Wave function:

Wave function is the quantity whose variation makes up the matter waves. Amplitude of matter wave is describes by wave function. It is denoted by ψ which consists of real and imaginary part.

$\Psi = A + iB$

Conjugate of ψ is $\psi^* = A - iB$

$\Psi^2 = A^2 + B^2$

Probability density :

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

$|\psi^2|$ at a particular place at a particular time is proportional to the probability of finding the particle there at that time.

Properties of Wave Function

1. Ψ must be continuous and single-valued everywhere.
2. $\partial\Psi / \partial x$, $\partial\Psi / \partial y$, $\partial\Psi / \partial z$ must be continuous and single-valued everywhere. (There may be exception in some special situations, we will discuss this later.)
3. $|\Psi|^2$ must go to zero as x, y, or z $\rightarrow \pm\infty$ so that $\int |\Psi|^2 dV$ remains finite
4. Ψ must be normalized. i.e. $\iiint_{-\infty}^{\infty} |\psi^2|\ dV = 1$
5. $\iiint_{-\infty}^{\infty} |\psi^2|\ dV = 0$ i.e. the particle does not exist but but $|\Psi|^2$ overall space must be finite i.e. the body is somewhere.

   Therefore $\iiint_{-\infty}^{\infty} |\psi^2|\ dV = 0\ , negative\ or\ complex\ is\ not\ possible$

Energy and Momentum Operator

In quantum Physics , the state of System is described by its wave function and the observables are represented by the operators .

Let us assume that Ψ for a particle moving freely in the +ve x direction is-

$\psi = Ae^{-i\omega\left(t-\frac{x}{v}\right)}$ ……….(1)

where $v = velocity, \omega = 2\pi\nu(nu),\ v(velocity) = \nu\lambda\ , \lambda = \frac{h}{P} = \frac{2\pi\hbar}{P}$

$\psi = Ae^{\left(-i2\pi\nu t + \frac{i2\pi}{\nu\lambda}\right)}$

$\psi = Ae^{-2\pi i}\left(\nu t - \frac{x}{\lambda}\right)$

$\psi = Ae^{-\frac{i}{\hbar}(Et-px)}$ ………………(2) This is the wave equation for a free particle.

On differentiating partially with respect to 't' we get

$\frac{\delta\psi}{\delta t} = -\frac{iE}{\hbar}\ Ae^{-\frac{i}{\hbar}(Et-px)}$

$\frac{\delta\psi}{\delta t} = -\frac{i}{\hbar}\ E\psi$

Or

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

Hence **energy operator** $\boldsymbol{E = i\hbar \frac{\delta}{\delta t}}$ **.............(3)**

Ψ is said to be eigen function of the operator $i\hbar \frac{\delta}{\delta t}$ and E is called corresponding eigen value. Now on differentiating partially with respect to 'x' we get

$$\frac{\delta\psi}{\delta x} = -\frac{iP}{\hbar} Ae^{-\frac{i}{\hbar}(Et- \quad)}$$

$$\frac{\delta\psi}{\delta x} = -\frac{iP}{\hbar}\psi$$

Or $P\psi = \frac{\hbar}{i}\frac{\delta\psi}{\delta x}$

Hence **momentum operator** $\boldsymbol{P = \frac{\hbar}{i}\frac{\delta}{\delta x}}$ **-...... (4)**

SCHRODINGER'S WAVE EQUATION

In 1926, Schrodinger gave a fundamental equation of wave mechanics in the same sense as the Newton's Second Law of Classical Mechanics. It is the differential equation of the de – Broglie wave associated with the particle and describes the motion of the particle.

Let us assume that Ψ for a particle moving freely in the +ve x direction is-

$$\psi = Ae^{-i\omega\left(t-\frac{x}{v}\right)} \text{ ....(1)}$$

where $v = velocity, \omega = 2\pi\nu(nu),\ v(velocity) = \nu\lambda\,, \lambda = \frac{h}{P} = \frac{2\pi\hbar}{P}$

$$\psi = Ae^{\left(-i2\pi\nu t+\frac{i2\pi\nu x}{\nu\lambda}\right)}$$

$$\psi = Ae^{-2\pi i}\left(\nu t - \frac{x}{\lambda}\right)$$

$\psi = Ae^{-\frac{i}{\hbar}(Et-px)}$ .... (2) This is the wave equation for a free particle.

As **energy operator** $\boldsymbol{E = i\hbar \frac{\delta}{\delta t}}$ and **momentum operator** $\boldsymbol{P = \frac{\hbar}{i}\frac{\delta}{\delta x}}$

Total energy E= K.E. + P.E. .... (3)

$$= \left(\frac{P^2}{2m}\right)\psi + V\psi \text{ .... (4)}$$

Putting the value of $E\psi$ and $P\psi$

$$i\hbar\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \text{ ....(5)}$$

This is the Schrodinger's time dependent wave equation in one dimension

In three dimension form $i\hbar\,\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi$ …………(6)

Schrodinger's Time independent wave equation :

Let us assume that Ψ for a particle moving freely in the +ve x direction is-

$\psi = Ae^{-i\omega\left(t-\frac{x}{v}\right)}$ ……….(1)

where $v = velocity, \omega = 2\pi\nu(nu),\ v(velocity) = \nu\lambda\,, \lambda = \frac{h}{P} = \frac{2\pi\hbar}{P}$

