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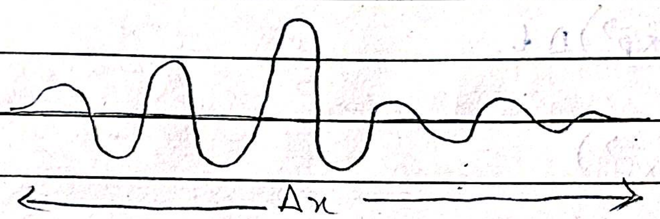
Ke

Unit - 3

Wave Packet :-

The material particles is represented by the wave function $\psi(x,t) = A e^{i(Kx - \omega t)}$. This wave spreads out over the infinite extend in one dimensional space in order to describe the particle localised in certain region (Δx). It is necessary that the wave function should be zero everywhere except in the region Δx where the particle is located a wave of finite extent is shown in the figure ~~is called wave packet~~.



In order to obtain a wave packet it is necessary to modulate the amplitude of the wave in such a way that it is non-zero region Δx and zero outside. This can be done by adding the number of waves of slightly different frequences and amplitude. If we suppose n numbers of waves then the function can be written as

$$\psi(x,t) = \sum_{i=1}^{N} A_i e^{i(k_i x - \omega_i t)}$$

$$\psi(x,t) = \int_{-\infty}^{+\infty} A(K) e^{i(Kx - \omega t)} dx$$

This wave function represents a wave packet which describe the localized particle. Hence we conclude that a localised particle is always associated with the wave packet.

Uncertainity principle :-

According to uncertainity principle it is impossible to measure simultaneously and precisely both the position and the momentum of the particle if Δx is the uncertainty in position and Δp is the uncertainity in momentum then

$$\Delta x . \Delta P_x \geq \hbar \qquad \boxed{\hbar = \frac{h}{2\pi}}$$

Which states that if we try to measure the position and the momentum of the particle simultaneously then the product of uncertanities Δx and Δp_x cannot be less then $\hbar$

$$\Delta P_x \geq \frac{\hbar}{\Delta x}$$

$$\Delta x = 0$$

$$\Delta P_x \geq \frac{\hbar}{0} \geq \infty$$

This means that the momentum of the particle is completely unknow

if $\Delta p_x = 0$

$$\Delta x \geq \frac{\hbar}{0}$$

$$\Delta x \geq \infty$$

Hence the particle is completely unlocalised and spreads out all over the ~~over~~ space.

In 3-D :-

The uncertainty principle becomes

$$\Delta y . \Delta P_y \geq \hbar$$

$$\Delta z . \Delta P_z \geq \hbar$$

The uncertainty principle indicates that we cannot find the exact position and momentum of the particles or atomic dimensions

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Born Interperation of wave function!!

Max. Born extend the concept of wave packets associated with the material particle the motion of the electron travelling in x direction with constant momentum is controlled by the metal wave associated with the wave function which is given by

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

The square of the wave function plays an important role in the metal waves it measures of the probability per unit length of finding the particle at position x and time t.

$|\psi^2|$

$$P = |\psi^2|$$

$\boxed{\psi^* \text{ Complex Conjugate}}$

$$P(x,t) = \psi(x,t)\,\psi^*(x,t)$$

Where P is the probability density

The Born interpertation of wave function means the local of the particle cannot be defined precisely but the wave function can predict only the probability density for finding the particle

Expectionvalue :-

The expection value is the average value of function in quantum mechanics the expection value of a function $f(x)$ is represented

$\langle\rangle$ notation

$$\langle f(x)\rangle = \int \psi^*(x,t)\,f(x)\,\psi(x,t)\,dx$$

Expectiona value of momentum :

The x component of expection value of momentum can be written as

$\langle P_x \rangle = \int \psi^*(x,t)\, P_x\, \psi(x,t)\, dx$ —— (1)

We know that the wave function of a free particle moving in x direction is given by

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

$\frac{\partial y}{\partial x} = A e^{i(kx-\omega t)} . ik$

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

$\frac{\partial y}{\partial x} = ik\, \psi(x,t)$

$P = \hbar k$

$k = \frac{P}{\hbar}$

$\frac{\partial \psi}{\partial x} = \frac{iP}{\hbar} \psi(x,t)$

$\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = P_x \psi(x,t)$

$P_x \psi(x,t) = \frac{\hbar}{i} \times \frac{i}{i} \frac{\partial \psi}{\partial x} = \frac{i\hbar}{i^2} \frac{\partial \psi}{\partial x}$

$P \psi(x,t) = -i\hbar \frac{\partial \psi}{\partial x}$

$P_x = i\hbar \frac{\partial}{\partial x}$

$\langle P_x \rangle = \int \psi^*(x,t) - i\hbar \frac{\partial}{\partial x} \psi(x,t)$

$\langle x \rangle = x$, $\langle y \rangle = y$, $\langle z \rangle = z$, $\langle P_x \rangle = -i\hbar \frac{\partial}{\partial x}$, $\langle E \rangle = i\hbar$

★ Probability Current :-

Consider a wave plane is represented by the wave function.

