PHYS-454

8 - The continuous spectrum of the potential wells.

Momentum eigenstates of a free particle.

- We can easily prove that the wave function

$$\psi = Ae^{ikx}$$

is an eigenfunction of the momentum operator

$$\hat{p} = -i\hbar d / dx$$

and describes particles which move with a specific momentum

$$p = \hbar k$$

The particle flux density-a

- In physics we know that the flux density of any physical quantity (mass, charge energy etc.) which is distribute in space with density ρ and moves with a velocity $\mathbf{v}$ is given by:

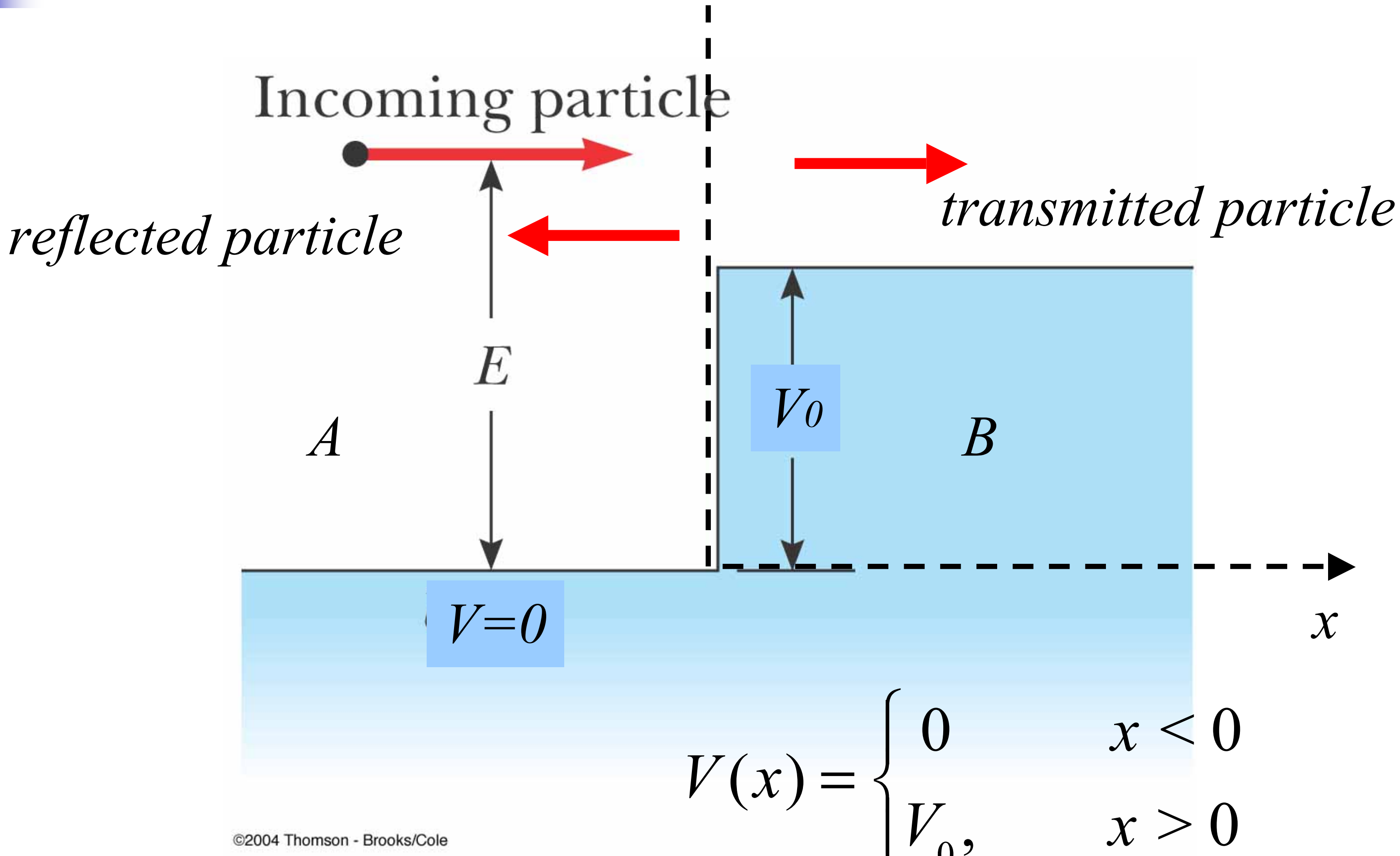
$$\mathbf{J} = \rho \mathbf{v}$$

The particle flux density-b

- In an experiment in quantum mechanics we have a flux of particles which make up a *beam*. Then the particle flux density (i.e. the number of particles that cross per second a unit surface perpendicular to the flux) will be given by:

$$J = |\psi|^2 v = |A|^2 \frac{\hbar k}{m}$$

The square potential step: The effect of reflection-a



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

The square potential step: The effect of reflection-b

- **A) The case where** $E > V_0$

The Schrödinger equation takes the form in the two regions A and B:

