21/10/19

Module-IV

→ In quantum mechanics physical system is characterised by a wave function which contains all information for probabilistic description of a system.

→ Any physical property of a system instead of having a exact value, can take a number of allowed values with different probabilities.

→ So, this probabilistic description is the basic characteristic of quantum physics and achieved by the wave function.

What is a wave function?
Wave functions are the mathematical representation of particles which contain all information required for the probabilistic description of the particle.

Characteristics of Wave Function -
→ Wave function is in general a mathematical function of space and time such that,

$$\psi(r,t) = \psi(x,y,z,t) = Ae^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

→ Wave function is in general a complex quantity such that,

$$\psi\psi^* = \psi^*\psi = |\psi|^2.$$

which determine the probability density and it is a real quantity.

→ 'ψ' must be finite every where.

→ It is a single valued function. It has one particular value at a point 'r' and at any time 't'. It vanishes at infinity.

→ The wave function 'ψ' and its first derivative $\left(\frac{\partial\psi}{\partial x}\right)$ is continuous everywhere.

if wave is in x-axis.

including boundaries.

→ Ψ satisfies Schrodinger's wave eqⁿ

→ Ψ must be normalizable or Ψ is a normalized wave function.

[Condition for normalization -
$$\int |\Psi|^2 dV = 1$$]

Probability Density ($|\Psi|^2$) -

It is the probability of finding the particle per unit volume and it is given by,

$$\Psi \Psi^* = \Psi^* \Psi = |\Psi|^2$$

So, the total probability $= \int |\Psi|^2 dV = 1$

Principle Of Superposition -

The wave function representing the actual state of a system is a linear superposition (combination) of different possible allowed states in which the system can exist.

Let $\Psi_1, \Psi_2, \Psi_3 \ldots\ldots \Psi_n$ represent ~~are~~ the different allowed states in which the system can exist.

Then $\Psi = C_1\Psi_1 + C_2\Psi_2 + C_3\Psi_3 + \ldots\ldots + C_n\Psi_n$

$$= \sum_{i=1}^{n} C_i \Psi_i$$

where, $C_1, C_2, C_3 \ldots\ldots C_n$ are the coeff. called as the probability amplitude.

C_i^2 is the probability of the system being in the state Ψ_i

Probability is the sq. of coeff of that particular state.

So, $C_1^2 + C_2^2 + C_3^2 + \dots\dots + C_n^2 = 1$

4/11/19 Operators, Eigen Values, Eigen Functions and Expectation Values-

Operators-
Any dynamical quantity like position, momentum energy etc. can be observed or measured. and known as observables.
To every observable quantity their exist an operator. So, every physical quantity is associated with a quantum mechanical operator.

Observables- (Physical quantity)	Operators 3-D	Operators 1-D
(i) Total Energy (E)	$i\hbar \frac{\partial}{\partial t}$	$i\hbar \frac{\partial}{\partial t}$
(ii) Linear Momentum (p)	$-i\hbar \nabla$	$-i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z}$
(iii) Kinetic Energy.	$\frac{-\hbar^2}{2m} \nabla^2$	$\frac{-\hbar^2}{2m} \frac{\partial}{\partial x}, \frac{-\hbar^2}{2m} \frac{\partial}{\partial y}, \frac{-\hbar^2}{2m} \frac{\partial}{\partial z}$
(iv) Potential Energy (V)	$V(r)$	$V(x), V(y), V(z)$
(v) Hamiltonian (H)	$\frac{-\hbar^2}{2m} \nabla^2 + V(r)$.	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$. $\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + V(y)$ $\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V(z)$.

Eigen Function -

The allowed quantum states of a physical system are called as eigen states and represented by a set of function called Eigen function.

The actual wave function of the system is the linear combination of Eigen function.

If $\psi_1, \psi_2, \psi_3 \ldots \psi_n$ are the Eigen function of a system with coeff. $c_1, c_2, c_3 \ldots c_n$ then the wave functions are,

$$\psi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \ldots + c_n\psi_n$$

Eigen Values-

The set of allowed values of a physical quantity for a given system is called Eigen values.

