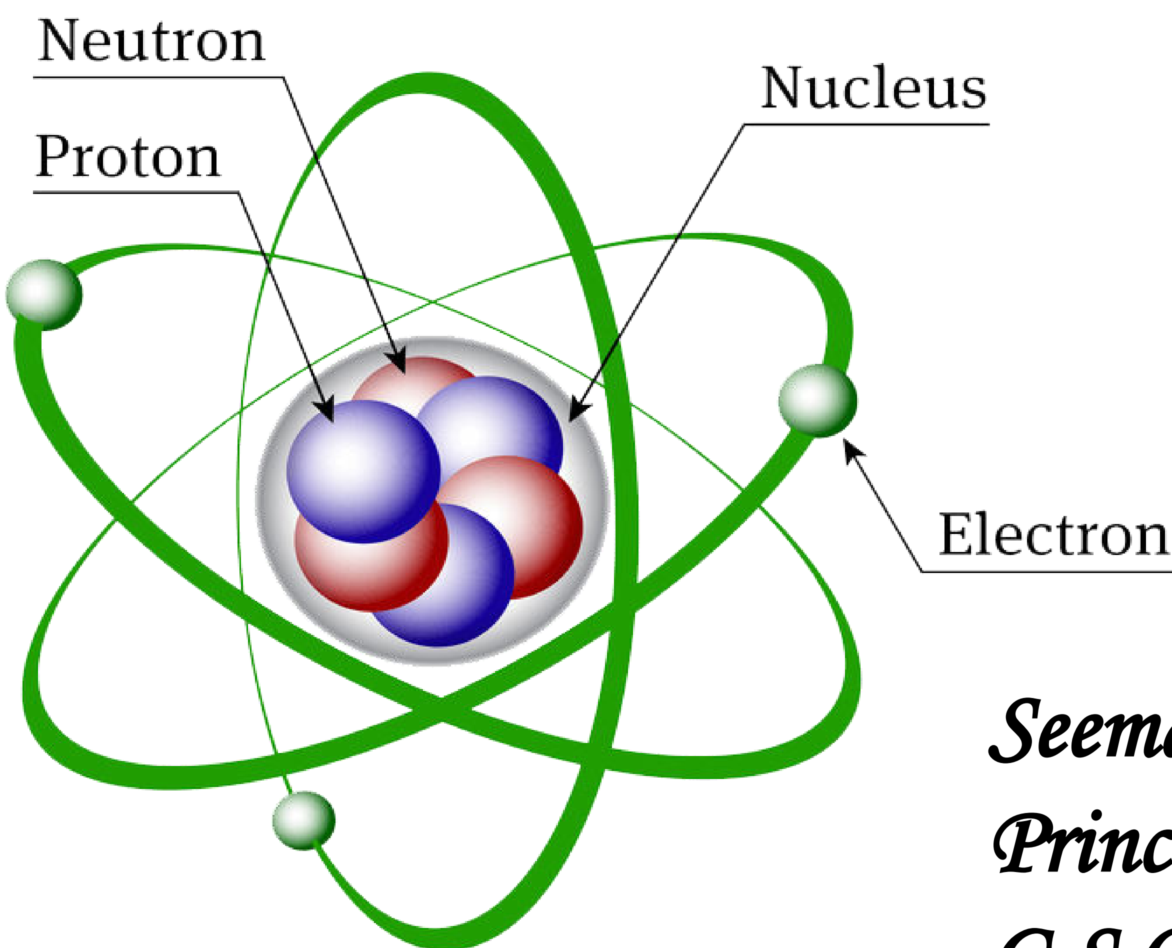
Structure Of Atom



Seema Saini
Principal
G.S.C Naya Nangal

SCHRODINGER WAVE EQUATION

- Schrodinger described the behaviour of electron in an atom by a mathematical equation known as Schrodinger wave equation.
- He used de Broglie idea to describe the motion of an electron in terms of electron wave.
- Though we cannot find the exact position or path of the electron we can calculate the energy of an electron.

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

m= mass of electron, E = total energy,
V= Potential energy, h = Planck's constant,
ψ = amplitude of electron wave (wave function)

$\frac{\partial^2\psi}{\partial x^2}$ = refers to second derivative of ψ w.r.t **x only**

$\frac{\partial^2\psi}{\partial y^2}$ =refers to second derivative of ψ w.r.t **y only**

$\frac{\partial^2 \psi}{\partial x^2}$ = refers to second derivativeof ψ w.r.t **z only**

