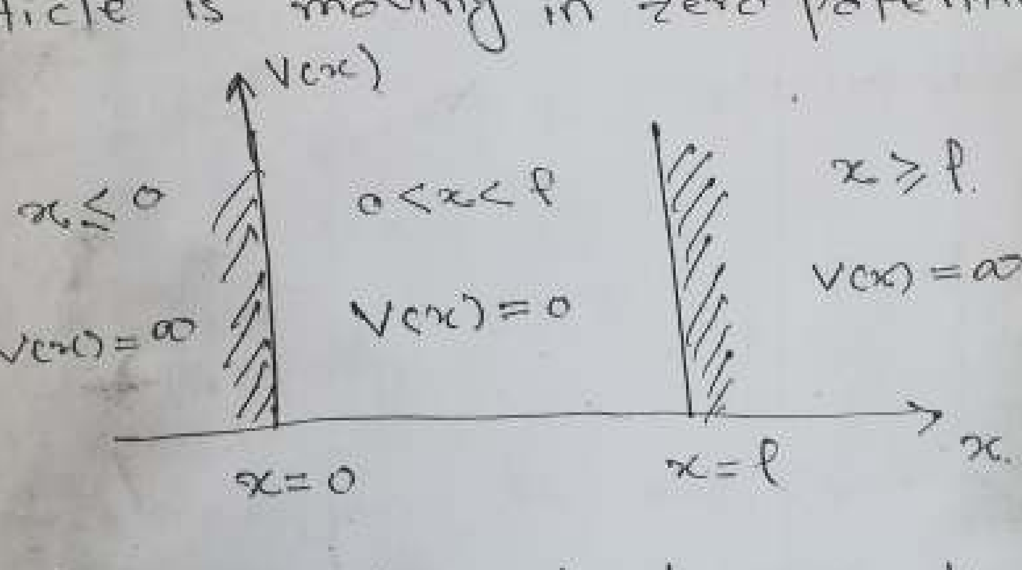
CH # 4, One-Dimensional Problems:

A Particle in a One-Dimensional Box:

The Free Particle:

Consider a particle of mass "m" moving freely along the x-axis b/w two rigid walls situated at $x = 0$ and $x = \ell$. For the free motion of the particle, we take $V(x) = 0$ i.e. the particle is moving in zero potential. inside the box.



The time independent Schrodinger equation is

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

or

$$\frac{\partial^2}{\partial x^2}\psi(x) + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

For the free motion inside the box.

$V(x) = 0$

$\Rightarrow$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0, \quad 0 < x < \ell$$

or we may write it as

$$\frac{\partial^2 \psi}{\partial x^2} + K^2 \psi(x) = 0, \quad \text{with } K^2 = \frac{2mE}{\hbar^2}$$

or

$$(D^2 + K^2)\psi(x) = 0$$

The most general solution is a combination of two linearly independent plane waves,.

$$\psi(x) = A_1 e^{iKx} + A_2 e^{-iKx} \quad \text{---} (1)$$

where A_1 and A_2 are two arbitrary constants. The first term, e^{iKx}, represents a wave traveling to the right, while the second term, e^{-iKx}, represents a wave traveling to the left.

Now equⁿ (1) can be written as

$$\psi(x) = A_1(\cos kx + i\sin kx) + A_2(\cos kx - i\sin kx)$$

or

$$= (A_1 + A_2)\cos kx + i(A_1 - A_2)\sin kx$$

$$= A\cos kx + B\sin kx$$

where $A = A_1 + A_2$

$B = i(A_1 - A_2)$

The boundary conditions for the problem are

$\psi(0) = 0$ ——— (i)

$\psi(l) = 0$ ——— (ii)

To satisfy the condition (i), we must have $A = 0$

Therefore,

$$\psi(x) = B\sin kx$$

Now using the condition (ii), we obtained

$$B\sin kl = 0$$

We can not set $B = 0$, as the wavefn ~~with~~ will then vanish. So the equⁿ $B\sin kl = 0$ is only satisfied if

$$kl = n\pi, \quad n = 1, 2, 3, \dots$$

The value $n=0$ is excluded because then $K=0$, i.e. $\psi=0$, $E=0$. A particle with $E=0$ cannot exist in the region.