Expectation Value-

In quantum mechanics every system is described in a probabilistic manner for a given state of a system the diff. eigen values of a quantity occur with diff relative probabilities. If $q_1, q_2, q_3 \ldots q_n$ are the eigen values of a physical quantity q and they occur with probabilities $P_1, P_2, P_3 \ldots P_n$ then the expectation value of q (Weighted avg. value) is represented by $\langle Q \rangle$

$$\langle Q \rangle = \frac{P_1q_1 + P_2q_2 + P_3q_3 + \ldots P_nq_n}{P_1 + P_2 + P_3 + \ldots P_n}$$

$$= \sum_{i=1}^{n} P_iq_i$$

By Integration Method-

ψ, ψ^*.

find the momentum expectation value.

$$\langle p \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx} = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx.$$

Q.1. The probability that a system can be represented by eigen function ψ_1, ψ_2, ψ_3 are $1/2$, $1/3$ and $1/6$ respectively write the wave function for the system.

If the energy eigen values for the above states are 4 eV, 6 eV and 9 eV then find energy expectation value.

Q.2. The wave function ψ of ~~of~~ a system is a linear combination of the eigen function $\phi_1, \phi_2, \phi_3, \phi_4$ and ϕ_5 and given by

$$\psi = \frac{1}{\sqrt{3}}\phi_1 + \frac{1}{\sqrt{3}}\phi_2 + \frac{1}{\sqrt{6}}\phi_3 + \frac{1}{\sqrt{24}}\phi_4 + \frac{1}{\sqrt{8}}\phi_5$$

What is the probability of the system being in the state ϕ_3.

Q.3. A particle is observed to have 5 quantum states i.e. $\psi_1, \psi_2, \psi_3, \psi_4$ and ψ_5 with relative probabilities, 0.2, 0.1, 0.3, 0.2 and 0.2 respectively. If the corresponding energy eigen values for this states are 2 eV, 3 eV, 3 eV, 1 eV and 1 eV. Calculate the ~~energy~~ energy expectation value.

2. $P_3 = \frac{1}{6}$

1. $\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{3}}\psi_2 + \frac{1}{\sqrt{6}}\psi_3$.

$\langle E \rangle = \frac{4 \times \frac{1}{2} + \frac{1}{3} \times 6 + \frac{1}{6} \times 9}{\frac{1}{2} + \frac{1}{3} + \frac{1}{6}} = 2 + 2 + \frac{3}{2} = 4 + \frac{3}{2} = \frac{11}{2}$ eV.

3. $\cancel{\psi = \frac{1}{\sqrt{2}}\psi_2 + \psi_2 + \frac{1}{\sqrt{3}}\psi_3 + \frac{1}{\sqrt{2}}\psi_4 + \frac{1}{\sqrt{2}}\psi_5}$

$\cancel{\langle E \rangle = \frac{.2 \times \frac{1}{2} + .1 \times 3 + .\frac{1}{3} \times 3 + .1 \times \frac{1}{2} + .1 \times \frac{1}{2}}{1}}$

$\cancel{= 1 + 3 + 1 + 1}$

$\cancel{= 6 \text{ eV}}$

3. $\psi = \frac{1}{\sqrt{5}}\psi_2 + \frac{1}{\sqrt{10}}\psi_2 + \sqrt{0.3}\,\psi_3 + \frac{1}{\sqrt{5}}\psi_4 + \frac{1}{\sqrt{5}}\psi_5$

$\langle E \rangle = 2 \times 0.2 + 0.1 \times 3 + 0.3 \times 3 + 0.2 \times 1 + 0.2 \times 1$

$= 0.4 + 0.3 + 0.9 + 0.2 + 0.2$

$\langle E \rangle = 2$ eV

Q.4 The wave function $\psi(x)$ is given by,
$\psi(x) = A_n \sin \frac{2n\pi x}{L}$ in the region $0 \le x \le L$.