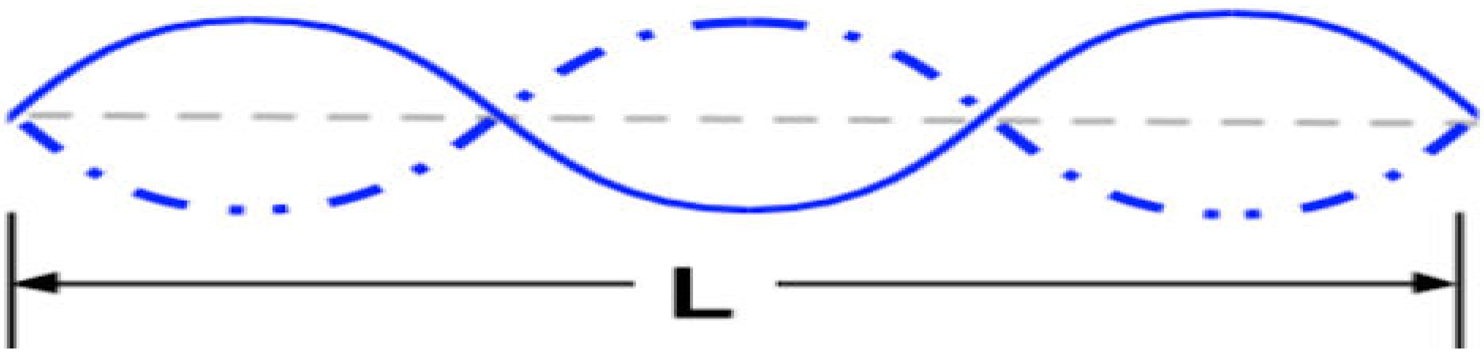
Schrodinger wave eqn. can also be written as

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

$$\nabla^2\psi = \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi$$

∇^2 = Laplacian operator

Formulation of Schrodinger wave equation:
Assumed that nucleus of atom is surrounded by vibrating electron wave similar to standing wave.



Stationary wave produced by vibrating string fixed between two fixed point

The general equation for such a wave in one direction (x- axis) is given as

$$\Psi = A\,\frac{\sin 2\pi x}{\lambda} \qquad \text{..................(iii)}$$

A= constant,

ψ= amplitude or wave function

x = distance from origin in one direction

λ= wavelength

On double differentiating Eq. (iii)

$$\frac{d\psi}{dx} = A\frac{2\pi}{\lambda}\cos\frac{2\pi x}{\lambda}$$

$$\frac{d^2\psi}{dx^2} = A\frac{2\pi}{\lambda}\cdot\frac{2\pi}{\lambda}(-)\sin\frac{2\pi x}{\lambda}.$$

$$= -\frac{4\pi^2}{\lambda^2}\cdot A\sin\frac{2\pi x}{\lambda}.$$

Subsitute the value of ψ. from equation 1

$$= -\frac{4\pi^2}{\lambda^2}\psi \quad \ldots\ldots \text{(iv)}$$

According to de Broglie

$$\lambda = \frac{h}{mv}$$

Subsitute the value of λ in equation (iv)

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2 m^2 v^2}{h^2}\psi \quad \ldots\ldots (v)$$

Consider electron as particle.

E = Total energy.

T = Kinetic energy

P = Potential energy.

Total energy of electron is

Total Energy = K.E (T) + P.E (V)

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

$$mv^2 = 2(E-V)$$

$$v^2 = \frac{2(E-V)}{m} \quad \ldots\ldots \text{(vi)}$$

Subsitute the value of v^2 from eq. 5 into eq. 4

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2 m^2 \times 2(E-V)^2}{h^2 \, m}\psi$$

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

Or

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

Above equation is Schrodinger wave equation for wave motion in one direction (x).

Similarly the Schrodinger wave equation for wave motion in y and z axis may be written as

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

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

So the schrodinger wave equation for wave motion of electron in three directions x, y and z may be written as

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

- The potential energy ‘V’ in S.W.E. can also be determined.
- The potential energy of an electron at rest and at infinite distance is taken as zero.
- Potential energy will have some value when the electron is at a distance ‘r’ from the nucleus and it is given as