then

$$K_n = \frac{n\pi}{l}$$

The solutions of the problem are therefore

$$\psi_n(x) = B \sin K_n x$$

where

$$K_n = \frac{n\pi}{l}, \quad n = 1, 2, 3, \ldots$$

The number 'n' is called the quantum number. The allowed values of K are discrete rather than continuous and the allowed values of energy are therefore,

$$E_n = \frac{p^2}{2m} = \frac{\hbar^2 K_n^2}{2m}, \quad p = \hbar K$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m l^2}, \quad n = 1, 2, 3, \ldots$$

The energy of the particle discussed in this problem is therefore quantized. The ground state of the particle is given by $n=1$ This is the lowest state:

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

This is the first energy level of the particle. The nth energy level is then

$$E_n = n^2 E_1 \quad , \quad n = 2, 3, 4, \ldots$$

The energy level diagram of the particle in a one-dimensional box is

The nth state of the particle is the ~~eigenvalue~~ eigenstate of the total energy with eigenvalue E_n i.e.

$$\hat{H}\psi_n = E_n \psi_n$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_n}{\partial x^2} = \frac{\hbar^2 K_n^2}{2m}\psi_n$$

The nth state is also an eigenstate of the momentum with eigenvalue $P_n = \hbar K_n$.

$$\hat{p}\psi_n = P_n \psi_n$$

$$-i\hbar \frac{\partial}{\partial x}\psi = \hbar K_n \psi$$

Let us normalized the wavefunction

$$\psi = B \sin Kx.$$

The total probability of finding the particle in the region $0 \leq x \leq l$ is unity i.e.

$$\int_0^l \psi^* \psi \, dx = 1$$

or

$$BB^* \int_0^l \sin^2 Kx \, dx = 1$$

or

$$BB^* \int_0^l \left(\frac{1 - \cos 2Kx}{2} \right) dx = 1$$

or

$$\frac{BB^*}{2} l = 1$$

$$BB^* = \frac{2}{l}$$

As B is complex, we write $\underline{\underline{B = a e^{i\theta}}}$

then

$$BB^* = a^2$$

Phase

So we have

$$a = \sqrt{\frac{2}{l}}$$

$\psi^* \psi$ is independent of θ, therefore we may take $B = \sqrt{\frac{2}{l}}$

Since

$$\psi^* \psi = B B^* \sin^2 kx.$$

$$= a^2 \sin^2 kx$$

$$\psi^* \psi = \sqrt{\frac{2}{l}} \sin^2 (kx)$$

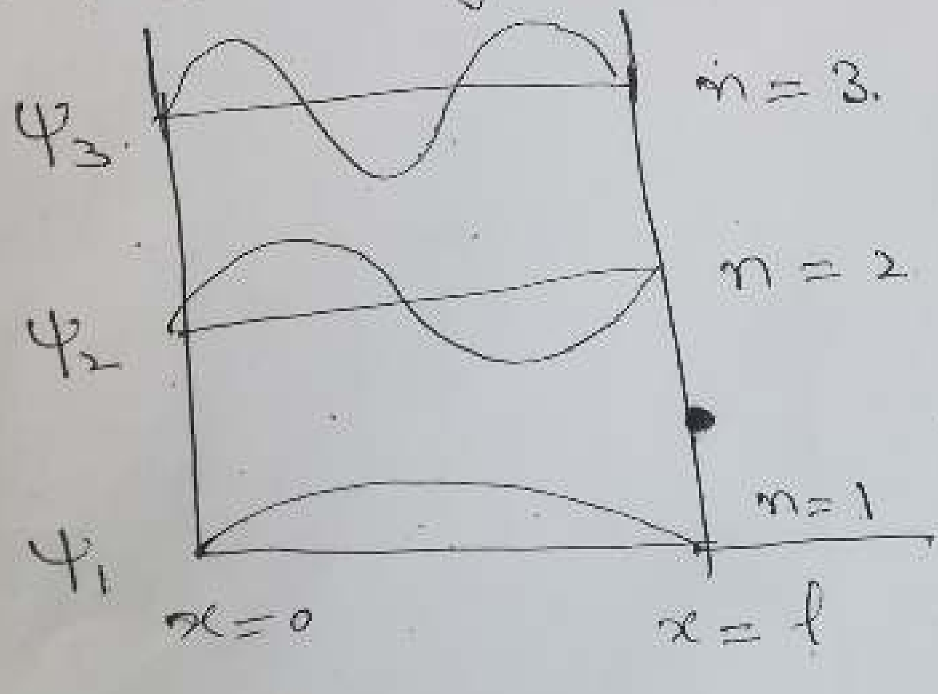
Hence the normalized wave fn.

