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

Phy851 Fall 2009

Continuity Theorem

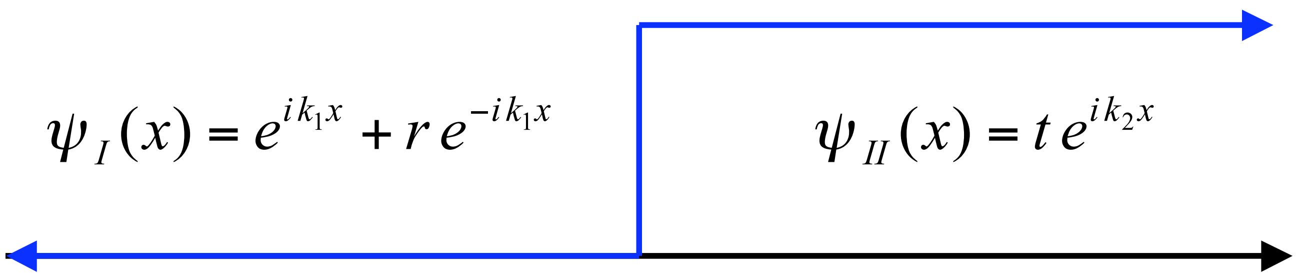
From previous Lecture:

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 → discontinuity in $\psi'(x)$ at $x=x_0$
    - $\delta'(x-x_0)$ potential → 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:



$$\psi_I(x) = e^{ik_1x} + r\,e^{-ik_1x} \qquad \psi_{II}(x) = t\,e^{ik_2x}$$

- As there is no δ *or* δ' potential, we need to impose two boundary conditions at $x=0$:

$$\psi_I(0) = \psi_{II}(0) \;\Longrightarrow\; 1 + r = t \qquad (1)$$

$$\psi_I'(0) = \psi_{II}'(0) \;\Longrightarrow\; ik_1(1-r) = ik_2t \qquad (2)$$

Insert (1) into (2) $$ik_1(1-r) = ik_2(1+r)$$

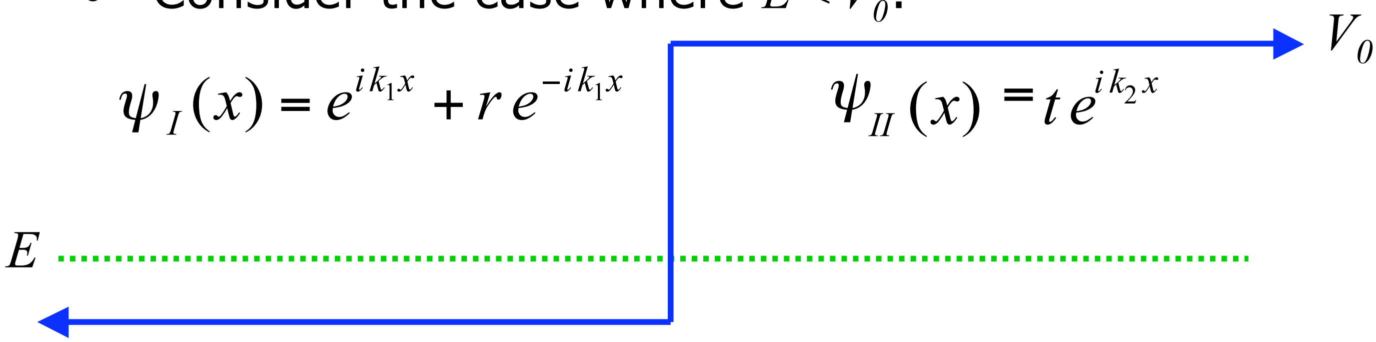
Collect r terms together $$-i(k_1+k_2)r = -i(k_1-k_2)$$

Solve for r $$r = \frac{k_1-k_2}{k_1+k_2}$$

Plug solutions into (1) and solve for t $$t = 1 + \frac{k_1-k_2}{k_1+k_2} \qquad t = \frac{2k_1}{k_1+k_2}$$

Case I: Tunneling into the Barrier

- Consider the case where $E < V_0$:



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

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

Q: why did we choose "+i", instead of "–i"?

A: If we had chosen "-i", solution would 'blow up' as x→∞.

