Lecture 15: Simple problems in 1D and Probability Current I

Phy851 Fall 2009
Continuity Theorem

From previous Lecture:

**Theorem:**
- the wavefunction and its first derivative must be everywhere continuous.
  - **Exception:** where there is a $\delta(x-x_0)$ or $\delta'(x-x_0)$ in the potential.
    - $\delta(x-x_0)$ potential $\rightarrow$ discontinuity in $\psi'(x)$ at $x=x_0$
    - $\delta'(x-x_0)$ potential $\rightarrow$ discontinuity in $\psi(x)$ at $x=x_0$
Solution to the Step Potential Scattering Problem

- Assuming an incoming flux from the left only, we make the ansatz:

\[ \psi_I(x) = e^{ik_1x} + re^{-ik_1x} \quad \psi_{II}(x) = t e^{ik_2x} \]

- As there is no \( \delta \) or \( \delta' \) potential, we need to impose two boundary conditions at \( x=0 \):

\begin{align*}
\psi_I(0) &= \psi_{II}(0) \quad \Rightarrow \quad 1 + r = t \quad (1) \\
\psi_I'(0) &= \psi_{II}'(0) \quad \Rightarrow \quad ik_1(1 - r) = ik_2t \quad (2)
\end{align*}

Insert (1) into (2)

\[ ik_1(1 - r) = ik_2(1 + r) \]

Collect \( r \) terms together

\[-i(k_1 + k_2)r = -i(k_1 - k_2) \]

Solve for \( r \)

\[ r = \frac{k_1 - k_2}{k_1 + k_2} \]

Plug solutions into (1) and solve for \( t \)

\[ t = 1 + \frac{k_1 - k_2}{k_1 + k_2} \quad t = \frac{2k_1}{k_1 + k_2} \]
Case I: Tunneling into the Barrier

- Consider the case where $E < V_0$:

$$\psi_I(x) = e^{ik_1x} + re^{-ik_1x} \quad \psi_{II}(x) = te^{ik_2x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} := k$$

$$k_2 = \frac{\sqrt{-2m(V_0 - E)}}{\hbar} = i\frac{\sqrt{2m(V_0 - E)}}{\hbar} := i\gamma$$

$$\psi_{II}(x) = te^{-\gamma x}$$

Q: why did we choose “+i”, instead of “-i”? A: If we had chosen “-i”, solution would 'blow up' as $x \to \infty$. That would describe a particle at $x = \infty$, but not the particle we are interested in.

$$r = \frac{k_1 - k_2}{k_1 + k_2} \quad \rightarrow \quad r = \frac{k - i\gamma}{k + i\gamma}$$

$$t = \frac{2k_1}{k_1 + k_2} \quad \rightarrow \quad t = \frac{2k}{k + i\gamma}$$

Note that: $|r|^2 = 1 \quad |t|^2 = \frac{4k^2}{k^2 + \gamma^2}$

Q: What is physical meaning of $|r|^2$ and $|t|^2$?
Case II: Quantum Reflection

- Consider the case where $E > V_0$:

\[
\psi_I(x) = e^{ik_1x} + re^{-ik_1x} \quad \psi_{II}(x) = te^{ik_2x}
\]

\[
k_1 = \frac{\sqrt{2mE}}{\hbar} := k
\]

\[
k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar} = \sqrt{k - \frac{2MV_0}{\hbar^2}} := \sqrt{k^2 - k_0^2}
\]

\[
r = \frac{k_1 - k_2}{k_1 + k_2} \quad t = \frac{2k_1}{k_1 + k_2}
\]

\[
|r|^2 = \frac{2k^2 - k_0^2 - 2k\sqrt{k^2 - k_0^2}}{2k^2 - k_0^2 + 2k\sqrt{k^2 - k_0^2}} \quad |t|^2 = \frac{4k^2}{2k^2 - k_0^2 + 2k\sqrt{k^2 - k_0^2}}
\]

