PHYS 357 Pset 10. Due 11:59 PM Thursday Nov. 28

1. Show that feeding the probability currnent (6.115) into the continuity equation (6.114) indeed gives $\frac{\partial}{\partial t}(\Psi^*\Psi)$ as expressed in 6.113.

2. A gaussian wave packet has $\Psi(x, t = 0) = c_0 \exp(ikx)\exp(-x^2/2\sigma^2)$. What is the probability current? We know from previous problem sets that a Gaussian wave packet spreads with time. Can you explain how that is consistent with the $k = 0$ result from the probability current?

3. Townsend 6.24

4. A way to estimate tunneling numerically is to start with a square well with a barrier in it, and add a wave packet on one side of the barrier. If you then solve Schrodinger's equation, you can calculate the probability as a function of time to find the particle on the right side of the barrier. If b is the width of the region to the left of the barrier, then particle hits the barrier something like every $2b/v$ seconds, where $v = p/m$. From that, you can estimate $T(k)$. Do this for a square barrier with a transmission probability of $\sim 1e-6$ and show you get a roughly sensible result. Then switch to a Gaussian barrier where Townsend 6.149 would predict the same tunneling probability. Do this for a) a Gaussian whose height is the same as the barrier and adjust the width, and b) for a gaussian with $\sigma = a/2$ (where a is the width of the square barrier) and adjust the height. How do you feel about the approximation in 6.149?

5. Quantum Snell's Law. Consider a 2-dimensional space where $V(x, y) = 0$ for $y < 0$, and $V(x, y) = V_0$ for $y > 0$ (note that V_0 could well be negative, but you may assume $E > V_0$). The momentum eigenstates in 2-d are $\exp(i\vec{k}\cdot\vec{x}) = \exp(i(k_x x + k_y y))$. The de Broglie relation carries straight over: $\vec{p} = \hbar\vec{k}$, and so the magnitude of k is just what we expect from 1D quantum mechanics. In particular $E - V = p^2/2m = \hbar^2(k_x^2 + k_y^2)/2m$.

   Now let's say we have an incoming wave $a\exp(i(k_x x + k_y y))$ for $y < 0$, we'll get a reflected wave $b\exp(i(k_x x - k_y y))$ for $y < 0$, and a transmitted wave $c\exp(i(k'_x x + k'_y y))$. Derive the three boundary conditions on b, c given that the combined wave function must be continuous and have continuous derivatves in both x and y at the $y = 0$ interface for all x.

a) Show that these conditions require $k'_x = k_x$

b) Solve for k'^2_y in terms of k_y, m and V_0.

c) If $k'^2_y < 0$, the wave can't penetrate the barrier since it will decay exponentially in y, even if $E > V_0$. This is the quantum version of total internal reflection. What is the condition for total internal reflection to happen?

d) Show that we recover Snell's law in quantum mechanics.

6. Bonus If you aren't sick of algebra yet, work out the reflection and transmission probabilities for Snell's law, and show that probability is conserved.

1. Show that feeding the probability currnent (6.115) into the continuity equation (6.114) indeed gives $\frac{\partial}{\partial t}(\Psi^*\Psi)$ as expressed in 6.113.

probability current (6.115) $j_x = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$

continuity equation (6.114) $\frac{\partial \psi^* \psi}{\partial t} = -\frac{\partial j_x}{\partial x}$

plugging in, we have: $-\frac{\partial}{\partial x}\left[\frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)\right]$

$$= \frac{-\hbar}{2mi}\left(\cancel{\frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}} + \psi^* \frac{\partial^2 \psi}{\partial x^2} - \cancel{\frac{\partial \psi}{\partial x}\frac{\partial \psi^*}{\partial x}} - \psi \frac{\partial^2 \psi^*}{\partial x^2}\right)$$

$$= \frac{-\hbar}{2mi}\left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2}\right)$$

Rearrange to the form of (6.113)

$$\frac{\partial(\psi^*\psi)}{\partial t} = \frac{-\psi}{\hbar i}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\right) + \frac{\psi^*}{\hbar i}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}\right)$$

2. A gaussian wave packet has $\Psi(x, t=0) = c_0 \exp(ikx)\exp(-x^2/2\sigma^2)$. What is the probability current? We know from previous problem sets that a Gaussian wave packet spreads with time. Can you explain how that is consistent with the $k=0$ result from the probability current?

