Wave Function

Wave Function :-

In matter waves, the quantity that varies periodically is called wave function. The wave function is represented by Ψ (psi). It has no direct physical significance. It is a complex number.

Def^n - A wave fun^n is a complex valued fun^n ψ defined on space and satisfying $|\psi|^2 = 1$

$\psi \longrightarrow$ Wave function $\rightarrow$ State of the System

$\psi(\vec{r},t)$ or $\psi(x,y,z,t)$

Significance :-

* ψ has no direct physical significance
* However $|\psi|^2$ gives the probability of finding the electron in certain area at a time.

i.e. prob of finding the e^- in small vol^m $d\tau$

$= \psi\psi^* d\tau$

where $d\tau = dx\,dy\,dz$)

* $\psi\psi^*$ is always positive & real.
* When $|\psi|^2$ value is high $\rightarrow$ Atomic orbital
* When $|\psi|^2$ value is zero $\rightarrow$ Node (i.e prob. of finding e^- is zero)
* $\int_{-\infty}^{\infty} \psi^* \psi \, d\tau = 1 \rightarrow$ Normalised cond^n.

If ψ is satisfied this condition, then ψ is normalised.

* $\int \psi_n^* \psi_m \, d\tau = 0, \; n \neq m \rightarrow$ orthogonal
* $\int \psi_m^* \psi_n \, d\tau = 0$, if $m \neq n$; $= 1$, if $n = m$ $\Big\} \rightarrow$ orthonormal condition.

Characteristics of ψ

* ψ must be finite, continuous & single valued
* $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ " " "
* ψ must be normalised.

Schrodinger's Time Dependent Equation

- Let us assume that wave function Ψ for a particle moving freely in the x-direction is specified by

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

- But $\omega = \frac{2\pi}{T} = 2\pi\upsilon = 2\pi\frac{E}{h} = \frac{E}{\hbar}$

  and $k = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$

- Now the wave function is $\boxed{\Psi = Ae^{-(i/\hbar)(Et-px)}}$

- Now differentiate above equation w.r.t t,

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

- Now differentiate above equation w.r.t x (twice)

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

- Now total energy of the particle is the sum of K.E and P.E, $\boxed{E = \frac{p^2}{2m} + U(x,t)}$

- Multiply ψ on both sides, $E\Psi = \frac{p^2\Psi}{2m} + U\Psi$

- Multiply ψ on both sides, Now substitute Eψ and p^2ψ into equation (1)

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U\Psi}$$ **(in 1D)**

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + U\Psi}$$

(in 3D)

Schrodinger's Time independent Equation

- In many situations the potential energy of a particle does not depend on time explicitly; the forces that act on it, and hence U, vary with the position of the particle only. When this is true, Schrodinger's equation may be simplified by removing all reference to t.

$$\boxed{\Psi = Ae^{-(i/\hbar)(Et-px)}} = Ae^{-(iE/\hbar)t}e^{+(ip/\hbar)x} = \psi e^{-(iE/\hbar)t}$$

- After substituting the value of Ψ into the time-dependent form of Schrödinger's equation, we find that

$$E\psi e^{-(iE/\hbar)t} = -\frac{\hbar^2}{2m} e^{-(iE/\hbar)t} \frac{\partial^2 \psi}{\partial x^2} + U\psi e^{-(iE/\hbar)t}$$

- Dividing through by the common exponential factor gives,

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

Steady-state Schrodinger equation in one dimension

- In 3D,

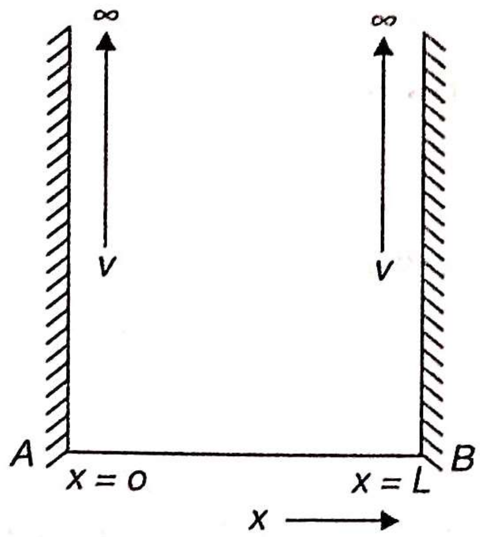
$$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0}$$

