SUBJECT - CHEMISTRY
CLASS - B.Sc(Hons) PART - III
PAPER - V
TOPIC - Schrodinger wave equation
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The Bohr's model violates the uncertainty principle, as it describes simultaneously both the position and momentum of an electron, Therefore the correct theory is expected to deal with the probability of finding an electron in a given space. This Concept led Schrodinger to think over the famous de-Broglie wave-particle duality principle and thus worked out a mathematical equation using the principle of quantum mechanics, which incorporates the requirements of uncertainty principle. Since electron behaves also as a wave hence Schrodinger used the following time independent one dimensional equation of linear waves i.e y w.r.t x axis to explain the behaviour of electron in an atom

$$\frac{d^2y}{dx^2} + \frac{4\pi^2 y}{\lambda^2} = 0$$

Since there is three dimensional distribution of charge density within an atom, hence y is replaced by psi (ψ) as the displacement function. Hence the above equation becomes-

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2\psi}{\lambda^2} = 0 \quad \text{--- (1)}$$

from de-Broglie relation $\lambda = \frac{h}{mv}$ or $\frac{1}{\lambda^2} = \frac{m^2v^2}{h^2}$ ... (2)

putting (2) in (1) we get,

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

further, if E = total energy of a particle and V = potential energy then

$$E = V + \frac{mv^2}{2} \quad \text{or} \quad v^2 = \frac{2(E-V)}{m} \quad \text{---} \quad (4)$$

putting (4) in (3), we have

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

This is the schrodinger wave equation in one dimension, where ψ is wave function. Now in three dimension. this equation becomes

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m(E-V)\psi}{h^2} = 0 \quad \text{---} \quad (6)$$

This is the general form of Schrodinger wave equation

To avoid repetition, the entire differential terms are shown by The symbol nabla or del ∇. Hence the above equation becomes-

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

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is known as Laplacian operator.