= \epsilon l^2 \langle m | \hat{a}^\dagger \hat{a}^\dagger + \hat{a} \hat{a}^\dagger | 0 \rangle$$

$$= \epsilon l^2 [\langle m | \hat{a}^\dagger \hat{a}^\dagger | 0 \rangle + \langle m | \hat{a} \hat{a}^\dagger | 0 \rangle]$$

$$= \epsilon^2 \left[\underbrace{\langle m|2\rangle}_{\delta_{m2}} \sqrt{2} + \underbrace{\langle m|0\rangle}_{\delta_{m0} = 0 \because m \neq 0} \right]$$

$$= \sqrt{2} \epsilon^2 \delta_{m2} \rightarrow \text{only non-zero when } m=2$$

$$\therefore |b\rangle = \sum_{m=1}^{\infty} \frac{\langle m| \hat{H} |0\rangle}{-(E_m - E_0)} |m\rangle$$

$$= \sum_{m=1}^{\infty} \frac{-\sqrt{2} \epsilon^2}{E_2 - E_0} |2\rangle = \frac{-\sqrt{2} \epsilon^2}{(2T_2 - \frac{1}{2})\hbar\omega} |2\rangle$$

$$= \cancel{\frac{\sqrt{2} \epsilon^2 \hbar}{2m\omega}} = \boxed{\frac{-\epsilon^2 \hbar}{\sqrt{2} \hbar \omega} |2\rangle} \quad \checkmark$$

$$(d) \quad \delta E_0^{(2)} = \sum_{m \neq 0} \frac{|\langle m | \hat{H} | 0 \rangle|^2}{E_0 - E_m}$$

$$= \frac{(\sqrt{2} \epsilon^2 \hbar)^2}{-2\hbar\omega} = - \frac{\frac{\epsilon^2 \hbar^2}{(2m\omega)^2}}{(\hbar\omega)}$$

$$= \boxed{\frac{-\epsilon^2 \hbar}{4m^2 \omega^3}} \quad \checkmark$$

$$2. \quad \hat{H}' = \hat{H}_0 + \delta \hat{H}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 + \varepsilon \hat{x}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \left(\hat{x}^2 + 2 \frac{\varepsilon}{m \omega^2} \hat{x} + \left(\frac{\varepsilon}{m \omega^2} \right)^2 \right) - \frac{1}{2} m \omega^2 \frac{\varepsilon^2}{m^2 \omega^4}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \underbrace{\left(\hat{x} + \frac{\varepsilon}{m \omega^2} \right)^2}_{\hat{x}^2} - \frac{\varepsilon^2}{2 m \omega^2} \quad \checkmark$$

$$= \frac{1}{2m} \left(\hat{p}^2 + m^2 \omega^2 \hat{x}^2 - \frac{\varepsilon^2}{\omega^2} \right) \quad \checkmark$$

$$(\hat{p} = -i\hbar \frac{\partial}{\partial x} = -i\hbar \frac{\partial}{\partial \hat{x}} \quad \therefore \frac{\partial}{\partial \hat{x}} = \frac{\partial}{\partial x})$$

$$\hat{H}' |n'\rangle = E_{n'} |n'\rangle$$

Ground state $\hat{H}' |0'\rangle = E_{0'} |0'\rangle$

$$E_{0'} = \left(\frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \right) |0'\rangle = \frac{1}{2} \hbar \omega |0'\rangle \quad \textcircled{1}$$

$$- \frac{\varepsilon^2}{2 m \omega^2} |0'\rangle = - \frac{\varepsilon^2}{2 m \omega^2} |0'\rangle \quad \textcircled{2}$$

$$\textcircled{1} + \textcircled{2} \Rightarrow \hat{H}' |0'\rangle = \left(\frac{1}{2} \hbar \omega - \frac{\varepsilon^2}{2 m \omega^2} \right) |0'\rangle$$

$$\therefore \boxed{\Delta E_0 = - \frac{\varepsilon^2}{2 m \omega^2}} \quad \checkmark$$

Physically $\delta \hat{H}$ represents the potential energy of a constant field. It shifts the equilibrium position from 0 to $-\frac{\varepsilon}{m \omega^2}$ and decreases the energy levels

by $\frac{\varepsilon^2}{2 m \omega^2}$ ✓

$$\delta E_0^{(1)} = \langle 0 | \delta \hat{H} | 0 \rangle = \cancel{\epsilon l} \langle 0 | \hat{a}^\dagger + \hat{a} | 0 \rangle$$

$$= \epsilon l \langle 0 | \hat{a} | 0 \rangle + \epsilon l \langle 0 | \hat{a}^\dagger | 0 \rangle$$

$$= \epsilon l \langle 0 | 1 \rangle = 0 \quad \checkmark$$

$$|\delta \psi_0^{(1)}\rangle = \sum_{m=1}^{\infty} \frac{\langle m | \delta \hat{H} | 0 \rangle}{E_0 - E_m} |m\rangle$$

$$\langle m | \delta \hat{H} | 0 \rangle = \epsilon l \langle m | \hat{a}^\dagger + \hat{a} | 0 \rangle$$

$$= \epsilon l \langle m | 0 \rangle = \epsilon l \delta_{m,1}$$

$$\rightarrow \cancel{|\delta \psi_0^{(1)}\rangle} =$$

$$|\delta \psi_0^{(1)}\rangle = \sum_{m=1}^{\infty} \frac{\epsilon l \cdot}{E_0 - E_1} |1\rangle$$

$$= - \frac{\epsilon l}{\hbar \omega} |1\rangle$$

$$= - \frac{\epsilon}{\hbar \omega} \left(\frac{\hbar}{2m\omega} \right)^{1/2} |1\rangle$$

$$= \cancel{\frac{\epsilon}{\hbar \omega} \left(\frac{\hbar}{2m\omega} \right)^{1/2}} |1\rangle = - \frac{\sqrt{\epsilon^2}}{\sqrt{2m\hbar\omega^3}} |1\rangle \quad \checkmark$$

$\therefore$ The perturbed ~~state~~ ground state

is $|0\rangle' = |0\rangle - \frac{\sqrt{\epsilon^2}}{\sqrt{2m\hbar\omega^3}} |1\rangle$ from perturbation

theory.

$$(|0\rangle'_p = |0\rangle - \frac{\epsilon l}{\hbar \omega} |1\rangle)$$

perturbed

The exact $\sqrt{}$ ground state is $|0\rangle'_e$, then

$$\langle X|0\rangle'_e = \langle X + \frac{\varepsilon}{m\omega^2} | 0 \rangle$$

$$= \frac{1}{(2\pi l^2)^{1/4}} \exp\left(-\frac{1}{4l^2} \left(x + \frac{\varepsilon}{m\omega^2}\right)^2\right)$$

~~$$= \frac{1}{(2\pi l^2)^{1/4}} \exp\left(-\frac{x^2}{4l^2}\right) \exp\left(-\frac{\varepsilon^2}{4m^2\omega^4 l^2}\right)$$~~

~~$$= \frac{1}{(2\pi l^2)^{1/4}}$$~~

$$= \frac{1}{(2\pi l^2)^{1/4}} \exp\left(-\frac{x^2}{4l^2}\right) \exp\left(-\frac{2\varepsilon x}{4m\omega^2 l^2}\right) \exp\left(-\frac{(\varepsilon/m\omega^2)^2}{4l^2}\right)$$

for ε and εx to be small

$$\exp\left(-\frac{(\varepsilon/m\omega^2)^2}{4l^2}\right) \sim \exp(0) \sim 1$$

$$\exp\left(-\frac{2\varepsilon x}{4m\omega^2 l^2}\right) \sim 1 - \frac{2\varepsilon x}{4m\omega^2 l^2} \sim 1 - \frac{\varepsilon x}{2m\omega^2 l^2}$$

~~$$\sim \frac{1}{2m\omega} \Rightarrow 2m\omega l^2 = \hbar$$~~

$$\Rightarrow 2m\omega l = \frac{\hbar}{l} \Rightarrow 2m\omega^2 l = \frac{\hbar\omega}{l}$$

$$\therefore \langle X|0\rangle'_e \approx \frac{1}{(2\pi l^2)^{1/4}} \exp\left(-\frac{x^2}{4l^2}\right) \left(1 - \frac{\varepsilon}{(2m\omega^2 l)} \frac{x}{l}\right)$$

$$= \frac{1}{(2\pi l^2)^{1/4}} \exp\left(-\frac{x^2}{4l^2}\right) - \frac{\varepsilon l}{\hbar\omega} \frac{1}{(2\pi l^2)^{1/4}} \frac{x}{l} \exp\left(-\frac{x^2}{4l^2}\right)$$

$$= \langle X|0\rangle - \frac{\varepsilon l}{\hbar\omega} \langle X|1\rangle$$

✓

Hence

$$|0\rangle_e' \sim |0\rangle - \frac{\epsilon l}{\hbar \omega} |1\rangle = |0\rangle_p' \quad \begin{matrix} \uparrow \\ \text{exact} \end{matrix} \quad \begin{matrix} \uparrow \\ \text{perturbation theory} \end{matrix}$$

under the assumption that ϵ is small
and ϵX is small.

$$\left(\frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - 1 \right) \langle 0 | \psi \rangle = \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

$$\frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - 1 \approx \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

