PHYS 4073 - Quantum Mechanics- Test 1 - Fall 2010

All problems are worth 25 points. Turn in solutions to four of the six problems to be graded. If you turn in more than four solutions, I will grade the first four. You are allowed to drop one-half of a test, so I will take the first two problems turned in as the first half-test and the second two problems turned in as the second half-test.

1 A particle is in the initial state $\psi(x,0) = A\exp(-ax)$ for $x > 0$ and $\psi = 0$ for $x < 0$. Compute the probability of finding the particle in the region $0 < x < 1/a$.

2 The initial state of a particle of mass m in an infinite square well is $\psi(x,0) = \frac{1}{\sqrt{2}}\phi_1(x) - \frac{1}{\sqrt{2}}\phi_2(x)$ where $\phi_n = \sqrt{\frac{2}{a}}\sin(n\pi x/a)$. Note, this initial state is already normalized. Compute the wave function as a function of time, $\psi(x,t)$. Compute the expectation value of x, $< x >$, as a function of time.

3 The initial state of a particle in an infinite square well that extends from 0 to a is $\psi(x,0) = A\sin(\pi x/a)$ for $0 < x < a/2$ and zero otherwise. Compute the probability of finding the particle in the ground state and the probability of finding the particle in the first excited state.

4 The wavefunction of a particle of mass m is $\psi(x,0) = A\sin(\pi x/b)$ for $0 < x < b$ and zero otherwise. Check the uncertainty relation for this state.

5 A particle is directed at a finite step potential where

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } 0 < x \end{cases}$$

Calculate the reflection coefficient from the time independent Schrodinger equation showing all steps for the $E > V_0$ case.

6 Model the hydrogen atom as a finite one-dimensional well of width $a = 1 \times 10^{-10}$m, two Bohr radii. The ground-state energy of hydrogen is $E_0 = 13.6$eV with 1eV $= 1.602 \times 10^{-19}$J. Using the Bohr model, this means the potential energy of hydrogen, $V = -V_0 = -27.2$eV. Compute the lowest energy bound state for the electron in this well. How many total bound states does the well have? Note you will not need E_0, that was just me thinking aloud.

① $\psi(x) = Ae^{-ax} \qquad x > 0$

<u>Normalize</u>

$$1 = \int_0^\infty \psi^* \psi \, dx = A^2 \int_0^\infty e^{-2ax} \, dx$$

$$= \frac{A^2}{-2a} e^{-2ax} \Big|_0^\infty = \frac{A^2}{2a}$$

$A = \sqrt{2a}$

<u>Compute $P(x \in [0, a])$</u>

$$P = \int_0^a \psi^* \psi \, dx = 2a \int_0^a e^{-2ax} \, dx$$

$$= \frac{2a}{-2a} e^{-2ax} \Big|_0^{1/a} = -e^{-2} + 1$$

$$= 1 - \frac{1}{e^2} = 0.86$$

(2) The energies of the infinite square well are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m} \frac{n^2\pi^2}{a^2} = n^2 E_1$$

$$E_1 = \frac{\hbar^2 \pi^2}{2ma^2} \qquad E_2 = 4E_1$$

The time dependent wave function is found by adding the appropriate phase factors to the expansion of the wave function in terms of the stationary states.

$$\psi(x,t) = c_1 \phi_1 e^{-i\frac{E_1 t}{\hbar}} + c_2 \phi_2 e^{-iE_2 t/\hbar}$$

Let $\omega = E_1/\hbar$

$$\psi(x,t) = \frac{1}{\sqrt{2}} \phi_1 e^{-i\omega t} - \frac{1}{\sqrt{2}} \phi_2 e^{-4i\omega t}$$

$$\rho(x,t) = \psi^*\psi = \left(\tfrac{1}{\sqrt{2}}\phi_1 e^{i\omega t} - \tfrac{1}{\sqrt{2}}\phi_2 e^{+4i\omega t}\right) \times$$

$$\left(\tfrac{1}{\sqrt{2}}\phi_1 e^{-i\omega t} - \tfrac{1}{\sqrt{2}}\phi_2 e^{-4i\omega t}\right)$$

$$= \frac{1}{2}\phi_1^2 + \frac{1}{2}\phi_2^2 - \frac{1}{2}\phi_1\phi_2\left(e^{-3i\omega t} + e^{3i\omega t}\right)$$

$$= \frac{1}{2}\phi_1^2 + \frac{1}{2}\phi_2^2 - \phi_1\phi_2 \cos 3\omega t$$

<u>Expectation Value</u>

$$\langle x \rangle = \int \rho(x,t)\, x \, dx$$

$$= \frac{1}{2}\int_0^a x\phi_1^2\, dx + \frac{1}{2}\int_0^a x\phi_2^2\, dx$$

$$- \cos 3\omega t \int_0^a \phi_1\phi_2\, x \, dx$$

The first two integrals yield $a/2$ as before

The last integral is

$$\int_0^a x\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\,dx = \frac{-16a}{9\pi^2}$$

says Alpha.