Quantum mechanical operators:

Physical properties		Operators	
Name of Operator	**Observables**	**Operators**	**Symbols**
Position	Position with x coordinate	x	x
Momentum	x component of momentum	$-i\hbar \frac{\partial}{\partial x}$	p_x
Angular momentum	z component of angular momentum	$-i\hbar \frac{\partial}{\partial \Phi}$	L_z
K.E operator	Kinetic energy	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$	T
P.E operator	Potential energy	$V_{(x)}$	V
Total energy (E)	Hamiltonian operator (Time-Independent)	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{(x)}$	$\hat{H}$
Total energy (E)	Hamiltonian operator (Time-dependent)	$+i\hbar \frac{\partial}{\partial t}$	$\hat{H}$

Particle in 1D box

- Consider a particle of mass m is confined in a 1D potential box and moving in x-axis only between 0 and L. The potential of the particle is shown below:



$$\boxed{\begin{array}{l} V = 0 \text{ for } 0 \leq x \leq L \\ V = \infty \text{ for } x < 0 \text{ and } x > L \end{array}}$$

The Schrödinger wave equation for the particle is given by

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\,\psi = 0$$

Inside the box, $V = 0$, therefore the above equation takes the form

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

$$\boxed{\frac{d^2\psi}{dx^2} + k^2\psi = 0} \quad (1)$$

Where, $2mE/\hbar^2 = k^2$

General solution of the above equation is

$$\boxed{\psi(x) = A \sin kx + B \cos kx} \quad (2)$$

As probability of finding the particles outside the boundary is zero, we get

$$\psi = 0 \text{ at } x = 0 \text{ and}$$

$$\psi = 0 \text{ at } x = L$$

- Apply boundary condition in general solution:
- For $\psi = 0$ at $x = 0$

$$0 = A \sin 0 + B \cos 0$$

$$\boxed{B = 0}$$

So we get from Eq (2), $\boxed{\psi = A \sin kx}$ ——— (3)

- For $\psi = 0$ at $x = L$,

So we get from Eq(3), $A \sin kL = 0$

(or) $\sin kL = 0$

$$kL = n\pi \qquad (n = 0, 1, 2, 3, \ldots)$$

$$\boxed{k = \frac{n\pi}{L}}$$

Now, the wave function ψ can be given as

$$\boxed{\psi(x) = A \sin \frac{n\pi x}{L}} \quad \text{——— (4)}$$

We have assumed that

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

So we get, $k^2 = \dfrac{n^2\pi^2}{L^2} = \dfrac{2mE}{\hbar^2}$

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

The discrete energy values are given by

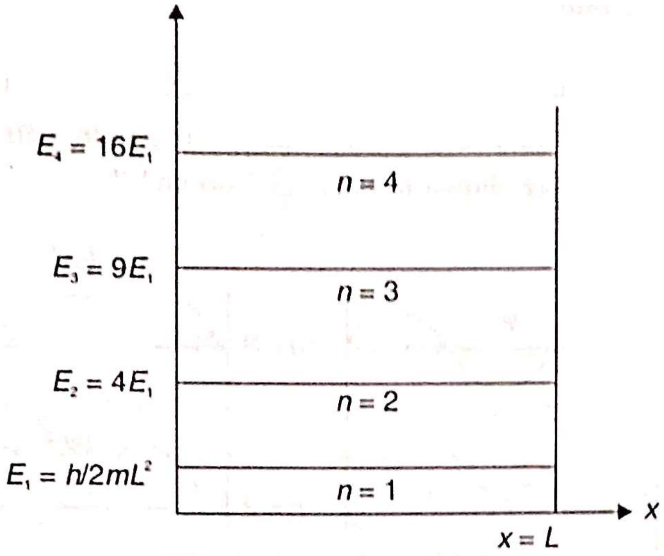
$$E_1 = \frac{h^2}{8mL^2} \text{ for } n = 1$$