① $\psi(x, t=0) = C_0 e^{ikx} e^{-x^2/2\sigma^2}$

② $J_x = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$

$\rightarrow \frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x}\left(C_0 e^{ikx} e^{-x^2/2\sigma^2}\right)$

$= C_0 (ik) e^{ikx} e^{-x^2/2\sigma^2} + C_0 e^{ikx}\left(\frac{-x}{\sigma^2}\right) e^{-x^2/2\sigma^2}$

$= C_0 e^{ikx} e^{-x^2/2\sigma^2}\left(ik - \frac{x}{\sigma^2}\right)$

$\rightarrow \frac{\partial \psi^*}{\partial x} = \frac{\partial}{\partial x}\left(C_0^* e^{-ikx} e^{-x^2/2\sigma^2}\right)$

$= C_0^* (-ik) e^{-ikx} e^{-x^2/2\sigma^2} + C_0^* e^{-ikx}\left(\frac{-x}{\sigma^2}\right) e^{-x^2/2\sigma^2}$

$= C_0^* e^{-ikx} e^{-x^2/2\sigma^2}\left(-ik - x/\sigma^2\right)$

so we have

$$j_x = \frac{\hbar}{2mi}\Big[\underbrace{C_0^* \cancel{e^{-ikx}} e^{-x^2/2\sigma^2}}_{\psi^*}\ \underbrace{C_0 \cancel{e^{ikx}} e^{-x^2/2\sigma^2}\left(ik - \frac{x}{\sigma^2}\right)}_{\partial_x \psi} - \underbrace{C_0 \cancel{e^{ikx}} e^{-x^2/2\sigma^2}}_{\psi}\ \underbrace{C_0^* \cancel{e^{-ikx}} e^{-x^2/2\sigma^2}\left(-ik - x/\sigma^2\right)}_{\partial_x \psi^*}\Big]$$

$= \frac{\hbar}{2mi}\left[|C_0|^2 e^{-x^2/\sigma^2}\left(ik - \frac{x}{\sigma^2}\right) - |C_0|^2 e^{-x^2/\sigma^2}\left(-ik - x/\sigma^2\right)\right]$

$= \frac{\hbar}{2mi}|C_0|^2 e^{-x^2/\sigma^2}\left(ik - \cancel{\frac{x}{\sigma^2}} + ik + \cancel{\frac{x}{\sigma^2}}\right)$

$= \frac{\hbar}{\cancel{2}m\cancel{i}}|C_0|^2 e^{-x^2/\sigma^2}\, \cancel{2i}k$

$\boxed{j_x = \frac{\hbar k}{m}|C_0|^2 e^{-x^2/\sigma^2}}$

③ for $k=0$, we have $j_x = 0$ so there's no net flow of probability and the spreading of the wave packet is due to the momentum uncertainty

6.24.

(a) Show that the transmission coefficient for scattering from the potential energy well

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

is given by

$$T = \left[1 + \frac{\sin^2 \sqrt{\frac{2m}{\hbar^2}(E+V_0)}\, a}{4\frac{E}{V_0}\frac{(E+V_0)}{V_0}} \right]^{-1}$$

Suggestion: What is the transcription required to change the wave function (6.142) into the one appropriate for this problem? What happens to the transmission coefficient (6.144) under this transcription?