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

That would describe a particle at x =∞, but not the particle we are interested in

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

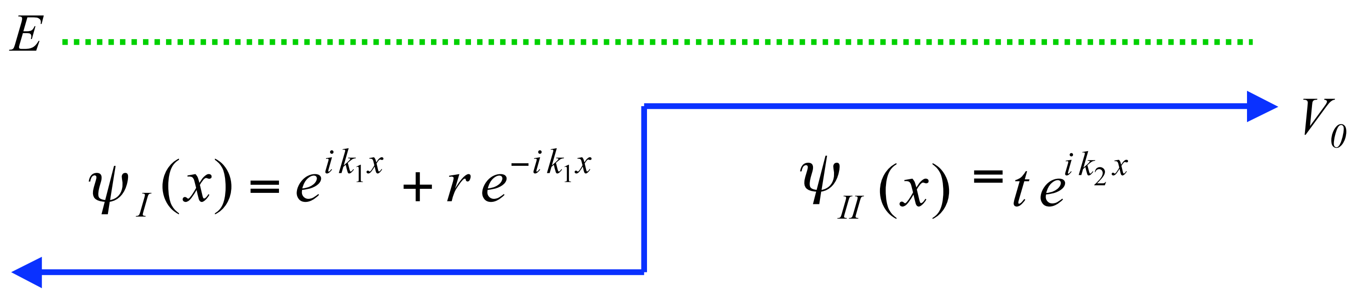
$$t = \frac{2k_1}{k_1 + k_2} \rightarrow \quad t = \frac{2k}{k + i\gamma}$$

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

Q: What is physical meaning of $|r|^2$ and $|t|^2$?

Case II: Quantum Reflection

- Consider the case where $E > V_0$:



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

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

Note that $k_2 < k_1$, as it should

$$r = \frac{k_1 - k_2}{k_1 + k_2} \rightarrow r = \frac{k - \sqrt{k^2 - k_0^2}}{k + \sqrt{k^2 - k_0^2}}$$

$$t = \frac{2k_1}{k_1 + k_2} \rightarrow t = \frac{2k}{k + \sqrt{k^2 - k_0^2}}$$

Quantum particle has non-zero probability to reflect!

$$|r|^2 = \frac{2k^2 - k_0^2 - 2k\sqrt{k^2 - k_0^2}}{2k^2 - k_0^2 + 2k\sqrt{k^2 - k_0^2}} \qquad |t|^2 = \frac{4k^2}{2k^2 - k_0^2 + 2k\sqrt{k^2 - k_0^2}}$$

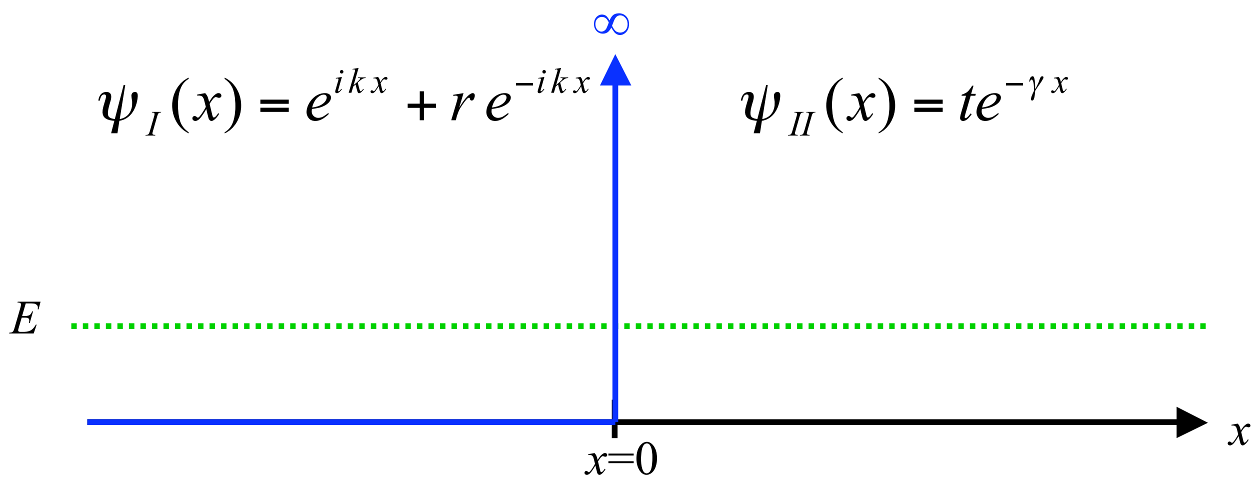
Note: $|r|^2 + |t|^2 \neq 1$

So $|r|^2$ and $|t|^2$ are not reflection and transmission probabilities !