$$E_2 = \frac{4 \cdot h^2}{8mL^2} = 4E_1 \text{ for } n = 2$$

$$E_3 = 9\frac{h^2}{8mL^2} = 9E_1 \text{ for } n = 3$$

$$E_4 = 16\frac{h^2}{8mL^2} = 16E_1 \text{ for } n = 4$$

$\vdots \quad \vdots$



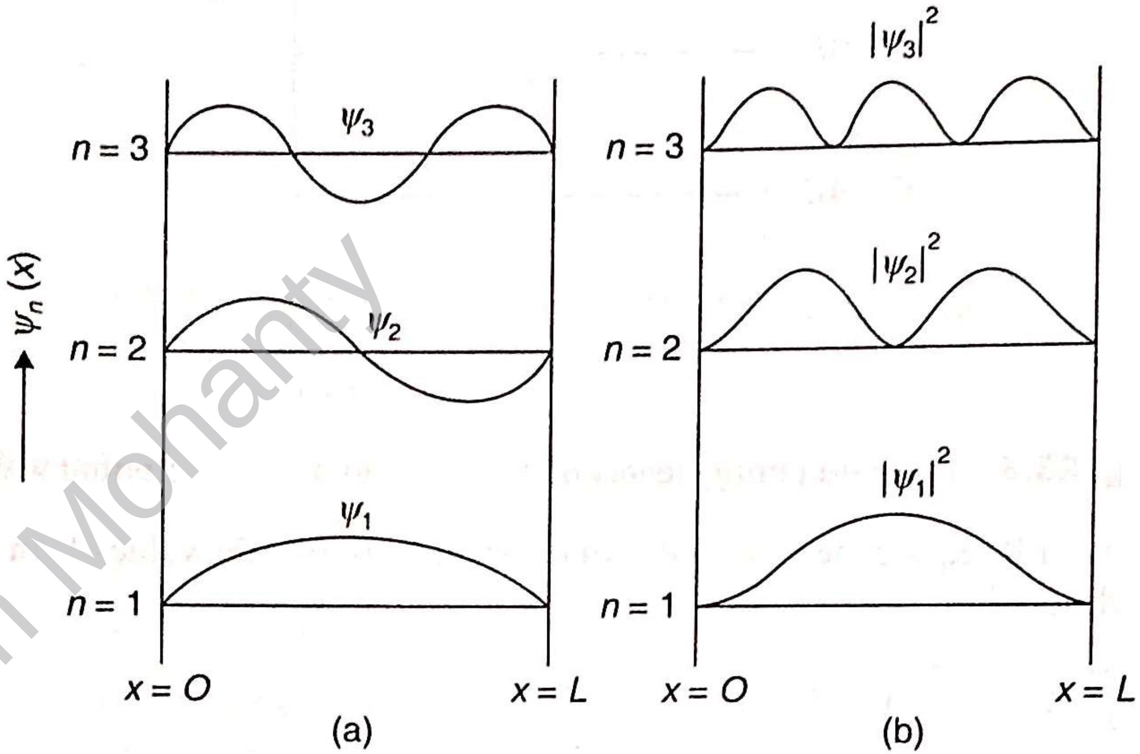
Discrete energy levels

- To find the value of A, we have to apply normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1$$

$$\int_0^L A^2 \sin^2 \frac{n\pi x}{L} dx = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

- So from Eq (4), $\boxed{\psi(x) = \sqrt{\left(\frac{2}{L}\right)} \sin \frac{n\pi x}{L}}$