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$$\frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - 1 \approx \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

$$\left(\frac{1}{2} \left(\frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - 1 \right) \right) \langle 0 | \psi \rangle = \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

$$\left(\frac{1}{2} \left(\frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - 1 \right) \right) \langle 0 | \psi \rangle = \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

$$\langle 0 | \psi \rangle \frac{\langle 0 | H | 0 \rangle}{\hbar \omega} - \langle 0 | \psi \rangle = \frac{\langle 0 | H | 1 \rangle}{\hbar \omega} \langle 1 | \psi \rangle$$

$$3. \quad \hat{H}' = \hat{H}_0 + \delta \hat{H}$$

$$\delta \hat{H} = \epsilon \hat{x}^4, \quad \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$$

$$\delta E = \delta E_n^{(1)} = \langle n | \delta \hat{H} | n \rangle$$

$$l = \sqrt{\frac{\hbar}{2m\omega}}$$

$$= \langle n | \epsilon \hat{x}^4 | n \rangle = \epsilon l^4 \langle n | (\hat{a}^\dagger + \hat{a})^4 | n \rangle$$

$$= \epsilon l^4 \langle n | (\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger + \hat{a}) | n \rangle$$

$$= \epsilon l^4 \left[\langle n | \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger | n \rangle + \langle n | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | n \rangle \right]$$

$$\sim \langle n | n+4 \rangle = 0$$

$$\sim \langle n | n+2 \rangle = 0$$

$$+ \langle n | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a}^\dagger | n \rangle + \langle n | \hat{a}^\dagger \hat{a} \hat{a}^\dagger \hat{a} | n \rangle$$

$$\sim \langle n | n+2 \rangle = 0$$

$$\sim \langle n | n+2 \rangle = 0$$

$$+ \langle n | \hat{a} \hat{a}^\dagger \hat{a}^\dagger \hat{a} | n \rangle + \langle n | \hat{a} \hat{a}^\dagger \hat{a} \hat{a} | n \rangle$$

$$\sim \langle n | n+2 \rangle = 0$$

$$\sim \sqrt{n} \sqrt{n-1} \sqrt{n-1} \sqrt{n} \langle n | n \rangle \sim n(n-1)$$

$$+ \langle n | \hat{a}^\dagger \hat{a} \hat{a}^\dagger \hat{a} | n \rangle + \langle n | \hat{a} \hat{a}^\dagger \hat{a}^\dagger \hat{a} | n \rangle$$

$$\sim \sqrt{n} \sqrt{n} \sqrt{n} \sqrt{n} = n^2$$

$$\sqrt{n} \sqrt{n} \sqrt{n+1} \sqrt{n+1} \sim n(n+1)$$

$$+ \langle n | \hat{a}^\dagger \hat{a} \hat{a} \hat{a}^\dagger | n \rangle + \langle n | \hat{a} \hat{a}^\dagger \hat{a} \hat{a}^\dagger | n \rangle$$

$$\sim \sqrt{n+1} \sqrt{n+1} \sqrt{n} \sqrt{n} \sim n(n+1)$$

$$\sim \sqrt{n+1} \sqrt{n+1} \sqrt{n+1} \sqrt{n+1} \sim (n+1)^2$$

$$+ \langle n | \hat{a} \hat{a} \hat{a}^\dagger \hat{a}^\dagger | n \rangle + \langle n | \hat{a}^\dagger \hat{a} \hat{a} \hat{a} | n \rangle$$

$$\sim \sqrt{n+1} \sqrt{n+2} \sqrt{n+2} \sqrt{n+1} \sim (n+1)(n+2)$$

$$\sim 0$$

$$+ \langle n | \hat{a} \hat{a}^\dagger \hat{a} \hat{a} | n \rangle + \langle n | \hat{a} \hat{a} \hat{a}^\dagger \hat{a} | n \rangle$$

$$\sim 0$$

$$\sim 0$$

$$+ \langle n | \hat{a} \hat{a} \hat{a}^\dagger \hat{a}^\dagger | n \rangle + \langle n | \hat{a}^\dagger \hat{a} \hat{a} \hat{a} | n \rangle$$

$$\sim 0$$

$$\sim 0$$

$$\Rightarrow \frac{\delta E}{\epsilon l^4} = n(n-1) + n^2 + n(n+1) + n(n+1) + (n+1)^2 + (n+1)(n+2)$$

$$= n^2 - n + n^2 + n^2 + n + n^2 + n + n^2 + 2n + 1 + n^2 + 3n + 2$$

$$= 6n^2 + 6n + 3 = 3(2n^2 + 2n + 1) \quad \because l = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\Rightarrow \delta E = 3(2n^2 + 2n + 1) \epsilon \left(\frac{\hbar}{2m\omega} \right)^2$$

4. infinite square well $\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(x)$

$$V(x) = \begin{cases} 0, & |x| < a \\ \infty, & |x| > a \end{cases}$$

then TISE $\hat{H}_0 \psi = E \psi$, $\psi(x) = 0$ for $|x| > a$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \quad \text{for } |x| < a$$

$$\therefore \psi'' + \frac{2mE}{\hbar^2} \psi = 0 \quad \text{let } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Rightarrow \psi(x) = A \cos(kx) + B \sin(kx)$$

~~ψ~~ Boundary Conditions: (ψ is continuous)

$$\psi(x=-a) = \psi(x=a) = 0$$

$$\Rightarrow A \cos(-ka) + B \sin(-ka) = 0 \quad (1)$$

$$A \cos(ka) + B \sin(ka) = 0 \quad (2)$$

$$(1) + (2) \Rightarrow 2A \cos(ka) = 0 \Rightarrow A = 0 \quad \text{or} \quad \cos(ka) = 0$$

$$(2) - (1) \Rightarrow 2B \sin(ka) = 0 \Rightarrow B = 0 \quad \text{or} \quad \sin(ka) = 0$$

$$\cancel{B \sin(ka)} \Rightarrow \cancel{\psi(x) = B \sin(ka)}$$

Even solution: ~~$A=0$~~ , $B=0$, $\cos(ka)=0$.

$$\rightarrow ka = (n + \frac{1}{2})\pi \quad (n = 1, 2, 3, \dots) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots$$

$$\therefore \psi(x) = A \cos\left(\frac{\pi x}{2a}\right), A \cos\left(\frac{3\pi x}{2a}\right), \dots$$

Odd solution : $A=0$, $\sin(ka)=0$

$$ka = n\pi \quad (n=1,2,3,\dots) = \pi, 2\pi, 3\pi, \dots$$

$$\therefore \psi(x) = B \sin\left(\frac{\pi x}{a}\right), B \sin\left(\frac{2\pi x}{a}\right), \dots$$

$$\text{Hence } ka = \frac{\pi}{2}, \frac{2\pi}{2}, \frac{3\pi}{2}, \frac{4\pi}{2}, \dots = \frac{n\pi}{2} \quad (n=1,2,3,\dots)$$

$$\therefore \text{Energy levels } E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{2}\right)^2$$

$$\rightarrow E_n = \frac{n^2}{8m} \left(\frac{\hbar\pi}{a}\right)^2 \quad (n=1,2,3,\dots)$$

The corresponding wavefunctions are

$$\psi = \psi(x) = A \cos\left(\frac{n\pi x}{2a}\right) \quad n=1,3,5,\dots$$

$$\psi(x) = B \sin\left(\frac{n\pi x}{2a}\right) \quad n=2,4,6,\dots$$

Normalise $\rightarrow$

for odd n .

$$\cancel{\int_{-a}^a} A^2 \int_{-a}^a \cos^2\left(\frac{n\pi x}{2a}\right) dx = 1$$

$$= A^2 \int_{-a}^a \left[\frac{1}{2} + \frac{1}{2} \cos\left(\frac{n\pi x}{a}\right) \right] dx$$

$$= A^2 \left[\frac{1}{2} (2a) \right] + \frac{A^2}{2} \left[\frac{a}{n\pi} \right] \left[\underbrace{\sin\left(\frac{n\pi x}{a}\right)}_0 \right]_{-a}^a$$

$$= aA^2 \quad \therefore A = \frac{1}{\sqrt{a}}$$

Similarly for even n , $B = \frac{1}{\sqrt{a}}$

$\therefore$ Eigenfunctions are:

$$\langle x|n\rangle = \psi_n(x) = \begin{cases} \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) & n=1,3,5,7,\dots \\ \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) & n=2,4,6,8,\dots \end{cases}$$

Perturbation $\hat{H}' = \hat{H}_0 + \delta\hat{H}$, $\delta\hat{H} = \frac{\epsilon}{a} \hat{x}$

First order change in energy

$$\begin{aligned} \delta E_n^{(1)} &= \langle n | \delta\hat{H} | n \rangle = \frac{\epsilon}{a} \langle n | \hat{x} | n \rangle \\ &= \int_{-a}^a x \psi_n^2(x) dx \end{aligned}$$

For odd n :

$$\begin{aligned} \delta E_n^{(1)} &= \frac{\epsilon}{a^2} \int_{-a}^a x \cos^2\left(\frac{n\pi x}{2a}\right) dx \\ &= \frac{\epsilon}{4\pi^2 n^2 a^2} \left(n\pi x \left(n\pi x + 2a \sin\left(\frac{n\pi x}{a}\right) \right) + 2a^2 \cos^2\left(\frac{n\pi x}{2a}\right) \right) \bigg|_{x=-a}^{x=a} \\ &= 0 \end{aligned}$$

For even n :

$$\delta E_n^{(1)} = \frac{\epsilon}{a^2} \int_{-a}^a x \sin^2\left(\frac{n\pi x}{2a}\right) dx = 0$$

$\therefore$ First order change in energy is 0

$$\frac{1}{2} |\delta\psi_1^{(1)}\rangle = \sum_{m=2}^{\infty} \frac{\langle m | \delta\hat{H} | 1 \rangle}{E_0 - E_m} |m\rangle$$

$$\psi_1'(x) = \psi_1(x) + \sum_{m=2}^{\infty} \frac{\langle m | \delta\hat{H} | 1 \rangle}{E_0 - E_m} \psi_m(x)$$

m is odd :

$$\langle m | \delta\hat{H} | 1 \rangle = \frac{\epsilon}{a^2} \int_{-a}^a x \cos\left(\frac{m\pi x}{2a}\right) \sin\left(\frac{\pi x}{2a}\right) dx$$

$$= 0$$

m is even :

$$\langle m | \delta\hat{H} | 1 \rangle = \frac{\epsilon}{a^2} \int_{-a}^a x \sin\left(\frac{m\pi x}{2a}\right) \cos\left(\frac{\pi x}{2a}\right) dx$$

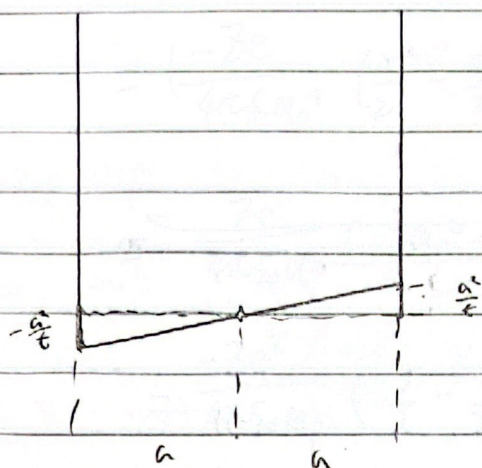
$$= \frac{\epsilon}{a^2} \frac{16na^2}{(n^2-1)^2} \frac{(-1)^{\frac{n}{2}+1}}{\pi^2} = \frac{16n\epsilon}{(n^2-1)^2} \frac{(-1)^{\frac{n}{2}+1}}{\pi^2}$$

$$\therefore \psi_1'(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) + \sum_{n=2,4,6,\dots} \frac{(-1)^{\frac{n}{2}+1} 16n\epsilon}{(n^2-1)^2} \frac{1}{\frac{16n\epsilon}{(n^2-1)^2} \frac{1}{\sqrt{a}} (1-n^2)E_1} \psi_1(x)$$

$$= \frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) + \sum_{n=2,4} (-1)^{\frac{n}{2}} \frac{16n\epsilon}{E_1(n^2-1)^3 \pi^2 \sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right)$$

$$= \left[\frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) + \frac{16\epsilon}{\pi^2 E_1 \sqrt{a}} \sum_{n=2,4,\dots} (-1)^{\frac{n}{2}} \frac{n}{(n^2-1)^3} \sin\left(\frac{n\pi x}{2a}\right) \right]$$

The perturbation $\delta\hat{H} = \frac{e}{a}\hat{x}$ destroys the symmetry ^{about $x=0$} of the Hamiltonian, so the wavefunction has no well-defined parity.