$$\psi_n(x) = \sqrt{\frac{2}{l}} \sin (K_n x)$$

or

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{l}} \sin \left(\frac{n\pi}{l} x\right)}$$

The wavefunctions for $n = 1, 2, 3$ are shown in the diagram.



The probability density is

$$P(x) = |\psi_n|^2 = \frac{2}{l} \sin^2\left(\frac{n\pi x}{l}\right)$$

$P(x)$ is maximum when

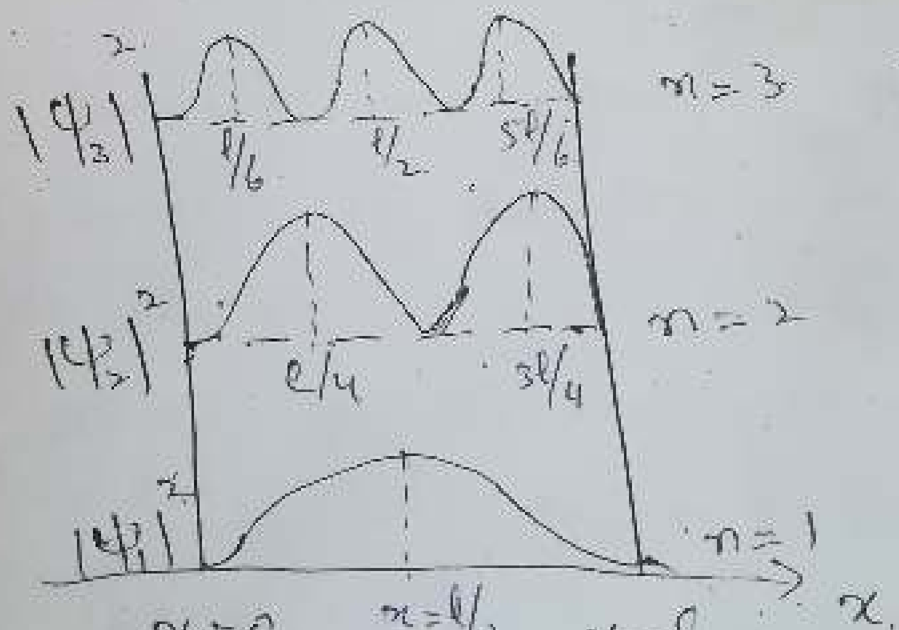
$$\frac{n\pi x}{l} = \pi/2,\ 3\pi/2,\ 5\pi/2 \ldots$$

or $$x = \frac{l}{2n},\ \frac{3l}{2n},\ \frac{5l}{2n}, \ldots$$

For the state $n=1$, the most probable position of the particle is at $x = l/2$.

for $n=2$, the most probable probable position is at $x = l/4$; and $x = 3l/4$.

