2011 Modern - 7 (QM)

7. Let H be a quantum mechanical Hamiltonian with eigenfunctions $|\phi_i\rangle$ and corresponding eigenvalues E_i with $i = 0, 1, 2, \cdots \infty$. Further assume that

$$E_0 < E_1 < E_2 < \cdots < E_\infty. \tag{3}$$

(a) Let $|\psi\rangle$ be a normalized wavefunction (not necessarily an eigenfunction of H). Prove that

$$\langle\psi|H|\psi\rangle \geq E_0. \tag{4}$$

Hint: Expand $|\psi\rangle$ in the eigenbasis of H.

(b) Prove that every attractive potential in one dimension, i.e., $V(x) < 0$ for all x, has at least one bound state. Hint: Consider the normalized wave function,

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha x^2}; \quad \alpha > 0 \tag{5}$$

and calculate,

$$E(\alpha) = \langle\psi_\alpha|H|\psi_\alpha\rangle; \quad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{6}$$

Show that $E(\alpha)$ can be made negative by a suitable choice of α.

a) $$|\psi\rangle = \sum_{n=0}^{\infty} c_n |\phi_n\rangle$$

$$\langle\psi|H|\psi\rangle = \left(\sum_{m=0}^{\infty} c_m^* \langle\phi_m|\right) H \left(\sum_{n=0}^{\infty} c_n|\phi_n\rangle\right)$$

$$= \left(\sum_{m=0}^{\infty} c_m^* \langle\phi_m|\right)\left(\sum_{n=0}^{\infty} c_n H|\phi_n\rangle\right)$$

$$= \left(\sum_{m=0}^{\infty} c_m^* \langle\phi_m|\right)\left(\sum_{n=0}^{\infty} c_n E_n |\phi_n\rangle\right)$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} c_m^* c_n E_n \langle\phi_m|\phi_n\rangle$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c_m^* c_n E_n \delta_{mn}$$

$$\langle \psi | H | \psi \rangle = \sum_{m=0}^{\infty} |c_m|^2 \underbrace{E_m}_{\substack{\hbar\omega \\ \geq E_0}}$$

$$\langle \psi | H | \psi \rangle \geq \sum_{m=0}^{\infty} |c_m|^2 E_0 = E_0 \sum_{m=0}^{\infty} |c_m|^2$$

Now, since $|\psi\rangle$ is normalized then,

$$\langle \psi | \psi \rangle = \sum_{m=0}^{\infty} |c_m|^2 = 1$$

Therefore, $\boxed{\langle \psi | H | \psi \rangle \geq E_0}$

b) $E(\alpha) = \langle \psi_\alpha | H | \psi_\alpha \rangle$

$$= \langle \psi_\alpha | \frac{\hat{p}^2}{2m} + U(x) | \psi_\alpha \rangle$$

$$= \langle \psi_\alpha | \frac{\hat{p}^2}{2m} | \psi_\alpha \rangle + \langle \psi_\alpha | V(x) | \psi_\alpha \rangle$$

$$E(\alpha) = \frac{1}{2m} \langle \psi_\alpha | \hat{p}^2 | \psi_\alpha \rangle + \langle \psi_\alpha | V(x) | \psi_\alpha \rangle$$

(1)

Since $\hat{p}$ is Hermitian

$$\langle \psi_\alpha | \hat{p}^2 | \psi_\alpha \rangle = \langle \psi_\alpha | \hat{p}^\dagger \hat{p} | \psi_\alpha \rangle$$

$$= \left(\langle \psi_\alpha | \hat{p}^\dagger \right) \left(\hat{p} | \psi_\alpha \rangle \right)$$

$$= \| \hat{p} \psi_\alpha \|^2$$

$$= \int_{-\infty}^{\infty} dx \, | \hat{p} \psi_\alpha(x) |^2$$

$$= \int_{-\infty}^{\infty} dx \, \left| -i\hbar \frac{d}{dx} \psi_\alpha(x) \right|^2$$

$$= \hbar^2 \int_{-\infty}^{\infty} dx \, \left| \left(\frac{\alpha}{\pi} \right)^{1/4} \frac{d}{dx} e^{-\frac{1}{2}\alpha x^2} \right|^2$$

$$= \hbar^2 \left(\frac{\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx \, \left| -\frac{1}{\cancel{2}} \alpha (\cancel{2}x) \, e^{-\frac{1}{2}\alpha x^2} \right|^2$$

$$= \hbar^2 \left(\frac{\alpha}{\pi}\right)^{1/2} \alpha^2 \int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2}$$

Note: $$\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

Take $\frac{d}{d\alpha}$ of both sides,

$$\int_{-\infty}^{\infty} dx\, (-x^2)\, e^{-\alpha x^2} = -\frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

$$\int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

Therefore,

$$\|\hat{p}\psi_\alpha\|^2 = \hbar^2 \left(\frac{\alpha}{\cancel{\pi}}\right)^{1/2} \alpha^2\, \frac{1}{2}\sqrt{\frac{\cancel{\pi}}{\alpha^3}}$$

$$= \frac{\hbar^2}{2}\, \alpha^{2+1/2-3/2}$$

$$\|\hat{p}\psi_\alpha\|^2 = \frac{\hbar^2 \alpha}{2} \qquad (2)$$

Inserting Eq. (2) into (1),

$$E(\alpha) = \frac{\hbar^2}{4m}\alpha + \langle\psi_\alpha|V(x)|\psi_\alpha\rangle \quad (3)$$

Since $V(x) < 0 \ \forall x \in \mathbb{R}$, then:

$$\langle\psi_\alpha|V(x)|\psi_\alpha\rangle = \int_{-\infty}^{\infty} dx\, |\psi_\alpha(x)|^2 V(x) < 0$$

Thus, if we take:

$$\alpha < \frac{4m|\langle\psi_\alpha|V(x)|\psi_\alpha\rangle|}{\hbar^2}$$

$$\Rightarrow E(\alpha) = \langle\psi_\alpha|H|\psi_\alpha\rangle < 0$$

and we have a bound state.