The particle must have larger probability ^{to be in} the ~~negative~~ region $-a < x < 0$ than in the region ~~the~~ $0 < x < a$.

The second order change in ground state ~~energy~~ energy should be negative.

This is because.
$$\delta E_1^{(2)} = \sum_{m=2}^{\infty} \frac{|\langle m | \delta\hat{H} | 1 \rangle|^2}{E_1 - E_m}$$

$E_m > E_1$ for all $m=2, 3, 4, \dots$

$\therefore \underline{\delta E_1^{(2)} < 0}$

5.

$$\delta \hat{V} = (\Phi(r) - \frac{Ze}{4\pi\epsilon_0 r}) (-e)$$

electric field inside sphere

$$= - \int_{a_p}^r \frac{Ze}{4\pi\epsilon_0 r'^2} \left(\frac{Ze r'}{4\pi\epsilon_0 a_p^3} \right) dr' + \frac{Ze}{4\pi\epsilon_0 a_p} - \frac{Ze}{4\pi\epsilon_0 r}$$

$$= \left(\frac{-Ze}{4\pi\epsilon_0 a_p^3} \left(\frac{r^2}{2} - \frac{a_p^2}{2} \right) + \frac{Ze}{4\pi\epsilon_0 a_p} - \frac{Ze}{4\pi\epsilon_0 r} \right) (-e)$$

$$= \frac{Ze}{4\pi\epsilon_0 a_p} \left(\frac{3}{2} - \frac{1}{2} \frac{r^2}{a_p^2} - \frac{a_p}{r} \right)$$

$$= \frac{-Ze^2}{4\pi\epsilon_0 a_p} \left(\frac{3}{2} - \frac{1}{2} \frac{r^2}{a_p^2} - \frac{a_p}{r} \right)$$

is the perturbation. for $r < a_p$ For $r \geq a_p$ $\delta V = 0$

$$\delta E_{100}^{(1)} = \langle 100 | \delta V | 100 \rangle$$

$$(r, \theta, \phi | 1, 0, 0) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

$$R(r) = 2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

$$= \int_0^{a_p} r^2 dr$$

$$= \int_0^{a_p} r^2 dr \left(\frac{Z}{a_0} \right)^3 e^{-2Zr/a_0} \frac{Ze}{4\pi\epsilon_0 a_p} \left(\frac{3}{2} - \frac{1}{2} \frac{r^2}{a_p^2} - \frac{a_p}{r} \right)$$

$$= - \left(\frac{Z}{a_0} \right)^3 \frac{Ze}{\pi\epsilon_0 a_p} \int_0^{a_p} r^2 dr e^{-2Zr/a_0} \left(\frac{3}{2} - \frac{1}{2} \frac{r^2}{a_p^2} - \frac{a_p}{r} \right)$$

$$\therefore a_p \sim 10^{-15} \text{ m} \ll a_0 \sim 10^{-10} \text{ m}, \text{ and } r < a_p$$

$$\therefore e^{-2Zr/a_0} \sim e^{-0} \sim 1$$

$$\therefore \delta E_{n0}^{(1)} = - \frac{Z^4 e^2}{\pi \epsilon_0 a_0^3 a_p} \int_0^{a_p} \left(\frac{3}{2} r^2 - \frac{2}{a_p^2} r^4 - a_p r \right) dr$$

$$= - \frac{Z^4 e^2}{\pi \epsilon_0 a_0^3 a_p} \left[\cancel{\frac{3}{2} r^3} \frac{1}{2} a_p^3 - \frac{a_p^5}{5 a_p^2} - \frac{1}{2} a_p^3 \right]$$

$$= \cancel{\frac{Z^4 e^2}{\pi \epsilon_0 a_0^3 a_p^2}} \boxed{\frac{Z^4 e^2 a_p^2}{10 \pi \epsilon_0 a_0^3}}$$

From the radial wavefunction of hydrogen we know that the leading order of the term $\frac{r}{a_0}$ in $U_n^l(r)$ is $(\frac{r}{a_0})^l$. Hence for $\frac{r}{a_0} \ll 1$

$$\Rightarrow U_n^l(r) \sim \left(\frac{r}{a_0}\right)^l$$

$\therefore$ the larger the value of l the smaller the magnitude of the change in energy because $U_n^l(r)$ is part of the integrand of $\delta E_{nlm}^{(1)} = \langle \psi_{nlm} | \delta V | \psi_{nlm} \rangle$

$$\delta E_{l00}^{(1)} \sim Z^4$$

$\Rightarrow$ larger ~~the~~ Z gives larger energy perturbation.

how about $\Delta E^{l=1}$?

~~of~~ ~~overlap~~

heavily elements higher perturbation

Z^4
↑
perturbation

Z^2
↑
energy levels

$$6. \quad \hat{H} = \frac{\hat{P}_x^2}{2m} + \frac{\hat{P}_y^2}{2m} + \frac{1}{2} m \omega^2 (x^2 + y^2)$$

$$= \left(\frac{\hat{P}_x^2}{2m} + \frac{1}{2} m \omega^2 x^2 \right) + \left(\frac{\hat{P}_y^2}{2m} + \frac{1}{2} m \omega^2 y^2 \right)$$

$$= \hat{H}_x + \hat{H}_y \quad \checkmark$$

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

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

$$\rightarrow \hat{H} |n_x, n_y\rangle = \hbar \omega (n_x + n_y + 1) |n_x, n_y\rangle$$

$$\text{Energy spectrum : } E_{n_x, n_y} = \boxed{(n_x + n_y + 1) \hbar \omega}$$

For the first excited level, $(n_x, n_y) = (1, 0)$ or $(0, 1)$

$$E_{1,0} = E_{0,1} = 2\hbar\omega$$

$$\text{Kets } \boxed{|1,0\rangle \text{ or } |0,1\rangle}$$

The n^{th} excited level.

$$\rightarrow n_x + n_y = n \rightarrow n_y = n - n_x$$

n_x can take values ~~independen~~ arbitrarily from $(0, 1, 2, \dots, n)$ and n_y takes $n - n_x$

$\Rightarrow$ the degeneracy equals to number of integers from 0 to n inclusive.

$$\rightarrow \text{degeneracy} = \boxed{n+1} \quad \checkmark$$

For the first excited level, perturbation $\delta V = \lambda xy$
 Find the eigenvector of the ^{following} V matrix in the degenerate subspace

$$\hat{V} = \begin{pmatrix} \langle 1,0 | \delta V | 1,0 \rangle & \langle 1,0 | \delta V | 0,1 \rangle \\ \langle 0,1 | \delta V | 1,0 \rangle & \langle 0,1 | \delta V | 0,1 \rangle \end{pmatrix} \quad \checkmark$$

$$\begin{aligned} \langle 1,0 | \lambda \hat{x} \hat{y} | 1,0 \rangle &= \lambda l^2 \langle 1,0 | (a_x^\dagger + a_x)(a_y^\dagger + a_y) | 1,0 \rangle \\ &= 0 \end{aligned}$$

$$\begin{aligned} \langle 1,0 | \lambda \hat{x} \hat{y} | 0,1 \rangle &= \lambda l^2 \langle 1,0 | (a_x^\dagger + a_x)(a_y^\dagger + a_y) | 0,1 \rangle \\ &= \lambda l^2 \end{aligned}$$

$$\begin{aligned} \langle 0,1 | \lambda \hat{x} \hat{y} | 1,0 \rangle &= \lambda l^2 \langle 0,1 | (a_x^\dagger + a_x)(a_y^\dagger + a_y) | 1,0 \rangle \\ &= \lambda l^2 \end{aligned}$$

$$\langle 0,1 | \lambda \hat{x} \hat{y} | 0,1 \rangle = 0$$

$$\therefore \hat{V} = \begin{pmatrix} 0 & \lambda l^2 \\ \lambda l^2 & 0 \end{pmatrix} \quad (l = \sqrt{\frac{\hbar}{2m\omega}})$$

$$\hat{V}|\psi\rangle = c|\psi\rangle \Rightarrow \det \begin{pmatrix} -c & \lambda l^2 \\ \lambda l^2 & -c \end{pmatrix} = 0$$

$$\therefore -c^2 - (\lambda l^2)^2 = 0$$

$$\Rightarrow c = \pm \lambda l^2$$

$$c = \lambda l^2 \Rightarrow$$

$$\text{eigenvector} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \checkmark$$

$$c = -\lambda l^2 \Rightarrow$$

$$\text{eigenvector} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \checkmark$$

∴ The energy corrections are

$$+ \lambda \lambda^2 = \cancel{\lambda^2} \frac{+\lambda \hbar}{2m\omega} \rightarrow E = 2\hbar\omega + \frac{\lambda \hbar}{2m\omega}$$

corresponds to state $\boxed{\frac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle)}$

$$\text{and } -\lambda^2 = -\frac{\lambda \hbar}{2m\omega} \rightarrow E = 2\hbar\omega - \frac{\lambda \hbar}{2m\omega}$$

corresponds to state $\boxed{\frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)}$

Mirror operator $\hat{M} : \langle x, y | \hat{M} | \psi \rangle = \langle y, x | \psi \rangle$

is a reflection about $y=x$. It ~~also~~ interchange

the x and y coordinates of ψ .

$$[M, H_1] \psi(x, y) = \hat{M} \hat{H}_1 \psi(x, y) - \hat{H}_1 \hat{M} \psi(x, y)$$

$$= \hat{M} (\lambda \hat{x} \hat{y} \psi(x, y)) - \lambda \hat{x} \hat{y} \psi(y, x)$$

$$= \lambda y x \psi(y, x) - \lambda x y \psi(y, x)$$

$$= 0 \rightarrow \text{for any arbitrary } \psi$$

$$\Rightarrow [\hat{M}, \hat{H}_1] = 0$$

$$(\hat{M} \hat{H}_1 - \hat{H}_1 \hat{M}) \psi = \hat{M} \hat{H}_x \psi(x, y) - \hat{H}_y \hat{M} \psi(x, y)$$

$$= \hat{M} \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2} m \omega^2 x^2 \right) \psi(x, y) - \hat{H}_y \psi(y, x)$$

$$= \frac{\hat{p}_y^2}{2m} \psi(y, x) + \frac{1}{2} m \omega^2 y^2 \psi(y, x) - \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2} m \omega^2 y^2 \right) \psi(y, x) = 0$$