① for $V = \begin{cases} 0 & x<0 \\ V_0 & 0<x<a \\ 0 & x>a \end{cases}$, (6.142) is $\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x<0 \\ Fe^{qx} + Ge^{-qx} & 0<x<a \\ Ce^{ikx} & x>a \end{cases}$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ & $q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

which gives (6.144) $T = \left[1 + \left(\frac{k^2+q^2}{2kq}\right)^2 \sinh^2 qa\right]^{-1}$

② Now we have $V(x) = \begin{cases} 0 & x<0 \\ -V_0 & 0<x<a \\ 0 & x>a \end{cases}$ so $V_0 \to -V_0$

$\Rightarrow k' = k = \sqrt{\frac{2mE}{\hbar^2}}$ and $q' = \sqrt{\frac{2m(-V_0-E)}{\hbar^2}} = i\sqrt{\frac{2m(V_0+E)}{\hbar^2}}$

③ The transmission coefficient becomes:

$$T' = \left[1 + \underbrace{\left(\frac{k'^2+q'^2}{2k'q'}\right)^2}_{①} \underbrace{\sinh^2 q'a}_{②}\right]^{-1}$$

① $\left[\left(\frac{2mE}{\hbar^2}\right) + i^2\left(\frac{2m(V_0+E)}{\hbar^2}\right)\right]^2 \cdot \left(\frac{1}{2i}\sqrt{\frac{\hbar^2}{2mE}}\sqrt{\frac{\hbar^2}{2m(V_0+E)}}\right)^2$

$= \left(\frac{\cancel{2mE} - 2mV_0 - \cancel{2mE}}{\hbar^2}\right)^2 \cdot \frac{-1}{4}\left(\frac{\hbar^2}{2mE}\right)\left(\frac{\hbar^2}{2m(V_0+E)}\right)$

$= \frac{-1}{4}\left(\frac{4m^2V_0^2}{\cancel{\hbar^4}}\right)\left(\frac{\cancel{\hbar^4}}{4m^2 E(V_0+E)}\right)$

$= \frac{-1}{4}\frac{V_0}{E}\frac{V_0}{(V_0+E)}$

② $\sinh^2 q'a = \left(\frac{e^{q'a} - e^{-q'a}}{2}\right)^2$

$\downarrow q'a = ai\sqrt{\frac{2m(V_0+E)}{\hbar^2}} \equiv aiq_0$ — I don't want to rewrite the $\sqrt{\ }$ ᵕ̈

$= \left(\frac{e^{iaq_0} - e^{-iaq_0}}{2}\right)^2$

$= (i\sin(aq_0))^2$

$= -\sin^2(aq_0)$

so $T' = \left[1 + \left(\frac{\cancel{-}1}{4}\frac{V_0}{E}\frac{V_0}{(V_0+E)}\right)(\cancel{1-}\sin^2 aq_0)\right]^{-1}$

$$T' = \left[1 + \frac{\sin^2 a\sqrt{\frac{2m(V_0+E)}{\hbar^2}}}{4\frac{E}{V_0}\frac{(V_0+E)}{V_0}}\right]^{-1}$$

(b) Show that for certain incident energies there is 100 percent transmission. Suppose that we model an atom as a one-dimensional square well with a width of 1 Å and that an electron with 0.7 eV of kinetic energy encounters the well. What must the depth of the well be for 100 percent transmission? This absence of scattering is observed when the target atoms are composed of noble gases such as krypton.

① 100% transmission $\rightarrow T=1$ so we have

$$\frac{\sin^2 a\sqrt{\frac{2m(V_0+E)}{\hbar^2}}}{4\frac{E}{V_0}\frac{(V_0+E)}{V_0}} = 0$$