Find the normalization constant and normalised wave function

$\psi(x) = A_n \sin \frac{2n\pi x}{L}$ $\psi^*(x) = A_n \sin \frac{2n\pi x}{L}$

Normalization Condition is. $A_n = \sqrt{\frac{2}{L}}$

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

$$\psi^* \psi = A_n^2 \sin^2 \frac{2n\pi x}{L}$$

$$\int_0^L A_n^2 \sin^2 \frac{2n\pi x}{L} = 1$$

$$\Rightarrow A_n = \sqrt{\frac{2}{L}}$$

6/11/19

1. Calculate the probability of finding the particle in the region $2 \leq x \leq 4$. if the wave function for the particle is given by $\psi = 0.25 e^{2ix}$

2. The normalized wave function for certain particle is $\psi(x) = \sqrt{\frac{3}{\pi}} \cos x$, $-\pi/2 < x < \pi/2$. Calculate the probability of finding the particle between $0 < x < \pi/4$.

3. Calculate the expectation value of linear momentum for the wave function $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ in the region $0 < x < L$ and $\psi(x) = 0$ for $|x| > L$.

4. Normalize the wave function in one dimension for $\psi(x) = A e^{-\alpha x}$ for $x > 0$ and $\psi(x) = A e^{\alpha x}$ for $x < 0$. here α is a positive constant.

1. $\psi = 0.25\, e^{2ix}$

$\psi^* = 0.25\, e^{-2ix}$

$\psi\psi^* = 0.0625$

$$\langle P \rangle = \int_2^4 \psi\psi^* \, dx = \int_2^4 0.0625 \, dx = 0.0625 \times 2$$

$$= 0.125$$

Probability of finding the particle in the above region is 12.5%.

2. $\psi = \sqrt{\frac{3}{\pi}} \cos x$. $\psi^* = \sqrt{\frac{3}{\pi}} \cos x$.

$\psi\psi^* = \frac{3}{\pi} \cos^2 x$.

$$\langle P \rangle = \int_0^{\pi/4} \frac{3}{\pi} \cos^2 x \, dx = \int_0^{\pi/4} \frac{3}{\pi} \left(\frac{1 + \cos 2x}{2} \right) dx$$

$$= \frac{3}{\pi} \left[\frac{1}{2} [x]_0^{\pi/4} \frac{1}{4} [\cos 2x]_0^{\pi/4} \right]$$

$$\frac{3}{\pi} \times \frac{\pi}{8} + \frac{3}{\pi} \times \frac{1}{4}$$

$$= \frac{3}{8} + \frac{3}{4\pi} = 0.613$$

Probability of finding the particle in the above region is 61.3%.

3. $\hat{p} = i\hbar \frac{\partial}{\partial x}$

$$\langle P \rangle = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \left\{ i\hbar \frac{\partial}{\partial x} \left(\sqrt{\frac{2}{L}} \sin \frac{\pi}{L} x \right) \right\} dx$$

$$= -i\hbar \frac{2}{L} \int_0^L \sin \frac{\pi x}{L} \cos \frac{\pi x}{L} \times \frac{\pi}{L} \, dx.$$

$$= \frac{-i\hbar}{L} \int_0^L \sin \frac{2\pi x}{L} \, dx$$

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$$\langle P\rangle = \frac{i\hbar}{L}\,\frac{L}{2\pi}\,[x]_0^L\left[\cos\frac{2\pi x}{L}\right]_0^L$$

$$\langle P\rangle = 0$$

Expression for momentum operator and Energy operator-

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\times\frac{2\pi}{\lambda} = \hbar k \quad — ①$$

$$E = \hbar\nu = \frac{h}{2\pi}\times\frac{2\pi\nu}{\nu} = \hbar\omega \quad — ②$$

Let us consider the wave propagating along x-axis within one-direction.

$$\psi = Ae^{i(kx-\omega t)} \quad — ③$$

$$\frac{\partial\psi}{\partial x} = ik\,Ae^{i(kx-\omega t)}$$

$$\Rightarrow \frac{\partial\psi}{\partial x} = ik\psi$$

From eqⁿ ①.

$$\frac{\partial\psi}{\partial x} = \frac{ip}{\hbar}\psi$$

$$\Rightarrow P\psi = \frac{\hbar}{i}\frac{\partial\psi}{\partial x} = \frac{\hbar i}{i^2}\frac{\partial\psi}{\partial x} = -\hbar i\frac{\partial\psi}{\partial x}$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

$$\frac{\partial\psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)}$$

$$\frac{\partial\psi}{\partial t} = -i\omega\psi$$

From eqⁿ ②

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \Rightarrow E\psi = -\frac{\hbar i}{i^2}\frac{\partial\psi}{\partial t}$$

$$E\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

In 3-Dimension.

