Below are solutions/hints on some of the questions. There is no guarantee of completeness or correctness; please watch out for typos.

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1. A particle on a one dimensional potential is subject to a potential that is constant for $x \notin [-a, a]$:

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

The Schroedinger equation for this system is found/known to have a solution with energy E with the following forms in the regions outside $[-a, a]$:

$$\begin{aligned} \psi(x) &= \alpha e^{ik_1x} + \beta e^{-ik_1x} && \text{for } x < -a \\ \psi(x) &= \gamma e^{ik_2x} && \text{for } x > a \end{aligned}$$

where

$$\alpha = \frac{k_1 + ik_2}{k_1 - ik_2} \qquad \beta = \frac{ik_1}{k_1 - ik_2} \qquad \gamma = \frac{\sqrt{k_1k_2}}{k_1 - ik_2}$$

(a) Express k_1 in terms of E.

Hint/Solution →
You can put in the wavefunction in the left ($x < a$) region into the Schroedinger equation with $V(x) = 0$. This will yield the following relation between E and k_1. However, you should actually already know the answer, since we worked this out a few times in class.

$$E = \frac{\hbar^2 k_1^2}{2m} \qquad \Longrightarrow \qquad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

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(b) Is E larger or smaller than V_0? Explain why.

Hint/Solution $\rightarrow$
$E > V_0$, because we have a plane wave solution in the region where $V(x) = V_0$. If $E < V_0$, we would have exponential solutions in this region.

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(c) Express k_2 in terms of E and V_0.

Hint/Solution $\rightarrow$
Again, you can insert $\psi(x) = \gamma e^{ik_2 x}$ in the Schroedinger equation for $x > a$, and this will give the relation

$$E - V_0 = \frac{\hbar^2 k_2^2}{2m} \qquad k_2 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

but you should in fact already know the answer.

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(d) If we want to interpret this as a scattering problem, which parts of the wavefunction would you interpret as incident wave, reflected wave, and transmitted wave?

Hint/Solution $\rightarrow$

incident	$\alpha e^{ik_1 x}$
reflected	$\beta e^{-ik_1 x}$
transmitted	$\gamma e^{ik_2 x}$

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(e) Calculate the reflection coefficient.

Hint/Solution →

$$R = \left|\frac{\beta}{\alpha}\right|^2 = \left|\frac{ik_1}{k_1+ik_2}\right|^2 = \frac{k_1^2}{k_1^2+k_2^2}$$

Note there are no momentum factors. This is explained in the following.

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(f) Calculate the transmission coefficient.
(Careful: remember momemntum factors.)

Hint/Solution →
The momentum factors appear because the transmission coefficient is the ratio of transmitted current to incident current, and the current density carried by a plane wave $Ae^{ipx/\hbar}$ is $|A|^2 p/m$. (Please do prove this to yourself using the definition of the current density.) Thus the transmission coefficient is

$$T = \frac{\text{transmitted current}}{\text{incident current}} = \frac{|\gamma|^2 \hbar k_2/m}{|\alpha|^2 \hbar k_1/m} = \left|\frac{\gamma}{\alpha}\right|^2 \times \frac{k_2}{k_1}$$

Note that, in the reflection coefficient, the momentum factors cancel (both are $\hbar k_1$) and hence are not needed.

$$T = \left|\frac{\gamma}{\alpha}\right|^2 \times \frac{k_2}{k_1} = \left|\frac{\sqrt{k_1 k_2}}{k_1 + ik_2}\right|^2 \frac{k_2}{k_1} = \frac{k_2^2}{k_1^2 + k_2^2}$$

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(g) Check that the sum of the two coefficients makes sense.

Hint/Solution →

$$R + T = \frac{k_1^2}{k_1^2 + k_2^2} + \frac{k_2^2}{k_1^2 + k_2^2} = 1$$

Interpreting the incident plane wave as a steady current/stream of particles, it's obvious that the particles either get reflected or they get transmitted. The sum of the reflected and transmitted currents should be equal to the incident current: otherwise particles are being created or destroyed. This means that the sum of reflection and transmission coefficients needs to be equal to unity.

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2. Suppose $\psi_0(x)$ is a properly-normalized wavefunction with

$$\langle \hat{x} \rangle_{\psi_0} = \langle \psi_0 | \hat{x} | \psi_0 \rangle = x_0 \qquad \langle \hat{p} \rangle_{\psi_0} = \langle \psi_0 | \hat{p} | \psi_0 \rangle = p_0$$

where x_0 and p_0 are constants. The subscript indicates the state in which the expectation values are being calculated. Define a new wavefunction

$$\psi_{new}(x) = e^{iqx/\hbar} \, \psi_0(x)$$

where q is a real quantity having dimensions of momentum.

(a) What is the expectation value $\langle \hat{x} \rangle_{\psi_{new}}$ in the state $\psi_{new}(x)$?