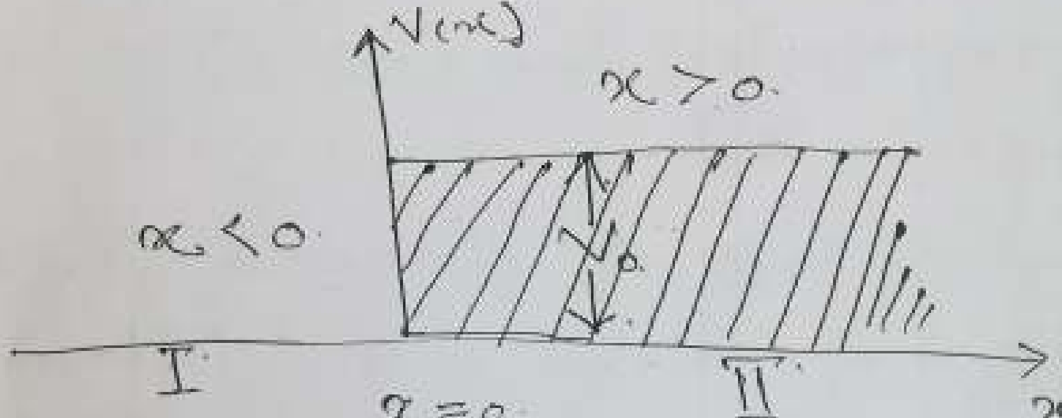
The variation of $P(x)$ with x for $n = 1, 2, 3$ is shown below.



The Potential Step:

A particle that is free everywhere, but beyond a particular point, i.e. $x = 0$, the potential increases sharply (i.e. it becomes repulsive or attractive). A potential of this type is called a potential step of the form

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



The potential is constant in region II.

In this problem, we analyse the dynamics of a flux of particles moving from left to right.

Let us consider the Schrodinger wave equation separately for region I $(x < 0)$ and region II $(x \geq 0)$.

we also distinguish the cases for the particle energy larger or smaller than V_0:

i). $E > V_0$

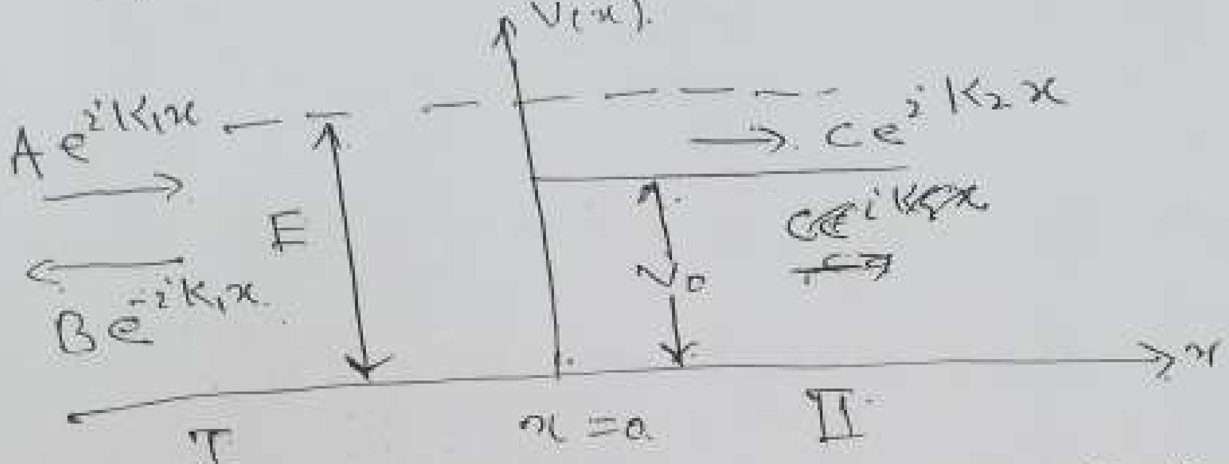
ii) $E < V_0$

Particle Energy Above the Potential Step: $(E > V_0)$

The particles are free for in region I $(x < 0)$ and feel a repulsive potential V_0 at $x = 0$ in region II $(x \geq 0)$. Classically the particle approach the potential step or barrier from the left with a constant momentum $\sqrt{2mE}$. As the particle enter the region II $(x \geq 0)$, where the potential is V_0, its momentum slow down to $\sqrt{2m(E-V_0)}$. Since the particles have enough energy to penetrate into the region II $(x \geq 0)$, there will be total transmission: all the particles will emerge to the right with a smaller kinetic energy $E - V_0$.

