Quantum Mechanics (P304H)
Part 2 – Lecture 11

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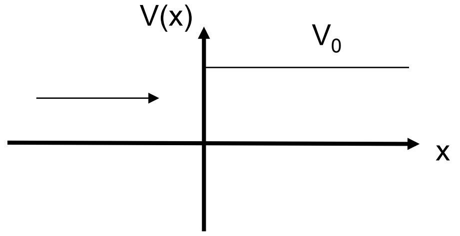
3. Potential Step ($E<V_0$)

- First example: Potential Step
  - The potential is defined as:

$$V(x)=\begin{cases}0 \text{ if } x<0\\ V_0 \text{ if } x\geq 0\end{cases}$$

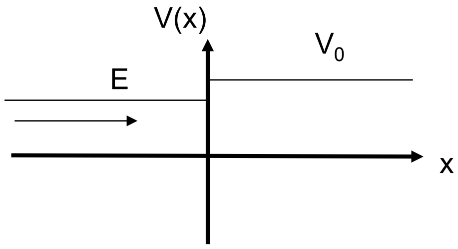


  - The 1D Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

3. Potential Step ($E<V_0$)

- Case 1: $E<V_0$



Equations:

$$\frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0 \quad \text{with} \quad k=\sqrt{\frac{2mE}{\hbar^2}}\,, \qquad x<0$$

$$\frac{d^2\psi(x)}{dx^2}-\kappa^2\psi(x)=0 \quad \text{with} \quad \kappa=\sqrt{\frac{2m}{\hbar^2}(V_0-E)}\,, \qquad x\geq 0$$

Solutions:

$$\psi(x)=Ae^{ikx}+Be^{-ikx}\;, x<0$$

$$\psi(x)=Ce^{\kappa x}+De^{-\kappa x}\;, x\geq 0$$

3. Potential Step ($E<V_0$)

One must apply boundary conditions:

1) At the limit $x\to\infty \Rightarrow Ce^{\kappa x}\to\infty$ so we must put $C=0$

2) The solutions have to be continuous in zero:

$$\left.\begin{array}{l} \psi(x) \text{ continuous in 0 (probability density conservation)} \Rightarrow A+B=D \\ \dfrac{d\psi(x)}{dx} \text{ continuous in 0 (momentum conservation)} \Rightarrow ik(A-B)=-\kappa D \end{array}\right\} \Rightarrow$$

$$\Rightarrow \quad A=\frac{1}{2}\left(1+\frac{i\kappa}{k}\right)D \quad \text{and} \quad B=\frac{1}{2}\left(1-\frac{i\kappa}{k}\right)D$$

And we can calculate the coefficient ratios:

$$\frac{B}{A}=\frac{k-i\kappa}{k+i\kappa}=e^{i\alpha} \quad \text{where we denoted} \quad \alpha=\arctan\left(\frac{2\kappa k}{\kappa^2-k^2}\right)$$

$$\frac{D}{A}=\frac{2ik}{ik-\kappa}=\frac{2k}{k+i\kappa}=\frac{k+i\kappa+k-i\kappa}{k+i\kappa}=1+e^{i\alpha}$$

3. Potential Step ($E<V_0$)

- Therefore, the solution for $x<0$ is:

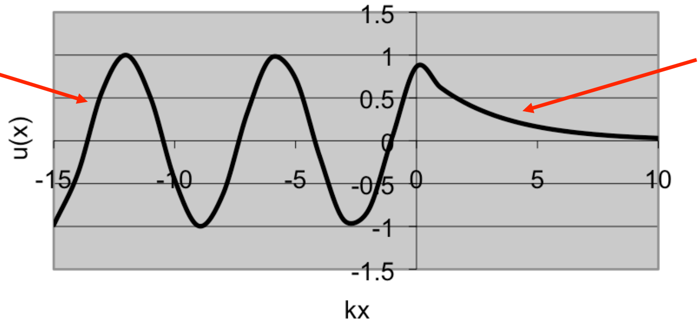
$$\psi(x) = Ae^{ikx} + Ae^{i\alpha}e^{-ikx} = Ae^{i\alpha/2}\left(e^{i(kx-\alpha/2)} + e^{-i(kx-\alpha/2)}\right) = 2Ae^{i\alpha/2}\cos\left(kx - \frac{\alpha}{2}\right)$$

