Homework 3, Quantum Mechanics 501, Rutgers

October 18, 2016

1) The normalized wave function $\psi(x,t)$ satisfies the time-dependent Schroedinger equation for a free particle of mass m moving in 1D. Consider a second wave function of the form $\phi(x,t) = exp(i(ax - bt))\psi(x - vt, t)$.

   – Show that $\phi(x,t)$ obeys the same time-dependent Schroedinger equation as $\psi(x,t)$ when constants a and b are choosen appropriately. What should the values of a and b be (express them in terms of v)?

     Answ.: We need to show that

$$i\hbar\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2}$$

     and we know that

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

     We first compute derivatives of ϕ using its given form:

$$\frac{d\phi}{dt} = -ib\phi - ve^{i(ax-bt)}\frac{\partial}{\partial x}\psi(x-vt,t) + e^{i(ax-bt)}\frac{\partial}{\partial t}\psi(x-vt,t) \quad (1)$$

$$\frac{\partial^2\phi}{\partial x^2} = -a^2\phi + 2iae^{i(ax-bt)}\frac{\partial}{\partial x}\psi(x-vt,t) + e^{i(ax-bt)}\frac{\partial^2}{\partial x^2}\psi(x-vt,t) \quad (2)$$

     When we plug these derivatives into the Schroedinger equation for ϕ and take into account that ψ satisfies the same equation, we get

$$i\hbar\left[-ib\phi - ve^{i(ax-bt)}\frac{\partial}{\partial x}\psi(x-vt,t)\right] = -\frac{\hbar^2}{2m}\left[-a^2\phi + 2iae^{i(ax-bt)}\frac{\partial}{\partial x}\psi(x-vt,t)\right] \quad (3)$$

     This is satisfies when the first (second) term on the rhs is equal to the first (second) term on the lhs, which gives

$$\hbar b = \hbar^2 a^2/(2m) \quad (4)$$

$$i\hbar v = ia\hbar^2/m \quad (5)$$

     and hence we need to require

$$a = \frac{mv}{\hbar}$$

$$b = \frac{mv^2}{2\hbar} \quad (6)$$

– Calculate the expectation value of position $\langle X \rangle$, momentum $\langle P \rangle$, and energy $\langle H \rangle$ for particle in the state $\phi(x,t)$ in terms of those for particle in the state $\psi(x,t)$. Show that uncertainty in the momentum is the same in both states.

Answ.:

$$\langle X \rangle_\phi = \int \phi^*(x) x \phi(x) dx = \int \psi^*(x - vt, t) x \psi(x - vt, t) dx = \\ = \int \psi^*(x', t)(x' + vt)\psi(x', t) dx' = vt + \langle X \rangle_\psi \tag{7}$$

$$\langle P \rangle_\phi = -i\hbar \int \phi^*(x) \frac{\partial}{\partial x} \phi(x) dx = -i\hbar \int \phi^* [ia\phi + e^{i(ax-bt)} \frac{\partial}{\partial x} \psi] dx = \\ = \hbar a + \langle P \rangle_\psi = mv + \langle P \rangle_\psi \tag{8}$$

$$\langle H \rangle_\phi = -\frac{\hbar^2}{2m} \int \phi^* [-a^2\phi + 2iae^{i(ax-bt)} \frac{\partial}{\partial x} \psi + e^{i(ax-bt)} \frac{\partial^2}{\partial x^2} \psi] dx = \\ = \frac{\hbar^2 a^2}{2m} + \frac{a\hbar}{m} \langle P \rangle_\psi + \langle H \rangle_\psi = \frac{1}{2} m v^2 + v \langle P \rangle_\psi + \langle H \rangle_\psi \tag{9}$$

$$(\Delta P)^2_\phi = 2m \langle H \rangle_\phi - \langle P \rangle^2_\phi = m^2 v^2 + 2mv \langle P \rangle_\psi + 2m \langle H \rangle_\psi - (mv + \langle P \rangle_\psi)^2 \\ = \langle P^2 \rangle_\psi - \langle P \rangle^2_\psi = (\Delta P)^2_\psi \tag{10}$$

– What physical interpretation can be given to the transformation from the state $\psi(x,t)$ to the state $\phi(x,t)$?

