Wave Function

- A wave is characterized by periodic variation in some physical quantity. For example – pressure varies periodically in sound waves whereas electric and magnetic fields vary periodically in an electromagnetic wave. Similarly whose periodic variations make up the matter wave is called wave function.
- Wave function in quantum mechanics accounts for the wave like properties of particle and is obtained by solving a fundamental equation called Schrödinger's equation.
- The wave functions vary with respect to both position co-ordinates of the physical system and the time (x, y, z & t) is called total wave function. It is denoted by the capital form of Greek letter 'Ψ'. If the wave function has variation only with position (x, y, z) it is denoted by the lower case Greek letter 'ψ'.
- The function ψ itself does not have any physical significance hence it is not an experimentally measurable quantity. The probability of finding a particle at some point in space at time 't' is a positive value between 0 & 1. But ψ can be positive or negative or complex. Hence ψ is not an observable quantity.

Physical Significance of Wave Function

The physical significance of ψ could be realized through its probabilistic nature in quantum mechanics in terms of probability density.

Probability Density

- In classical mechanics, the square of wave amplitude associated with electromagnetic radiation is interpreted as measure of intensity. This suggests there will be a similar interpretation for de-Broglie waves associated with electron or any particle.
- Let τ be a volume inside which a particle is present, but where exactly the particle is situated inside τ is not known "If ψ is the wave function associated with the particle then the probability of finding the particle in certain volume $d\tau$ of τ is equal to $|\psi|2\ d\tau$. So $|\psi|2$ is called the probability density".

$$|\psi|^2\, d\tau$$

- This interpretation was first given by Max Born in 1926.
- If the value of $|\psi|2$ is large, then the probability of finding the particle at the point at that time is more. If $|\psi|2 = 0$, then the probability of finding the particle is zero or less. Therefore the total wave function can be represented by the equation,

$$\Psi = Ae^{i(kx-\omega t)} \rightarrow (1)$$

where A is a constant, ω is angular frequency of the wave

The complex conjugate of Ψ is given by,

$$\Psi^* = Ae^{-i(kx-\omega t)} \rightarrow (2)$$

From equation (1) and (2), ΨΨ* is real and positive quantity which is called the probability density. ψψ *

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

Normalization

- According to Born's interpretation the probability of finding the particle within an element of volume is $I\psi I^2$ dv , since the particle is certainly present somewhere inside the volume dv.
- Therefore "The integral of the square of the wave function over the entire volume in space must be equal to unity" and mathematically it is represented as,

$$\int_{-\infty}^{\infty} |\psi|^2 \, dv = 1$$

Where, the wave function satisfying the above relation is the normalized wave function.

Very often Ψ is not a normalized wave function. If this function Ψ is multiplied by a constant *A*, then the new wave function *A*Ψ is also a solution of the wave equation. Hence the new wave function is a normalized wave function.

$$\int_{-\infty}^{\infty} |A\psi^*||A\psi|\,dv = 1 \quad \text{or} \quad A^2 \int_{-\infty}^{\infty} \psi\psi^*\,dv = 1$$

$$|A|^2 = \frac{1}{\int_{-\infty}^{\infty} \psi^*\psi\,dv}$$

Where IAI^2 is known as normalizing constant, the quantity IAΨI^2 represents probability. Therefore the process of constructing AΨ from Ψ is called normalization of the wave function.

The interpretation of the wavefunction

The interpretation of the wavefunction is commonly called the Born interpretation:

- The probability that a particle will be found in the volume element dt at the point r is proportional to $I\psi(r^2)Id\tau$.
- As we know that, in one dimension the volume element is dx. In three dimensions the volume element is dxdydz. It follows from this interpretation that $I\psi(r^2)Id\tau$ is a probability density, in the sense that it yields a probability when multiplied by the volume $d\tau$ of an infinitesimal region.
- The wavefunction itself is a probability amplitude, and has no direct physical meaning. Note that whereas the probability density is real and non negative, the wavefunction may be complex and negative. It is usually convenient to use a normalized wavefunction; then the Born interpretation becomes an equality rather than a proportionality.

Properties of Wave Functions

Physically acceptable wave function Ψ must satisfy the following conditions,

1. Ψ is single valued everywhere, If Ψ has more than one value at any point, it would mean more than one value of probability of finding the particle at that point which is obviously ridiculous. Therefore Ψ must be single valued everywhere.
2. Ψ is finite everywhere. If Ψ is infinite at a point there will be large probability of finding the particle at that point this violet the uncertainty principle therefore Ψ must be finite or zero value at any point and hence $|\psi|^2$ represents probability.
3. Ψ and its first derivatives $d\psi/dx$ with respect to its variables are continuous

Everywhere This is necessary from Schrödinger's equation itself which shows that $d\psi/dx$ must be finite everywhere. Further, the existence of is continuous function, which implies that the function of Ψ is also continuous everywhere.

Time Independent One Dimensional Schrodinger's Wave Equation

Based on de-Broglie idea of matter waves, Schrödinger developed a mathematical theory for a particle of mass 'm' moving with a velocity 'v' along x-direction associated with a wave of wavelength,

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

Where, p = mv is the momentum of the particle.
Let a wave function Ψ describing the de-Broglie wave travelling in +ve x-direction is given by,

$$\psi = Ae^{i(kx-\omega t)} \quad \rightarrow (1)$$

Where Ψ is a total wave function, *A* is a constant and ω is angular frequency of wave.
Let us differentiate Ψ (in equation 1) twice with respect to 'x' then

$$\frac{d\psi}{dx} = A(ik)e^{i(kx-\omega t)}$$

$$\frac{d^2\psi}{dx^2} = A(ik)^2 e^{i(kx-\omega t)}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad or \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \rightarrow (2) \quad \because i^2 = -1$$

$$But \quad k = \frac{2\pi}{\lambda} \qquad and \qquad \lambda = \frac{h}{mv}$$

$$\therefore k = \frac{2\pi mv}{h} \quad \text{or} \quad k^2 = \frac{4\pi^2 m^2 v^2}{h^2}$$

Hence equation (2) becomes.

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \qquad \rightarrow (3)$$

The total energy E of the particle is the sum of kinetic energy T and potential energy V,

$$\therefore E = T + V$$

$$\text{But} \quad T = \frac{1}{2}mv^2 \qquad \therefore \frac{1}{2}mv^2 = mv^2 \quad \text{or} \quad mv^2 = 2(\mathrm{E} - \mathrm{V})$$

Substitute this value of mv^2 in equation (3) we get

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \rightarrow (5)$$

This is known as time independent 1 - dimensional Schrödinger equation.

Equation (5) can also be extended for 3-dimensional space as,

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \rightarrow (6)$$

$$or \quad \nabla^2\psi + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \rightarrow (7)$$

$$where \quad \nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

Equation (6) and (7) are the 3-dimensional time independent Schrödinger wave equation, where Ψ is $\Psi(x, y, z)$.