- The solution for $x \geq 0$ is:

$$\psi(x) = A\left(1+e^{i\alpha}\right)e^{-\kappa x} = Ae^{i\alpha/2}\left(e^{-i(\alpha/2)} + e^{i(\alpha/2)}\right)e^{-\kappa x} = 2Ae^{i\alpha/2}\cos\left(\frac{\alpha}{2}\right)e^{-\kappa x}$$

- For example, we can put $A = \frac{1}{2}e^{-i\alpha/2}$ (α is determined by V_o and E) and do a plot:

Oscillation Behaviour due to interference of incident and reflected wave



Finite probability of finding particle in classically forbidden region at x>0

3. Potential Step ($E<V_0$)

- The probability:

$$P(x) = |\psi(x)|^2 = \begin{cases} 4|A|^2\cos^2\left(kx - \frac{\alpha}{2}\right), & x<0 \\ 4|A|^2\cos^2\left(\frac{\alpha}{2}\right)e^{-2\kappa x}, & x \geq 0 \end{cases}$$

- The probability current density is zero everywhere:

Standing wave ↴

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x<0 \\ De^{-\kappa x}, & x \geq 0 \end{cases} \Rightarrow$$

$$J(x,t) = \mathrm{Re}\left[\psi^* \frac{\hbar}{im}\frac{\partial}{\partial x}\psi\right] = v\left(|A|^2 - |B|^2\right) = 0, x<0$$

$$J(x,t) = \mathrm{Re}\left[\psi^* \frac{\hbar}{im}\frac{\partial}{\partial x}\psi\right] = 0,\ x \geq 0$$

No net flow of particles (since $\psi(x) = De^{-\kappa x}$ is real)

- If we define the reflection coefficient as the ratio of the intensity of the reflected wave to that of the incident wave:

$$R = \frac{v|B|^2}{v|A|^2} = \frac{|B|^2}{|A|^2} = 1 \qquad v = \frac{\hbar k}{m}$$

The wave is totally reflected, even though there is a non-zero probability of finding the particle at x>0, and the net probability current density is zero.

3. Potential Step ($E<V_0$)

- Physical interpretation of solution at $x \geq 0$:
  - Classically there is no solution at $x \geq 0$ since energy $E<V_0$.
  - In Quantum Mechanics we see a non-zero solution at $x \geq 0$. This is called barrier penetration

We can calculate

$$\langle x \rangle = \frac{\int_0^\infty De^{-i\kappa} x D^* e^{-i\kappa}\, dx}{\int_0^\infty De^{-i\kappa} D^* e^{-i\kappa}\, dx} = \frac{\cancel{|D|^2} \int_0^\infty x e^{-2i\kappa}\, dx}{\cancel{|D|^2} \int_0^\infty e^{-2i\kappa}\, dx} = \frac{\frac{1}{(2\kappa)^2}}{\frac{1}{2\kappa}} = \frac{1}{2\kappa} \quad \text{and} \quad \langle x^2 \rangle = \frac{2}{(2\kappa)^2}$$

Then the uncertainty in position is

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle \overline{x} \rangle^2} = \frac{1}{2\kappa}$$

And according to Heisenberg's uncertainty relation:

$$\Delta p_x \geq \frac{\hbar}{2\Delta x} \sim \hbar\kappa = \left[2m\left(V_0 - E\right)\right]^{1/2}$$

3. Potential Step ($E<V_0$)

- The corresponding uncertainty in energy is:

$$\Delta E = \Delta\left(\frac{p_x^2}{2m}\right) = \frac{p_x}{m}\Delta p_x = 2\left(V_0 - E\right)$$

- Therefore, we can no longer state with certainty that the energy E of the particle is less than V_0, so there is some probability of the particle penetrating into the barrier.