The Schrodinger wave equ: in one-dimension is

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi = 0$$



Hence the S.W.E in region I ($x<0$) is,

I $$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_1 = 0 \qquad \because V_0 = 0$$

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0$$

where $$K_1 = \frac{\sqrt{2mE}}{\hbar}$$

In region II, the equ will be

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

or

$$\frac{d^2\psi_2}{dx^2} + K_2^2 \psi_2 = 0$$

where $K_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

The most general solutions of the above equations in region I $(x<0)$ and in region II $(x \geq 0)$ are,

$\underline{\underline{I}}$ $\psi_1 = A e^{iK_1 x} + B e^{-iK_1 x}$ — $(x<0)$

$\underline{\underline{II}}$ $\psi_2 = C e^{iK_2 x} + D e^{-iK_2 x}$ — $(x \geq 0)$

In region II $(x \geq 0)$, the term $D e^{-iK_2 x}$ represents the reflected wave in the negative x-direction.

Since, there is no such wave, therefore, $D = 0$, So ~~the~~ solutions are now.

$\underline{\underline{I}}$ $\psi_1 = A e^{iK_1 x} + B e^{-iK_1 x}$ — $(x<0)$

$\underline{\underline{II}}$ $\psi_2 = C e^{iK_2 x}$ — $(x \geq 0)$

Here, Ae^{iK_1x}, Be^{-iK_1x}, and Ce^{iK_2x} represent the incident, the reflected, and the transmitted waves, respectively. Since $V(x)$ is finite everywhere ~~and~~ therefore any wave fn and its derivative are continuous at $x=0$.

Therefore, one can write

i). $\psi_1(0) = \psi_2(0)$, gives.

$$A+B = C. \quad \text{——} (1)$$

ii) $$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

as. $$\psi_1(x) = Ae^{iK_1x} + Be^{-iK_1x}$$

$$\frac{d\psi_1(x)}{dx} = iK_1Ae^{iK_1x} - iK_1Be^{-iK_1x}$$

at $x=0$

$$\frac{d\psi_1(0)}{dx} = AiK_1 - BiK_1$$

Also $$\psi_2(x) = Ce^{iK_2x}$$

$$\frac{d\psi_2(x)}{dx} = iK_2Ce^{iK_2x}$$

at. $x=0$.

$$\frac{d\psi_2(0)}{dx} = iK_2C.$$

Now,
$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx} \text{ gives.}$$

$$iK_1A - iK_1B = iK_2C.$$

$$K_1A - K_1B = K_2C \text{ ——— (2)}$$

By putting the value of "C" from (1) in (2), one can get.

$$K_1A - K_1B = K_2(A+B).$$

$$K_1A - K_2A = K_1B + K_2B.$$

$$A(K_1 - K_2) = B(K_1 + K_2)$$

$$\boxed{\frac{B}{A} = \frac{K_1 - K_2}{K_1 + K_2}}$$

Now, we know

$$A + B = C.$$

$$\Rightarrow B = C - A, \text{ put in equ: (2)}$$

$$K_1A - K_1(C - A) = K_2C$$

$$\Rightarrow \boxed{\frac{C}{A} = \frac{2K_1}{K_1 + K_2}.}$$

Let us calculate the reflection "R" and transmission "T" co-efficients as.

$$R = \left| \frac{\text{reflected current density}}{\text{incident current density}} \right| = \left| \frac{J_r}{J_i} \right|$$

and

$$T = \left| \frac{\text{transmitted current density}}{\text{incident current density}} \right| = \left| \frac{J_t}{J_i} \right|$$

"R" represents the ratio of reflected to the incident beams and "T" the ratio of the transmitted to the incident beams.

where J_i, J_r, and J_t, represent the incident, reflected, and transmitted current densities (flux), respectively and defined as.

$$J_i = \frac{\hbar}{2mi}\left(\psi_i^* \frac{\partial \psi_i}{\partial x} - \psi_i \frac{\partial \psi_i^*}{\partial x} \right) \text{ - incident}$$

$$J_r = \frac{\hbar}{2mi}\left(\psi_r^* \frac{\partial \psi_r}{\partial x} - \psi_r \frac{\partial \psi_r^*}{\partial x} \right) \text{ - reflected}$$

$$J_t = \frac{\hbar}{2mi}\left(\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x} \right) \text{ - transmitted}$$