Note: $|r|^2 + |t|^2 \neq 1$

So $|r|^2$ and $|t|^2$ are not reflection and transmission probabilities!
Limiting case: Infinite Barrier

- Consider an infinitely high potential barrier:

\[ \psi_I(x) = e^{ikx} + re^{-ikx} \quad \psi_{II}(x) = te^{-\gamma x} \]

\[ \gamma = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{\sqrt{2m(\infty - E)}}{\hbar} = \infty \]

\[ r = -\frac{(\gamma + ik)}{(\gamma - ik)} = -1 \]

\[ t = -\frac{2ik}{\gamma - ik} = 0 \]

\[ \psi_I(x) = \sin(kx) \quad \text{(up to a constant)} \]

\[ \psi_{II}(x) = 0 \quad \text{Wave function goes to zero at infinite barrier} \]
Bound states: Infinite Square Well Solution

- Extend this result to the infinite square well

\[ \psi_I(x) = 0 \quad \text{II} \quad \psi_\text{III}(x) = 0 \]

From continuity of \( \psi \):

\[ \psi_\text{II}(0) = 0 \quad \psi_\text{II}(L) = 0 \]

Most general free-space solution:

\[ \psi_\text{II}(x) = a e^{ikx} + b e^{-ikx} = a \sin(kx) + b \cos(kx) \]

Apply boundary conditions:

\[ \psi_\text{II}(0) = 0 \rightarrow b = 0 \]

\[ \psi_\text{II}(L) = 0 \rightarrow k = \frac{n\pi}{L}; \quad n = 1, 2, 3, \ldots \]

- Momentum and Energy are quantized by the boundary conditions at 0 and L:

\[ k_n = \frac{n\pi}{L} \quad \text{Bound States are normalizable:} \]

\[ E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \quad \varphi_n(x) = \sqrt{\frac{2}{L}} \sin\left( \frac{n\pi x}{L} \right) \]
Probability Current

- From studying quantum reflection at a step potential, we saw that $|r|^2 + |t|^2 = 1$ is not always true
  - Let $R :=$ reflection probability
  - Let $T :=$ transmission probability
  - Clearly we must have $R + T = 1$
  - So $R = |r|^2$ and $T = |t|^2$ must not always be correct

- The problem is that in this case the velocity in region I is not the same as in II
- This suggests that we need to think in terms of a *probability current*

- Derivation of probability current:
  - Start from the probability density:
    $$ \rho(x,t) = |\psi(x,t)|^2 $$
  - Consider a tiny region of length $2\varepsilon$ located a position $x$:
    $$ P(x,t) = \rho(x,t)2\varepsilon $$
  - Imagine currents are flowing through points $x-\varepsilon$ and $x+\varepsilon$: (A positive current flows from left to right)

\[
\frac{dP(x,t)}{dt} = j(x - \varepsilon) - j(x + \varepsilon)
\]

Current at $-\varepsilon$  Current at $+\varepsilon$
Continuity Equation

\[ j(x - \varepsilon) - j(x + \varepsilon) = \frac{dP(x,t)}{dt} \]

\[ j(x - \varepsilon) - j(x + \varepsilon) = \frac{d\rho(x,t)2\varepsilon}{dt} \]

\[ \frac{j(x - \varepsilon) - j(x + \varepsilon)}{2\varepsilon} = \frac{d\rho(x,t)}{dt} \]

\[-\frac{d}{dx} j(x,t) = \frac{d}{dt} \rho(x,t)\]

- This is the standard continuity equation, valid for any kind of fluid

- For energy eigenstates (stationary states), we need:
  \[ \frac{d}{dt} \rho(x,t) = 0 \Rightarrow \rho(x,t) = \rho(x,0) \]
  \[ \frac{d}{dt} j(x,t) = 0 \Rightarrow j(x,t) = j(x,0) \]

- This gives:
  \[ \frac{d}{dx} j(x,t) = 0 \Rightarrow j(x,0) = j_0 \]

- Must have \textit{spatially uniform} current in steady state (of course \( j_0 \) can be zero)