Wave function and probability density

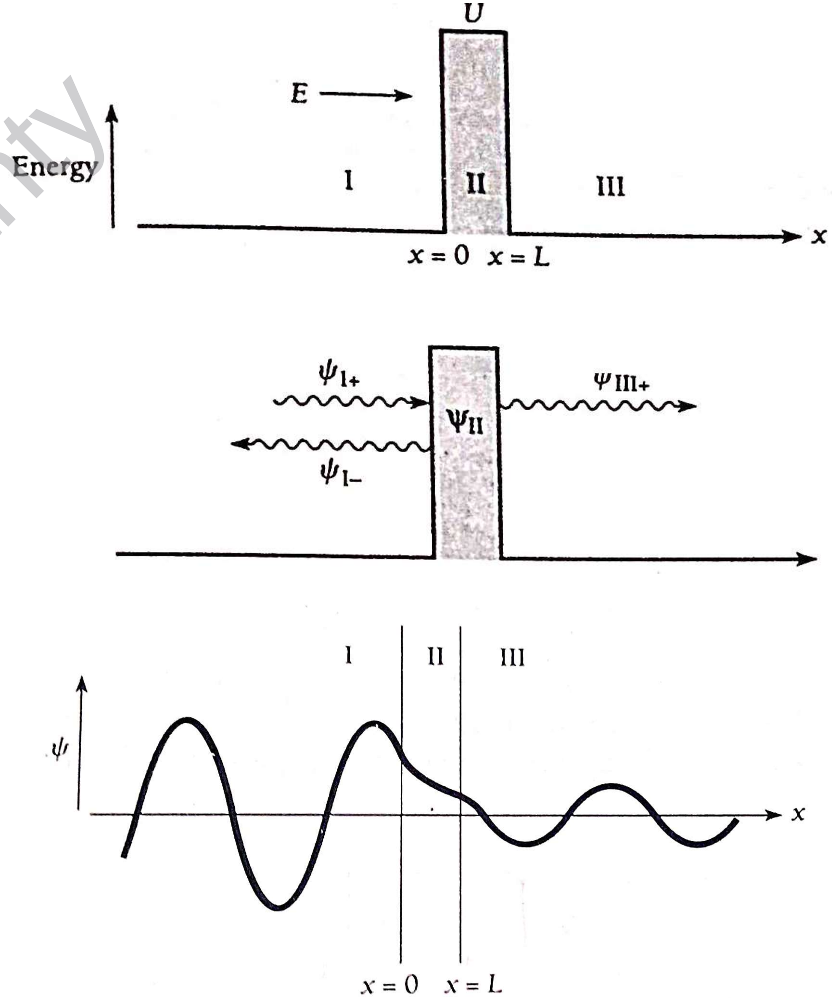
$$\psi_1 = \sqrt{\left(\frac{2}{L}\right)} \sin\left(\frac{\pi x}{L}\right) \qquad \psi_2 = \sqrt{\left(\frac{2}{L}\right)} \sin\left(\frac{2\pi x}{L}\right)$$

and so on ----

Tunnel Effect

- A particle without the energy to pass over a potential barrier may still tunnel through it !!
- When a particle that strikes a potential barrier of height U, again with E < U, but here the barrier has a finite width. What we will find is that the particle has a certain probability not necessarily great but not zero either –of passing through the barrier and emerging on other sides.
- When a particle of energy E < U approaches a potential barrier, according to classical mechanics the particle must be reflected. In quantum mechanics, the de Broglie waves that correspond to the particle are partly reflected and partly transmitted, which means that the particle has a finite chance of penetrating the barrier.
- Approximate Transmission probability is: $\boxed{T = e^{-2k_2 L}}$

Where, $k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$



- Which of the following are the Eigen function of the operator $\frac{\partial^2}{\partial x^2}$? Find the approximate Eigen value.

A. $\sin^2 x$

B. e^{2x}

Given that $f(x) = e^{2x}$

Operating $\frac{\partial^2}{\partial x^2}$ on $f(x)$, we get

$$\frac{\partial^2}{\partial x^2}(e^2 x) = 2 \times 2e^{2x} = 4 f(x)$$

Hence, e^{2x} is an eigenfunction having eigenvalue +4.

Given that $f(x) = \sin^2 x$

Operating $\frac{\partial^2}{\partial x^2}$ on $f(x)$, we get

$$\frac{\partial^2}{\partial x^2}(\sin^2 x) = 2 - 4 \sin^2 x$$

Hence, it is not an eigenfunction for $f(x) = \sin^2 x$.

- Normalize the eigenfunction $\phi(x) = e^{icx}$ within the region $-a \leq x \leq a$.