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

$$\hat{p} = -i\hbar \nabla$$

7/11/19

Schrondinger's Wave Eqn-

1-D.

1. Time dependent S. wave eqn for a free particle along x-axis.

Let the wave function associated with the particle be represented by,

$$\psi(x,t) = A e^{i(kx-\omega t)} \quad \text{—— (1)}$$

$$\frac{\partial \psi}{\partial x} = ikA e^{i(kx-\omega t)} = ik\psi \quad \text{—— (2)}$$

$$\frac{\partial \psi}{\partial t} = -i\omega\psi \quad \text{—— (3)} \Rightarrow \psi = \frac{-1}{i\omega}\frac{\partial \psi}{\partial t}.$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2\psi \quad \text{—— (4)}$$

$$p = \frac{h}{\lambda} = \hbar k$$

$$E = h\nu = \hbar\omega \qquad E = \frac{p^2}{2m} \Rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m}$$

Substituiting the value of ψ in eqn (4) from eqn (3).

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-k^2}{-i\omega}\frac{\partial \psi}{\partial t}$$

$$\Rightarrow -\frac{\omega}{k^2}\frac{\partial^2 \psi}{\partial x^2} = \frac{-1}{i}\frac{\partial \psi}{\partial t}$$

$$\Rightarrow -\frac{\omega}{k^2}\frac{\partial^2\psi}{\partial x^2} = \frac{i^2}{i}\cdot\frac{\partial\psi}{\partial t}$$

$$\Rightarrow -\hbar\frac{\omega}{k^2}\frac{\partial^2\psi}{\partial x^2} = \hbar i\frac{\partial\psi}{\partial t}$$ (Multiply $\hbar$ both sides)

$$\left(\hbar\omega = \frac{\hbar^2 k^2}{2m}\right)$$

$$\Rightarrow -\frac{\hbar^2 k^2}{2mk^2}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t}.$$

$$\Rightarrow \boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}}$$ → (5) 1-D time dependent S. wave eq^n for a free particle along x-axis.

2. For any particle-

Let the particle moves under a potential. V(x)

$$E = \frac{p^2}{2m} + V(x)$$

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi(x)}$$ → (6) 1-D time dependent S. wave eq^n for any particle along x-axis

In 3-D

(i) Time dependent S-wave eq^n for a free particle

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi}$$

(ii) Time dependent S. wave eq^n for any particle.

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi(\vec{r})}$$

2. 1-D

(i) Time Independent S. wave Eq^n for free particles:

As we know

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

So, $E\Psi = i\hbar \frac{\partial \Psi}{\partial t}$

Substitute this in eq^n 5

$$E\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}$$

$$\Rightarrow \frac{2mE\Psi}{\hbar^2} = -\frac{\partial^2 \Psi}{\partial x^2}$$

$$\Rightarrow \boxed{\frac{\partial^2 \Psi}{\partial x^2} + \frac{2mE\Psi}{\hbar^2} = 0} \quad \text{--- (7)}$$

This is time independent S. wave eq^n for free particle along x-axis

(ii) Time Independent S. Wave eq^n for any particle along x-axis:

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

$$\Rightarrow (E - V)\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}.$$

$$\Rightarrow \boxed{\frac{2m}{\hbar^2}(E - V)\Psi = -\frac{\partial^2 \Psi}{\partial x^2}}$$

3-D

(i) Time Independent S. wave Eq^n for free particle.

$$\boxed{\nabla^2 \Psi + \frac{2mE\Psi}{\hbar^2} = 0}$$

(ii) Time Independent S. Wave Eq^n for any particle.

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

Time independent S wave Eq^n -
(Derivation fo in independent way)

1-D.

for ~~free~~ any particle.