→ for ~~arbitrary~~ arbitrary ψ

$$\therefore \underline{\hat{M}\hat{H}_x = \hat{H}_y\hat{M}} \xrightarrow{\text{by symmetry}} \hat{M}\hat{H}_y = \hat{H}_x\hat{M}$$

$$[\hat{M}, \hat{H}] = [\hat{M}, \hat{H}_x] + [\hat{M}, \hat{H}_y]$$

$$= \hat{M}\hat{H}_x - \hat{H}_x\hat{M} + \hat{M}\hat{H}_y - \hat{H}_y\hat{M}$$

$$= \underbrace{(\hat{M}\hat{H}_x - \hat{H}_x\hat{M})}_0 + \underbrace{(\hat{M}\hat{H}_y - \hat{H}_y\hat{M})}_0 = 0$$

$\therefore \hat{M}$ commutes with $\hat{H}$ ✓

$\therefore$ The system has symmetry of $\hat{M}$ ✓

$\Rightarrow$ The system ~~has is symmetrical about~~
 ~~$y=x$~~ has reflection symmetry about
 $y=x$ and ~~has the~~ states have
well-defined mirror-states because eigenstates
of $\hat{H}$ is also eigenstates of $\hat{M}$

$$\hat{M} \frac{1}{\sqrt{2}} (|1,0\rangle + |0,1\rangle) = (1) \frac{1}{\sqrt{2}} (|0,1\rangle + |1,0\rangle)$$

eigenvalue = 1

$$\hat{M} \frac{1}{\sqrt{2}} (|1,0\rangle - |0,1\rangle) = (-1) \frac{1}{\sqrt{2}} (|0,1\rangle - |1,0\rangle)$$

$$= (-1) \frac{1}{\sqrt{2}} (|1,0\rangle - |0,1\rangle)$$

eigenvalue = -1

7. (a)

$$\hat{H} = \hat{H}_0 + \epsilon \delta \hat{H} = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} + \epsilon \begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix}$$

$$\hat{H}_0 |1\rangle = A_1 |1\rangle \Rightarrow |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad E_1 = A_1$$

$$\hat{H}_0 |2\rangle = A_2 |2\rangle \Rightarrow |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad E_2 = A_2$$

$$\begin{aligned} \delta E_1^{(1)} &= \epsilon \langle 1 | \delta H | 1 \rangle = \epsilon (1, 0) \begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \epsilon (1, 0) \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \epsilon B_1 \end{aligned}$$

$$\underline{E_1' = A_1 + \epsilon B_1} \quad \underline{E_1' = A_1 + \epsilon B_2} \quad \underline{E_1' = A_1 + \epsilon (B_1 + B_2)}$$

$$\begin{aligned} \delta E_2^{(1)} &= \epsilon \langle 2 | \delta H | 2 \rangle = \epsilon (0, 1) \begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \epsilon (0, 1) \begin{pmatrix} B_2 \\ 0 \end{pmatrix} = \boxed{0} \end{aligned}$$

$$\underline{E_2' = A_2}$$

(b) $\hat{H}_0 = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}$ for $A_1 = A_2 = A$

~~Diagonalize~~ Find eigenvectors of $\begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix}$

$$\det \begin{pmatrix} B_1 - \lambda & B_2 \\ B_2 & -\lambda \end{pmatrix} = 0$$

$$\Rightarrow (\lambda - B_1)\lambda - B_2^2 = 0$$

$$\lambda^2 - B_1\lambda - B_2^2 = 0$$

$$\Rightarrow \lambda = \frac{B_1 \pm \sqrt{B_1^2 + 4B_2^2}}{2}$$

$$\lambda = \frac{B_1 + \sqrt{B_1^2 + 4B_2^2}}{2}$$

$$\frac{B_1 - \sqrt{B_1^2 + 4B_2^2}}{2}$$

$$\begin{pmatrix} B_2 & -\frac{B_1 - \sqrt{B_1^2 + 4B_2^2}}{2} \\ \frac{\sqrt{B_1^2 + 4B_2^2}}{2} - B_1 & B_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\frac{\sqrt{B_1^2 + 4B_2^2}}{2} x_1 = B_2 x_2$$

$$\therefore \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} B_2 \\ \frac{\sqrt{B_1^2 + 4B_2^2} - B_1}{2} \end{pmatrix}$$

Normalise

$$= B_2^2 + \frac{(\frac{\sqrt{B_1^2 + 4B_2^2} - B_1}{2})^2}{2}$$

$$= B_2^2 + \frac{B_1^2 + 4B_2^2}{4} + \frac{B_1^2}{4} - \frac{1}{2} B_1 \sqrt{B_1^2 + 4B_2^2}$$

$\therefore$ Energy levels :

$$E_1 = A + \frac{\hbar^2}{2}$$

$$E_1 = A + \frac{\hbar^2}{2} (B_1 + \sqrt{B_1^2 + 4B_2^2})$$

$$E_2 = A + \frac{\hbar^2}{2} (B_1 - \sqrt{B_1^2 + 4B_2^2})$$

Exact eigenvalues:

$$\det \begin{pmatrix} A_1 + B_1 \epsilon - C & B_2 \epsilon \\ B_2 \epsilon & A_2 - C \end{pmatrix} = 0$$

$$\rightarrow (A_1 + B_1 \epsilon - C)(A_2 - C) - B_2^2 \epsilon^2 = 0.$$

$$\rightarrow C^2 - (A_1 + A_2 + B_1 \epsilon)C + (A_1 A_2 + B_1 A_2 \epsilon - B_2^2 \epsilon^2) = 0$$

$$C = \frac{1}{2} \left[(A_1 + A_2 + B_1 \epsilon) \pm \sqrt{(A_1 + A_2 + B_1 \epsilon)^2 - 4(A_1 A_2 + B_1 A_2 \epsilon - B_2^2 \epsilon^2)} \right]$$

$$= \frac{1}{2} \left[(A_1 + A_2 + B_1 \epsilon) \pm \left(A_1^2 + A_2^2 + B_1^2 \epsilon^2 + 2A_1 A_2 + 2A_1 B_1 \epsilon + 2A_2 B_1 \epsilon - 4A_1 A_2 - 4B_1 A_2 \epsilon + 4B_2^2 \epsilon^2 \right)^{\frac{1}{2}} \right]$$

$$= \frac{1}{2} \left[(A_1 + A_2 + B_1 \epsilon) \pm (A_1^2 + A_2^2 - 2A_1 A_2 + 2B_1(A_1 - A_2)\epsilon + (B_1^2 + 4B_2^2)\epsilon^2)^{\frac{1}{2}} \right]$$

$$= \frac{1}{2} \left[(A_1 + A_2 + B_1 \epsilon) \pm \sqrt{(A_1 - A_2)^2 + 2B_1(A_1 - A_2)\epsilon + (B_1^2 + 4B_2^2)\epsilon^2} \right]$$

$$\text{If } A_1 = A_2 = A, \quad A_1 - A_2 = 0$$

$$C = E = \frac{1}{2} A + \frac{\epsilon}{2} (B_1 \pm \sqrt{B_1^2 + 4B_2^2}).$$

$\rightarrow$ consistent

If $A_1 \neq A_2$

$$C = E = \frac{1}{2} [A_1 + A_2 + B_1 \epsilon \pm \cancel{A_1 A_2} (A_1 - A_2) \left[1 + \frac{2B_1 \epsilon}{A_1 - A_2} + \frac{B_1^2 + 4B_2^2}{(A_1 - A_2)^2} \epsilon^2 \right]^{\frac{1}{2}}]$$

$$\approx \frac{1}{2} [A_1 + A_2 + B_1 \epsilon \pm \cancel{A_1 A_2} (A_1 - A_2) \left[1 + \frac{B_1 \epsilon}{A_1 - A_2} \right]]$$

expand in small ϵ ,
ignore ϵ^2

$$= \frac{1}{2} [A_1 + A_2 + B_1 \epsilon \pm (A_1 - A_2) + B_1 \epsilon]$$

$\therefore E_1 = \frac{1}{2} [A_1 + A_2 + B_1 \epsilon + A_1 - A_2 + B_1 \epsilon]$

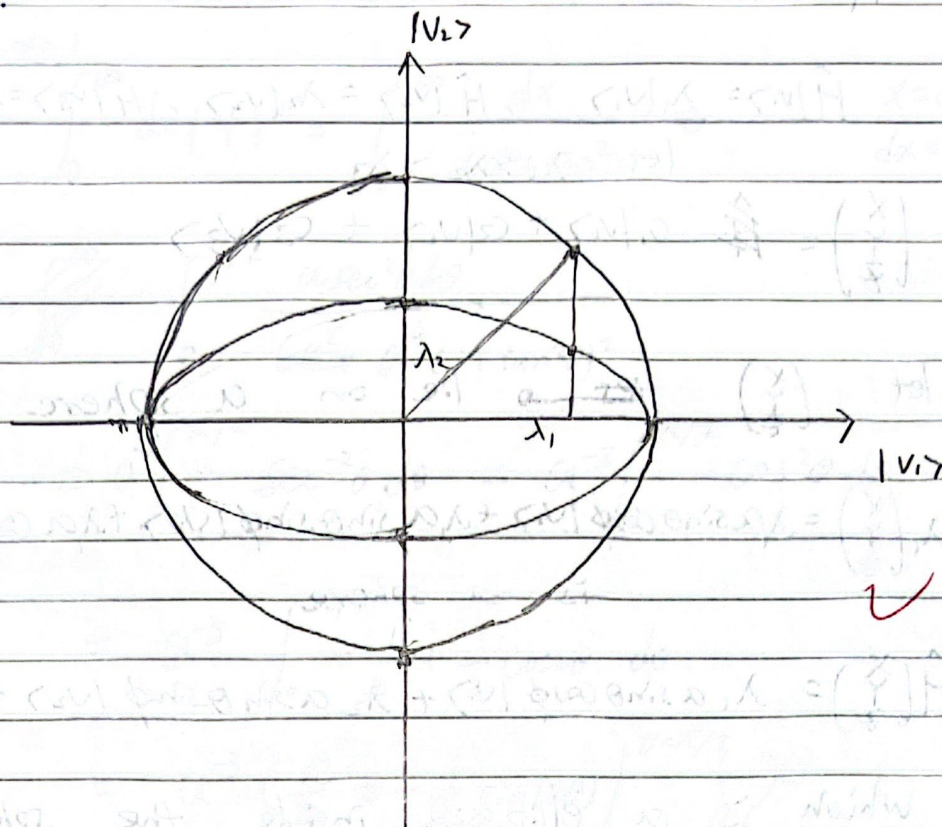
$$= \underline{A_1 + B_1 \epsilon}$$

$$E_2 = \frac{1}{2} [A_1 + A_2 + B_1 \epsilon - \cancel{A_1 + A_2} - B_1 \epsilon]$$

$$= \underline{A_2}$$

→ consistent.

