Quantum Mechanics I_ 2nd Exam: Solutions (2008 fall)

1. For a particle moving under a one-dimensional potential V(x), show that any two bounded states ψ_1 and ψ_2 are orthogonal, based on the time-independent Schrödinger equation.

Solutions:

If ψ_1 and ψ_2 are two bound states with energy E_1 and E_2, respectively, then

$$\psi_1'' = \frac{2m}{\hbar}[V(x) - E_1]\psi_1$$

$$\psi_2^{*}'' = \frac{2m}{\hbar}[V(x) - E_1]\psi_2^{*}$$

and $\psi_2^{*}\psi_1'' - \psi_1\psi_2^{*}'' = \frac{d}{dx}(\psi_2^{*}\psi_1' - \psi_1\psi_2^{*}') = \frac{2m}{\hbar}[E_2 - E_1]\psi_2^{*}\psi_1$

such that

$$\int \frac{2m}{\hbar}(E_2 - E_1)\psi_2^{*}\psi_1 dx = \frac{2m}{\hbar}(E_2 - E_1)\int \psi_2^{*}\psi_1 dx$$

$$= \int \frac{d}{dx}(\psi_2^{*}\psi_1' - \psi_1\psi_2^{*}')dx = (\psi_2^{*}\psi_1' - \psi_1\psi_2^{*}')\Big|_{-\infty}^{\infty} = 0$$

2. An electron is moving freely inside a one-dimensional infinite potential well with wall at x = 0 and x = a. If the electron is initially in the ground state (n = 1) of the well [with energy $E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}$ and $\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$] and if we suddenly quadruple the size of the well (from *a* to 4*a*), Calculate the probability of finding the electron in:

(a) the ground state of the new well.

(b) the first excited state of the new well

Solution:

Initially, the electron is in the ground state of the box x = 0 and x = a; its energy and wave function are

$$E_1 = -\frac{\pi^2\hbar^2}{2ma^2} \text{ and } \phi_1(x) = \sqrt{\frac{2}{a}}\sin(\frac{\pi x}{a})$$

(a) Once in the new box, x = 0 and x = 4a, the ground state and wave function of the electron are

$$E_1^{'} = -\frac{\pi^2\hbar^2}{2m(4a)^2} \text{ and } \psi_1(x) = \sqrt{\frac{1}{2a}}\sin(\frac{\pi x}{4a})$$

The probability of finding the electron in ψ_1(x) in the original state $\phi_1(x)$ is

$$P(E_1^{'}) = \left|\langle\psi_1|\phi_1\rangle\right|^2 = \left|\int_0^a \psi_1^{*}(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin(\frac{\pi x}{4a})\sin(\frac{\pi x}{a})dx\right|^2$$

$$= \frac{1}{a^2}\left|\frac{1}{2}\int_0^a [\cos(\frac{3\pi x}{4a}) - \cos(\frac{5\pi x}{4a})]dx\right|^2 = \frac{128}{15^2\pi^2} = 0.058 = 5.8\%$$

(b) If the electron is in the first excited state of the new box, its energy and wave function are

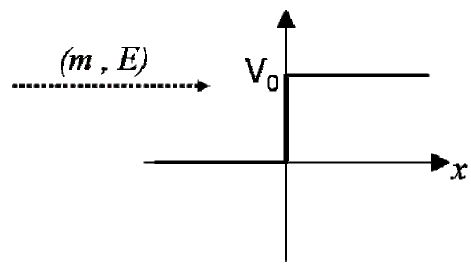
$$E_2^{'} = -\frac{\pi^2\hbar^2}{8ma)^2} \text{ and } \psi_2(x) = \sqrt{\frac{1}{2a}}\sin(\frac{\pi x}{2a})$$

The corresponding probability is

$$P(E_2^{'}) = \left|\langle \psi_2 | \phi_1 \rangle\right|^2 = \left|\int_0^a \psi_2^*(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin(\frac{\pi x}{2a})\sin(\frac{\pi x}{a})dx\right|^2$$

$$= \frac{16}{9\pi^2} = 0.18 = 18\%$$

3. A particle, with a mass *m* and an energy *E*, moves from left to right across a one-dimensional potential step shown in the figure. Find (a) The probability distribution in the classically forbidden region ($x > 0$) $P(x, t)$. Does it changes with time? Why? (b) The reflection and transmission coefficient.



Solution:

(a) For x < 0, $\frac{d^2}{dx^2}\psi + \frac{2mE}{\hbar^2}\psi = 0$ such that $\psi(x) = e^{ikx} + re^{-ikx}$

where *r* is a constant and $k = \sqrt{\frac{2mE}{\hbar^2}}$.

For x > 0 $\frac{d^2}{dx^2}\psi + \frac{2m(E - V_0)}{\hbar^2}\psi = 0$

If $E < V_0$, we have

$$\frac{d^2}{dx^2}\psi - \frac{2m(V_0 - E)}{\hbar^2}\psi = 0 .$$

And the physical solution is $\psi(x) = Ae^{-k^{'}x}$ where *A* is constant and $k^{'} = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$.

The probability for $x > 0$ is given by $P(x) = |\psi(x)|^2$ such that

$$P(x) = |\psi(x)|^2 = |A|^2 \exp(-2k' x)$$

A is determined through the normalization of the incident wave. Obviously it does not change with time since this is a stationary case!