$$\langle x\rangle = \frac{1}{2}\frac{a}{2} + \frac{1}{2}\frac{a}{2} - \cos 3\omega t\left(\frac{-16a}{9\pi^2}\right)$$

$$= \frac{a}{2} + \frac{16a}{9\pi^2}\cos 3\omega t$$

$$= \frac{a}{2}\left(1 + \frac{32}{9\pi^2}\cos 3\omega t\right)$$

$$= \frac{a}{2}\left(1 + 0.36\cos 3\omega t\right) \rightarrow$$ Particle stays in well.

WolframAlpha

integrate x sin(Pi x/a) sin(2 Pi x/a) (2/a) from x=0 to a

Definite integral:

$$\int_0^a \frac{2\,x \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right)}{a}\,dx = -\frac{16\,a}{9\,\pi^2}$$

(3) $\psi(x,0) = A \sin \frac{\pi x}{a} \qquad x < a/2$

<u>Normalize</u>

$$1 = \int \psi^* \psi \, dx = A^2 \int_0^{a/2} \sin^2 \frac{\pi x}{a} \, dx$$

$$= A^2 \left[\frac{a}{4} \right]$$

$$A = \frac{2}{\sqrt{a}}$$

<u>Probability In Ground State</u>

$$P(E_1) = c_1^* c_1 \qquad \phi_1 = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$$

$$c_1 = \int_{-\infty}^{\infty} \phi_1^* \psi(x,0)$$

$$= \int_0^{a/2} \left(\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \right) \left(\frac{2}{\sqrt{a}} \sin \frac{\pi x}{a} \right)$$

$$= \frac{2\sqrt{2}}{a} \int_0^{a/2} \sin^2 \left(\frac{\pi x}{a} \right) dx = \frac{2\sqrt{2}}{a} \cdot \frac{a}{4}$$

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

$$P(E_1) = c_1^* c_1 = \frac{1}{2}$$

Probability in First Excited State

$$c_2 \cancel{P(E_2)} = \int \phi_2^* \psi(x,0)\,dx$$

$$= \int_0^{a/2} \sqrt{\frac{2}{a}} \sin\frac{2\pi x}{a} \sin\frac{\pi x}{a} \cdot \frac{2}{\sqrt{a}}\,dx$$

$$= \frac{2\sqrt{2}}{a} \int_0^{a/2} \sin\frac{2\pi x}{a} \sin\frac{\pi x}{a}\,dx$$

$$= \frac{2\sqrt{2}}{a}\left(\frac{2a}{3\pi}\right)$$

$$c_2 = \frac{4}{3}\frac{\sqrt{2}}{\pi} = 0.6$$

$$P(E_2) = c_2^* c_2 = 0.36$$

WolframAlpha computational knowledge engine

integrate sin(Pi x/a)^2 from x=0 to a/2

Definite integral:

$$\int_0^{\frac{a}{2}} \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{a}{4}$$

WolframAlpha computational knowledge engine

integrate sin(Pi x/a) sin(2 Pi x/a) from x=0 to a/2

Definite integral:

$$\int_0^{\frac{a}{2}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2 \pi x}{a}\right) dx = \frac{2 a}{3 \pi}$$

(4) By comparison with infinite square well the normalized wave function is

$$\psi(x) = \sqrt{\frac{2}{b}} \sin\left(\frac{\pi x}{b}\right)$$

$$\langle x \rangle = \int x \psi^* \psi \, dx = \frac{b}{2}$$ center of well.