Hint/Solution $\rightarrow$

$$\begin{aligned}
\langle \hat{x} \rangle_{\psi_{new}} &= \langle \psi_{new} | \hat{x} | \psi_{new} \rangle = \int_{-\infty}^{\infty} x \left| \psi_{new}(x) \right|^2 dx \\
&= \int_{-\infty}^{\infty} x \left| e^{iqx/\hbar} \psi_0(x) \right|^2 dx = \int_{-\infty}^{\infty} x \left| e^{iqx/\hbar} \right|^2 \left| \psi_0(x) \right|^2 dx \\
&= \int_{-\infty}^{\infty} x \left| \psi_0(x) \right|^2 dx = \langle \hat{x} \rangle_{\psi_0} = x_0
\end{aligned}$$

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(b) What is the expectation value $\langle \hat{p} \rangle_{\psi_{new}}$ in the state $\psi_{new}(x)$?

Hint/Solution $\rightarrow$

$$\begin{aligned}
\langle \hat{p} \rangle_{\psi_{new}} &= \langle \psi_{new} | \hat{p} | \psi_{new} \rangle = \int_{-\infty}^{\infty} \psi_{new}(x)^* \hat{p} \psi_{new}(x) dx \\
&= -i\hbar \int_{-\infty}^{\infty} \psi_{new}(x)^* \frac{d}{dx} \psi_{new}(x) dx
\end{aligned}$$

Now

$$\frac{d}{dx} \psi_{new}(x) = \frac{d}{dx} \left[e^{iqx/\hbar} \, \psi_0(x) \right] = \frac{iq}{\hbar} e^{iqx/\hbar} \, \psi_0(x) + e^{iqx/\hbar} \frac{d}{dx} \psi_0(x)$$

so that

$$\psi_{new}(x)^* \frac{d}{dx}\psi_{new}(x)$$
$$= \left[e^{-iqx/\hbar}\,\psi_0(x)^*\right]\left(\frac{iq}{\hbar}e^{iqx/\hbar}\,\psi_0(x) \;+\; e^{iqx/\hbar}\frac{d}{dx}\psi_0(x)\right)$$
$$= \frac{iq}{\hbar}\,|\psi_0(x)|^2 + \psi_0(x)^*\frac{d}{dx}\psi_0(x)$$

Thus

$$\langle\hat{p}\rangle_{\psi_{new}} \;=\; -\,i\hbar\frac{iq}{\hbar}\int_{-\infty}^{\infty}|\psi_0(x)|^2\,dx \;-\; i\hbar\int_{-\infty}^{\infty}\psi_0(x)^*\frac{d}{dx}\psi_0(x)dx$$
$$= q \;+\; \int_{-\infty}^{\infty}\psi_0(x)^*\hat{p}\psi_0(x)dx \;=\; q \;+\; \langle\hat{p}\rangle_{\psi_0} \;=\; q \;+\; p_0$$

A ‘COMMON’ MISTAKE $\longrightarrow$
Here's a WRONG calculation:

$$|\psi_{new}\rangle \;=\; e^{iqx/\hbar}\;|\psi_0\rangle$$
$$\Longrightarrow\; \langle\hat{p}\rangle_{\psi_{new}} \;=\; \langle\psi_{new}|\hat{p}|\psi_{new}\rangle$$
$$= e^{-iqx/\hbar}\langle\psi_0|\hat{p}|\psi_0\rangle e^{iqx/\hbar} \qquad \text{WRONG}$$
$$= \langle\psi_0|\hat{p}|\psi_0\rangle \;=\; p_0 \qquad \text{WRONG}$$

Where did we go wrong? We mixed the abstract bra-ket notation with the specific real-space representation by writing expressions mixing $e^{iqx/\hbar}$ (specific real-space expression) and bra's and ket's (in which the real-space dependence is hidden away). Clearly a bad idea. While the first line above is maybe not necessarily incorrect by itself, it is susceptible to mistreatment due to the mixing of notation.

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(c) Based on your results, interpret in one sentence the physical significance of multiplying a wavefunction by the factor $e^{iqx/\hbar}$.

Hint/Solution $\rightarrow$
Multiplying by this phase factor $e^{iqx/\hbar}$ keeps the average of the position unchanged, and shifts the momentum by the quantity q.
Multiplying by such a phase factor is sometimes informally called ‘boosting’ the wavefunction.

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3. Consider a particle with mass m in the state described by wavefunction $\psi(x)$, which we write in amplitude-phase form:

$$\psi(x) = A(x)e^{i\theta(x)}$$

(a) Write down the definition of the probability current density.

Hint/Solution →

$$j(x) = \frac{\hbar}{m}\text{Im}\left[\psi(x)^*\frac{\partial}{\partial x}\psi(x)\right]$$

or

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

The first form is usually easier to calculate with, but of course both should give the same answer. I use the first form below, but students should try out both ways to get the same result.

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(b) Show that the probability current density is given by

$$j(x) = [A(x)]^2\,\frac{\hbar}{m}\,\partial_x\theta(x)$$

i.e., the probability current is proportional to the *gradient* of the phase.