$\psi = Ae^{i(kx-\omega t)}$

$$\frac{\partial\psi}{\partial x} = ik\psi$$

$$\frac{\partial\psi}{\partial t} = -i\omega\psi$$

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi \Rightarrow E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

$p = \hbar k.$ $\Rightarrow \boxed{E\psi = i\hbar\frac{\partial\psi}{\partial t}}$

$E = \hbar\omega$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{p^2}{\hbar^2}\psi \Rightarrow \boxed{p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}}$$

Total Energy $= \frac{p^2}{2m} + V$

Operate every term on the wave function ψ.

$$E\psi = \frac{p^2}{2m}\psi + V\psi$$

$$\boxed{p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}}$$

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

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

For free particle,

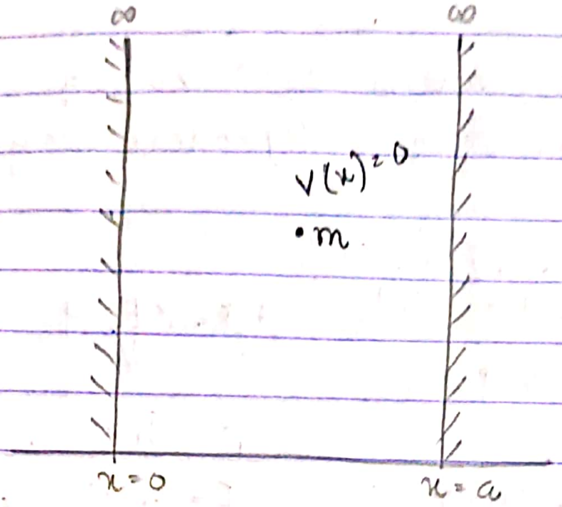
$V = 0$

$$\boxed{\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0}$$

11/11/19

Application Of Sch. Wave Eqn

1. **Potential Well (Box)** (Particle in a 1-D well/Box of infinite height)



Let us consider the case of a particle of mass 'm' moving along x-axis b/w the two walls at $x = 0$ and at $x = a$. The particle is free to move b/w the walls.
When the particle strikes any of the wall it is reflected back immediately as the walls are perfectly rigid. The potential function is defined as,

$$V(x) = 0 \quad , \quad 0 < x < a$$

$$\text{and} \quad V(x) = \infty \quad , \quad x \leq 0 \ \text{and} \ x \geq a$$

Since the height of the potential well is ∞. So the probability of finding the particles at the rigid walls and outside the rigid walls vanishes.

Inside the well, the Sch. wave eqn can be written as,

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

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{--- (2)} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar}}$$

The sol^n of eq^n (2) can be written as

$$\psi(x) = A \sin kx + B \cos kx. \quad \text{--- (3)}$$

where A and B are arbitrary constant. and can be found out by using boundary conditions.

Boundary Condition. ← [Characteristic of wave function. ⇓ point (v)]

$\psi(0) = 0.$	, $\psi(a) = 0.$
Putting in eq^n (3)	$0 = A \sin ka + B \cos ka$
$0 = 0 + B.$	$0 = A \sin ka.$
$\Rightarrow \boxed{B = 0}$	$\sin ka = 0.$ as $A \neq 0.$
	$ka = \pm n\pi.$ $n \neq 0$
	$n = 1, 2, 3 \ldots$

Energy eigen value –

$$ka = \pm n\pi$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\frac{n^2 \pi^2}{a^2} = \frac{2mE}{\hbar^2}$$

$$E = \frac{\hbar^2}{2m} \frac{n^2 \pi^2}{a^2}$$

$$E = \frac{h^2}{4\pi^2 \times 2m} \frac{n^2 \pi^2}{a^2}$$

$$\boxed{E_n = \frac{h^2}{8ma^2} \times n^2.} \quad \text{where } n = 1, 2, 3 \ldots$$

$$E_1 = \frac{h^2}{8ma^2}, \quad E_2 = \frac{h^2}{8ma^2} \times 4, \quad E_3 = \frac{h^2}{8ma^2} \times 9 \ldots$$

So, energy is quantised.

