Simple Harmonic Oscillator (one dimensional) or Linear Harmonic Oscillator.

The time-independent Schrodinger wave equation for linear motion of a particle along the x-axis is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

or $$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad ; \text{———} (1)$$

where E is the total energy of the particle,

V is the potential energy.

ψ is the wave function for the particle, which is the function of x alone.

For the linear oscillator along the x-axis with the angular frequency ω under a restoring force proportional to the displacement x,

The potential energy is given by

$$V = \frac{1}{2}m\omega^2x^2 \quad ; \text{———} (2)$$

Putting the value of V from (2) in equation (1)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2x^2\right)\psi = 0 \quad ; \text{———} (3)$$

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2x^2}{\hbar^2}\right)\psi = 0 \quad \text{———} (4)$$

To simplify equation (4) we introduce a dimensionless independent variablee y which is related to x by the equation:

$$y = \sqrt{\frac{m\omega}{\hbar}}\, x \quad ; \text{———} (5)$$

so that $x = \sqrt{\frac{\hbar}{m\omega}}\, y$

Now we have

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\cdot\frac{dy}{dx} = \frac{d\psi}{dy}\cdot\sqrt{\frac{m\omega}{\hbar}}$$

and $$\frac{d^2\psi}{dx^2} = \frac{d^2\psi}{dy^2}\cdot\frac{dy}{dx}\sqrt{\frac{m\omega}{\hbar}} = \frac{d^2\psi}{dy^2}\cdot\frac{m\omega}{\hbar} = \frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2} ; \text{—} ($$

Putting the values of $\frac{d^2\psi}{dx^2}$ from equation (6) and x^2 from equation (5) in (4) we get

$$\frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}\cdot\frac{\hbar}{m\omega}y^2\right)\psi = 0$$

or $$\frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - \frac{m\omega}{\hbar}y^2\right)\psi = 0$$

or $$\frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2} + \frac{m\omega}{\hbar}\left(\frac{\hbar}{m\omega}\cdot\frac{2mE}{\hbar^2} - y^2\right)\psi = 0$$

or $$\frac{d^2\psi}{dy^2} + \left(\frac{2E}{\hbar\omega} - y^2\right)\psi = 0 \; ; \text{———} \; (7)$$

or $$\frac{d^2\psi}{dy^2} + (\lambda - y^2)\psi = 0$$

———(8)

where $\lambda = \frac{2E}{\hbar\omega}$

For large values of y, such that $y^2 >> \lambda$, we may neglect λ. Therefore, equation (7) is transformed to the form

$$\frac{d^2\psi}{dy^2} - y^2\psi = 0 \; ; \text{———} \; (9)$$

For large ~~value of y, the approp approximate solution of this equation is~~ ~~$\psi =$~~ Its general solution is

$$\psi = e^{\pm y^2/2}$$

Since $\psi \to 0$, when $y \to \infty$, we reject the form $e^{+y^2/2}$

Then the equation becomes

$$\psi = e^{-y^2/2} \; ; \text{———} \; (10)$$

~~Substituting this equation into equation (9), we get~~

~~$\frac{d^2\psi}{dy^2}$~~ Equation (10) contains the term $e^{-y^2/2}$ as a factor.

The accurate solution of equation (7) must be of the form

$$\psi = e^{-y^2/2} H(y) \quad \text{———} \; (11)$$

where $H(y)$ is a finite polynomial in y.

~~Diffe~~ change of dependent variable from ψ to $H(y)$ in equation (7).

To change the differential equation (7) into a differential equation for the dependent variable $H(y)$

Differentiating equation (11) w.r.t y, we get

$$\frac{d\psi}{dy} = e^{-y^2/2}\frac{dH}{dy} + He^{-y^2/2}(-y)$$

$$\frac{d\psi}{dy} = \left(\frac{dH}{dy} - Hy\right)e^{-y^2/2}$$

Scanned with CamScanner

Now differentiating this equation w.r.t y again, we get

$$\frac{d^2\psi}{dy^2} = \left(\frac{d^2H}{dy^2} - y\frac{dH}{dy} - H\right)e^{-y^2/2} + \left(\frac{dH}{dy} - Hy\right)e^{-y^2/2}(-y)$$

$$\frac{d^2\psi}{dy^2} = \left[\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} - H + Hy^2\right]e^{-y^2/2}$$

Now substituting the expression for $\frac{d^2\psi}{dy^2}$ and the expression for ψ in equation (8) we get

$$\left[\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} - H + Hy^2\right]e^{-y^2/2} + (\lambda - y^2)He^{-y^2/2} = 0$$

or $$\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + (\lambda-1)H = 0 \quad ; \text{———} (12)$$

This is a well known Hermite's differential equation.