Incident Current Density:

$$J_i = \frac{\hbar}{2mi}\left(\psi_i^* \frac{\partial \psi_i}{\partial x} - \psi_i \frac{\partial \psi_i^*}{\partial x}\right)$$

Now

$$\psi_i = A e^{ik_1x}, \quad \psi_i^* = A e^{-ik_1x}$$

$$\frac{\partial \psi_i}{\partial x} = ik_1 A e^{ik_1x}$$

and

$$\frac{\partial \psi_i^*}{\partial x} = -ik_1 A e^{-ik_1x}$$

put in above equ' on get

$$J_i = \frac{\hbar}{2mi}\left(A e^{-ik_1x} ik_1 A e^{ik_1x} - A e^{ik_1x} \times (-ik_1 A e^{-ik_1x})\right)$$

$$\boxed{J_i = \frac{\hbar k_1}{m} |A|^2}$$

Transmitted Current Density:

$$J_t = \frac{\hbar}{2mi}\left(\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x}\right)$$

Now

$$\psi_t = C e^{ik_2x}, \quad \psi_t^* = C e^{-ik_2x}$$

then

$$\frac{\partial \psi_t}{\partial x} = i k_2 C e^{i k_2 x}.$$

and

$$\frac{\partial \psi_t^*}{\partial x} = -i k_2 C e^{-i k_2 x}.$$

Then

$$J_t = \frac{\hbar}{2mi}\left(C e^{-i k_2 x}\, i k_2 C e^{i k_2 x} - C e^{i k_2 x} \times (-i C k_2 e^{-i k_2 x})\right).$$

$$J_t = \frac{\hbar}{m} k_2 |C|^2$$

Now we know

$$\frac{C}{A} = \frac{2k_1}{k_1+k_2}$$

$$C = \frac{2k_1}{k_1+k_2} A.$$

So

$$|C|^2 = \frac{4k_1^2}{(k_1+k_2)^2} |A|^2$$

Hence

$$\boxed{J_t = \frac{\hbar}{m} \frac{4k_1^2}{(k_1+k_2)^2} k_2 |A|^2}$$

Reflected Current Density:

Define as:

$$J_r = \frac{\hbar}{2mi}\left(\psi_r^* \frac{\partial \psi_r}{\partial x} - \psi_r \frac{\partial \psi_r^*}{\partial x}\right)$$

Now:

$$\psi_r = Be^{-ik_1x}, \quad \psi_r^* = Be^{ik_1x}$$

$$\frac{\partial \psi_r}{\partial x} = -iBK_1 e^{-ik_1x}$$

and

$$\frac{\partial \psi_r^*}{\partial x} = iBK_1 e^{ik_1x}$$

So:

$$J_r = \frac{\hbar}{2mi}\left[Be^{ik_1x}\times\left(-iBK_1 e^{-ik_1x}\right) - Be^{-ik_1x}\times\left(iK_1B e^{ik_1x}\right)\right]$$

$$= -\frac{\hbar}{m} K_1 |B|^2$$

we know that

$$\frac{B}{A} = \frac{K_1 - K_2}{K_1 + K_2}$$

$$B = \frac{K_1 - K_2}{K_1 + K_2}$$

then

$$\boxed{J_r = \frac{-\hbar}{m}\frac{(k_1-k_2)^2}{(k_1+k_2)^2}k_1|A|^2}$$

The transmission co-efficient "T" is ~~an~~ defined as

$$T = \left|\frac{J_t}{J_i}\right|$$

By putting the value of J_t and J_i

one gets

$$\boxed{T = \frac{4k_1k_2}{(k_1+k_2)^2}}$$

The reflection co-efficient "R" is.

