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T.Y. B.Sc. Physics Sem IV. (CBSC pattern 2021-2022)

Paper II- PHY 362 Quantum Mechanics

Unit-3 Applications of Schrodinger's Equation

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CHAPT # 3

Applications of Schrödinger's equation

Free particle:

The Force acting on a particle is zero, the particle is a free particle

(As $V(x) =$ constant
Force $F = -\frac{dV}{dx}$ to be zero)

Consider the schrödinger's time independent equation.

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

with $V=0$, it is

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{—— (1)}$$

or $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{—— (2)} \quad \left(k^2 = \frac{2mE}{\hbar^2}\right)$$

The solutions of this equation are eigen functions. They can be e^{-ikx} & e^{+ikx}

The solution of time part is $\phi(t) = e^{-\frac{iEt}{\hbar}}$

As $E = h\nu$, $\phi(t) = e^{-i\omega t}$

The wave function is

$$\Psi(x,t) = \psi(x)\cdot\phi(t)$$
$$= e^{ikx} \cdot e^{-i\omega t}$$
$$\Psi(x,t) = e^{i(kx-\omega t)} \quad \text{—— (3)}$$

or $$\Psi(x,t) = e^{-ikx} \cdot e^{-i\omega t}$$
$$= e^{-i(kx+\omega t)} \quad \text{—— (4)}$$

Eqn (3) represents wave propagating along positive x axis.

Eqn (4) represents wave propagating along negative x axis.

For a wave propagating along positive x axis and having A as normalisation constant the wave function is

$$\psi(x,t) = A e^{i(kx-\omega t)}$$

The probability density is $\psi^*\psi = A^*A = \text{Const}$

∴ the particle is equally likely to be found everywhere.

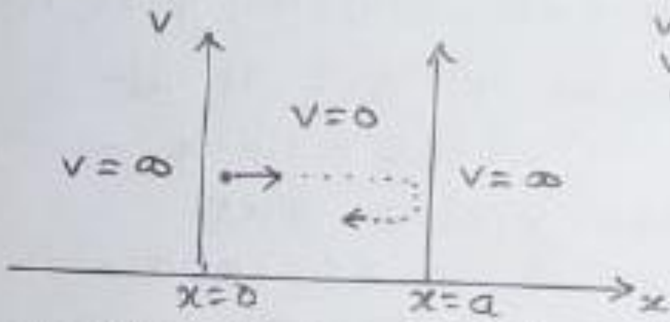
Energy of the free particle is $E = \frac{p^2}{2m}$.

The energy spectrum of the free particle is continuous.

** Particle in infinitely deep potential well (one dimensional case)

Here the particle has one dimensional motion along x axis between two points $x=0$ and $x=a$. It can not go to the left of $x=0$ and to the right of $x=a$.

Potential	Region
$V=\infty$	$x \le 0$
$V=0$	$0<x<a$
$V=\infty$	$x \ge a$



This particle is also called a particle in one dimensional rigid box.

Schrödinger's time independent equation is

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \qquad \text{—(1)}$$

As $V=0$ for $0<x<a$,

the equation becomes

$$\frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0 \qquad \text{—(2)}$$

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad \left(k^2=\frac{2mE}{\hbar^2}\right) \qquad \text{—(3)}$$

The general solution to this second order linear homogeneous differential equation can be written as

$$\psi(x)=A\sin kx+B\cos kx \qquad \text{—(4)}$$

where, A & B are arbitrary constants and can be obtained by using boundary conditions on ψ.

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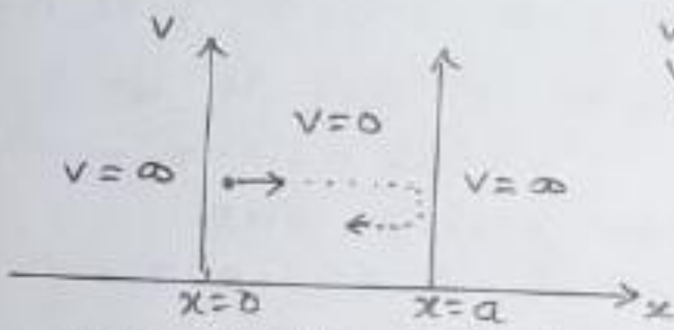

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$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

From eq (8) it can be seen that certain allowed energy values ... are possible with the values of integer n. This integer n is called a quantum number.

The ground state is obtained with $n=1$.