HW

Q. Show that momentum is quantised.

$$E = \frac{p^2}{2m}.$$

$\hbar = \frac{h}{2\pi}$

de-Broglie's wave length:

(Q. Prove that width of the potential box is half-integral multiple of de-Broglie wavelength)

$p = \frac{h}{\lambda}$

$p = \hbar k = \hbar \frac{n\pi}{a}$

$= \frac{h}{2\pi} \times \frac{n\pi}{a}$

$\Rightarrow \frac{h}{\lambda} = \frac{h}{2} \times \frac{n}{a}$

$\boxed{\lambda = \frac{2a}{n}}$ $\boxed{a = \frac{n\lambda}{2}}$

So, the allowed bound states are possible for the energies, for which the width of the potential well is equal to half integral multiple of the wavelength.

Eigen functions-

The normalization condition.

$$\int |\psi|^2 dx = 1.$$

$\psi(x) = A \sin kx.$

Here the corresponding eq^n.

$$\int_0^a A^2 \sin^2 kx = 1. \qquad A = \sqrt{\frac{2}{a}}.$$

$$\Rightarrow A^2 \int_0^a \left(\frac{1 - \cos 2kx}{2}\right) \cdot dx = 1.$$

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Now the normalized wave function,

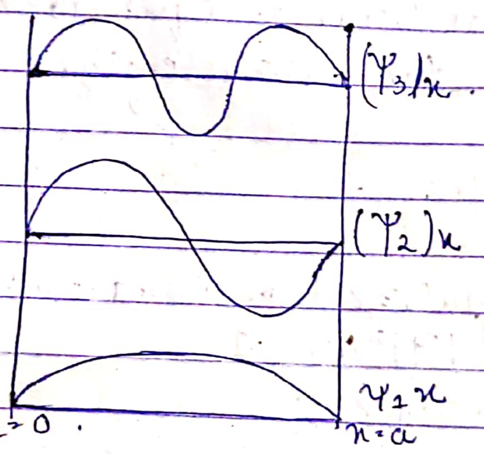
$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x} \quad n = 1, 2, 3 \ldots$$

$\psi_1(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi}{a} x$ Eigen function for ground state.

$\psi_2(x) = \sqrt{\frac{2}{a}} \sin \frac{2\pi}{a} x$ Eigen function for 1st state

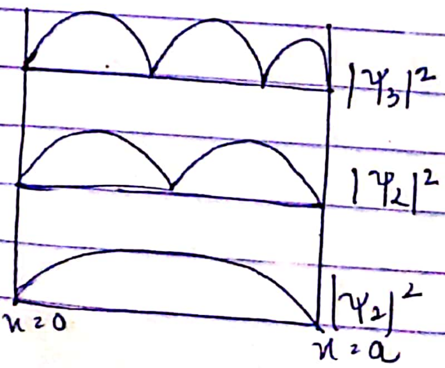
⋮



$$|\psi_n|^2 = \frac{2}{a} \sin^2 \frac{n\pi x}{a}$$

$$|\psi_1|^2 = \frac{2}{a} \sin^2 \frac{\pi x}{a}, \quad |\psi_2|^2 = \frac{2}{a} \sin^2 \frac{2\pi x}{a}$$

$$|\psi_3|^2 = \frac{2}{a} \sin^2 \frac{3\pi x}{a}$$



$$\boxed{E_n = \frac{h^2}{8ma^2} \cdot n^2}$$

The ground state energy $E_1 = \frac{h^2}{8ma^2}$ which is minimum energy of the particle and non-zero.

$$E_n = E_1 n^2$$

The energy of higher allowed levels are the multiple of E_1 and $E_n \propto n^2$. So, values of the energy lying b/w the allowed state is forbidden.

The energy levels are ~~yet~~ not equispaced. The spacing b/w two successive level increases with increase in 'n'.

Potential Barrier-

For a free particle.

Let the particle move freely in x-axis.

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0.$$

$$\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0. \qquad k = \sqrt{\frac{2mE}{\hbar}}.$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}.$$

where,

Ae^{ikx} - This is the plane wavefunction which represent movement of particle in positive x-axis.

Be^{-ikx} - It represents the plane wave function which represents movement of particle in negative x-axis.