$$\sin^2 a\sqrt{\frac{2m(V_0+E)}{\hbar^2}} = 0$$

$$a\sqrt{\frac{2m(V_0+E)}{\hbar^2}} = n\pi \quad \text{for } n=0,1,\ldots$$

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

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

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 - V_0$$

② $a = 1$ Å

$E = 0.7$ eV

$m = m_e$

choose $n=1$

$\longrightarrow$ $V_0 = \frac{\hbar^2}{2m_e}\left(\frac{\pi}{a}\right)^2 - E$

$\downarrow$ wolfram

$V_0 = 36.9$ eV

5. Quantum Snell's Law. Consider a 2-dimensional space where $V(x, y) = 0$ for $y < 0$, and $V(x, y) = V_0$ for $y > 0$ (note that V_0 could well be negative, but you may assume $E > V_0$). The momentum eigenstates in 2-d are $\exp(i\vec{k} \cdot \vec{x}) = \exp(i(k_x x + k_y y))$. The de Broglie relation carries straight over: $\vec{p} = \hbar\vec{k}$, and so the magnitude of k is just what we expect from 1D quantum mechanics. In particular $E - V = p^2/2m = \hbar^2(k_x^2 + k_y^2)/2m$.

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a) Show that these conditions require $k'_x = k_x$

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d) Show that we recover Snell's law in quantum mechanics.

① $V(x,y) = \begin{cases} 0 & y<0 \\ V_0 & y>0 \end{cases}$ with $V_0 < E$

momentum eigenstates: $e^{i\vec{k}\cdot\vec{x}} = e^{ik_x x + ik_y y}$

$\vec{p} = \hbar\vec{k}$

$E - V = \frac{p^2}{2m} = \frac{\hbar^2(k_x^2 + k_y^2)}{2m}$

Incoming wave: $\psi_I = ae^{ik_x x + ik_y y}$ $\quad y<0$

Reflected wave: $\psi_R = be^{ik_x x - ik_y y}$ $\quad y<0$

transmitted wave: $\psi_T = ce^{ik_x' x + ik_y' y}$ $\quad y>0$

② Boundary conditions:

- continuous wave fxns: $\psi_I + \psi_R = \psi_T$ at $y=0$

$ae^{ik_x x} + be^{ik_x x} = ce^{ik_x' x}$ for all x

$\rightarrow a + b = c$ ①

- continuous derivatives: (in x) $\partial_x(\psi_I + \psi_R) = \partial_x \psi_T$

$ik_x(ae^{ik_x x + ik_y y} + be^{ik_x x - ik_y y}) = ik_x' ce^{ik_x' x + ik_y' y}$ for all x, at y=0

$ik_x e^{ik_x x}(a+b) = ik_x' ce^{ik_x' x}$

$\rightarrow k_x \underbrace{(a+b)}_{=c \text{ from condition ① above}} = k_x' c$ ②

$k_x c = k_x' c$

$k_x = k_x'$

part a)

(in y) $\partial_y(\psi_I + \psi_R) = \partial_y \psi_T$

$ik_y(ae^{ik_x x + ik_y y} - be^{ik_x x - ik_y y}) = ik_y' ce^{ik_x' x + ik_y' y}$ for all x, at y=0

$ik_y e^{ik_x x}(a-b) = ik_y' ce^{ik_x' x}$

$\rightarrow k_y(a-b) = k_y' c$

b) we know $E-V=\frac{\hbar^2(K_x^2+K_y^2)}{2m}$ so $E=\begin{cases}\frac{\hbar^2(K_x^2+K_y^2)}{2m} & y<0 \quad (\text{since } V=0) \quad ① \\ \frac{\hbar^2(K_x'^2+K_y'^2)}{2m}+V_0 & y>0 \quad (\text{since } V=V_0) \quad ②\end{cases}$

from ①, we have: $E=\frac{\hbar^2(K_x^2+K_y^2)}{2m}$

$$\frac{2mE}{\hbar^2}-K_y^2=K_x^2$$

substituting $K_x=K_x'$ in ②, we get: $E=\frac{\hbar^2(K_x^2+K_y'^2)}{2m}+V_0$

$$\frac{2m(E-V_0)}{\hbar^2}=K_x^2+K_y'^2$$

$$\downarrow K_x^2=\frac{2mE}{\hbar^2}-K_y^2$$

$$\cancel{\frac{2mE}{\hbar^2}}-\frac{2mV_0}{\hbar^2}=\cancel{\frac{2mE}{\hbar^2}}-K_y^2+K_y'^2$$