$$A: \quad \psi''_A + \varepsilon\psi_A = \psi''_A + k^2\psi_A = 0$$

$$B: \quad \psi''_B + (\varepsilon - U_0)\psi_B = \psi''_B + k'^2\psi_B = 0$$

$$\varepsilon = \frac{2mE}{\hbar^2}, \qquad U_0 = \frac{2mV_0}{\hbar^2}$$

$$k^2 = \varepsilon, \qquad k'^2 = \varepsilon - U_0 > 0$$

The square potential step: The effect of reflection-c

In this case the general solutions of Schrödinger equations are:

$$\psi_A = A_+ e^{ikx} + A_- e^{-ikx}$$

$$\psi_B = B_+ e^{ik'x} + B_- e^{-ik'x}$$

The index + is for the constant of the wave exp(*ikx*) which travel to the right and the index - for the constant of the wave exp(-*ikx*) which goes to the left.

The square potential step: The effect of reflection-d

- Here there is an important point: The wave functions of the free particle are everywhere finite **but not** square integrable since they are not zero at infinity!
- Their physical meaning is that they are proper of describing *scattering* problems.
- The problem we study here is a scattering problem.
- This means that in the region B we must have only particles that go to the right .

The square potential step: The effect of reflection-e

- The coefficients A determine the densities of the incident and reflected beams respectively.
- Since the incident beam is regulated by us we can chose $A_+ = 1$
- Thus we can chose the following conditions of scattering from the left

$$A_+ = 1 \qquad B_- = 0$$

The square potential step: The effect of reflection-f

- The general solution takes the form:

$$\psi_A = e^{ikx} + Ae^{-ikx}, \qquad \psi_B = Be^{ik'x}$$

- In an experiment we care about the coefficients of reflection R and transmission T, given by

$$R = \frac{J_R}{J_I}, \qquad T = \frac{J_T}{J_I}$$

- where

J_I = the flux of incident beam

J_R = the flux of reflected beam

J_T = the flux of transmitted beam

The square potential step: The effect of reflection-g

- The coefficients of reflection and transmission satisfy the relation

$$R + T = 1$$

- We can prove that the coefficients take the form

$$R = \left(\frac{k - k'}{k + k'}\right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right)^2$$

$$T = \frac{4kk'}{\left(k + k'\right)^2} = \frac{4\sqrt{E\left(E - V_0\right)}}{\left(\sqrt{E} + \sqrt{E - V_0}\right)^2}$$

Graphical solutions of the eigenvalues-d

- **B) The case where** $E < V_0$

The Schrödinger equation takes the form in the two regions A and B:

$$A: \quad \psi_A'' + \varepsilon \psi_A = \psi_A'' + k^2 \psi_A = 0$$

$$B: \quad \psi_B'' + \left(\varepsilon - U_0\right)\psi_B = \psi_B'' - \gamma^2 \psi_B = 0$$

$$\varepsilon = \frac{2mE}{\hbar^2}, \qquad U_0 = \frac{2mV_0}{\hbar^2}$$

$$k^2 = \varepsilon, \qquad \gamma^2 = U_0 - \varepsilon > 0$$

Graphical solutions of the eigenvalues-e

In this case the general solutions of Schrödinger equations are:

$$\psi_A = e^{ikx} + Ae^{-ikx}$$

$$\psi_B = Be^{-\gamma x}$$

$$A = \frac{k - i\gamma}{k + i\gamma}, \qquad B = \frac{2k}{k + i\gamma}$$

Graphical solutions of the eigenvalues-f

- In this case the coefficients of reflection and transmission are:

$$R = \left|A\right|^2 = \left|\frac{k - i\gamma}{k + i\gamma}\right|^2 = 1 \qquad T = 0$$

- This is not a surprising result. In region B the wave function is a decreasing exponential so the particle has no probability to reach the infinity and to be detected there.

Discussion-a
The effect of reflection

- The most exciting aspect of the solution is the possibility of a particle to be reflected even if it has the required energy to go ahead. This is a consequence of the discontinuity of the potential at $x=0$.
- It is the analogue of the discontinuity of the refractive index when an e/m wave passes at the boundary of two transparent media.

Discussion-b
The transmission coefficient at high energies

- When the energy E is very large the coefficient of transmission becomes equal to 1. This is not a surprise. At high energies the wavelength of a particle is very small, so the classical behavior prevails.

Discussion-c
A paradox!

- A very strange result is that the coefficients of reflection **do not depend** on Planck's constant. This is a paradox since it is a quantum mechanical result.
- The origin of this paradox is the non-natural discontinuity of the potential at x=0. The wave behavior of matter is dominant when the wavelength is comparable in size with the discontinuity. But since the discontinuity has a zero "length" it will be always far smaller of the particle's wavelength.