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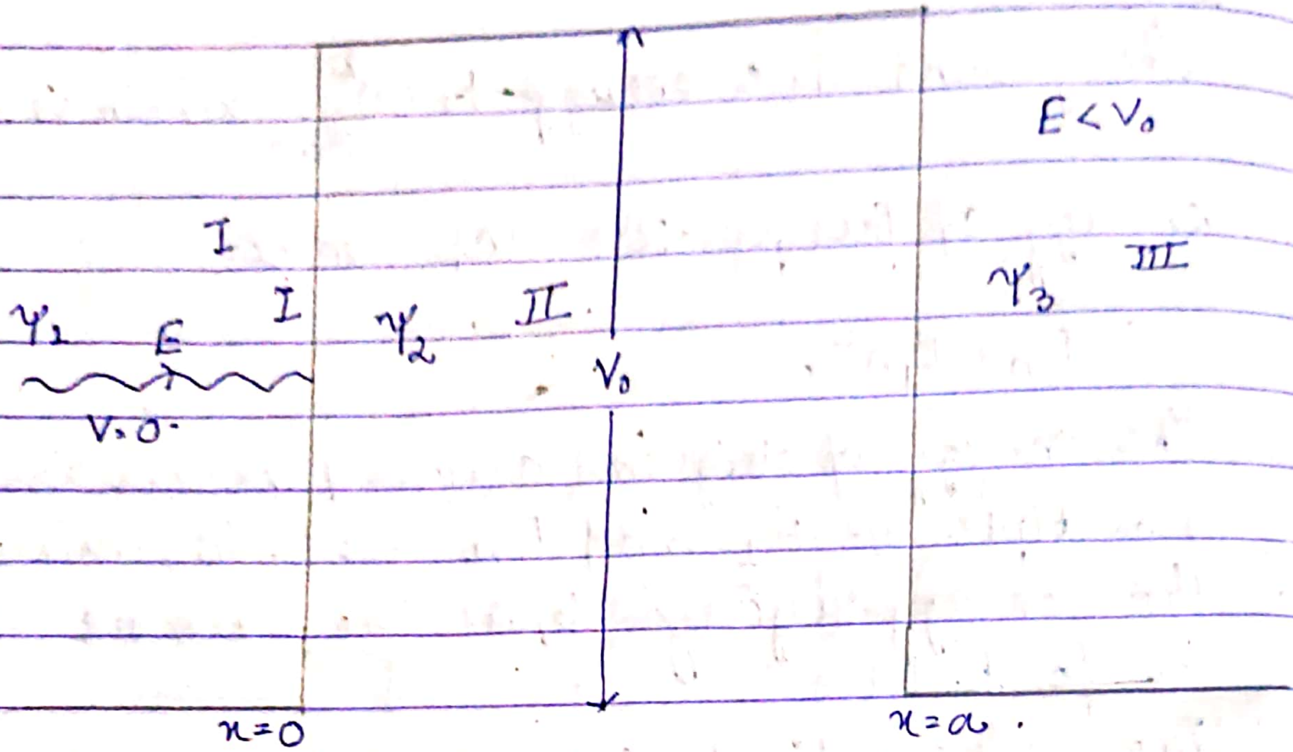

It is a region of finite height and finite width in which the potential is significantly higher than the point either side of it, so that the particle requires energy to pass through it.

So, potential function is defined as the

$$V(x) = 0 \quad x < 0,\ x > a$$
$$V(x) = V_0 \quad 0 \le x \le a.$$

14/11/19

Classical Physics tells particle cannot cross through the barrier and total reflection occurs as $E < V_0$ but quantum mechanics predicts that, the particle has a non-zero probability of crossing the barrier and will reach at region III even if its energy is less than the height of the barrier which is called as quantum mechanical Tunnelling.

For Region-I-

The time independent Sch. wave eq^n.

$$\frac{\partial^2 \psi_1}{\partial x^2} + \frac{2mE\psi_1}{\hbar^2} = 0. \quad \text{——} (1)$$

$$\frac{\partial^2 \psi_1}{\partial x^2} + k^2\psi_1 = 0 \quad \text{——} (2) \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

The sol^n of eq^n (2).

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

A and B are arbitrary constant can be found out by the boundary condition.