Answ.:

ϕ describes the same state as ψ, except from a coordinate system that is moving towards the left with velocity v. In that coordinate system, the system seems to be moving to the right with additional velocity v and therefore additional momentum mv. The total kinetic energy increases accordingly.

2) A particle is in the ground state of a box of length L with infinitely high walls. Suddenly, the box expands (symmetrically) to length 2L, leaving the wave function momentarily undisturbed. Calculate the probability that measuring the energy of the system afterwards yields as result the ground state energy of the new box.

Ans.: The ground state wave function of the box with length L is

$$\psi_{0,L} = \sqrt{\frac{2}{L}} \sin(\pi \frac{x}{L} + \pi/2). \tag{11}$$

Here we set zero at the midpoint of the box. The expanded box has the ground state equal to

$$\psi_{0,2L} = \sqrt{\frac{2}{2L}} \sin(\pi \frac{x}{2L} + \pi/2). \tag{12}$$

The probability to find the final ground state $\psi_{0,2L}$ when we start with $\psi_{0,L}$ is $P = |\langle\psi_{0,L}|\psi_{0,2L}\rangle|^2$.

The integral is

$$\langle\psi_{0,L}|\psi_{0,2L}\rangle = \frac{\sqrt{2}}{L}\int_{-L/2}^{L/2} \sin(\pi\frac{x}{L} - \frac{\pi}{2}) \sin(\pi\frac{x}{2L} - \frac{\pi}{2})dx = \frac{8}{3\pi} \tag{13}$$

hence the probability $P = (\frac{8}{3\pi})^2$.

3) Consider the Gaussian wave packet of the form

$$\psi(x, t = 0) = \frac{1}{(\pi\Delta^2)^{1/4}} e^{ip_0x/\hbar} e^{-\frac{x^2}{2\Delta^2}} \tag{14}$$

Calculate the probability current j_x for every point x at time $t = 0$. Calculate explicitely the probability density, $P(x,t)$, at finite t using Hamiltonian of a free particle. Next, use this probability density to explicitely verify the validity of continuity equation at $t = 0$ ($\frac{\partial P(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}$).

Ans.: The current is computed by

$$j_x = -\frac{i\hbar}{2m}\left(\psi^* \frac{d}{dx}\psi - \psi\frac{d}{dx}\psi^*\right) \tag{15}$$

For Gaussian packet we get

$$j_x = \frac{p_0}{m\sqrt{\pi\Delta^2}} e^{-x^2/\Delta^2}$$

The time dependent probability density is

$$P(x,t) = \frac{1}{\sqrt{\pi\Delta^2}} \frac{1}{\sqrt{1 + \frac{\hbar^2 t^2}{m^2\Delta^4}}} e^{-\frac{(x-p_0t/m)^2}{(\Delta^2+\hbar^2t^2/(m^2\Delta^2))}} \tag{16}$$

Taking the time derivative of $P(x,t)$ and x-derivative of current j_x, it can be verified that

$$\frac{dP(x,t=0)}{dt} = -\frac{dj_x(x,t=0)}{dx}$$

4) An atom of mass 4 10^9 eV/c^2 has its position measured within 2 nm accuracy. Assume that it is in a Gaussian wave packet state afterwards. How much time will elapse before the uncertainty of our knowledge about its position has doubled? How about a 1 g speck of matter that has been located to within 1 m?

Ans.: The uncertainty in momentum and position satisfies $\Delta x\ \Delta p = \hbar/2$ hence, the velocity uncertainty at the beginning is

$$\Delta v = \frac{\hbar}{2(\Delta x)_0 m} \approx 3.7\frac{m}{s} \tag{17}$$

The uncertainties are adding in quadrature, hence after time t is ellapsed, the uncertainty increases to

$$(\Delta x)^2 \approx (\Delta x)_0^2 + (\Delta v t)^2,$$

which gives for time of doubling

$$t \approx \frac{\sqrt{(2\Delta x)_0^2 - (\Delta x)_0^2}}{(\Delta v)} \approx 10^{-9} s$$