The solution of equation (12) is expressed in the form of power series of y.

$$H(y) = \sum_{n=0}^{\infty} A_n y^n \quad ; \text{———} (13)$$

$$H(y) = A_0 + A_1 y + A_2 y^2 + A_3 y^3 + A_4 y^4 + \cdots \text{———} (14)$$

Differentiating equation (14) w.r.t y

$$\frac{dH}{dy} = A_1 + 2A_2 y + 3A_3 y^2 + 4A_4 y^3 + \cdots \text{———} (15)$$

Multiplying this equation by $-2y$

$$-2y\frac{dH}{dy} = -2(A_1 y + 2A_2 y^2 + 3A_3 y^3 + \cdots)$$

$$-2y\frac{dH}{dy} = \sum_{n=0}^{\infty} -2n A_n y^n \text{———} (16)$$

Differentiating equation (15) w.r.t y

$$\frac{d^2H}{dy^2} = 2A_2 + 3\cdot 2A_3 y + 4\cdot 3A_4 y^2 + \cdots$$

$$= \sum_{n=0}^{\infty} (n+2)(n+1)A_{n+2} y^n \text{———} (17)$$

Multiplying both the sides of equation (13) by $(\lambda-1)$

$$(\lambda-1)H(y) = \sum_{n=0}^{\infty} (\lambda-1)A_n y^n \quad ; \text{———} (18)$$

Putting (16), (17) & (18) in equation (12), we get

$$\sum_{n=0}^{\infty}\left[(n+2)(n+1)A_{n+2} - 2nA_n + (\lambda-1)A_n\right]y^n = 0$$

or $\sum_{n=0}^{\infty} \left[(n+1)(n+2) A_{n+2} - (2n+1-\lambda) A_n\right] y^n = 0$

This equation must be true for all values of y and therefore, the coefficient of each power of y must vanish separately.

Hence we have

$$(n+2)(n+1) A_{n+2} - (2n+1-\lambda) A_n = 0$$

or
$$\boxed{A_{n+2} = \frac{2n+1-\lambda}{(n+1)(n+2)} \cdot A_n} \quad (19)$$

This is known as Recursion formula

Eigen values of Harmonic Oscillator

In order to obtain a satisfactory wavefunction the series given in equation (19) should break off after a finite number of terms. In equation (19) the term $2n+1-\lambda$ must be zero so that the series break off after the nth i.e. the finite term.

$$\therefore \quad 2n+1-\lambda = 0$$
$$\text{or} \quad \lambda = 2n+1 \quad \text{———} \ (20)$$

Here λ is dimensionless eigen value

But $\lambda = \frac{2E}{\hbar\omega}$

$$\therefore \frac{2E}{\hbar\omega} = (2n+1)$$
$$2E = (2n+1)\hbar\omega$$
$$E = \left(n+\frac{1}{2}\right)\hbar\omega$$

~~Putting $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi$~~

In general we get

$$\boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega} \ ; \text{———} \ (21)$$

Putting $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi\nu$

$$\boxed{E_n = \left(n+\frac{1}{2}\right)h\nu} \ , \text{———} \ (22)$$

where $n = 0, 1, 2, \ldots\ldots$

From equation (21) we get the following conclusions:

(i) The lowest energy of the oscillator is obtained by putting $n=0$ in equation (21)

$$\boxed{E_0 = \frac{1}{2}\hbar\omega} \ ; \text{———} \ (23)$$

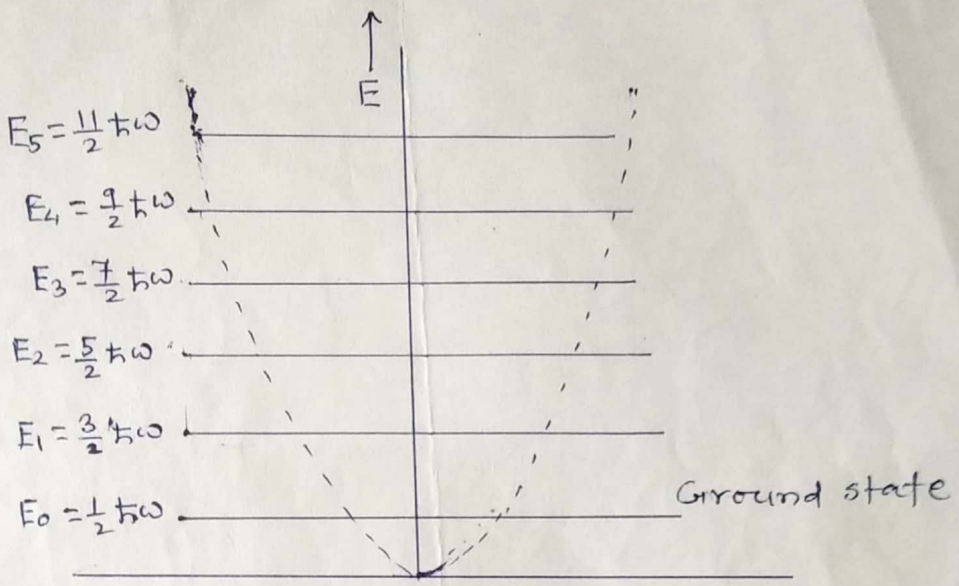
This energy is called the ground state energy or the zero point vibration energy of the harmonic oscillator. The zero point energy is the characteristic result of quantum mechanics. The values of E_n in terms of E_0 are given by $E_n = (2n+1) E_0$; ——— (24)

where $n = 0, 1, 2, 3, \ldots\ldots$

(ii) The eigen values of the total energy depend only on the quantum number n.

Therefore all the energy levels of the oscillator are non-degenerate.

(iii) The successive energy-levels are equally spaced. i.e the separation between two adjacent energy levels being $\hbar\omega$. The energy level diagram for the harmonic oscillator is shown as —



[Energy Level diagram of Harmonic oscillator]

Scanned with CamScanner