$$K_y'^2=K_y^2-\frac{2mV_0}{\hbar^2}$$

c) total internal reflection when $K_y'^2<0 \iff K_y^2-\frac{2mV_0}{\hbar^2}<0$

$$K_y^2<\frac{2mV_0}{\hbar^2}$$

using $|\vec{K}|^2=K_x^2+K_y^2$, we can also rewrite this as $K^2-K_x^2<\frac{2mV_0}{\hbar^2}$

$$K_x^2>K^2-\frac{2mV_0}{\hbar^2}$$

d) we have $\vec{K}=(K_x,K_y)=\vec{K_I}$ (incident wave) & $\vec{K}'=(K_x',K_y')=\vec{K_T}$ (transmitted)

$\rightarrow K_y=K\sin\theta_I$ & $K_y'=K'\sin\theta_T$ with $K^2=K_x^2+K_y^2$ and $K'^2=K_x'^2+K_y'^2=K_x^2+K_y'^2$

so $K'^2=K_x^2+K_y^2-\frac{2mV_0}{\hbar^2}$

$$K'^2=K^2-\frac{2mV_0}{\hbar^2}$$

$$\frac{K'^2}{K^2}=1-\frac{2mV_0}{\hbar^2K^2} \qquad K^2=P^2/\hbar^2$$

$$=1-\frac{2mV_0}{P^2}$$

$$\Rightarrow \frac{\sin\theta_I}{\sin\theta_T}=\frac{K_y}{K}\cdot\frac{K'}{K_y'}$$

$$\sin\theta_I=\frac{K_y}{\sqrt{K_y-\frac{2mV_0}{\hbar}}}\cdot\sqrt{1-\frac{2mV_0}{P^2}}\ \sin\theta_T$$

6. Bonus If you aren't sick of algebra yet, work out the reflection and transmission probabilities for Snell's law, and show that probability is conserved.

① from Q5, we know $a+b=c$ and $k_y(a-b)=k_y'c$

$$\rightarrow k_y(a-b)=k_y'(a+b)$$
$$k_y a-k_y b=k_y' a+k_y' b$$
$$(k_y-k_y')a=b(k_y+k_y')$$
$$b=a\,\frac{k_y-k_y'}{k_y+k_y'}$$

$$\rightarrow c=a+b$$
$$c=a+a\,\frac{k_y-k_y'}{k_y+k_y'}$$
$$c=a\left(1+\frac{k_y-k_y'}{k_y+k_y'}\right)$$
$$c=a\cdot\frac{2k_y}{k_y+k_y'}$$

② $R=\left|\frac{b}{a}\right|^2$ and $T=\frac{k_y'}{k_y}\left|\frac{c}{a}\right|^2$

$$\boxed{R=\left(\frac{k_y-k_y'}{k_y+k_y'}\right)^2}$$

$$=\frac{k_y'}{k_y}\left(\frac{2k_y}{k_y+k_y'}\right)^2$$
$$\boxed{T=\frac{4k_yk_y'}{(k_y+k_y')^2}}$$

③ check that $R+T=1$:

$$R+T=\left(\frac{k_y-k_y'}{k_y+k_y'}\right)^2+\frac{4k_yk_y'}{(k_y+k_y')^2}$$
$$=\frac{(k_y-k_y')^2+4k_yk_y'}{(k_y+k_y')^2}$$
$$=\frac{k_y^2-2k_yk_y'+k_y'^2+4k_yk_y'}{(k_y+k_y')^2}$$
$$=\frac{k_y^2+2k_yk_y'+k_y'^2}{(k_y+k_y')^2}$$
$$=\frac{(k_y+k_y')^2}{(k_y+k_y')^2}$$
$$=1$$