Solution

Given that $\phi(x) = e^{icx}$

In order to normalize the wave function $\phi(x)$, let us multiply it by k. Thus,

$$\phi(x) = ke^{icx}$$

To find out the value of c, we apply normalization condition as

$$\int_{-a}^{a} \phi(x)\phi^*(x)dx = 1$$

$$\phi(x) = ke^{icx} \text{ and } \phi^*(x) = ke^{-icx}$$

Now, using these values in the above equation, we get

$$k^2 \int_{-a}^{a} e^{icx} e^{-icx} dx = 1$$

$$k^2 \int_{-a}^{a} dx = 1$$

$$k^2 [x]_{a}^{a} = 1$$

or $k^2 \cdot 2a = 1$

or $k = \dfrac{1}{\sqrt{2a}}$

Hence, the normalized wave function can be given as $\phi(x) = \dfrac{1}{\sqrt{2a}} \cdot e^{icx}$

- Find the energy of an electron moving in one-dimension in an infinitely high potential box of width 1 Å. (Mass of the electron is 9.1×10^{-31} kg and $h = 6.63 \times 10^{-34}$ Js.)

Solution

From the expression of energy of a particle in a deep potential box of width L, we have

$$E_n = \frac{n^2h^2}{8mL^2}$$

where $n = 1, 2, 3, ...$

Particle is generally found in the ground state, which occurs corresponding to $n = 1$.

Hence, $$E = \frac{h^2}{8mL^2}$$

$$= \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2} = \frac{43.96 \times 10^{-68}}{72.8 \times 10^{-51}} = 6.038 \times 10^{-18} \text{ J}$$

$$= \frac{6.038 \times 10^{-18}}{1.6 \times 10^{-19}} \text{ eV}$$

$$= 37.74 \text{ eV}$$

Quantum Computing

- Aim to use quantum mechanical phenomena that have no classical counterpart for computational purposes.
- Central research tasks include:
  - ✓ Building devices — with a specified behaviour.
  - ✓ Designing algorithms — to use the behaviour.
- Mediating these two are models of computation.

Why look at QC ??

➢ The world is quantum

– classical models of computation provide a level of abstraction

– discrete state systems

➢ Devices are getting smaller

– Moore's law

– the only descriptions that work on the very small scale are quantum

➢ Exploit quantum phenomena

– using quantum phenomena may allow us to perform computational tasks that are not otherwise possible/efficient

– understand capabilities/resources

Bits

A building block of classical computational devices is a two-state system.

$$0 \longleftrightarrow 1$$

Indeed, any system with a finite set of *discrete, stable* states, with controlled transitions between them will do.

Qubits

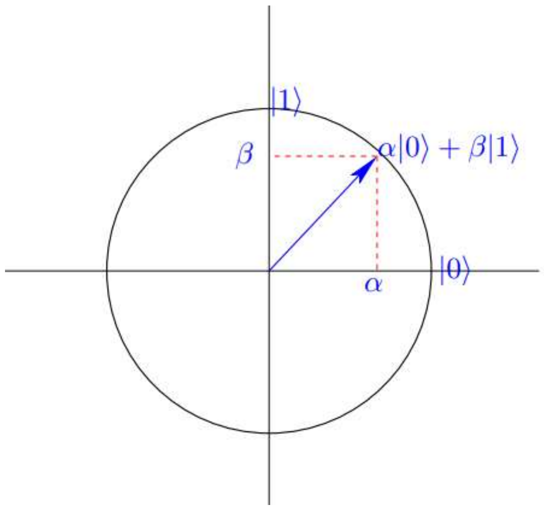
Quantum mechanics tells us that any such system can exist in a *superposition* of states.

In general, the state of a *quantum bit* (or *qubit* for short) is described by:

$$\alpha|0\rangle + \beta|1\rangle$$

where, α and β are complex numbers, satisfying $|\alpha|^2 + |\beta|^2 = 1$

and $|0\rangle$ with probability $|\alpha|^2$, and $|1\rangle$ with probability $|\beta|^2$



A qubit may be visualised as a unit vector on the plane.

In general, however, α and β are *complex* numbers.

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$ where $|\ \rangle$— a *ket*, Dirac notation for vectors.

Thank You