

## Step Potential:-

Consider a particle of mass  $m$  and energy  $E$  moving along  $x$ -axis from left to right towards a region having a potential step as shown in Fig-1. described by

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

We assume that  $E < V_0$ . The motion of the particle is governed by time-independent Schrödinger equation

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0 \dots (1)$$

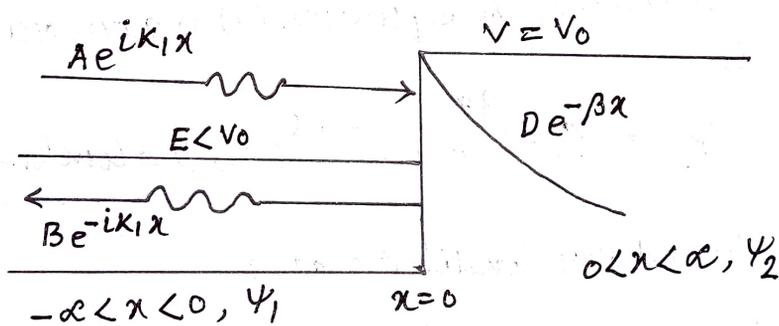


Fig-1.

Region  $-\infty < x < 0$ :  $\psi = \psi_1$ ,  $V = 0$  ( $E < V_0$ ):

Schrödinger equation for region  $-\infty < x < 0$  is

$$\frac{d^2 \psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0 \Rightarrow \frac{d^2 \psi_1}{dx^2} + K_1^2 \psi_1 = 0; K_1^2 = \frac{2mE}{\hbar^2} \dots (2)$$

The equation (2) is a simple harmonic equation having oscillatory solution given by

$$\psi_1(x) = A e^{ik_1x} + B e^{-ik_1x} = \psi_{in} + \psi_{ref}; A, B = \text{constants} \dots (3)$$

$K_1$  is a real quantity.

(2)

Region  $0 < x < \infty$ :  $\Psi = \Psi_2$  and  $V = V_0$

Schrodinger equation for region  $0 < x < \infty$  is

$$\frac{d^2 \Psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \Psi_2 = 0$$

$$\Rightarrow \frac{d^2 \Psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \Psi_2 = 0$$

$$\Rightarrow \frac{d^2 \Psi_2}{dx^2} - \beta^2 \Psi_2 = 0; \quad \beta^2 = \frac{2m}{\hbar^2} (V_0 - E) \dots (4)$$

$\beta$  is a real quantity as  $E < V_0$ :

The solution of the equation (4) is non-oscillatory and is

$$\Psi_2 = C e^{\beta x} + D e^{-\beta x}; \quad C, D = \text{constants} \dots (5)$$

The boundary conditions are:

- (i)  $\Psi = 0$  at  $x = \pm \infty$
- (ii)  $\Psi$  is continuous at the boundary (at  $x=0$ )
- (iii)  $\frac{d\Psi}{dx}$  is continuous at the boundary (at  $x=0$ )

Imposing boundary condition (i) on equation (5) we get

$$\begin{aligned} 0 &= C e^{\beta(\infty)} + D e^{-\beta(\infty)} \quad [ \because x = +\infty ] \\ &= C e^{\infty} \end{aligned}$$

To prevent R.H.S of eqn (5) from diverging we choose  $C = 0$

Hence equation (5) becomes

$$\Psi_2 = D e^{-\beta x} \text{ for } 0 < x < \infty \dots\dots (6)$$

Hence the solutions for wavefunctions for  $E < V_0$  are

$$\left. \begin{aligned} \Psi_1 &= A e^{ik_1 x} + B e^{-ik_1 x} = \Psi_{in} + \Psi_{ref} \quad (-\infty < x < 0) \\ \Psi_2 &= D e^{-\beta x} \quad (0 < x < \infty) \end{aligned} \right\} \dots\dots (7)$$

A, B and D are determined from the boundary conditions (ii) and (iii) and they are found to be

$$\left. \begin{aligned} B &= \frac{k_1 - i\beta}{k_1 + i\beta} A \\ \text{and } D &= \frac{2k_1}{k_1 + i\beta} A \end{aligned} \right\} \dots\dots (8)$$

The position probability current densities of  $\Psi_{in}$ ,  $\Psi_{ref}$  and  $\Psi_2$  are given by (using eqn 12).

$$J_{in} = \frac{\hbar k_1}{m} |A|^2, \quad J_{ref} = -\frac{\hbar k_1}{m} |A|^2 \text{ and}$$

$$J_{transmitted} = 0 \text{ for } \Psi_2$$

Reflection coefficient represents the probability of reflection and is given by

$$R = \left| \frac{J_{ref}}{J_{in}} \right| = \left| \frac{-\frac{\hbar k_1}{m} |A|^2}{\frac{\hbar k_1}{m} |A|^2} \right| = 1.$$

Transmission coefficient is

$$T = \left| \frac{J_{transmission}}{J_{in}} \right| = \left| \frac{0}{\frac{\hbar k_1}{m} |A|^2} \right| = 0.$$

(4)

$$\therefore R + T = 1 + 0 = 1$$

$\therefore \boxed{R + T = 1}$  This is the expression of Conservation of probability.