Limiting case: Infinite Barrier

- Consider an infinitely high potential barrier:

$$\psi_I(x) = e^{ikx} + r\,e^{-ikx} \qquad \psi_{II}(x) = te^{-\gamma x}$$



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

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

π phase-shift upon reflection.

$$t = -\frac{2ik}{\gamma - ik} = 0$$

no tunneling

$$\psi_I(x) = \sin(kx)$$

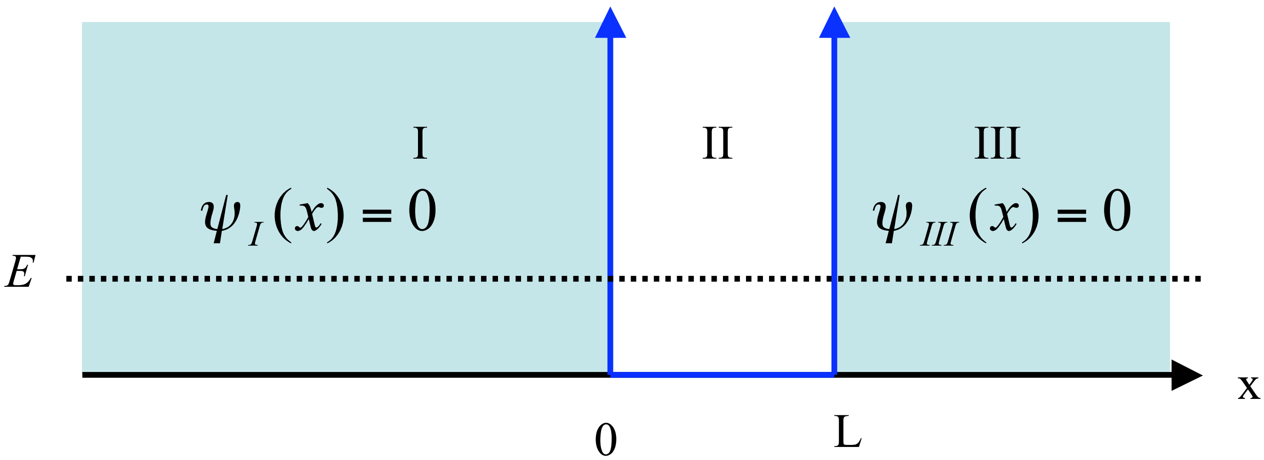
(up to a constant)

$$\psi_{II}(x) = 0$$

Wave function goes to zero at infinite barrier

Bound states: Infinite Square Well Solution

- Extend this result to the infinite square well



From continuity of ψ:

$$\psi_{II}(0) = 0 \qquad \psi_{II}(L) = 0$$

Most general free-space solution:

$$\psi_{II}(x) = \bar{a}e^{ikx} + \bar{b}e^{-ikx} = a\sin(kx) + b\cos(kx)$$

Apply boundary conditions:

$$\psi_{II}(0) = 0 \rightarrow b = 0$$

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

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

$$k_n = \frac{n\pi}{L}$$

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

Bound States are normalizable:

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

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:

$$\rho(x,t)=\left|\psi(x,t)\right|^2$$

  - Consider a tiny region of length 2ε located a position x:

$$P(x,t)=\rho(x,t)2\varepsilon$$

  - Imagine currents are flowing through points $x\text{-}\varepsilon$ and $x+\varepsilon$: (A positive current flows from left to right)

Probability in region can increase or decrease

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

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: $$\frac{d}{dx}j(x,t)=0\quad\Rightarrow\quad j(x,0)=j_0$$

- Must have ***spatially uniform*** current in steady state (of course j_0 can be zero)