PH3102 Midsem

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Q1 $V = \frac{-V_0}{\sigma\sqrt{\pi}} e^{-x^2/\sigma^2}$

Take ground state
$\psi = A e^{-\alpha x^2}$

$A = \left(\frac{2\alpha}{\pi}\right)^{1/2}$.

$\psi = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$

We'll use variational principle.

$\psi = \sum c_n \psi_n$

$\langle \psi | H | \psi \rangle = \sum |c_n|^2 E_n \geq E_0 \sum |c_n|^2$
$= E_g$

We vary parameter α till we get minimum

$\langle \psi | T | \psi \rangle = -\frac{\hbar^2}{m} \int \psi^* \frac{d^2\psi}{dx^2} \psi \, dx$

$\Rightarrow \langle T \rangle = \frac{3\hbar^2 \alpha}{4m}$

$\langle V \rangle = A^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(\frac{-V_0}{\sqrt{\pi}\sigma} e^{-x^2/\sigma^2} \right) e^{-\alpha x^2} dx$

$= \frac{-V_0}{\sigma} \left(\frac{2\alpha}{2\alpha + 1/\sigma^2} \right)^{1/2}$

$\langle H \rangle = \langle T \rangle + \langle V \rangle$

$\frac{d\langle H \rangle}{d\alpha} = 0 \Rightarrow$

~~$\frac{3\hbar^2}{}$~~

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Q2 Hamiltonian has real eigenvalues

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

$$\int (H\psi)^* \psi \, dx = \int \left(\left(\frac{p^2}{2m} + V(x) \right) \psi \right)^* \psi \, dx$$

$$= \frac{1}{2m} \int (p^2 \psi)^* \psi \, dx + \int dx \, (V(x)\psi)^* \psi$$

$$= \frac{1}{2m} \int \psi^* p^2 \psi \, dx + \int dx \, \psi^* V(x) \psi$$

$$= \frac{1}{2m} \int \psi^* H \psi \, dx$$

$\Rightarrow$ Hamiltonian is Hermition.

Now it's sufficient to prove the spectral theorem.

$$\hat{H}\psi = a\psi$$

$$\int (H\psi)^* \psi \, dx = \int (a\psi)^* \psi \, dx = a^* \int \psi^* \psi \, dx$$

and also $\int \psi^* H \psi \, dx = a \int \psi^* \psi \, dx$

$$\Rightarrow (a^* - a) \int \psi^* \psi \, dx = 0$$

as $\int \psi^* \psi \, dx \neq 0$

$$\Rightarrow a^* - a = 0 \Rightarrow a = a^*$$

$$\Rightarrow a \in R$$

$\Rightarrow$ ~~Ham~~ Hermition operators have real eigenvalues

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Q3 $$V(x) = \begin{cases} \infty & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > a \end{cases}$$

~~The energy levels cannot go beyond V_0 or they escape~~ For bound, $E < 0$

Schrodinger's equation.

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - V_0\psi(x) = E\psi(x) & 0 < x < a \\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) & a < x. \end{cases}$$

~~Let $k^2 = 2m$~~

$$\Rightarrow \begin{cases} \frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2m}{\hbar^2}(E+V_0)\psi(x) & 0 < x < a \\ \frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) & x > a \end{cases}$$

$$k^2 = \frac{2m}{\hbar^2}(E+V_0), \quad q^2 = -\frac{2mE}{\hbar^2} = \frac{2m|E|}{\hbar^2}$$

$$\Rightarrow \begin{cases} \frac{\partial^2}{\partial x^2}\psi = -k^2\psi \\ \frac{\partial^2}{\partial x^2}\psi = +q^2\psi \end{cases}$$

$$\Rightarrow \begin{cases} \psi = 0 \\ \psi = Ae^{ikx} + Be^{-ikx} \\ \psi = Ce^{qx} + De^{-qx} \end{cases}$$

Now Boundary conditions

$\psi(0) = 0$, $\psi(x \to \infty) = 0$, $\psi(a^-) = \psi(a^+)$

$\psi'(a^-) = \psi'(a^+)$

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to satisfy the bondary $\psi(0)=0$, $\psi(\to\infty)=0$

$$\psi = \begin{cases} 0 & x \le 0 \\ A\sin(\cancel{k}x) & x \in (0,a) \\ Be^{-qx} & x > a. \end{cases}$$

Now we match, bomdary.

$A\sin(ka) = Be^{-qa} \Rightarrow B = A\sin(ka)e^{qa}$.