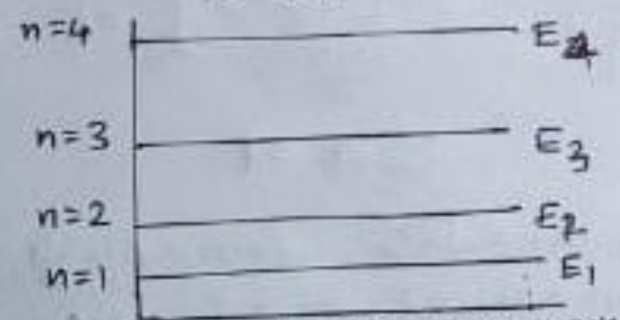
$$\therefore \quad E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad \text{—— (9)}$$

This is also known as zero point energy. (classically it is zero, but quantum mechanically it is non-zero.)

$$E_2 = 4\frac{\pi^2\hbar^2}{2ma^2} = 4E_1$$

$$E_3 = 9E_1$$

$$\therefore \quad E_n = n^2 E_1$$



Energy spectrum -

wave functions:

$$\psi_n(x) = A \sin\left(\frac{n\pi}{a} x\right) \quad \text{---(10)}$$

Normalisation condition for it is

$$\int_0^a |\psi_n(x)|^2 dx = 1$$

$$\therefore |A|^2 \int_0^a \sin^2\left(\frac{n\pi}{a} x\right) dx = 1 \quad \text{---(11)}$$

From $\sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$, eqn (11) becomes

$$|A|^2 \int_0^a \frac{1}{2}\left[1 - \cos\left(\frac{2n\pi}{a} x\right)\right] dx = 1$$

$$\frac{|A|^2}{2} \int_0^a \left[1 - \cos\left(\frac{2n\pi}{a} x\right)\right] dx = 1$$

$$\frac{|A|^2}{2} \int_0^a \left[dx - \cos\left(\frac{2n\pi x}{a}\right) dx\right] = 1$$

$$\frac{|A|^2}{2} \left[x - \frac{\sin\left(\frac{2n\pi x}{a}\right)}{\frac{2n\pi}{a}}\right]_0^1 = 1$$

$$\therefore \frac{|A|^2}{2} a = 1$$

$$\therefore |A| = \sqrt{2/a} \quad \text{(normalisation constant)}$$

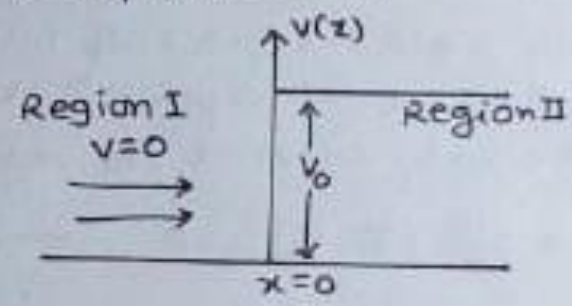
Hence normalised wave function is

$$\psi_n(x) = \sqrt{2/a} \sin\left(\frac{n\pi}{a} x\right) \quad \text{---(12)}$$

For ground state, $n=1$

$$\therefore \psi_1(x) = \sqrt{2/a} \sin\left(\frac{\pi}{a} x\right) \quad \text{---(13)}$$

* Step potential



Potential Region

$V(x) = 0$ for $x \leq 0$

$= V_0$ for $x > 0$

A particle of energy E is considered to be moving along the positive direction of x axis.

<u>Classical Treatment</u>:

<u>Case I</u> : $E > V_0$

For particle with energy $E > V_0$, the reflection probability $R = 0$ and transmission probability $T = 1$

<u>Case II</u> : $E < V_0$

$R = 1$ and $T = 0$

<u>Quantum mechanical treatment</u>:

The potential is independent of time. So the time independent Schrödinger's equation can be used.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{—— (1)}$$

For region I, $V=0$ (wave function is ψ_1)

$$\therefore \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0 \quad \text{—— (2)}$$

$$\therefore \frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0 \quad \text{—— (3)} \quad \text{where } k_1^2 = \frac{2mE}{\hbar^2}$$

The solution of this equation is

$$\psi_1 = A e^{ik_1x} + B e^{-ik_1x} \quad \text{—— (4)}$$

The first term Ae^{ik_1x} represents incident wave.
The second term Be^{-ik_1x} represents reflected wave.
The Schrödinger's equation for region II is

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0 \quad \text{———} (5)$$

Case I: $E > V_0$

$$k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$\therefore$ eqn (5) becomes

$$\frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 = 0 \quad \text{———} (6)$$

Solution for this is

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \quad \text{——} (7)$$

In region II, Ce^{ik_2x} represents transmitted wave.