8.



$$\hat{H}|v_1\rangle = \lambda_1|v_1\rangle \quad \hat{H}|v_2\rangle = \lambda_2|v_2\rangle$$

$$\text{let } \begin{pmatrix} x \\ y \end{pmatrix} = c_1|v_1\rangle + c_2|v_2\rangle \quad (|v_1\rangle, |v_2\rangle \text{ form a complete set of basis})$$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \hat{H} \begin{pmatrix} x \\ y \end{pmatrix} = c_1\lambda_1|v_1\rangle + c_2\lambda_2|v_2\rangle$$

$$\begin{pmatrix} x \\ y \end{pmatrix} \text{ lies on a circle} \therefore \text{let } c_1 = a \cos \theta \quad c_2 = a \sin \theta$$

$$\text{then } \begin{pmatrix} x \\ y \end{pmatrix} = a\lambda_1 \cos \theta |v_1\rangle + a\lambda_2 \sin \theta |v_2\rangle$$

which is an ellipse. inside the circle
~~described~~ described by $\lambda_1 \begin{pmatrix} x \\ y \end{pmatrix} = a\lambda_1 \cos \theta |v_1\rangle + a\lambda_2 \sin \theta |v_2\rangle$

~~For~~

If $\hat{H}$ is a 3×3 matrix then

$$\hat{H}|v_1\rangle = \lambda_1|v_1\rangle, \quad \hat{H}|v_2\rangle = \lambda_2|v_2\rangle, \quad \hat{H}|v_3\rangle = \lambda_3|v_3\rangle.$$

let $\lambda_1 > \lambda_2 > \lambda_3$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \cancel{\frac{1}{a}} c_1|v_1\rangle + c_2|v_2\rangle + c_3|v_3\rangle$$

let $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ ~~lies~~ lie on a sphere, then

$$\lambda_1 \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \lambda_1 a \sin\theta \cos\phi |v_1\rangle + \lambda_1 a \sin\theta \sin\phi |v_2\rangle + \lambda_1 a \cos\theta |v_3\rangle$$

is a sphere

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \hat{H} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \lambda_1 a \sin\theta \cos\phi |v_1\rangle + \lambda_2 a \sin\theta \sin\phi |v_2\rangle + \lambda_3 a \cos\theta |v_3\rangle$$

which is an ellipsoid inside the sphere. ✓

• Expectation of $\hat{H}$ in state $\begin{pmatrix} x \\ y \end{pmatrix}$ is

$$\begin{aligned} \langle X, Y | \begin{pmatrix} x \\ y \end{pmatrix} \rangle &= (c_1 \langle v_1 | + c_2 \langle v_2 |) (c_1 \lambda_1 |v_1\rangle + c_2 \lambda_2 |v_2\rangle) \\ &= c_1^2 \lambda_1 + c_2^2 \lambda_2 = \lambda_1 a^2 \cos^2\theta + \lambda_2 a^2 \sin^2\theta \end{aligned}$$

which attains stationary values when $\theta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$.

$$0, \pi \Rightarrow \langle \hat{H} \rangle = \lambda_1 \quad \text{state} = |v_1\rangle$$

$$\frac{\pi}{2}, \frac{3\pi}{2} \Rightarrow \langle \hat{H} \rangle = \lambda_2 \quad \text{state} = |v_2\rangle$$

This corresponds to the variational theorem, which states that the stationary points of the expectation value of an Hermitian operator occur at the eigenstates of that operator. Also, all eigenstates provide stationary value points of the operator.

9. $\psi(x) = (a^2 + x^2)^{-\alpha}$

For $\alpha = 1$

$$\int_0^{\infty} dx |\psi|^2 = \int_0^{\infty} \frac{dx}{(a^2 + x^2)^2}$$

$$x = a \tan \theta$$

$$dx = a \sec^2 \theta d\theta$$

$$= \int_0^{\pi/2} \frac{a \sec^2 \theta d\theta}{a^4 (1 + \tan^2 \theta)^2}$$

$$= a^{-3} \int_0^{\pi/2} \sec^{-2} \theta d\theta = a^{-3} \int_0^{\pi/2} \cos^2 \theta d\theta$$

$$= a^{-3} \int_0^{\pi/2} \left(\frac{1}{2} + \frac{1}{2} \cos 2\theta \right) d\theta$$

$$= a^{-3} \left(\frac{\pi}{4} - \frac{1}{4} \sin(2\theta) \right) \bigg|_{\theta=0}^{\theta=\pi/2}$$

$$= \frac{1}{4} \pi a^{-3}$$

$$\int_0^{\infty} dx x^2 |\psi|^2 = \int_0^{\infty} \frac{x^2 dx}{(a^2 + x^2)^2} = \int_0^{\pi/2} \frac{a^3 \tan^2 \theta \sec^2 \theta d\theta}{a^4 \sec^4 \theta}$$

$$= \frac{1}{a} \int_0^{\pi/2} \sin^2 \theta d\theta$$

$$= \frac{1}{a} \left[\frac{\pi}{2} - \int_0^{\pi/2} \cos^2 \theta d\theta \right] = \frac{1}{4} \pi a^{-1}$$

$$\hat{p}\psi = -i\hbar \frac{\partial}{\partial x} \psi(x) = i\hbar \alpha (a^2 + x^2)^{-\alpha-1} (2x)$$

$$= 2i\hbar \alpha (a^2 + x^2)^{-\alpha-1} (2x)$$

When $\alpha=1$ $\hat{p}\psi = 2i\hbar (a^2 + x^2)^{-2} (2x)$

$$\therefore |\hat{p}\psi|^2 = 4\hbar^2 (a^2 + x^2)^{-4} (2x)^2 = \frac{16\hbar^2 x^2}{(a^2 + x^2)^4}$$

$$\therefore \int_0^\infty dx |\hat{p}\psi|^2 = \int_0^\infty \frac{16\hbar^2 x^2 dx}{(a^2 + x^2)^4} = \frac{16\hbar^2}{4} \int_0^{\pi/2} \frac{\tan^2 \theta \sec^2 \theta d\theta}{\sec^8 \theta}$$

$$= 4\hbar^2 \int_0^{\pi/2} \frac{\tan^2 \theta \sec^2 \theta d\theta}{\sec^8 \theta}$$

$$= 4\hbar^2 \int_0^{\pi/2} \tan^2 \theta \sec^{-6} \theta d\theta$$

$$= 4\hbar^2 \int_0^{\pi/2} \sin^2 \theta \cos^4 \theta d\theta$$

$$\hat{p}\psi = -i\hbar \frac{\partial}{\partial x} \psi(x) = i\hbar \alpha (a^2 + x^2)^{-\alpha-1} (2x)$$

$$= 2i\hbar \alpha x (a^2 + x^2)^{-\alpha-1}$$

When $\alpha=1$ $\hat{p}\psi = 2i\hbar \frac{x}{(a^2 + x^2)^2}$

$$\therefore |\hat{p}\psi|^2 = 4\hbar^2 \frac{x^2}{(a^2 + x^2)^4}$$

$$\therefore \int_0^{\infty} dx |\hat{p}\psi|^2 = 4\hbar^2 \int_0^{\infty} \frac{x^2 dx}{(a^2 + x^2)^4}$$

$$= 4\hbar^2 \int_0^{\pi/2} \frac{a^3 \tan^2 \theta \sec^2 \theta d\theta}{a^8 \sec^8 \theta}$$

$$= 4\hbar^2 a^{-5} \int_0^{\pi/2} \tan^2 \theta \sec^{-6} \theta d\theta$$

$$= 4\hbar^2 a^{-5} \int_0^{\pi/2} \sin^2 \theta \cos^4 \theta d\theta$$

$$= 4\hbar^2 a^{-5} \int_0^{\pi/2} \frac{1}{2} (1 - \cos 2\theta) \frac{1}{2} (1 + \cos^2 2\theta) \frac{1}{2} (1 + \cos 2\theta) d\theta$$

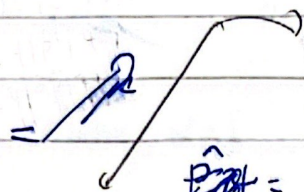
$$= \frac{4\hbar^2 a^{-5}}{8} \int_0^{\pi/2} (1 - \cos^2 2\theta) (1 + \cos 2\theta) d\theta$$

$$= \frac{\hbar^2 a^{-5}}{2} \int_0^{\pi/2} 1 + \cos^2 2\theta - \cos^2 2\theta - \cos^3 2\theta d\theta$$

$$= \frac{\hbar^2 a^{-5}}{2} \left[\underbrace{\int_0^{\pi/2} d\theta}_{\pi/2} + \underbrace{\int_0^{\pi/2} \cos 2\theta d\theta}_0 - \underbrace{\int_0^{\pi/2} \cos^2 2\theta d\theta}_{\pi/4} - \underbrace{\int_0^{\pi/2} \cos^3 2\theta d\theta}_0 \right]$$

$$= \frac{1}{8} \pi \hbar^2 a^{-5}$$

$$\langle H \rangle_a = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{-\infty}^{\infty} \psi^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi dx}{\int_{-\infty}^{\infty} |\psi|^2 dx}$$



$\hat{P}$ is hermitian

$$\langle \psi | \hat{P}^2 | \psi \rangle$$

$$= \langle \psi | \hat{P} \hat{P} | \psi \rangle$$

$$= (\hat{P} | \psi \rangle)^\dagger \hat{P} | \psi \rangle$$

$$= |\hat{P} | \psi \rangle|^2$$

factors of 2

come from

$|\psi|^2, x^2 |\psi|^2$

and $|\psi|^2$ all

being even functions.

$$= \frac{\frac{1}{2m} \left(\frac{1}{8} \pi \hbar^2 a^{-5} \right) + \frac{1}{2} m \omega^2 \left(\frac{1}{4} \pi a^{-1} \right)}{\frac{1}{4} \pi a^{-3}}$$

$$= \frac{\hbar^2}{4m} a^{-2} + \frac{1}{2} m \omega^2 a^2$$

minimize $\langle H \rangle_a$: $\frac{d\langle H \rangle_a}{da} = 0$

$$\Rightarrow 0 = \frac{\hbar^2}{4m} (-2) a^{-3} + m \omega^2 a$$

$$\therefore a^4 = \frac{\hbar^2}{2m} = m \omega^2 a^4$$

$$\therefore a^4 = \frac{1}{2} \frac{\hbar^2}{m^2 \omega^2} = 2 \left(\frac{\hbar}{2m\omega} \right)^2$$

$$\rightarrow a = 2^{1/4} \sqrt{\frac{\hbar}{2m\omega}} = \boxed{2^{1/4} l}$$

$$(l \equiv \sqrt{\frac{\hbar}{2m\omega}}).$$

Substitute this back $a^2 = \sqrt{2} l^2$ $a^{-2} = \frac{1}{\sqrt{2} l^2}$.