- Note that if the potential barrier is infinite: $V_0 \to \infty$, then:

$$\lim_{V_0 \to \infty} \frac{B}{A} = -1 \text{ and } \lim_{V_0 \to \infty} \frac{D}{A} = 0 \Rightarrow \Psi(x) = \begin{cases} A\left(e^{ikx} - e^{-ikx}\right), & x<0 \\ 0 & , \quad x \geq 0 \end{cases}$$

***i.e.* the wave function vanishes at the barrier and there is absolutely no penetration.**

(The slope of the wave function becomes discontinuous – this corresponds to an infinite force)

3. Potential Step ($E>V_0$)

- Case 2: $E>V_0$

$$\frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0 \text{ with } k=\left(\frac{2mE}{\hbar^2}\right)^{1/2}, x<0$$

$$\frac{d^2\psi(x)}{dx^2}+k'^2\psi(x)=0 \text{ with } k'=\left[\frac{2m}{\hbar^2}(E-V_0)\right]^{1/2}, x\geq 0$$

Solution:

$$\psi(x)=\begin{cases} Ae^{ikx}+Be^{-ikx} & ,x<0 \\ Ce^{ik'x}+De^{-ik'x} & ,x\geq 0 \end{cases}$$

Particles are incident from the left ⇒ $D=0$

No wave coming from the right and nothing to reflect $Ce^{ik'x}$

Continuity conditions require:

$$A+B=C \quad \text{and} \quad ik(A-B)=ik'C$$

$$\Rightarrow \frac{B}{A}=\frac{k-k'}{k+k'} \quad \text{and} \quad \frac{C}{A}=\frac{2k}{k+k'}$$

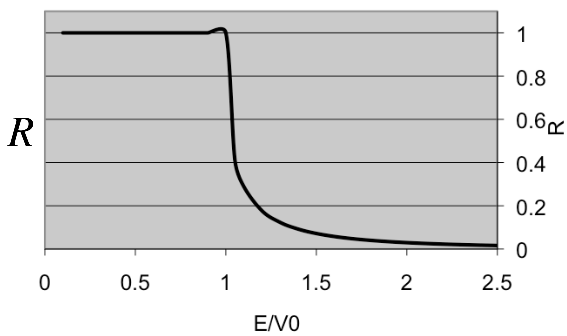
3. Potential Step ($E>V_0$)

Probability current density:

$$J(x,t)=\begin{cases} v\left[|A|^2-|B|^2\right], x<0 & v=\frac{\hbar k}{m} \\ v'|C|^2, x\geq 0 & v'=\frac{\hbar k'}{m} \end{cases}$$

Reflection coefficient:

$$R=\frac{|B|^2}{|A|^2}=\frac{(k-k')^2}{(k+k')^2}=\frac{\left[1-(1-V_0/E)^{1/2}\right]^2}{\left[1+(1-V_0/E)^{1/2}\right]^2}$$



Transmission coefficient:

$$T=\frac{v'|C|^2}{v|A|^2}=\frac{4kk'}{(k+k')^2}=\frac{4(1-V_0/E)^{1/2}}{\left[1+(1-V_0/E)^{1/2}\right]^2}$$

$$\Rightarrow R+T=1$$

Potential step can reflect particles even if $E>V_0$, due to wave-like nature of particles.

Similar to wave optics:

$$n=\frac{\lambda}{\lambda'}=\frac{k'}{k}$$

$$\Rightarrow R=\left(\frac{1-n}{1+n}\right)^2$$

The probability current density is constant

$$\frac{|B|^2}{|A|^2}+\frac{v'}{v}\frac{|C|^2}{|A|^2}=\frac{(k-k')^2}{(k+k')^2}+\frac{4kk'}{(k+k')^2}=1 \quad \Rightarrow \quad v'|C|^2=v\left(|A|^2-|B|^2\right)$$