(Fig-2)

We consider the energy of the particle  $E > V_0$ :

Schrödinger equation in region  $0 < x < \infty$  is

$$\frac{d^2 \psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_2 = 0$$

$$\Rightarrow \frac{d^2 \psi_2}{dx^2} + k_2^2 \psi_2 = 0 ; k_2^2 = \frac{2m}{\hbar^2} (E - V_0) \dots (9)$$

$k_2 = \text{real quantity}$

The solution is oscillator and does not have any reflected part as the wave travels along +ve x-direction and is given by

$$\psi_2 = \psi_{\text{transmitted}} = G e^{ik_2 x} ; G = \text{constant} \dots (10)$$

Hence the solution for wave function for  $E > V_0$

$$\left. \begin{aligned} \psi_1 &= A e^{ik_1 x} + B e^{-ik_1 x} ; -\infty < x < 0 \\ \psi_2 &= G e^{ik_2 x} ; 0 < x < \infty \end{aligned} \right\} \dots (11)$$

Applying the boundary conditions (ii) and (iii) on  $\psi_1, \psi_2, d\psi_1/dx$  and  $d\psi_2/dx$ , the constants are found to be

$$B = \frac{k_1 - k_2}{k_1 + k_2} A \text{ and } G = \frac{2k_1}{k_1 + k_2} A$$

The position probability current density is given by

$$J = \frac{\hbar}{2im} \left( \psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \dots (12)$$

Using equation (12) we have

$$J_{in} = \frac{\hbar k}{m} |A|^2 \dots (13)$$

$$J_{ref} = -\frac{\hbar k_1}{m} \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2 |A|^2 \dots (14)$$

$$\text{and } J_{tr} = \frac{4\hbar k_1^2 k_2}{m(k_1 + k_2)^2} |A|^2 \dots (15)$$

Reflection Coefficient is defined as

$$\begin{aligned} R &= \left| \frac{J_{ref}}{J_{in}} \right| = \frac{\left| -\frac{\hbar k_1}{m} \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2 |A|^2 \right|}{\left| \frac{\hbar k_1}{m} |A|^2 \right|} \\ &= \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2 \\ &= \left| \frac{k_1 \left( 1 - \frac{k_2}{k_1} \right)}{k_1 \left( 1 + \frac{k_2}{k_1} \right)} \right|^2 = \left| \frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}} \right|^2 \end{aligned}$$

$$\text{Now } \frac{k_2}{k_1} = \frac{\sqrt{\frac{2m}{\hbar^2} (E - V_0)}}{\sqrt{\frac{2m}{\hbar^2} E}} = \sqrt{\frac{E - V_0}{E}} = \sqrt{1 - \frac{V_0}{E}}$$

$$\therefore R = \left| \frac{1 - \sqrt{1 - \frac{V_0}{E}}}{1 + \sqrt{1 - \frac{V_0}{E}}} \right|^2 \dots (16)$$

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Transmission Coefficient is defined as

$$\begin{aligned}
 T &= \left| \frac{J_{tr}}{J_{in}} \right| = \frac{\left| \frac{4\hbar K_1^2 K_2}{m(K_1+K_2)^2} |A|^2 \right|}{\left| \frac{\hbar K_1}{m} |A|^2 \right|} \\
 &= \frac{4 K_1 K_2}{(K_1+K_2)^2} \\
 &= \frac{4 \sqrt{\frac{2m}{\hbar^2} E} \cdot \sqrt{\frac{2m}{\hbar^2} (E-V_0)}}{\left( \sqrt{\frac{2m}{\hbar^2} E} + \sqrt{\frac{2m}{\hbar^2} (E-V_0)} \right)^2} \\
 &= \frac{4 \sqrt{E(E-V_0)}}{(\sqrt{E} + \sqrt{E-V_0})^2} \\
 &= \frac{4 \sqrt{E^2(1-\frac{V_0}{E})}}{\left[ \sqrt{E} \left( 1 + \sqrt{\frac{E-V_0}{E}} \right) \right]^2} \\
 T &= \frac{4 \sqrt{1-V_0/E}}{\left( 1 + \sqrt{1-V_0/E} \right)^2} \quad \dots \dots (17)
 \end{aligned}$$

$$\therefore R+T = \frac{(1-\sqrt{1-V_0/E})^2}{(1+\sqrt{1-V_0/E})^2} + \frac{4\sqrt{1-V_0/E}}{(1+\sqrt{1-V_0/E})^2}$$

$$= 1$$

$$\therefore \boxed{R+T=1}$$

The eqn (1) represents conservation of probability.

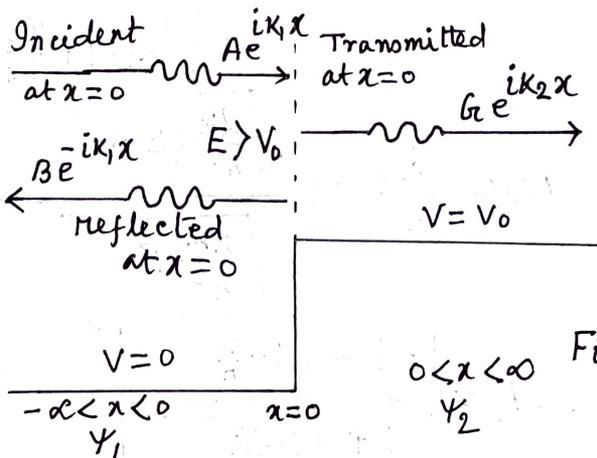


Fig-2