Ae^{ikx} — incident wave in region I

Be^{-ikx} — Reflected wave in region I

For region-II-

The time idependent Sch. wave eq^n

$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0.$$

$$\frac{\partial^2 \psi_2}{\partial x^2} - \alpha^2 \psi_2 = 0 \quad \text{——} (3). \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

The sol^n of eq^n (3).

$$\psi_2(x) = Ce^{\alpha x} + De^{-\alpha x}$$

$Ce^{\alpha x}$ when $x \to \infty$. $\to$ Not exist.

$\psi_2(x) = De^{-\alpha x}$.

For region-III

The time independent Sch. wave eqⁿ

$$\frac{\partial^2 \psi_3}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_3 = 0.$$

$$\underbrace{\frac{\partial^2 \psi_3}{\partial x^2} + k^2\psi_3 = 0}_{(4)}, \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

Solⁿ of eqⁿ (4)

$\psi_3(x) = Fe^{ikx} + \underbrace{Ge^{-ikx}}_{\text{Not exist}}$

$\psi_3(x) = Fe^{ikx} \longrightarrow$ Transmitted wave.

Using the boundary condition the arbitrary constant A, B, D and F canbe found out. Then the transmission coeff;

$$T = \frac{16E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\alpha a} \longrightarrow \text{(For derivation)}$$

$$\simeq e^{-2\alpha a} \longrightarrow \text{(For numerical)}$$

The transmitⁿ probability increases with the decrease in height V_0 and width 'a' of the potential barrier.

Quantum Mechanical Tunnelling.
(Tunnelling Effect)

It is the penetration of the particle of lower energy to a region of higher potential with finite probability and then escaping them from the potential region is called as tunnelling.

The phenomenon of barrier penetration or quantum mechanical tunnelling suggests that microscopic particle trapped in a deep potential have a non zero probability of escaping them from the potential well even if they donot have enough energy to climb over the well.

Ex: (i) α-particle scattering
(ii) Nuclear fusion

Q.1 $e^{\ominus}$s with energy 3 eV are incident on a potential barrier of 10 eV high and 4 A° wide. Find the transmission probability

Q.2. If 20×10^{6} $e^{\ominus}$s with energy 2 eV are incident on a potential barrier of 8 eV high and 0.5 nm width. then calculate. how many $e^{\ominus}$s ~~to~~ will tunnel through the barrier.

1. $T = e^{-2\alpha a}$ $\qquad$ $\alpha = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$

$m = 9.1 \times 10^{-31}$.

$V_0 = 10$ eV. $\qquad$ $(V_0 - E) = 7 \times 1.6 \times 10^{-19}$.

$E = 3$ eV.

$\hbar = 1.054 \times 10^{-34}$

$$\alpha = \frac{\sqrt{2 \times 9.1 \times 10^{-31} \times 7 \times 1.6 \times 10^{-19}}}{1.054 \times 10^{-34}}$$

$= 1.354 \times 10^{10}$

1.354
$\times 8$
10.832

$T = e^{-2 \times 1.354 \times 10^{10} \times 4 \times 10^{-10}}$

$\therefore T = e^{-8 \times 1.354} = e^{..}$

$= 33.8 \times 10^{-2}$.

2. $E = 2\,eV$

$V_0 = 8\,eV$

$a = 0.5 \times 10^{-9}$

$$\alpha = \frac{\sqrt{2 \times 9.1 \times 10^{-31} \times 6 \times 1.6 \times 10^{-19}}}{1.054 \times 10^{-34}}$$

$\alpha = 1.254 \times 10^{10}$

$2\alpha a = 2 \times 1.254 \times 10^{10} \times 0.5 \times 10^{-9}$

$= 1.254 \times 10 = 12.54$

$T = e^{-2\alpha a} = e^{-12.54} = 3.58 \times 10^{-6}$

$n_{in} = 20 \times 10^{6}$

$n_{Tran} = n_{inc} \times T$

$= 20 \times 10^{6} \times 3.58 \times 10^{-6}$

$= 71.6$

$\begin{array}{r} 42 \\ -21 \\ \hline 34 \\ -21 \\ \hline 13 \end{array}$

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