

Unit-III

\* Quantum Mechanical treatment of linear Harmonic Oscillator :-

Since the potential energy of oscillation at any point 'x' is -

$$2\pi^2 \nu_0^2 M x^2$$

The Hamiltonian operator for a harmonic oscillator is given by -

$$\hat{H} = \frac{-h^2}{8\pi^2 M} \frac{d^2}{dx^2} + 2\pi^2 \nu_0^2 M x^2$$

The Schrödinger equation  $\hat{H}\psi = E\psi$  for such a motion may be written as -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 M}{h^2} (E - 2\pi^2 \nu_0^2 M x^2) \psi = 0 \quad \text{--- (4)}$$

Let,

$$\alpha = \frac{8\pi^2 M E}{h^2} \quad \& \quad \beta = \frac{4\pi^2 \nu_0^2 M}{h} \quad \text{--- (5)}$$

So, eqs - (4) becomes -

$$\frac{d^2\psi}{dx^2} + (\alpha - \beta x^2) \psi = 0 \quad \text{--- (6)}$$

Let,  $y = \sqrt{\beta} x$

So,  $dx = \frac{dy}{\sqrt{\beta}}$  &  $\frac{d^2\psi}{dx^2} = \beta \frac{d^2\psi}{dy^2}$

Substituting these values in eqs - (6) we get,

$$\beta \cdot \frac{d^2\psi}{dy^2} + (\alpha - \beta y^2) \psi = 0$$

or, 
$$\frac{d^2\psi}{dy^2} + \left(\frac{\alpha}{\beta^2} - y^2\right)\psi = 0 \quad \text{--- (7)}$$

\* Solution of this equation :-

let  $y \gg \frac{\alpha}{\beta}$

then eq<sup>n</sup> - (7) reduces to

$$\frac{d^2\psi}{dy^2} - y^2\psi = 0$$

The solution of this equation may be as  $\psi = \exp(\pm y^2/2)$

but the solution  $\psi = \exp(\pm y^2/2)$  is not acceptable because in that case  $\psi$  will be rapidly increase tending to  $\infty$  as  $y$  approaches  $\pm\infty$ . so, the other solution is

$$\psi = \exp(-y^2/2)$$

So, the general solution for eq<sup>n</sup> - (7) may be written as

$$\psi = F(y)\exp(-y^2/2) \quad \text{--- (8)}$$

where,  $F(y)$  or  $F$  is same function of  $y$  whose form has to be determined by finding its differential eq<sup>n</sup> for it. differentiating eq<sup>n</sup> - (8) w.r.t  $y$ , we obtain,

$$\frac{d^2\psi}{dy^2} = \left\{ \frac{d^2F}{dy^2} - 2y \frac{dF}{dy} + (y^2 - 1)F \right\} \exp(-y^2/2) \quad \text{--- (9)}$$

Hence, by substituting for  $\psi$  and  $\frac{d^2\psi}{dy^2}$  from eqs (8) & (9)

respectively in the eqn - (6), we get

$$\left[ \frac{d^2 F}{dy^2} - 2y \frac{dF}{dy} + (y^2 - 1) F \right] \exp(-y^2/2) + \left[ \frac{\alpha}{\beta} - y^2 \right] \exp(-y^2/2) F = 0$$

$$\therefore, \left[ \frac{d^2 F}{dy^2} - 2y \frac{dF}{dy} + \left( \frac{\alpha}{\beta} - 1 \right) F \right] \exp(-y^2/2) = 0 \quad \text{--- (10)}$$

Since,  $\exp(-y^2/2) \neq 0$  except  $y = \pm\infty$

the expression within brackets must be zero.

$$\text{i.e. } \frac{d^2 F}{dy^2} - 2y \frac{dF}{dy} + \left( \frac{\alpha}{\beta} - 1 \right) F = 0 \quad \text{--- (11)}$$

This eqn - (11) is known as Hermite's differential Equation.

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