$D = 0$ as there is no flow of particles in negative x direction.

$$\therefore \psi_2 = Ce^{ik_2x} \quad (8)$$

Boundary conditions:

At $x = 0$ $\quad \psi_1 = \psi_2$

$$\therefore A + B = C \quad \text{———} (9)$$

and $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ (at $x = 0$)

$$\therefore k_1(A - B) = k_2C \quad \text{———} (10)$$

multiplying eqn (9) by k_1 & adding to eqn (10)

$$2k_1A = (k_1 + k_2)C$$

$$\therefore C = \frac{2k_1}{(k_1 + k_2)}A \quad \text{—} (11)$$

Substituting in (9), we get

$$B = \frac{k_1 - k_2}{k_1 + k_2} A \quad \text{—— (12)}$$

The wave function for incident waves is

$$\psi_{in} = A e^{ik_1x}$$

$$\therefore \psi_{in}^* = A^* e^{-ik_1x}$$

Probability current density

$$J_{in} = \frac{\hbar}{2mi}\left(\psi_{in}^* \frac{d\psi_{in}}{dx} - \psi_{in}\frac{d\psi_{in}^*}{dx}\right)$$

$$\therefore \boxed{J_{in} = \frac{\hbar k_1}{m}|A|^2} \quad \text{—— (13)}$$

The wavefunction for reflected waves is

$$\psi_{ref} = B e^{-ik_1x}$$

$$\therefore \psi_{ref}^* = B^* e^{ik_1x}$$

$$\therefore \boxed{J_{ref} = \frac{\hbar k_1}{m}|B|^2} \quad \text{—— (14)}$$

For transmitted wave

$$\psi_2 = \psi_{tr} = C e^{ik_2x}$$

$$\therefore \boxed{J_{tr} = \frac{\hbar k_2}{m}|C|^2} \quad \text{—— (15)}$$

Transmission probability T is given by

$$T = \frac{J_{tr}}{J_{in}} = \frac{k_2|C|^2}{k_1|A|^2}$$

using eqn (11)

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

$$\therefore T = \frac{4k_1k_2}{(k_1+k_2)^2} \quad \text{—— (16)}$$

Reflection probability R is given by

$$R = \frac{J_{ref}}{J_{in}}$$

$$= \frac{|B|^2}{|A|^2} \quad \left(\text{using eq}^n (13) \& (14)\right)$$

$$\therefore R = \frac{(K_1 - K_2)^2}{(K_1 + K_2)^2} \quad \left(\text{using eq}^n (12)\right) \quad \text{——} (17)$$

$$\therefore R + T = \frac{(K_1 - K_2)^2}{(K_1 + K_2)^2} + \frac{4K_1K_2}{(K_1 + K_2)^2} \quad \left(\text{using eq } 16 \& 17\right)$$

$$\therefore R + T = 1$$

Case II : $E < V_0$

Here, $$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0 \quad \text{——} (18)$$

$$\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

$$\therefore \frac{d^2\psi_2}{dx^2} - \alpha^2\psi_2 = 0 \quad \text{——} (19)$$

$\therefore$ solution, $$\psi_2 = \psi_{tr} = Ce^{-\alpha x} \quad \text{——} (20)$$

Current density, $$J_{tr} = \frac{\hbar}{2mi}\left(\psi_{tr}^* \frac{d\psi_{tr}}{dx} - \psi_{tr}\frac{d\psi_{tr}^*}{dx}\right)$$

As $\psi_{tr} = Ce^{-\alpha x}$, $\psi_{tr}^* = C^* e^{-\alpha x}$

$$\therefore J_{tr} = 0$$

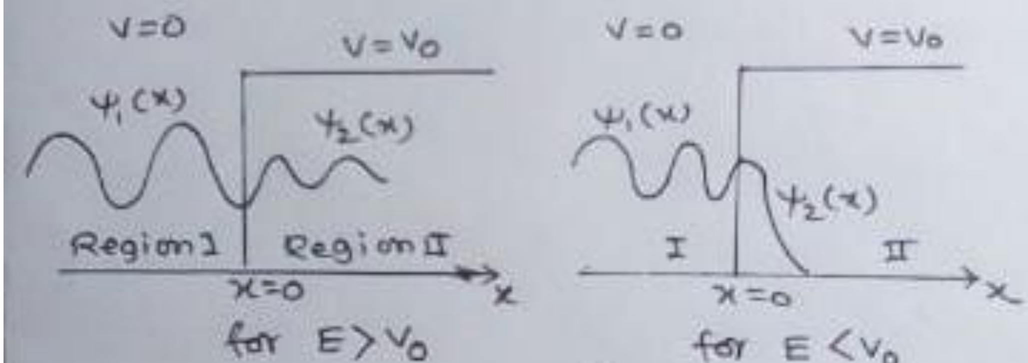
$$\therefore T = 0$$

As $R + T = 1$, $R = 1$ indicates complete reflection.

This shows that quantum mechanical results are the same as those of classical results for this case.

However, the function has a tail into the classically forbidden region. It is represented by $e^{-\alpha x}$.

The tail becomes shorter and shorter as E becomes smaller & smaller as compared to V_0. There is small probability of finding the particle in region $x > 0$. This phenomenon is called barrier penetration.



wave functions.