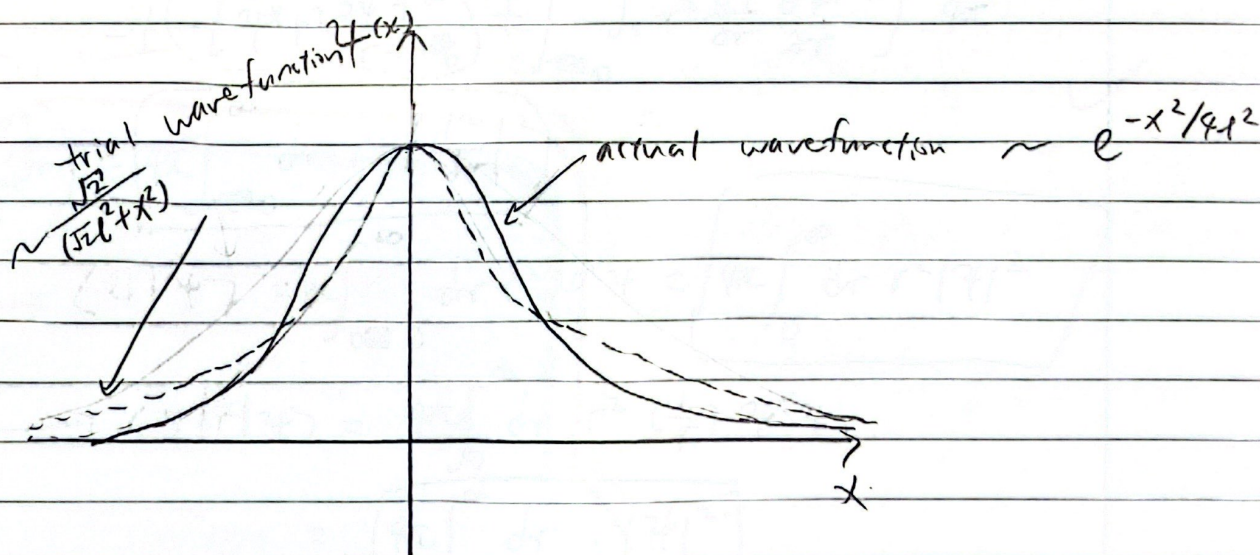
$$\langle H \rangle_{\min} = \frac{\hbar^2}{4m} \frac{1}{\sqrt{2} l^2} + \frac{1}{2} m \omega^2 \sqrt{2} l^2.$$

$$= \frac{\hbar^2}{2 \cdot 4m} \frac{1}{\sqrt{2}} \frac{2m\omega}{\hbar} + \frac{1}{2} m \omega^2 \sqrt{2} \frac{\hbar}{2m\omega}$$

$$= \frac{\hbar^2}{2} \frac{\omega}{\hbar} + \frac{1}{2\sqrt{2}} \hbar \omega + \frac{\sqrt{2}}{4} \hbar \omega$$

$$= \frac{\hbar \omega}{\sqrt{2}}$$

is the upper limit of E_0



Increasing α makes the shape of trial function more and more like a gaussian

$\rightarrow$ we should increase α .

10. For gross structure of hydrogen.

$$\hat{H} = \frac{\hat{p}^2}{2m_e} + \frac{\hbar^2 \nabla^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\langle \psi | \hat{H} | \psi \rangle = \frac{\hbar^2}{2m_e} \langle \psi | \nabla^2 | \psi \rangle + \underbrace{\frac{Ze^2}{4\pi\epsilon_0} \langle \psi | \frac{1}{r} | \psi \rangle}_{0 \text{ for spherical symmetric } \psi(r)}$$

$$\Rightarrow \langle \psi | \hat{H} | \psi \rangle = \frac{\hbar^2}{2m_e} \langle \psi | \nabla^2 | \psi \rangle - \frac{Ze^2}{4\pi\epsilon_0} \langle \psi | \frac{1}{r} | \psi \rangle$$

$$\rightarrow \langle \psi | \nabla^2 | \psi \rangle = - \int_0^\infty r^2 dr \psi^* \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) (4\pi)$$

$$= - \int_0^\infty dr \psi^* \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) (4\pi)$$

$$= \left[- \left[\psi^* r^2 \frac{\partial \psi}{\partial r} \right]_0^\infty + \int_0^\infty dr r^2 \frac{\partial \psi}{\partial r} \frac{\partial \psi^*}{\partial r} \right] 4\pi$$

$$= 4\pi \int_0^\infty dr r^2 \left| \frac{d\psi}{dr} \right|^2$$

$$\rightarrow \langle \psi | \psi \rangle = 4\pi \int_0^\infty dr r^2 \psi^* \psi = \left[4\pi \int_0^\infty dr r^2 |\psi|^2 \right]$$

$$\rightarrow \langle \psi | \frac{1}{r} | \psi \rangle = 4\pi \int_0^\infty dr r^2 \left(\frac{1}{r} \right) \psi^* \psi$$

$$= \left[4\pi \int_0^\infty dr r |\psi|^2 \right]$$

$$\therefore \langle H \rangle = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\left(\frac{\hbar^2}{2m_e} \int_0^\infty dr r^2 \left| \frac{d\psi}{dr} \right|^2 - \frac{e^2}{4\pi\epsilon_0} \int_0^\infty dr r |\psi|^2 \right)}{\int_0^\infty dr r^2 |\psi|^2}$$

(Z=1 for hydrogen)

trial wave function.

~~$\langle H \rangle$~~

$$\int dr r^2 |4|^2 = \int dr r^2 e^{-2br}$$

$$\begin{aligned} \text{let } u &= 2br \\ du &= 2b dr \quad 2dr \\ r^2 &= \frac{u^2}{4b^2} \\ dr &= \frac{du}{2b} \end{aligned}$$

$$= \int \frac{du}{2b} \left(\frac{u^2}{4b^2} \right) e^{-u}$$

$$= \frac{1}{(2b)^3} \int du \underbrace{u^2 e^{-u}}_{2!}$$

$$= \frac{1}{4b^3}$$

$$\int dr r^2 \left| \frac{d\psi}{dr} \right|^2 = \int dr r^2 b^2 e^{-2br} = \frac{1}{4b}$$

$$\int dr r |4|^2 = \int \frac{du}{2b} \frac{u}{2b} e^{-u} = \frac{1}{4b^2} \int e^{-u} \underbrace{u du}_{1!} = \frac{1}{4b^2}$$

$$\therefore \langle H \rangle = 4b^3 \left[\frac{1}{4b} \frac{\hbar^2}{2me} - \frac{e^2}{4\pi\epsilon_0} \frac{1}{4b^2} \right]$$

$$= \left[\frac{\hbar^2 b^2}{2me} - \frac{e^2 b}{4\pi\epsilon_0} \right]$$

Find the minimum of $\langle H \rangle_b$.

$$\text{Set } 0 = \frac{d\langle H \rangle_b}{db}$$

We have :

$$0 = \frac{\hbar^2 b}{me} - \frac{e^2}{4\pi\epsilon_0}$$

$$\Rightarrow b = \frac{e^2}{4\pi\epsilon_0} \frac{me}{\hbar^2} = \frac{mee^2}{4\pi\epsilon_0\hbar^2}$$

$$a_0 \equiv \frac{1}{b} = \frac{4\pi\epsilon_0\hbar^2}{mee^2} \quad \text{is the Bohr radius}$$

$\rightarrow \psi_{\min} = e^{-r/a_0}$ is the ground state wavefunction of hydrogen.

Substitute $b = \frac{mee^2}{4\pi\epsilon_0\hbar^2}$ back in to $\langle H \rangle_b$ gives

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2me} \frac{(4\pi\epsilon_0\hbar^2)^2}{(mee^2)^2} - \frac{e^2}{4\pi\epsilon_0} \frac{mee^2}{4\pi\epsilon_0\hbar^2}$$

$$= -\frac{1}{2}me\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \equiv -R \quad \text{Rydberg Constant.}$$

Where R is the Rydberg constant.

11. $\hat{H} = \hat{H}_0 + \delta \hat{H}$

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

expand $|\psi\rangle = \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = (\hat{H}_0 + \delta \hat{H}) |\psi\rangle$$

$$= \sum_n (E_n |n\rangle + \delta \hat{H} |n\rangle) a_n e^{-iE_n t/\hbar}$$

$\hat{H}$ is an operator!

$$= \sum_n \left(i\hbar \frac{da_n}{dt} + E_n a_n \right) e^{-iE_n t/\hbar} |n\rangle$$

$$\langle a_k | \cdot \Rightarrow i\hbar \frac{da_k}{dt} e^{-iE_k t/\hbar} = \sum_n a_n e^{-iE_n t/\hbar} \langle k | \delta \hat{H} | n \rangle$$

Initial conditions: $a_0 = 1$ ~~$a_{n \neq 0} = 0$~~

$$\begin{aligned} a_0(0) &= 1 & a_{n \neq 0}(0) &= 0 \\ a_0(-\infty) &= 1 & a_{n \neq 0}(-\infty) &= 0 \end{aligned}$$

at early times the term $a_0 \gg a_{n \neq 0}$
assume that is true for all times $-\infty \leq t \leq \infty$

$$\therefore \frac{da_k}{dt} \approx -\frac{i}{\hbar} e^{i(E_k - E_0)t/\hbar} \langle k | \delta \hat{H} | 0 \rangle$$

For $k=2$: $\frac{da_2}{dt} = -\frac{i}{\hbar} e^{i(E_2 - E_0)t/\hbar} \langle 2 | \delta \hat{H} | 0 \rangle$

$$\langle 2 | \delta \hat{H} | 0 \rangle = \xi e^{-t^2/\kappa^2} \langle 2 | \hat{x} | 0 \rangle$$

$$= \xi e^{-t^2/\kappa^2} \langle 2 | \hat{a}^\dagger + \hat{a} | 0 \rangle = 0$$

$\downarrow$ $\downarrow$
 $\langle 2 | 1 \rangle = 0$ $\hat{a} | 0 \rangle = 0$

$$\therefore \frac{da_2}{dt} \approx 0 \quad \therefore a_2(t=0) = 0 \quad \therefore a_2(t) = 0$$