$Ak\cos(ka) = -Bqe^{-qa} = -Aq\sin(ka)$

$$\Rightarrow \cot(ka) = -\frac{q}{k}.$$

$$\Rightarrow \psi = \begin{cases} 0 & x<0 \\ A\sin(kx) & 0<x<a \\ A\sin(ka).e^{q(a-x)} & x > a. \end{cases}$$

To find eigenvalue for bound states one must have just one bound state.

Now for a zero point energy state

$q \to 0$, $k \to \frac{\sqrt{2mV_0}}{\hbar}$

and $\cot(ka) = -\frac{q}{k} = 0$

(ii) $\Rightarrow \cot\left(\left(\frac{\sqrt{2mV_0}}{\hbar}\right)a\right) = 0$

$\Rightarrow \sqrt{2mV_0}\,\frac{a}{\hbar} = \frac{\pi}{2}$ for exactly one energy eigenvalue.

$\Rightarrow a^2V_0 > \frac{\pi^2\hbar^2}{8m}$ for just one bound state energy to exist for large V_0.

$k \rightarrow \infty$

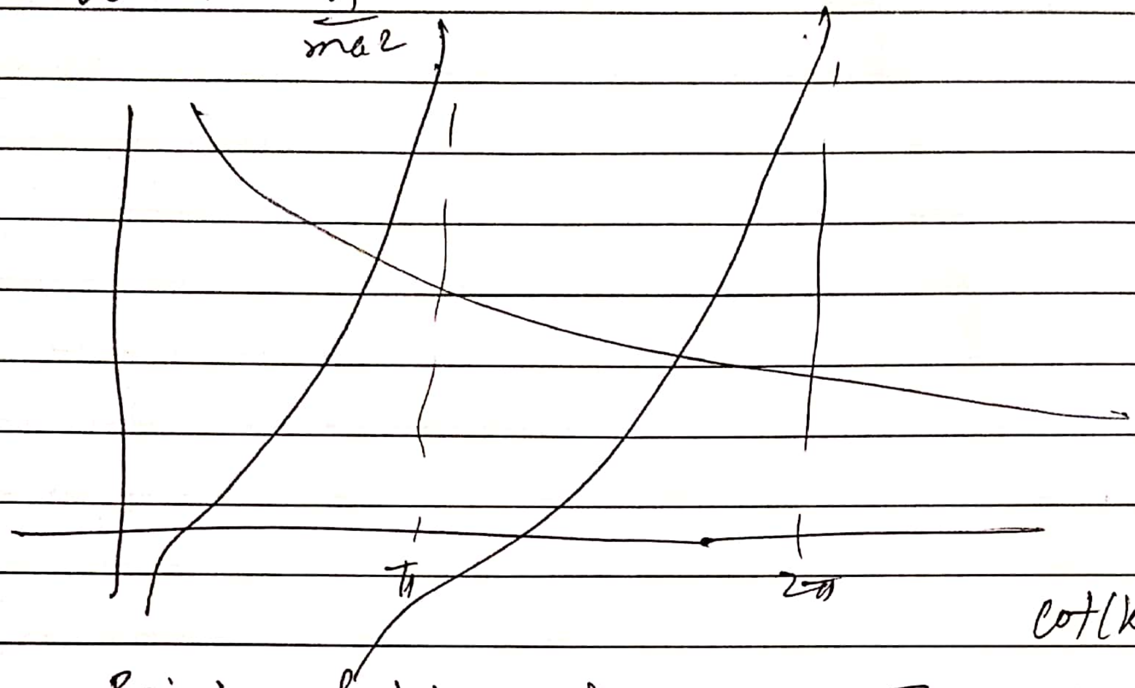
$\cot(ka) = -q/k \simeq 0$

$$\cot\left(\frac{\sqrt{2m(E+V_0)}}{\hbar} a\right) = \left(n+\frac{1}{2}\right)\pi$$

$$\Rightarrow \quad E+V_0 = \left(n+\frac{1}{2}\right)^2 \frac{\pi^2\hbar^2}{2a^2 m}$$

$$E+V_0 \longrightarrow \frac{n^2\pi^2\hbar^2}{(2a)^2 2m}$$

(iii) for $V_0 \gg \frac{\hbar^2}{ma^2}$



$\cot(ka) = -\frac{q}{k}$

Point of intersection. $z_n = n\pi$

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

energy eigen $E_n + V_0 = \frac{n^2\pi^2\hbar^2}{(2a)^2(2m)}$