5) A point-like particle of mass m sits in a one-dimensional potential well. The potential is infinitely high for $x < -s$ and for $x > +s$, while it is at a constant value of $V_0 > 0$ for $-s \leq x < 0$ and zero for $0 \leq x \leq s$. The particle is in the ground state (lowest energy eigenstate of the Hamiltonian) with energy $E_0 > V_0$.
Question: What is the probability that the particle can be found in the left half ($x < 0$) of the potential well? Outline how you would solve this problem step by step, without actually solving the (transcendental) equations that you encounter:

1.) Write down the one-dimensional Schrooedinger equation for this problem.
Ans.:

$$x < 0 : \psi'' = -\frac{2m(E - V_0)}{\hbar^2}\psi \quad (18)$$

$$x > 0 : \psi'' = -\frac{2mE}{\hbar^2}\psi \quad (19)$$

2.) Find the generic stationary solutions in the left and the right half of the potential well (you may assume $E > V_0$).
Ans.:

$$x < 0 : \psi_A(x) = A\sin(k_1 x + \delta) \quad (20)$$

$$x > 0 : \psi_B(x) = B\sin(kx + \delta') \quad (21)$$

where $k^2 = 2mE/\hbar^2$ and $k_1^2 = 2m(E - V_0)/\hbar^2$.

3.) List all boundary conditions that must be fulfilled (there are 4 of them!)
Ans.:

$$\psi_A(-s) = 0 \quad (22)$$

$$\psi_B(s) = 0 \quad (23)$$

$$\psi_A(0) = \psi_B(0) \quad (24)$$

$$\psi'_A(0) = \psi'_B(0) \quad (25)$$

4.) Rewrite your two half-solutions from item 2. above to explicitly fulfill as many of the boundary conditions as possible.
Ans.:

$$x < 0 : \psi_A(x) = A\sin(k_1(x + s)) \quad (26)$$

$$x > 0 : \psi_B(x) = B\sin(k(x - s)) \quad (27)$$

5.) Outline how you would find the lowest energy (ground state eigenvalue E) that solves the one- dimensional Schrodinger equation. No closed algebraic solution is possible or required for this part - just explain which equation needs to be solved.

The second two boundary conditions require

$$A\sin(k_1 s) = -B\sin(ks) \tag{28}$$
$$Ak_1\cos(k_1 s) = Bk\cos(ks) \tag{29}$$

which is satisfied when

$$k_1\cot(k_1 s) = -k\cot(ks) \tag{30}$$

We can write $k_1 = \sqrt{k^2 - k_0^2}$, where $k_0^2 = 2mV_0/\hbar$ is a known constant. The transcedental equation is then

$$\cot(s\sqrt{k^2 - k_0^2})\sqrt{k^2 - k_0^2} = -k\cot(ks) \tag{31}$$

This has a solution at $ks = \pi/2 + y(V_0)$, where y is a small positive number, which depends on the potential strength V_0.

6.) Assuming you have E, how would you determine the normalization constants for the two half- solutions?

$$\int_{-s}^{0}\sin^2(k_1(x+s))dx + \frac{\sin^2(k_1 s)}{\sin^2(ks)}\int_0^s \sin(k(x-s))dx = 1/A^2 \tag{32}$$

The integration can be completed, and leads to

$$\left(1 - \frac{\sin^2(2k_1 s)}{2k_1 s}\right) + \frac{\sin^2(k_1 s)}{\sin^2(ks)}\left(1 - \frac{\sin^2(2ks)}{2ks}\right) = \frac{1}{A^2 s/2} \tag{33}$$

7.) Once you have those in hand as well, how can you answer the original question?

Answ.: The probability of finding a particle on the left side is $P_L = \int_{-s}^{0}|\psi(x)|^2 dx = A^2\int_{-s}^{0}\sin^2(k_1(x+s))dx = A^2\frac{s}{2}(1 - \frac{\sin(2k_1 s)}{2k_1 s})$ hence

$$P_L = \frac{1 - \frac{\sin(2k_1 s)}{2k_1 s}}{\left(1 - \frac{\sin^2(2k_1 s)}{2k_1 s}\right) + \frac{\sin^2(k_1 s)}{\sin^2(ks)}\left(1 - \frac{\sin^2(2ks)}{2ks}\right)} \tag{34}$$