$$\langle x^2 \rangle = \int x^2 \psi^* \psi \, dx = \frac{2}{b} \int_0^b x^2 \sin^2\left(\frac{\pi x}{b}\right) dx$$

$$= \frac{1}{12}\left(2 - \frac{3}{\pi^2}\right) b^3 \cdot \frac{2}{b} = \frac{1}{6}\left(2 - \frac{3}{\pi^2}\right) b^2$$

$$\langle p \rangle = \int \psi^* \frac{\hbar}{i} \frac{d}{dx} \psi \, dx = \frac{\hbar}{i} \frac{2}{b} \frac{\pi}{b} \int_0^a \sin\left(\frac{\pi x}{b}\right) \cos \frac{\pi x}{b} dx$$

$$= 0$$

$$\langle p^2 \rangle = \int \psi^* \frac{\hbar^2}{i^2} \frac{d^2}{dx^2} \psi \, dx = + \frac{2\hbar^2}{b} \frac{\pi^2}{b^2} \underbrace{\int_0^a \sin^2 \frac{\pi x}{b} dx}_{\frac{b}{2}}$$

$$= \frac{2\hbar^2}{b} \cdot \frac{\pi^2}{b^2} \cdot \frac{b}{2} = \frac{\hbar^2 \pi^2}{b^2}$$

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

$$= \sqrt{\frac{1}{6}\left(2 - \frac{3}{\pi^2}\right)b^2 - \frac{b^2}{4}}$$

$$= b\sqrt{\frac{1}{3} - \frac{1}{4} - \frac{3}{6\pi^2}} \qquad = b\sqrt{\frac{1}{12} - \frac{3}{6\pi^2}}$$

$$= b\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}}$$

$$\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{\hbar\pi}{b}$$

$$\sigma_p\sigma_x = \hbar\pi\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} = 0.57\hbar > \frac{1}{2}\hbar$$

5 From my lecture notes.

Consider $E_2 > V$

Solutions to TISE, with particle incident from left

$$\phi(x) = \begin{cases} \underbrace{A_I e^{ik_1 x}}_{\text{incident}} + \underbrace{A_{II} e^{-ik_1 x}}_{\text{reflected}} & x<0 \\ \underbrace{B_I e^{ik_2 x}}_{\text{transmitted}} & x>0 \end{cases}$$

* No negatively traveling wave if incident wave is from left.

For $x<0$, $k_1 = \sqrt{\frac{2m(E-V)}{\hbar^2}} = \sqrt{\frac{2mE}{\hbar^2}}$

For $x>0$, $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

Now solve for R, T. Note, since particles are conserved at the boundary

$$1 = R + T$$

so we can solve for R, then trivally compute T.

Impose Boundary Conditions

ϕ Continuous at $x=0$

$$A_I + A_{II} = B_I \qquad (1)$$

Derivative ϕ continuous at $x=0$

$$ik_1 A_I - ik_1 A_{II} = ik_2 B_I \qquad (2)$$

Solve for A_{II}/A_I - Substitute (1) into (2)

$$k_1 A_I - k_1 A_{II} = k_2 (A_I + A_{II})$$

$$(k_1 - k_2) A_{I} = (k_1 + k_2) A_{II}$$

$$\frac{A_{II}}{A_{I}} = \frac{k_1 - k_2}{k_1 + k_2}$$

Reflection Coefficient

$$R = \frac{A_{II}^{*} A_{II}}{A_{I}^{*} A_{I}} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^{*} \left(\frac{k_1 - k_2}{k_1 + k_2}\right) = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^{2}$$

Transmission Coefficient

$$T = 1 - R = 1 - \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^{2}$$

$$= \frac{k_1^2 + 2k_1 k_2 + k_2^2 - (k_1^2 - 2k_1 k_2 + k_2^2)}{(k_1 + k_2)^2}$$

$$= \frac{4 k_1 k_2}{(k_1 + k_2)^2}$$

(6) Finite Square Well

$$z_0^2 = \frac{2 m V_0 a^2}{\hbar^2} = \frac{2(9.11\times10^{-31}\,kg)(4.35\times10^{-18}\,J)(10^{-10}\,m)^2}{(1.05\times10^{-34}\,J\cdot s)^2}$$

$$= 7.18$$

$$V_0 = 27.2\,eV = 4.35\times10^{-18}\,J$$

$$z_0 = 2.68 \qquad \frac{\pi}{2} < z_0 < \pi$$

$\Rightarrow$ One even and one odd bound state

Solve

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

$$\Rightarrow \quad z = 1.13$$

$$z^2 = \frac{2m(E+V_0)}{\hbar^2} a^2$$

$$E = \frac{\hbar^2 z^2}{2ma^2} - V_0 = -3.56\times10^{-18}\,J$$

$$= -22\,eV$$

WolframAlpha computational knowledge engine

solve tan(z)=sqrt((2.68/z)^2-1) for z

Input interpretation:

solve $\tan(z) = \sqrt{\left(\frac{2.68}{z}\right)^2 - 1}$ for z

Result:

$z \approx 1.13392528880346\ldots$