∴ The Probability of transition to $|2\rangle$ is $\boxed{0}$

For $k=1$

$$\begin{aligned} \langle 1 | \hat{H} | 0 \rangle &= \langle 1 | \epsilon l e^{-t^2/k^2} \langle 1 | \hat{a}^\dagger + \hat{a} | 0 \rangle \\ &= \epsilon l e^{-t^2/k^2} (1 + 0) = \epsilon l e^{-t^2/k^2} \end{aligned}$$

$$E_1 - E_0 = \hbar \omega$$

$$\begin{aligned} \therefore \frac{da_1}{dt} &= -\frac{i}{\hbar} e^{i\omega t} \epsilon l e^{-t^2/k^2} \\ &= -\frac{i}{\hbar} \epsilon l e^{i\omega t - t^2/k^2} \end{aligned}$$

$$\therefore a_1(0) = 0$$

$$\therefore a_1 = -\frac{i}{\hbar} \epsilon l \int_0^t e^{i\omega t - t^2/k^2} dt.$$

$$\approx -\frac{i}{\hbar} \epsilon l \int_0^t e^{i\omega t} \left(1 - \frac{t^2}{k^2}\right) dt.$$

$$= -\frac{i}{\hbar} \epsilon l \int_0^t e^{i\omega t} dt + \frac{i}{\hbar} \epsilon l \frac{1}{k^2} \int_0^t t^2 e^{i\omega t} dt.$$

$$\int_0^t e^{i\omega t} dt = -\frac{i}{\omega} e^{i\omega t} \Big|_0^t = -\frac{i}{\omega} (e^{i\omega t} - 1)$$

$$\begin{aligned} \int_0^t t^2 e^{i\omega t} dt &= \frac{1}{\omega^3} [e^{i\omega t} [-it^2\omega^2 + 2\omega t + 2i]] \Big|_0^t \\ &= \frac{1}{\omega^3} [e^{i\omega t} [-it^2\omega^2 + 2\omega t + 2i]] - \end{aligned}$$

$$\frac{da_1}{dt} = -a_1(-\omega) \quad \therefore a_1(-\infty) = 0$$

$$\therefore a_1 = -\frac{i}{\hbar} \mathcal{E} l \int_{-\infty}^{\infty} e^{i\omega t - t^2/\tau^2} dt.$$

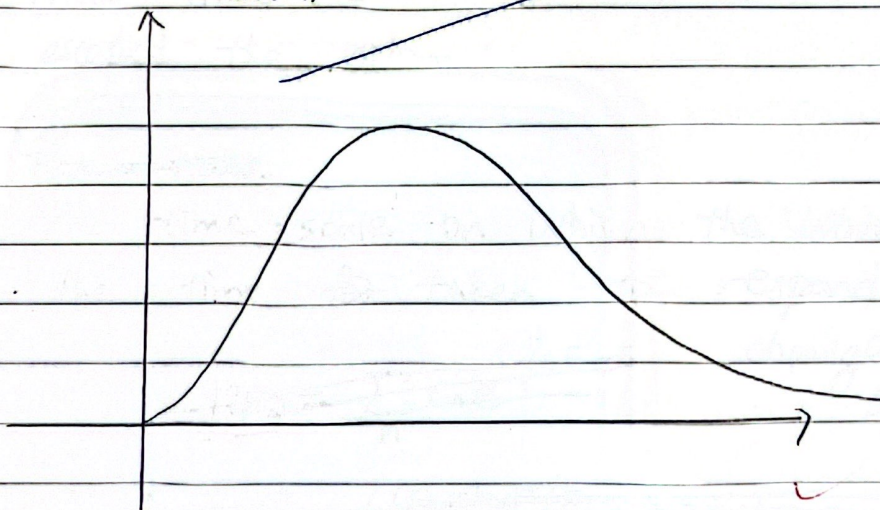
Gaussian integral formula

$$\int_{-\infty}^{\infty} dx e^{-(b^2 x^2 + ax)} = \frac{\sqrt{\pi}}{b} e^{a^2/4b^2}$$

$$\rightarrow a_1 = -\frac{i}{\hbar} \mathcal{E} l \frac{\sqrt{\pi}}{\tau} (\sqrt{\pi} \tau) e^{-\omega^2 \tau^2/4}$$

$$\therefore P_1 = |a_1|^2 = \frac{\mathcal{E}^2}{\hbar^2} \frac{\hbar}{2m\omega} \pi \tau^2 e^{-\omega^2 \tau^2/2}.$$

$$= \frac{\pi \mathcal{E}^2 \tau^2}{2m\hbar\omega} e^{-\omega^2 \tau^2/2}$$



As $\omega\tau \rightarrow 0$ or $\omega\tau \rightarrow \infty$, the probability for the oscillator to be excited vanishes.

why?

small

$\tau\omega \rightarrow$ peaks very sharp. no time for interaction.

$\tau\omega$ large.

$\rightarrow$ adiabatic. system remains in eigenstate.

beta particle 3 body problem
energy may be different

12. kinetic energy of emitted electron.

$$T = 16 \times 10^3 \text{ eV} = 2.56 \times 10^{-15} \text{ J}$$

Speed ~~velocity~~ of electron

$$v = \sqrt{\frac{2T}{m}} = 7.5 \times 10^7 \text{ m/s} \sim 0.25c.$$

$\gamma \sim 1.03$ can be approximated to 1.

$\therefore$ time ~~we~~

At time around $t = 5 \times 10^{-17} \text{ s}$.

electron has escaped $r_e = 3.75 \times 10^{-9} \text{ m}$

$r_e \gg 5.29 \times 10^{-11} \text{ m} = a_0 = \text{the Bohr radius}$

$\therefore$ After time $t \sim 5 \times 10^{-17} \text{ s}$, the electron has escaped the atom

~~the time~~

the time-scale on which the wavefunction changes is the time ~~for~~ taken to respond to the changes of the system

~~$$\frac{1}{\tau} = \sum_n \frac{1}{\hbar} \langle E_n | V | E \rangle$$~~

~~$$\frac{1}{\tau} = \frac{1}{\hbar} \langle E_k | V | E_n \rangle$$~~

~~a change~~

this is given by $\Delta t \sim \frac{\hbar}{\Delta E}$

by the uncertainty principle of Energy-time.

the smallest ΔE for hydrogen ~~is~~ that is associated with the ground state is

$$\Delta E = E_{n=2} - E_{n=1} = -R\left(\frac{1}{2^2} - \frac{1}{1^2}\right) = \frac{3}{4}R$$

$$= \frac{3}{4} \times 13.6 \text{ eV} = 10.2 \text{ eV}$$

$$= 1.63 \times 10^{-18} \text{ J}$$

$$\therefore \Delta t = \frac{\hbar}{\Delta E} = \underline{6.44 \times 10^{-17} \text{ s}}$$

$\therefore \Delta t \lesssim \Delta t$ ^{even} ~~the~~ after the electron has escaped the atom the wavefunction of the system can hardly change ✓

→ the perturbation is sudden.

The ground state of H^3 is $|100\rangle_{\text{H}}$.

~~$|100\rangle_{\text{H}}$~~

After the decay, by sudden approximation, the state of the ~~system~~ electron remains unchanged, so it is still $|100\rangle_{\text{H}}$

We can then expand this state as a superposition of ~~hydrogen~~ ^{Helium} states:

$$|100\rangle_{\text{H}} = \sum_{n,l,m} |nlm\rangle_{\text{He}} C_{nlm}$$

The probability amplitude ~~of~~ for the electron to remain in the ground state of helium is

$$\langle 100_{\text{He}} | 100_{\text{H}} \rangle$$

$$\hat{H}_{\text{H}} = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad (Z=1)$$

$$\hat{H}_{\text{He}} = -\frac{\hbar^2}{2m} \nabla^2 - \frac{2e^2}{4\pi\epsilon_0 r} \quad (Z=2)$$

$$\rightarrow \langle 100_{\text{He}} | 100_{\text{H}} \rangle = \int_0^\infty r^2 dr U_{n=1}^{l=0}(r, Z=2) \times U_{n=1}^{l=0}(r, Z=1)$$

$$= \frac{2}{(a_0)^{3/2}} \times \frac{2}{(a_0/2)^{3/2}} \int_0^\infty dr r^2 e^{-r/a_0} e^{-2r/a_0}$$

$$= 2^{7/2} a_0^{-3} \int_0^\infty dr r^2 e^{-3r/a_0}$$

$$= 2^{7/2} a_0^{-3} \left(\frac{a_0}{3} \right)^3 \int_0^\infty \underbrace{u^2 e^{-u}}_{2!} du$$

$$\begin{aligned} u &= \frac{3}{a_0} r \\ du &= \frac{3}{a_0} dr \\ dr &= \frac{a_0}{3} du \\ r^2 &= \left(\frac{a_0}{3} \right)^2 u^2 \end{aligned}$$

$$= 2^{9/2} \left(\frac{1}{3} \right)^3$$

$$\therefore \text{Probability} = |\langle 100_{\text{He}} | 100_{\text{H}} \rangle|^2$$

$$= \frac{2^9}{3^6} = 2^3 \left(\frac{2}{3} \right)^6 \sim 0.7$$

1	2	3	4	5	6	7	8	9	10	11	12	13
100	100	100	100	90	100	100	100	100	100	90	100	

$$(1-5/10)^{10} \times N \times (5/10)^{10} = 100 \times (1-5/10)^{10} \times (5/10)^{10}$$

$$\begin{aligned} \frac{S}{N} &= N \\ \frac{S}{N} &= N \times \frac{S}{N} \\ \frac{S}{N} &= N \times \frac{S}{N} \end{aligned}$$

$$F.O \sim \left(\frac{1}{2}\right)^{10}$$

FQM ~~For~~ Tutorial

$$(1,2) \quad |b\rangle = \sum_{m \neq 0} \frac{\langle m | \delta V | 0 \rangle}{E_0 - E_m} |E_m\rangle$$

the crucial thing is that we assume $|b\rangle$ can be expressed as L.C. of $|E_m\rangle$.

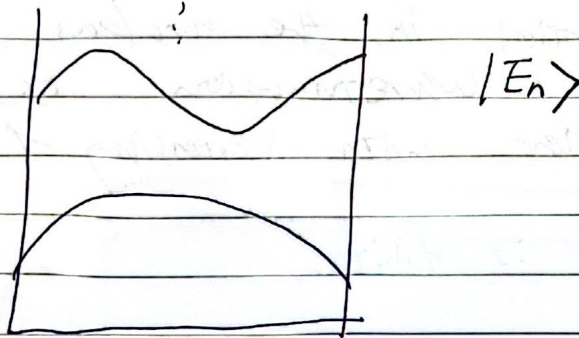
$$H_0 + \delta V, E_0: \{|E_{0,i}\rangle, i \in I\}$$

$$\hat{H}_0 |E_{0,i}\rangle = E_0 |E_{0,i}\rangle$$

$$SV_{ij} = \langle E_{0,j} | \delta V | E_{0,i} \rangle$$

$$|E_{0,i}'\rangle = \hat{U} |E_{0,i}\rangle$$

(4)



$$\hat{P} |E_n\rangle = (-1)^{n+1} |E_n\rangle$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$$

$[\hat{H}, \hat{P}] = 0 \rightarrow$ eigenfunctions of $\hat{H}$ can be chosen such that they have definite parity.

$$\therefore [\hat{H}, \hat{p}] = 0$$

$$\rightarrow E^{(1)} = \langle E_n | X | E_n \rangle$$

$$= \int_{-\infty}^{\infty} |\psi|^2 x dx$$

if ψ is even or odd

then $|\psi|^2$ is even

since x is odd

$$\text{the } E^{(1)} = 0$$

(5)

$$\Delta E^{l=1} ?$$

overlap between perturbation potential in the nucleus and the wavefunction is smaller with increasing l .