$$R = \left|\frac{J_r}{J_i}\right|$$

By putting the values of J_r ad. J_i,

one gets

$$\boxed{R = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}}$$

The sum of T and R is equal to 1

$$R+T = \frac{4k_1k_2}{(k_1+k_2)^2} + \frac{(k_1-k_2)^2}{(k_1+k_2)^2} = 1$$

when $\underline{E \leq V_0}$

then

$$\left.\begin{array}{l} T = 0 \\ R = 1 \end{array}\right\}$$ every thing is reflected

when

$\underline{\underline{E \gg V_0}}$ (V_0 can be neglected)

then

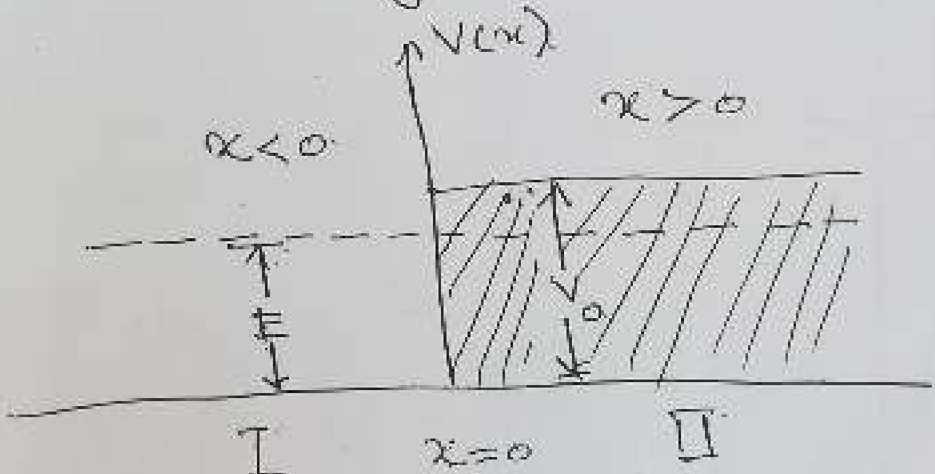
$$\left.\begin{array}{l} T = 1 \\ R = 0 \end{array}\right\}$$ every thing is Transmitted

Particle Energy Below the Potential Step: ($E < V_0$)

Classically, when the particle reaches to potential step with energy $E = P^2/2m$ less than the energy of the barrier height i.e. $E < V_0$, will stop at $x = 0$ and then

~~part~~ will bounce back with same energy. Hence, in this case, there is total reflection of the particle occurs.

Quantum mechanical picture is different from classical one. The S.W.E for the two regions $x<0$ and $x>0$ are



In region I $(x<0)$

I. $$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0$$

where

$$K_1 = \frac{\sqrt{2mE}}{\hbar}$$

(11a)

In region II $(x \geq 0)$

II

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

$$\frac{d^2\psi_2}{dx^2} - K^2\psi_2 = 0$$

where $K = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

The solutions are

I $\psi_1 = Ae^{iK_1x} + Be^{-iK_1x} \Rightarrow (x < 0)$

II $\psi_2 = Ce^{Kx} + De^{-Kx} \Rightarrow (x \geq 0)$

Since, the wavefn must be finite everywhere, but the term e^{Kx} produce divergence at $x \to \infty$, therefore we need to put $\boxed{C = 0}$

Continuity of ψ_1 and ψ_2 and also their derivatives implies that

$$\psi_1(0) = \psi_2(0)$$

$$A + B = D \quad \text{——} \; (1)$$

and

$$\frac{d\psi_1(0)}{dx} = \frac{d}{dx}\psi_2(0) \rightarrow$$

$$iK_1 A - iK_1 B = -KD \quad \text{——} \; (2)$$

By putting the value of "D" from (1) in (2), one gets

$$iK_1 A - iK_1 B = -K(A+B) = -KA - KB$$

$$\boxed{\frac{B}{A} = \frac{iK_1 + K}{iK_1 - K}}$$

Now putting the value of "B" from (1) in (2) one obtain

$$\boxed{\frac{D}{A} = \frac{2iK_1}{iK_1 - K}}$$

Hence, the resulting wave fns are

$$\psi_1 = A\left[e^{ik_1x} + \frac{ik_1+K}{ik_1-K}\, e^{-ik_1x}\right]$$

$$\psi_2 = A\, \frac{2ik_1}{ik_1-K}\, e^{-Kx}$$

Incident Current Density:

$$J_i = \frac{\hbar}{2mi}\left(\psi_i^* \frac{\partial \psi_i}{\partial x} - \psi_i \frac{\partial \psi_i^*}{\partial x}\right)$$