$\psi = Ae^{\left(-i2\pi\nu t+\frac{i2\pi\nu x}{\nu\lambda}\right)}$

$\psi = Ae^{-2\pi i}\left(\nu t - \frac{x}{\lambda}\right)$

$\psi = Ae^{-\frac{i}{\hbar}(Et-px)}$ ……………… (2) This is the wave equation for a free particle $\psi = e^{-\frac{i}{\hbar}(Et)}\boldsymbol{Ae^{\frac{i}{\hbar}(px)}}$

$\psi = \psi_0 e^{-\frac{i}{\hbar}(Et)}$ ……..(3)

Where $\psi_0 = \boldsymbol{Ae^{\frac{i}{\hbar}(px)}}$ **…….(4)**

Partially Differentiating equation (3) with respect to 't'

$\frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar}\psi_0 e^{-\frac{i}{\hbar}(Et)}$ ……………..(5)

Double differentiate partially with respect to 'x'

$\frac{\partial^2\psi}{\delta x^2} = \frac{\partial^2\psi_0}{\delta x^2} e^{-\frac{i}{\hbar}(Et)}$ …………(6)

Now we put the values of equation 4,5,and 6 in Schrodinger's time dependent equation . i.e.

$$i\hbar\,\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

$$i\hbar\left\{\frac{-iE}{\hbar}\psi_0 e^{-\frac{i}{\hbar}(Et)}\right\} = -\frac{\hbar^2}{2m}\left\{\frac{\partial^2\psi_0}{\delta x^2} e^{-\frac{i}{\hbar}(Et)}\right\} + V\left\{\psi_0 A e^{-\frac{i}{\hbar}(Et)}\right\}$$

$$E\psi_0 = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_0}{\delta x^2} + V\,\psi_0\right\}$$

$\frac{\delta^2\psi_0}{\delta x^2} + \frac{2m}{\hbar^2}(E-V)\psi_0 = 0$ In One dimension

$\nabla^2\psi_0 + \frac{2m}{\hbar^2}(E-V)\psi_0 = 0$ *Where* $\nabla^2 = \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}$ **In three dimension**

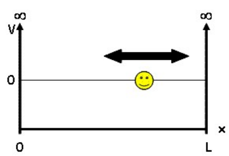
Application of Schrodinger Wave equation

1. **Particle in a box (Innfinite square well)**

A particle in a 1dimensional box is a fundamental quantum mechanical approximation describing the translational motion of a single particle confined inside an infinitely deep well f rom which it *cannot escape*.

Let us consider a particle moving inside a box along the X- Direction. The particle is bouncing back and forth between the walls of the box. 'L' is the width of the box

The potential energy is *0 inside the box* (V=0 for 0<x<L) and goes to infinity at the walls of th e box (V=∞ for x<0 or x>L). We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box.



Particle cannot exist outside the box so its wave function $\psi = 0$ for $x \leq 0$ and $x \geq L$

Within the box , the Schrodinger equation becomes

$$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}(E)\psi = 0 \quad \text{(V= 0 for free particle inside the box)} \quad \cdots\cdots (1)$$

Consider $K = \sqrt{\frac{2mE}{\hbar^2}}$

Equation –(1) becomes

$$\frac{\delta^2\psi}{\delta x^2} + K^2\psi = 0 \quad \cdots\cdots..(2)$$

The general solution of this equation is

$$\psi = A\sin Kx + Cos\ Kx \quad ……………..(3)$$

Using Boundary condition

$$\psi = 0 \ \ at \ \ x = 0$$

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

i.e. B= 0 …………….(4)

Applying II Boundary condition

$\psi = 0 \;\; at \;\; x = L$

$0 = A \sin KL$

$A \neq 0$

i.e. $\sin KL = 0$

i.e. $\sin KL = \sin n\pi$

$K = \frac{n\pi}{L}$

$\psi_n(x) = A \sin \frac{n\pi}{L} x$ ……….(4) where n= 1,2,3,……….

Energy Level $E_n = \frac{K^2\hbar^2}{2m}$

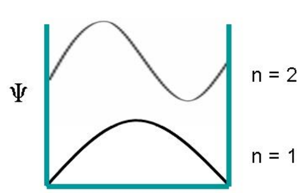
$\hbar = \frac{h}{2\pi}$

Eigen Value $E_n = \left(\frac{n\pi}{L}\right)^2 \left(\frac{h}{2\pi}\right)^2 \frac{1}{2m}$

$E_n = \frac{n^2h^2}{8mL^2}$ …………(5) n= 0,1,2,3,4…………

Equation –(5) reveals that

1. The energy of a particle is quantized .i.e. the particle cannot have an arbitrary energy but can have only certain discrete energy corresponding to n = 1,2,3,…..
2. The lowest possible energy of a particle is **NOT** zero. This is called the **zero-point energy** and means the particle can never be at rest because it always has some kinetic energy.
3. Each permitted energy is called eigen value of the particle and constitutes the energy level of the system.
4. Each permitted energy is called eigen value of the particle and constitutes the energy level of the system. The wave function ψ corresponding to each eigen value are called eigen functions.
5. The wavefunction for a particle in a box at the n=1 and n=2 energy levels look like this:



To find the Eigen functions of the particle using eq.(4) and applying normalization condition

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

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

$$\int_0^L \left| A \sin \frac{n\pi}{L} x \right|^2 dx = 1$$

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

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

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

$$\frac{A^2}{2} [L] = 1$$

$$A = \sqrt{\frac{2}{L}}$$

Eigen Function $\boldsymbol{\psi_n(x)} = \sqrt{\frac{2}{L}} \,\mathbf{sin} \frac{\boldsymbol{n\pi}}{\boldsymbol{L}} \boldsymbol{x}$ n= 1,2,3……