(b) This is a trivial question. Since $\psi(x) = Ae^{-k'x} \to 0$ as $x \to \infty$, the transmission coefficient will be zero and reflection coefficient will be 1.

4. (optional) Solve the time-independent Schrödinger equation for a centered infinite square well with a delta-function barrier in the middle:

$$V(x) = \begin{cases} V_0\,\delta(x) & |x| < a \\ \infty & |x| \geq a \end{cases}$$

Treat the odd and even function separately. Don't bother to normalize them. Find the allowed energies (graphically, if necessary). Explain why the odd solutions are not affected by the delta function barrier. Discuss on the limiting cases $V_0 \to 0$ and $V_0 \to \infty$.

Solution:

Since $V(x) \to \infty$ when $\psi \to 0$, the boundary condition is given by

$$\psi(x) = 0 \; for \, |x| \geq a$$

In the potential well ($|x| \leq a$), we have

$$\psi'' + \frac{2m}{\hbar^2}[E - V_0\delta(x)]\psi = 0 \quad \text{--------(1)}$$

and the "jump" condition of the derivative of the wave function at $x = 0$ is give as

$$\psi'(0^+) - \psi'(0^-) = \frac{2mV_0}{\hbar^2}\psi(0) \quad \text{-----(2)}$$

though the wave function should be continuous at $x = 0$. Since $V(x)$ is an even function so every eigenstate should be a certain value of parity. Assume that

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

For $x \neq 0$, Eq. (2) becomes

$\psi'' + k^2\psi = 0$ for ($-a < x < 0, 0 < x < a$) ------ (3)

and a special solution is give by

$\psi = \sin kx$ or $\psi = \cos kx$

1) For the odd states: $\psi(-x) = -\psi(x)$ and $\psi(0) = 0$ such that the condition in Eg (2) is satisfied automatically and the energy levels and wave functions are the same as these in the symmetric infinite well without δ-potential barrier. Therefore we have

$$E = E_n = \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2 \quad \text{where n = 1, 2, 3…}$$

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\frac{n\pi x}{a} \quad \text{--------(4)}$$

2) for the even states: $\psi(-x) = \psi(x)$ we have solution for Eq (3) as

$\psi(x) = A\cos kx + B\sin kx$ for 0 < x < a

$\psi(x) = A\cos kx - B\sin kx$ for -a < x < 0

The boundary condition and the "jump" condition gives

$$A\cos ka + B\sin ka = 0 \quad \text{-----------(5)}$$

$$Bk = mV_0 A/\hbar^2 \text{ or } \frac{A}{B} = \frac{\hbar^2 k}{mV_0}$$

By putting this ratio into eq (5) we obtain

$$\tan ka = -\frac{\hbar^2}{mV_0}k = -\frac{b}{a}ka \quad \text{-------(6)}$$

where $b \equiv \frac{\hbar^2}{mV_0}$ is the characteristic length of δ-potential barrier. Using graphic method one can find the solution for k so as the energy levels.

DISCUSSION:

a) When $V_0 \gg \frac{n\pi\hbar^2}{ma}$ or $V_0 \to \infty$, Eq.(6) becomes approximately

$\tan ka \approx 0$ or $ka \approx n\pi$ with n = 1, 2, 3 ….

Such that $E \approx \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2$

with n = 1, 2, 3 …. This looks like that the δ-potential barrier is un-penetrated thin wall and the well is divided in two symmetric well.

b) When $V_0 \ll \frac{n\pi\hbar^2}{ma}$ or $V_0 \to 0$, Eq. (6) becomes approximately

$\cot ka \approx 0$ or $ka \approx (n+\frac{1}{2})\pi$ with n = 0, 1, 2, …

So that the energy levels are given by

$$E \approx \frac{1}{2m}\left(\frac{(2n+1)\pi\hbar}{2a}\right)^2$$

This is like that the δ-potential barrier disappears so the energy levels is these in the even states of an infinitive potential well.

5. (Optional) in the momentum space, (a) what is the time-independent Schrödinger equation for a one dimensional harmonic oscillator? (b) Find the energy levels and wave functions in momentum space (You do not need to solve the equation but simply comparing with them in the real space).

Solution:

In the representation in momentum space we have

$$\hat{p} = p \quad \text{and} \quad \hat{x} = i\hbar\frac{\partial}{\partial p}$$

such the one-dimensional time-independent Schrödinger equation is expressed as

$$[\frac{p^2}{2m} + V\left(i\hbar\frac{\partial}{\partial p}\right)]\varphi(p) = E\varphi(p)$$

For a one-dimensional harmonic oscillator, we have

$$[\frac{p^2}{2m} - \frac{m\omega^2\hbar^2}{2}\frac{d^2}{dp^2}]\varphi(p) = E\varphi(p)$$

Define $\xi \equiv \frac{p}{\sqrt{m\omega\hbar}}$ and $K \equiv \frac{2E}{\omega\hbar}$, then we have

$$\frac{d^2\varphi}{d^2\xi} = (\xi^2 - K)\varphi$$

This is in the exactly the same format as the simplified Schrödinger equation (see Eq. 2.72 in the textbook) in the configuration space. Therefore the energy levels should be exactly the same as in the representation in real space, that is

$E = E_n = (n + \frac{1}{2})\hbar\omega$ with n = 0, 1, 2, ….

And the wave function is given as

$$\varphi_n(p) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{p}{\sqrt{m\omega\hbar}}\right)e^{-\xi^2/2}$$