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matter wave

(BAS-201)

UNIT 1

QUANTUM MECHANICS

TOPICS- TIME-DEPENDENT SCHRODINGER WAVE EQUATIONS

PREPARED BY: LALIT SIR

Schrodinger Wave Equation:

Schrodinger wave equation is a mathematical expression, describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom.

Time-dependent Schrodinger wave equations:

The Schrodinger equation has two ‘forms’, one in which time explicitly appears, and so describes how the wave function of a particle will develop in time. In general, the wave function behaves like a wave, and so the equation is often referred to as the time dependent Schrodinger wave equation. The other is the equation in which the time dependence has been ‘removed’ and hence is known as the time independent Schrodinger equation.

The time-dependent Schroedinger equation is used to describe how a system changes over time. This is the most common form of the equation, and it is used in many different fields of physics.

Time-dependent Schrodinger wave equations:

In the derivation of time-independent schrodinger eqn. potential is taken as independent of time. If however in the system potential energy also does depend on time, the total energy is also time dependent. Therefore, one has to consider time dependent wave function and eqn. will be referred to as time dependent schrodinger wave eqn.

For simplicity, the differential eqn. representing a one-dimension wave motion is given as,

$$\frac{\partial^2 Q}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 Q}{\partial t^2} \quad \text{——} \quad (1)$$

Here $v \rightarrow$ wave velocity moving along x-axis

The general solu. of eqn (1) is given as,

$$Q = A e^{i\omega(t - x/v)}$$

$A \rightarrow$ const. Amplitude

$\omega \rightarrow$ angular velocity

Since the wave equivalent to a free particle moving along +ve x-direction may be expressed by a corresponding eqn. as,

$$\psi(x,t) = A e^{i\omega(t - x/v)} \quad \text{——} \quad (2)$$

Since we know that, $\omega = 2\pi\nu$ & $\nu = \frac{v}{\lambda} \Rightarrow v = \lambda\nu$

$$\psi(x,t) = A \cdot e^{-i2\pi\nu(t - x/v\lambda)}$$

$$= A \cdot e^{-i2\pi(\nu t - x\cancel{\nu}/\cancel{\nu}\lambda)}$$

$$= A \cdot e^{-i2\pi(\nu t - x/\lambda)}$$

$$= A \cdot e^{-i2\pi\left(\frac{E}{h} \cdot t - \frac{px}{h}\right)}$$

$$= A \cdot e^{-i\frac{2\pi}{h}(Et - px)}$$

$$\psi(x,t) = A \cdot e^{-\frac{i}{\hbar}(Et - px)} \qquad \text{———— (3)}$$

Since, we know that $E = h\nu \Rightarrow \nu = \frac{E}{h}$, $\lambda = \frac{h}{p}$

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

Now partially diff. eqn. (3) twice w.r.t 'x' then we get

$$\frac{\partial \psi}{\partial x} = A\left[-\frac{i}{\hbar}(0-p)\right] \cdot e^{-i/\hbar(Et-px)} \qquad \frac{\partial}{\partial x} e^{x} = e^{x} \cdot (1)$$

$$\frac{\partial^2 \psi}{\partial x^2} = A\left[-\frac{i}{\hbar}(0-p)\right]^2 \cdot e^{-i/\hbar(Et-px)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = A \frac{i^2}{\hbar^2} \cdot p^2 \cdot e^{-i/\hbar(Et-px)} = \underline{A \cdot e^{-i/\hbar(Et-px)}} \cdot \frac{\overset{\to -1}{i^2}}{\hbar^2} \cdot p^2$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \cdot \psi \Rightarrow p^2 = -\frac{\hbar^2}{\psi} \cdot \frac{\partial^2 \psi}{\partial x^2} \quad \text{——— (4)}$$

Now partially diff. eqn. (3) w.r.t 't' then we get,

$$\frac{\partial \psi}{\partial t} = A e^{-i/\hbar(Et-px)} \left[-\frac{i}{\hbar}(E-0)\right]$$

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

$$\frac{\partial\psi}{\partial t} = \frac{E}{i\hbar} \cdot \psi \Rightarrow E = \frac{i\hbar}{\psi} \cdot \frac{\partial\psi}{\partial t} \quad \text{--- (5)}$$

Since, we know that,

Total energy = K.E + V

$$E = \frac{1}{2}mv^2 + V = \frac{m^2v^2}{2m} + V$$

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

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

$$\frac{i\hbar}{\cancel{\psi}} \cdot \frac{\partial\psi}{\partial t} = \frac{1}{\cancel{\psi}}\left[\frac{-\hbar^2}{2m} \cdot \frac{\partial^2\psi}{\partial x^2} + \psi V\right]$$

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

Now putting values of E & p2

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

time dependent wave eqn when particle moving in 1-D (along x-axis)

If particle is moving into three-dimensional space then eqn. can be written as,

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

Let $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\nabla^2$

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

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

time dependent wave eqn. when particle moving into 3-D


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