$$V = -\frac{(+Ze)(e)}{r} = -\frac{Ze^2}{r}$$

where,

+Ze = charge on the nucleus

Z = atomic number

e = charge on the electron

So, the equation can be written as

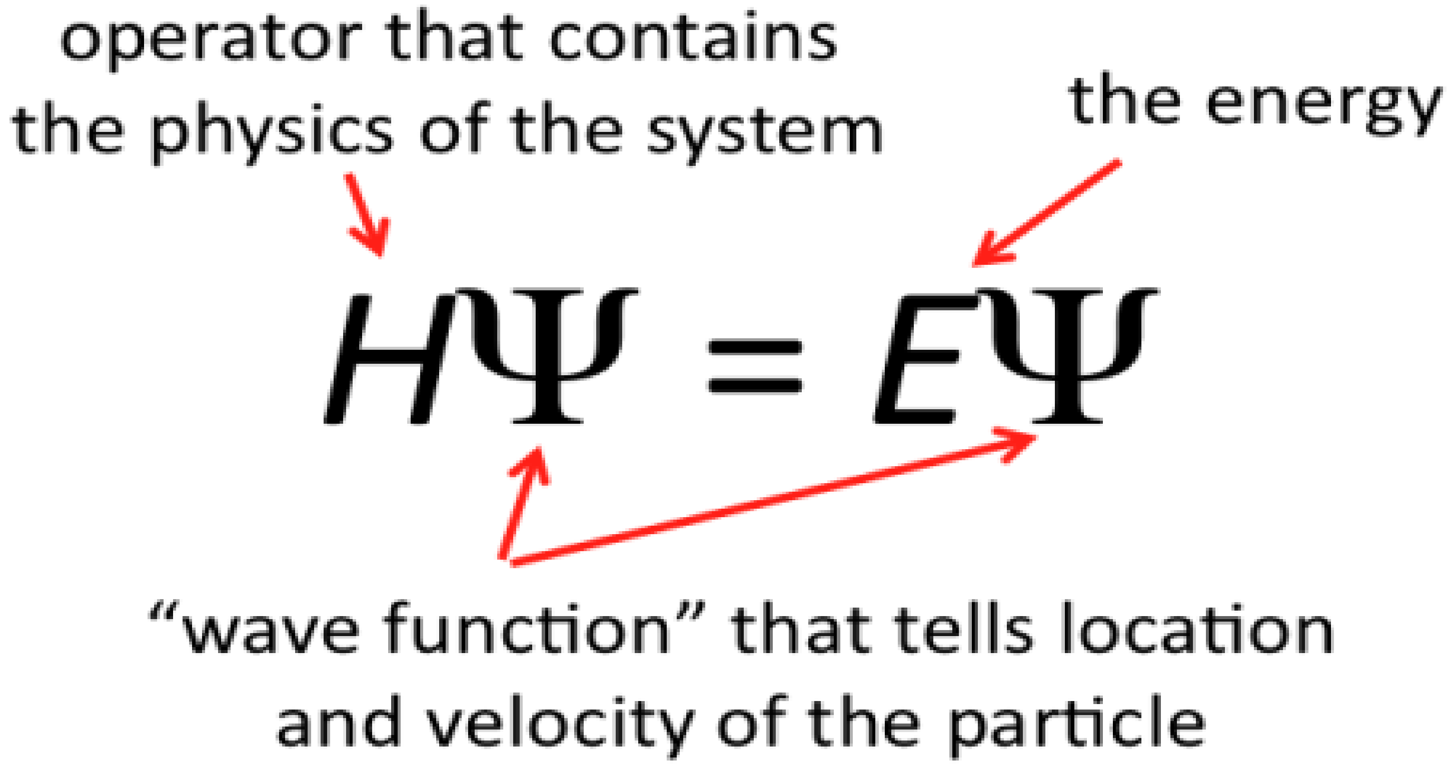
$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}(E+\frac{Ze^2}{r})\psi=0$$

- This eqn. is the basis of wave mechanical model of atom.

- Dependence on all three coordinates suggests that quantum mechanical model considers that the charge on electron is distributed about the nucleus in three dimensions.

- It is not confined to planar orbits as in Bohr model .

Schrodinger wave equation for a system whose energy does not change with time can be written as



H is the **Hamiltonian operator** which is vector sum of kinetic and potential energy.

Takes into account K.E of all sub atomic particle(electron , nuclei) and attractive potential between nuclei and electron and repulsive potential between nuclei and electron.

Solution of Schrodinger equation gave value of E and ψ

SOLUTIONS OF S.W.E :

- Have **large number** of solutions in terms of wave function (**Ψ**)
- All solutions **are not acceptable** as they do not have any physical significance.
- Solutions which **satisfy certain conditions** and have physical significance are acceptable.
- These are called **eigen functions** of the system.

CONDITIONS FOR WAVE FUNCTION (Ψ) TO SATISFY :

1. **Ψ must be single valued .**

2. **The wave function ψ must be continuous.**

3. **Ψ must have finite value.**

4. **Ψ must be normalised.**

5. **ψ must become zero at infinity**

EIGEN FUNCTIONS : Are the solution of Schrodinger wave equation which have physical significance and corresponds to definite energy values (eigen values).

EIGEN VALUE : Are the definite values of total energy for solutions of Schrodinger wave equation which have physical significance .

Application of Schrodinger wave equation to Hydrogen Atom

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E + \frac{Ze^2}{r})\psi = 0$$

$$E_n = -\frac{2\pi^2 m e^4 Z^2}{n^2 h^2}$$

$$E_n = -R[\frac{Z^2}{n^2}]$$

where , $R = \frac{2\pi^2 m e^4}{h^2}$

R= Rydberg's constant

$E_n = -\frac{\mathbf{2.17 \times 10^{-18}}}{\mathbf{n^2}}$ **J per mole**

$E_n = -\frac{1311.8}{n^2}$ $kJmol^{-1}$

Identical with Bohr equation for energy of electron in hydrogen atom