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

The time dependent schrondinger wave equation :

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi \quad \text{--- (1)}$$

Multiply by ψ^* on both sides

$$i\hbar \psi^* \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \psi^* \nabla^2 \psi + \psi^* V \psi \quad \text{--- (2)}$$

Taking the Complex conjugate of the above equation -

$$-i\hbar \psi \frac{\partial \psi^*}{\partial t} = \frac{-\hbar^2}{2m} \psi \nabla^2 \psi^* + \psi V \psi^* \quad \text{--- (3)}$$

Subtract the eq (3) from eq (2)

$$i\hbar \psi^* \frac{\partial \psi}{\partial t} + i\hbar \psi \frac{\partial \psi^*}{\partial t} = + \frac{\hbar^2}{2x} (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*) + \cancel{\psi^* V \psi} - \cancel{\psi V \psi^*}$$

$$i\hbar \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) = \frac{\hbar^2}{2m} \left(\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right)$$

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

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

$$i \frac{\partial}{\partial t} (\rho) = -\frac{\hbar}{2m} \nabla (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

$$\frac{\partial \rho}{\partial t} = \frac{i^2 \hbar^2}{2m} \nabla (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

$$\frac{\partial \rho}{\partial t} = \frac{-i\hbar}{2m} \nabla (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

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$$\frac{\partial \rho}{\partial t} = -\frac{i\hbar}{2m} \nabla\left(\psi^* \nabla\psi - \psi\nabla\psi^*\right)$$

$$\frac{\partial \rho}{\partial t} + \nabla \frac{i\hbar}{2m}\left(\psi^* \nabla\psi - \psi\nabla\psi^*\right) = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla J = 0$$

$$J = \frac{i\hbar}{2m}\left(\psi^* \nabla\psi - \psi\nabla\psi^*\right)$$

Time independent schrodinger wave equation:-

The one dimensional time dependent mutual wave equation is

$$i\hbar \frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad [V(x)\psi(x,t)] \quad \text{——} \quad (1)$$

In quantum mechanics the potential energy in not a function of In such case, it is possible to separate space and time variable in the wave equation. Let us assume $\psi(x,t)$ is a product of functions

$$\psi(x,t) = \psi(x)T(t)$$

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

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

Divide the above eqn by $\psi(x)T(t)$

$$i\hbar\,\psi(x)\frac{\partial T}{\partial t} = -\frac{\hbar^2}{2m}T(t)\frac{\partial^2\psi}{\partial x^2} + \frac{V(x)\cancel{\psi(x)T(t)}}{\cancel{\psi(x)T(t)}}$$

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

In the above equation left hand side is a function of T(t) only and the right hand side is a function of x only. Therefore, we can write

$$\frac{i\hbar}{T(t)}\frac{\partial T}{\partial t} = E$$

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

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

$$\frac{\partial^2 \psi}{\partial x^2}\cdot\frac{\hbar^2}{2m} + [E - V(x)]\,\psi(x) = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x)]\,\psi(x) = 0$$

In per dimension $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{2m}{\hbar}\left[E - V(x)\right]\psi(x) = 0$

$$\nabla^2\psi + \frac{2m}{\hbar^2}[E - V(1)]\,\psi(x) = 0$$

Linear Harmonic Oscillator :-

A system in which ~~linear harmonic~~ the force is directly proportional to displacement from the equilibrium position and is directed opposite to the displacement is called linear harmonic oscillator. If $x = 0$ is the equilibrium position then f is proportional to $-x$.

$$f \propto -x$$

$$f = -kx \quad \text{--- (1)}$$

Where k is the constant of proportionality

f is known as the force constant

V is the potential energy function then we know that

$$f = -\frac{dV}{dx} \quad \text{--- (2)}$$

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from eqn (1) & (2)

$$Kx = \frac{dV}{dx}$$

$$dV = Kx\,dx$$

$$V = \int_0^x K\,x\,dx$$

$$V = \frac{1}{2}Kx^2$$

This gives the potential energy of the linear harmonic oscilla
The time independent wave equation is given by

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

$$V = \frac{1}{2}Kx^2$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi = 0$$

$K = \omega^2 m$ [for harmonic oscillator]

$$\frac{\partial^2 \psi}{\partial x^2} + \left(\frac{2m}{\hbar^2}E - \frac{\omega^2 m x^2}{2}\right)\psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \left(\beta^2 - \alpha^2 x^2\right)\psi = 0 \quad \text{——— (A)}$$

$$\beta^2 = \frac{2mE}{\hbar^2}, \quad \alpha^2 = \frac{\omega^2 m^2}{\hbar^2}$$

On solving the equation - (A) we obtain

$$\frac{\beta}{\alpha} = 2n+1, \quad n = 0, 1, 2 \ldots\ldots$$

$$= \frac{\frac{2mE}{\cancel{\hbar^2}}}{\frac{\omega^2 m^2}{\cancel{\hbar^2}}} = 2n+1$$

$$= \frac{2E}{\hbar\omega} = 2n+1$$

$$E = \frac{\hbar\omega}{2}(2n+1)$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

This gives the energy of the linear harmonic oscillator.

$$n = 0$$

$$\cancel{E_0 = \frac{1}{2}\hbar\omega} \quad E_0 = \frac{1}{2}\hbar\omega$$

This energy is known as zero point energy.

Hence the particle executing simple harmonic ~~osc~~ motion can have only series

Discrete energies of LHO