Hint/Solution →

$$\partial_x\psi = \partial_x\left[Ae^{i\theta}\right] = (\partial_x A)\,e^{i\theta} + A\partial_x e^{i\theta}$$
$$= (\partial_x A)\,e^{i\theta} + Ae^{i\theta}i\partial_x\theta$$

Multiplying by $\psi(x)^* = Ae^{-i\theta}$,

$$\psi^*\partial_x\psi = A\,(\partial_x A) + iA^2\partial_x\theta$$

so that

$$j = \frac{\hbar}{m}\text{Im}\left[A\,(\partial_x A) + iA^2\partial_x\theta\right] = \frac{\hbar}{m}A^2\partial_x\theta = \frac{\hbar}{m}\,[A(x)]^2\,\partial_x\theta(x)$$

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(c) Show that there is no current in a region where the wavfunction is real.

Hint/Solution →
In a region where the function is real, $\theta(x) = 0$, so that $\partial_x\theta(x) = 0$, which implies from the above result:

$$j = 0$$

Alternatively, using the longer definition $j = \frac{i\hbar}{2m}(\psi\partial_x\psi^* - \psi^*\partial_x\psi)$, we find that when the wavefunction is real ($\psi = \psi^*$), the current becomes

$$j \;=\; \frac{i\hbar}{2m}\left(\psi\partial_x\psi - \psi\partial_x\psi\right) \;=\; 0$$

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4. Consider the time-dependent Schroedinger equation (TDSE) for a single particle on a one-dimensional line:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \;+\; V(x)\psi(x,t)$$

The potential $V(x)$ is real-valued, i.e., $V^*(x) = V(x)$.

(a) Using the TDSE, show that the probability density $\rho(x,t) \;=\; \psi^*\psi$ and the probability current density $j(x,t)$ satisfy the one-dimensional continuity equation

$$\frac{\partial j}{\partial x} \;=\; -\frac{\partial \rho}{\partial t}$$

Hint/Solution →
Because this is cumbersome, I omit the dependences on x and t, e.g., write ψ and ρ and j instead of $\psi(x,t)$ and $\rho(x,t)$ and $j(x,t)$.

Using the definition of j,

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

On the other hand, using $\rho = \psi^*\psi$, we obtain

$$-\partial_t\rho = -\partial_t\left(\psi^*\psi\right) = -\partial_t\left(\psi^*\psi\right) = -\left(\partial_t\psi^*\right)\psi - \psi^*\left(\partial_t\psi\right)$$

We can now use the TDSE and its complex conjugate, i.e,

$$\partial_t\psi = -\frac{\hbar}{2mi}\partial_x^2\psi + \frac{V\psi}{i\hbar}\,, \qquad \partial_t\psi^* = +\frac{\hbar}{2mi}\partial_x^2\psi^* - \frac{V\psi^*}{i\hbar}$$

Using these expressions, we obtain for ρ

$$-\partial_t\rho = -\left(+\frac{\hbar}{2mi}\partial_x^2\psi^* - \frac{V\psi^*}{i\hbar}\right)\psi - \psi^*\left(-\frac{\hbar}{2mi}\partial_x^2\psi + \frac{V\psi}{i\hbar}\right)$$
$$= -\frac{\hbar}{2mi}\left(\psi\partial_x^2\psi^* - \psi^*\partial_x^2\psi\right) + \frac{V\psi\psi^*}{i\hbar} - \frac{V\psi\psi^*}{i\hbar}$$
$$= \frac{i\hbar}{2m}\left(\psi\partial_x^2\psi^* - \psi^*\partial_x^2\psi\right)$$

Thus we have shown that

$$\partial_x j = -\partial_t\rho$$

i.e., the one-dimensional continuity equation for probability density and probability current.

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(b) Guess the form of the continuity equation for the probability density, for the case of a particle in three spatial dimensions.

Hint/Solution →
The single spatial derivative $\partial_x j$ of one dimension is replaced by a divergence in three dimensions. Also, the current density becomes a 3-vector. Thus

$$\nabla \cdot \vec{j} \;=\; -\,\partial_t \rho$$

for three spatial dimensions.
This is familiar from electromagnetism. However, here ρ and $\vec{j}$ are the probability density and probability current, instead of the charge density and the charge current.

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(c) What does the continuity equation imply physically?

Hint/Solution →
The continuity equation means that the quantum probability of a particle on a line can change only continuously, in the sense that if it decreases in some region, then there must be some probability current carrying it away, and if it increases in some region, then there must be some probability current carrying it into that region.
The probability density shares this property with the charge density in electrodynamics, and with the mass density in fluid dynamics.
Of course, the probability is conserved in total — because we are dealing with a single particle system, the probability of finding the particle somewhere in space must be conserved (= 1). You also know this because the norm of a wavefunction does not change with time.
But the continuity equation tells us something more — that the probability density also locally satisfies continuity. The probability can continuously move or flow from one region to another, but cannot discontinuously jump from one region to another.

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