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(BAS-201)

UNIT 1

QUANTUM MECHANICS

TOPICS- TIME-INDEPENDENT SCHRODINGER WAVE EQUATIONS

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SYLLABUS

Quantum Mechanics: Inadequacy of classical mechanics, Planck's theory of black body radiation(qualitative), Compton effect, de-Broglie concept of matter waves, Davisson and Germer Experiment, Phase velocity and group velocity, Time-dependent and time-independent Schrodinger wave equations, Physical interpretation of wave function, Particle in a one-Dimensional box. Numericals

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Where to Use the Schroedinger Wave Equation

In quantum mechanics, the Schroedinger wave equation is used to describe the behavior of a particle in a given potential field.

The equation is named after Erwin Schroedinger, who first derived it in 1926. It is a wave equation that describes the wave-like behavior of a particle in a given potential field. The equation has both time-dependent and time-independent versions, depending on the application.

The Schroedinger wave equation has many applications in physics and chemistry. It is used to describe the behavior of electrons in atoms and molecules. It is also used in the study of semiconductors and other solid-state materials.

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.

Schrodinger's time-independent wave equation describes the standing waves. Sometimes the potential energy of the particle does not depend upon time, and the potential energy is only the function of position.

Time-independent Schrodinger wave equations: OR

Steady-state Schrodinger wave Equation:

Acc. to classical wave optics the differential eqⁿ of a wave when it is in motion is given by

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = \frac{1}{c^2} \cdot \frac{\partial^2 \phi}{\partial t^2} \quad \text{--- (1)}$$

In analogy with optics, the differential eqⁿ of a wave motion of particle can be written as, ψ, v

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \psi}{\partial t^2} \quad \text{--- (2)}$$

$\psi \rightarrow$ wave funⁿ of matter wave

The wave fun. $\psi(x,y,z,t)$ of the particle can be seperated into space dependent (x,y,z) and time dependent t.

$$\psi(x,y,z,t) = \psi(x,y,z)\cdot f(t) \quad \text{——} \quad (3)$$

for the wave, the fun. $f(t)$ ~~was~~ must be a periodic fun. so that $f(t) = e^{i\omega t}$ $\qquad \omega = 2\pi\nu$

$$\psi(x,y,z,t) = \psi(x,y,z)\cdot e^{i\omega t} \quad \text{——} \quad (4)$$

(Partially diff.)

Now diff. eqn. (4) twice w.r.t 'x, y, z, t' respectively,

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\psi}{\partial x^2}\cdot e^{i\omega t} \qquad \frac{\partial^2\psi}{\partial y^2} = \frac{\partial^2\psi}{\partial y^2}\cdot e^{i\omega t} \qquad \frac{\partial^2\psi}{\partial z^2} = \frac{\partial^2\psi}{\partial z^2}\cdot e^{i\omega t}$$

$$\psi(x,y,z,t) = \psi(x,y,z)\cdot e^{i\omega t}$$ w.r.t 't' twice

$$\frac{\partial \psi}{\partial t} = \psi\cdot(i\omega)\cdot e^{i\omega t} \Rightarrow \frac{\partial^2 \psi}{\partial t^2} = \psi(i\omega)^2 e^{i\omega t} \qquad i^2 = -1$$

$$\frac{\partial^2 \psi}{\partial t^2} = \psi(-\omega^2)\cdot e^{i\omega t} = -\omega^2\cdot e^{i\omega t}\cdot\psi$$

Now putting the values of $\frac{\partial^2 \psi}{\partial x^2}, \frac{\partial^2 \psi}{\partial y^2}, \frac{\partial^2 \psi}{\partial z^2}$ & $\frac{\partial^2 \psi}{\partial t^2}$ into eqⁿ (2)

then we get,

$$\frac{\partial^2 \psi}{\partial x^2}\cdot\cancel{e^{i\omega t}} + \frac{\partial^2 \psi}{\partial y^2}\cdot\cancel{e^{i\omega t}} + \frac{\partial^2 \psi}{\partial z^2}\cdot\cancel{e^{i\omega t}} = -\frac{\omega^2}{v^2}\cdot\cancel{e^{i\omega t}}\cdot\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{\omega^2}{v^2}\cdot\psi \qquad (5)$$

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

Now eqn. (5) becomes, $\nabla^2\psi = -\frac{\omega^2}{v^2}\psi$

$$\boxed{\nabla^2\psi + \frac{\omega^2}{v^2}\psi = 0} \quad \text{——— (6)}$$

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

then $\omega = \frac{2\pi v}{\lambda} \Rightarrow \frac{\omega}{v} = \frac{2\pi}{\lambda} \Rightarrow \frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2}$

since $\lambda = \frac{h}{p}$ $\quad \frac{\omega^2}{v^2} = \frac{4\pi^2 p^2}{h^2}$ ——— (7)

If E and V are the velocity of the wave associated with the particle (p is the momentum, λ is wavelength)

K.E (T) = E − V $\quad$ Since, $T = \frac{p^2}{2m} \Rightarrow p^2 = 2mT$

Now eqn. (7) becomes, $\frac{\omega^2}{v^2} = \frac{4\pi^2}{h^2}2m(E-V)$ $\quad p^2 = 2m(E-V)$

$$\frac{\omega^2}{v^2} = \frac{8\pi^2}{h^2} m(E-V) \qquad \hbar = \frac{h}{2\pi} \Rightarrow \hbar^2 = \frac{h^2}{4\pi^2}$$

$$\frac{\omega^2}{v^2} = \frac{2}{\hbar^2} m(E-V) = \frac{2m}{\hbar^2}(E-V) \quad \text{——} \quad (8)$$

Now putting this value into eqn. (6) then we get,

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

steady state wave eqn.

Schrodinger time-independ. wave eqn.

For free particle $V=0$ then

$$\nabla^2\psi + \frac{2m}{\hbar^2}\cdot E\psi = 0$$

This is a wave eqn. for free particle.

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