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Unit-2 Schrodinger's equation (A)

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Ch#2 SCHRÖDINGER'S EQUATION

✓ In Classical physics, the motion of a body is governed by the Newton's laws of motion. The position, momentum, angular momentum can be measured precisely at any instant of time.

✓ In Quantum mechanics, instead of measurements we talk in terms of probability.

The mathematical function which describes wave group is the wave function $\psi(x, y, z, t)$. As the particle moves under the action of external forces, the wave function changes with time. The motion of a particle is described by the wave function ψ.

* Wave function and its physical interpretation

The wave function ψ may be positive, negative or complex. The probability density is important here. The square of absolute magnitude of wave function $|\psi|^2$ is probability density. At a particular place, particular time it is proportional to the probability of finding the particle there at that time.

$$|\psi|^2 \rightarrow \psi\psi^* \quad (\psi^* \text{ is complex conjugate of } \psi)$$

max Born in 1926 gave interpretation for this.

If at an instant t, a measurement is made to locate a particle having wave function $\psi(x,t)$, then the probability $P(x,t)$ of finding the particle in a range between x and $x+dx$ will be equal to —

$$\psi(x,t)\,\psi^*(x,t)\,dx.$$

The integral of $|\psi|^2$ or $\psi\psi^*$ should be a finite quantity if the wave function ψ has to describe the real particle.

$$\therefore \int |\psi|^2 dV = 1 \quad \text{or} \quad \int \psi\psi^* dv = 1$$

This condition on ψ is called the — <u>normalisation condition</u>.

✓ If the wave function is not normalised, multiply it by some constant A and .....

$$\int A\psi (A\psi^*) dv = 1$$

$$AA^* \int \psi\psi^* dv = 1$$

$$|A|^2 = \frac{1}{\int \psi\psi^* dV}$$

where A is called normalisation constant and it is the positive square root of above equation.

Schrodinger's time dependent equation:

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

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

$$E = h\nu = \frac{h}{2\pi} \cdot 2\pi\nu = \hbar\omega$$

$$\therefore k = \frac{p}{\hbar} \quad \text{and} \quad \omega = \frac{E}{\hbar}$$

$$\therefore \psi = A e^{\frac{i}{\hbar}(px - Et)}$$

Differentiating w.r.t. x we get,

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

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

$$p^2\psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad \text{—— (1)}$$

Differentiating w.r.t. t we get,

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} A e^{i/\hbar(px - Et)}$$

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

$$\therefore E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad \text{—— (2)}$$

The total energy of a particle is the sum of KE and PE ($V(x)$).

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

$$\therefore E\psi = \frac{p^2}{2m}\psi + V\psi \quad \text{——— (3)}$$

using eq (1) and eq (2) in eq (3) we get,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad (4)$$

It was first obtained by Schrödinger in the year 1926. The equation is called Schrödinger's wave equation.

It is time dependent one dimensional equation -

In two dimensions, the equation is

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

In three dimensions, the equation is

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

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

* Schrödinger's time independent equation:
(Steady state equation)

One dimensional schrödinger's equation

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

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

Using method of seperation of variables..

$$\psi(x,t) = \psi(x)\,\phi(t) \quad \text{—(2)}$$

Using (2) in (1) we get

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

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

Dividing by $\psi\phi$ to this equation

$$i\hbar \frac{1}{\phi}\frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial x^2} + V \quad \text{—(3)}$$

In this equation LHS is a function of t only and RHS is a function of x only. So RHS & LHS are equal to some constant E.

$$\therefore \; -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial x^2} + V = E \quad \text{—(4)}$$

and $$i\hbar \frac{1}{\phi}\frac{\partial \phi}{\partial t} = E \quad \text{—(5)}$$

According to Gauss's divergence theorem-

$$\int \bar{J}\cdot d\bar{s} = \int \bar{\nabla}\cdot\bar{J}\, d\tau$$

$$\therefore \int \frac{\partial \rho}{\partial t} d\tau = -\int_{\tau} \bar{\nabla}\cdot\bar{J}\, d\tau$$

or $$\int_{\tau} \left(\bar{\nabla}\cdot\bar{J} + \frac{\partial \rho}{\partial t}\right) d\tau = 0$$

This is true for any arbitrary volume,

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

This is equation of continuity.

✓ Physical significance of equation of continuity

1. If $\frac{\partial \rho}{\partial t}$ is positive, $\bar{\nabla}\cdot\bar{J}$ is negative.
2. If $\frac{\partial \rho}{\partial t}$ is negative, $\bar{\nabla}\cdot\bar{J}$ is positive
3. If $\frac{\partial \rho}{\partial t} = 0$, $\bar{\nabla}\cdot\bar{J} = 0$, ($\rho$ independent of time)

If $\bar{\nabla}\cdot\bar{J}$ is negative, there is net inward flow of the probability current & there is increase in total probability density in region in side.

If $\bar{\nabla}\cdot\bar{J}$ is positive, there is net outward flow of the probability current & there is decrease in total probability density in the given volume.

★ Operator in Quantum Mechanics:

An operator $\hat{O}$, is a mathematical operator when applied to a function $f(x)$, changes that to another function $g(x)$.

$$\therefore \hat{O} f(x) = g(x)$$

e.g. $\frac{d}{dx}(x^3+2) = 3x^2$

Here operator $\frac{d}{dx}$ operates on function x^3+3.

✓ Operators in Quantum mechanics:

$$\psi(x,t) = A e^{i/\hbar (px - Et)} \quad \text{--- (1) a wave fn.}$$

Differentiating w.r.t. x

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

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

$\therefore$ momentum operator p is $-i\hbar\frac{\partial}{\partial x}$

It can be written as $\hat{p} = -i\hbar\frac{\partial}{\partial x}$

or $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$, $\hat{p}_y = -i\hbar\frac{\partial}{\partial y}$, $\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$,

In three dimensions, $\hat{p} = -i\hbar\nabla$.

Differentiating (1) w.r.t t

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

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

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

Schrödinger's time independent equation is...

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

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

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = E\psi$$

$$H\psi = E\psi$$

Where, $H = -\frac{\hbar^2}{2m}\nabla^2 + V$ is the differential operator called Hamiltonian operator.