$|\psi|_{l=0}^2$ is finite

$|\psi|_{l \neq 0}^2$ is 0

Classically
orbit

higher L circular

lower L , elliptical orbit
sharp.

$$(5) \quad \hat{H}_0 \gg \delta \hat{V} \quad X.$$

$$\langle \psi_0 | \hat{H}_0 | \psi_0 \rangle \gg \langle \psi_0 | \delta \hat{V} | \psi_0 \rangle.$$

for the sake of your interest.

$$\frac{1}{r} e^{-r} \quad \text{at } r \rightarrow 0$$

$\rightarrow 0.$

To: Felix Tennie

Further Quantum I

Ziyan Li

13. For a single particle in a 3-D box:

The TISE gives $(-\frac{\hbar^2}{2m} \nabla^2 + V) \psi = E \psi$

$$\text{and } V = \begin{cases} 0 & -\frac{L}{2} < x, y, z < \frac{L}{2} \\ \infty & \text{otherwise} \end{cases}$$

$$\Rightarrow -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi = E \psi \quad \text{for } -\frac{L}{2} < x, y, z < \frac{L}{2}$$

Use separation of variables, try $\psi(x, y, z) = X(x) Y(y) Z(z)$

$$\Rightarrow -\frac{\hbar^2}{2m} \left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} \right) = E$$

$$\Rightarrow \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\frac{2mE}{\hbar^2} = -k^2 \quad (k = \sqrt{\frac{2mE}{\hbar^2}})$$

$\therefore \frac{X''}{X}$ is a function only of x , ~~and~~ similarly

~~let~~ $\frac{Y''}{Y}$ of only of y and $\frac{Z''}{Z}$ only of z .

$$\Rightarrow X'' + k_x^2 X = 0, \quad Y'' + k_y^2 Y = 0, \quad Z'' + k_z^2 Z = 0$$

$(k_x^2 + k_y^2 + k_z^2 = k^2)$

For periodic solutions we take k_x, k_y, k_z to be real.

$$X'' + k_x^2 X = 0 \rightarrow X(x) = C_x e^{ik_x x} + D_x e^{-ik_x x}$$

$$\text{Similarly } \rightarrow Y(y) = C_y e^{ik_y y} + D_y e^{-ik_y y}$$

$$Z(z) = C_z e^{ik_z z} + D_z e^{-ik_z z}$$

General Solution : Apply the principle of superposition.

$$\psi(x, y, z) = X Y Z = \sum_{k_x^2 + k_y^2 + k_z^2 = k^2} A_{k_x, k_y, k_z} e^{ik_x x} e^{ik_y y} e^{ik_z z}$$

Boundary conditions (periodic)

wavefunction
vanish at the edge
of the box.

$$\psi(-\frac{L}{2}, y, z) = \psi(\frac{L}{2}, y, z) = 0$$

$$\rightarrow 0 = \sum A_{k_x, k_y, k_z} e^{ik_x L/2} e^{ik_y y} e^{ik_z z}$$

$$= \sum A_{k_x, k_y, k_z} e^{-ik_x L/2} e^{ik_y y} e^{ik_z z}$$

$$\rightarrow \sum A_{k_x, k_y, k_z} (e^{ik_x L/2} - e^{-ik_x L/2}) e^{ik_y y} e^{ik_z z} = 0$$

this is true for any $-\frac{L}{2} < y, z < \frac{L}{2}$

$$\rightarrow e^{ik_x L/2} = e^{-ik_x L/2} \rightarrow e^{ik_x L} = 1$$

$$\rightarrow k_x L = 2\pi n_x \rightarrow k_x = \frac{2\pi}{L} n_x$$

Similarly $\rightarrow k_y = \frac{2\pi}{L} n_y$
 $k_z = \frac{2\pi}{L} n_z$

(n_x, n_y, n_z are integers, can be either +ve or -ve and satisfy $k^2 = k_x^2 + k_y^2 + k_z^2$)

The wave number vector $\vec{k}$ is

$$\vec{k} = \left(\frac{2\pi}{L} n_x, \frac{2\pi}{L} n_y, \frac{2\pi}{L} n_z \right) = (k_x, k_y, k_z)$$

∴ The volume ~~is~~ per ~~part~~ particle in $\vec{k}$ -space is

$$\Delta V = \left(\frac{2\pi}{L} \right)^3 \cdot \text{a volume element}$$

$$dV = \cancel{k^2 dk} k^2 \sin\theta dk d\theta d\phi = k^2 dk d^3\Omega$$

of particle with ~~momentum~~ $[k, k+dk]$ within $d^3\Omega$ is then given by

$$g(k) dk d^3\Omega = \frac{dV}{\Delta V} = \left(\frac{L}{2\pi} \right)^3 k^2 dk d^3\Omega$$

$$\therefore \text{Ezr } k = \sqrt{\frac{2mE}{\hbar^2}} \quad \therefore E = \frac{\hbar^2 k^2}{2m}$$

$$\therefore \cancel{dE} dk = \frac{\sqrt{m}}{2\hbar^2} dE \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\therefore g(E) dE d^3\Omega = \left(\frac{L}{2\pi} \right)^3 \frac{2mE}{\hbar^2} \frac{\sqrt{m}}{2\hbar^2} dE$$

$$= \boxed{\left(\frac{L}{2\pi} \right)^3 \frac{m^{3/2}}{\hbar^3} \sqrt{2E} dE d^3\Omega}$$

Form: Golden Rule

$$\sum_k P_k = \frac{2\pi t}{\hbar} g(E_{\text{out}}) |\langle \text{out} | V | \text{in} \rangle|^2$$

the transition rate is

$$\begin{aligned} \frac{d}{dt} (\sum_k P_k) &= \frac{2\pi}{\hbar} g(E_{\text{out}}) |\langle \text{out} | V | \text{in} \rangle|^2 \\ &= \frac{2\pi}{\hbar} \left(\frac{L}{2\pi}\right)^3 \frac{m^{3/2}}{\hbar^3} \sqrt{2E} |\langle \text{out} | V | \text{in} \rangle|^2 \end{aligned}$$

$$\langle \vec{x} | \text{out} \rangle = \frac{1}{L^{3/2}} e^{-i\vec{k}' \cdot \vec{x}}$$

$$\langle \vec{x} | \text{in} \rangle = \frac{1}{L^{3/2}} e^{i\vec{k} \cdot \vec{x}}$$

} needs $V(\vec{x})$ to be weak
so for the beam to remain
in its original state. ?

$$\begin{aligned} \langle \text{out} | V | \text{in} \rangle &= L^3 \int d^3\vec{x} e^{-i\vec{k}' \cdot \vec{x}} V(\vec{x}) e^{i\vec{k} \cdot \vec{x}} \\ &= \frac{1}{L^3} \int d^3\vec{x} e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} V(\vec{x}) \end{aligned}$$

Consider the ~~initial~~ ^{incident} wavefunction

$$\langle \vec{x} | \text{in} \rangle_t = \frac{1}{L^{3/2}} e^{i\vec{k} \cdot \vec{x} - \frac{E}{\hbar} t} = \psi$$

then probability flux :

$$\vec{j} = \frac{i\hbar}{2m} [\nabla \psi^* \psi - \psi^* \nabla \psi]$$

$$= \frac{i\hbar}{2mL^3} (-i\hbar - i\vec{k}' - 0 - i\hbar)$$

$$= \frac{\hbar \vec{k}}{mL^3}$$

$$\begin{aligned} |\vec{j}| &= \frac{\hbar k}{mL^3} = \frac{\hbar}{mL^3} \sqrt{\frac{2mE}{\hbar^2}} \\ &= \frac{m^{1/2}}{\hbar L^3} \sqrt{2E} \end{aligned}$$

For ~~elastic~~ elastic scattering $E' = E$

$$\rightarrow \text{the } \frac{d\sigma}{d^2\Omega} = \frac{\text{transition rate}}{|j|}$$

$$= \frac{\frac{2\pi}{\hbar} \frac{L^3}{(2\pi)^3} \frac{m^{3/2}}{\hbar^3} \sqrt{2/E'} \frac{1}{L^3} \left| \int d^3\vec{x} e^{i(\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) \right|^2}{\frac{m^{-1/2}}{L^3} \sqrt{2/E}}$$

$$\rightarrow \boxed{d\sigma = \frac{m^2}{(2\pi)^2 \hbar^4} d^2\Omega \left| \int d^3\vec{x} e^{i(\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) \right|^2} \quad \checkmark$$

The potential has to be weak because.
+ for weak potential we can assume that the eigenstates are only slightly modified by V .
So we can use the original eigenkets of the incident ~~to~~ beam (free ~~par~~ eigenkets of free particle Hamiltonian) ✓

Form 1

13.

$$g(E) dE d\Omega^2 = \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega$$

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

$$dk = \frac{2mE}{\hbar^2} \frac{1}{k} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$dk = \frac{m}{\hbar^2 k} dE \approx$$

$$\rightarrow \left(\frac{L}{2\pi}\right)^3 \frac{2mE}{\hbar^2} \frac{m}{\hbar^2} \sqrt{\frac{\hbar^2}{2mE}} dE d\Omega \dots \text{the result.}$$

~~Fermi's~~ Fermi's Golden rule

$$\dot{P} = \frac{2\pi}{\hbar} g(E) d^2\Omega \underbrace{|\langle 0|V|i\rangle|^2}$$

$$\frac{1}{L^3} \int d^3x e^{-i\mathbf{k}' \cdot \mathbf{x}} V(\mathbf{x}) e^{i\mathbf{k} \cdot \mathbf{x}}$$

$$d\sigma = \frac{P}{\text{incoming flux}} \Rightarrow \frac{\hbar k}{mL^3}$$

$$\psi_0 \longrightarrow$$

$$\psi_0 \longrightarrow$$

$$\begin{array}{c} \uparrow \\ 0 \longrightarrow \\ x \end{array}$$

$$\frac{1}{\sqrt{2}} (|+,x\rangle + |-,x\rangle)$$