Now

$$\psi_i = A\, e^{ik_1x}, \quad \psi_i^* = A\, e^{-ik_1x}$$

$$\frac{\partial \psi_i}{\partial x} = A\, ik_1\, e^{ik_1x}$$

and

$$\frac{\partial \psi_i^*}{\partial x} = -ik_1 A\, e^{-ik_1x}$$

then

$$\boxed{J_i = \frac{\hbar}{m}\, k_1\, |A|^2}$$

Transmitted Current Density:

$$J_t = \frac{\hbar}{2mi}\left(\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x}\right)$$

So

$$\psi_t = D e^{-Kx}, \quad \psi_t^* = D e^{-Kx}$$

$$\frac{\partial \psi_t}{\partial x} = -DK e^{Kx}, \quad \frac{\partial \psi_t^*}{\partial x} = -DK e^{-Kx}$$

Hence

$$\boxed{J_t = 0}$$

Reflected Current Density:

$$J_r = \frac{\hbar}{2mi}\left(\psi_r^* \frac{\partial \psi_r}{\partial x} - \psi_r \frac{\partial \psi_r^*}{\partial x}\right)$$

so

$$\psi_r = B e^{-ik_1x}, \quad \psi_r^* = B e^{ik_1x}$$

$$\frac{\partial \psi_r}{\partial x} = -B ik_1 e^{-ik_1x}, \quad \frac{\partial \psi_r^*}{\partial x} = ik_1 B e^{ik_1x}$$

then

$$J_r = -\frac{\hbar}{m} k_1 |B|^2$$

The transmission Co-efficient "T" is

$$\boxed{T = \left|\frac{J_t}{J_i}\right| = 0}$$

and the reflection co-efficient "R" is

$$R = \left|\frac{J_r}{J_i}\right|$$

$$R = \frac{\hbar/2m \; K_1 |B|^2}{\hbar/2m \; K_1 |A|^2}$$

$$R = \frac{|B|^2}{|A|^2} = \frac{B^* B}{A^* A}$$

Now

$$\frac{B}{A} = \frac{iK_1 + K}{iK_1 - K}$$

$$B = \left(\frac{iK_1 + K}{iK_1 - K}\right) A$$

$$B^* = \frac{K - iK_1}{(-iK_1 - K)} A^*$$

then

$$\boxed{R = 1}$$

As $R + T = 1$

$\boxed{R = 1}$, $T = 0$

There is total reflection, no transmission which is in accordance with the classical mechanics; But, we know that, $\psi_t = D e^{-kx}$

$D = \frac{2ik_1}{ik_1 - k} A$

$$\psi_t = \frac{2ik_1}{ik_1 - k} A e^{-kx}$$

Hence, the probability of finding the particle in region II $(x > 0)$ is

$$P(x) = \psi_t^* \psi_t = |\psi_t|^2$$

$$\psi_t^* = \frac{-2ik_1}{-ik_1 - k} A e^{-kx}$$

$$P(x) = \frac{-2ik_1}{-ik_1 - k} A e^{-kx} \cdot \frac{2ik_1}{ik_1 - k} A e^{-kx}$$

$$= \frac{-4i^2 k_1^2}{-(ik_1 + k)(ik_1 - k)} |A|^2 e^{-2kx}$$

$$= \frac{4k_1^2}{-[(ik_1)^2 - (k)^2]} |A|^2 e^{-2kx}$$

$$P(x) = \frac{4K_1^2}{K_1^2+K^2} |A|^2 e^{-2Kx}$$

One can observe that the probability of finding the particle in region II ($x \geq 0$) is not zero. Although the reflection co efficient is one i.e. $\boxed{R=1}$, still there is some probability of finding the particle in classically forbidden region II. It means that reflection does not take place at $x = 0$.

The behaviour of the probability density is shown below, which falls exponentially to small values as x becomes larger.