# UNIT-V

# APPLIED QUANTUM PHYSICS

## INTRODUCTION

- In this chapter Schrodinger's time independent wave equation can be applied to a system and then solved to find the energy and wave function of the system under given conditions.
- We also aim at learning characteristic properties of solutions of this equation and comparing the predictions of quantum mechanics with those of Newtonian mechanics.
- As simple applications of Schrodinger's time independent wave equation, here we shall discuss the problem of Harmonic oscillator, Barrier penetration and Quantum tunneling, Finite potential wells.

## 5.1. HARMONIC OSCILLATOR.

Definition

A particle undergoing simple harmonic motion is called a harmonic oscillator. In harmonic oscillator, the force applied is directly proportional to the displacement and is always directed towards the mean position.

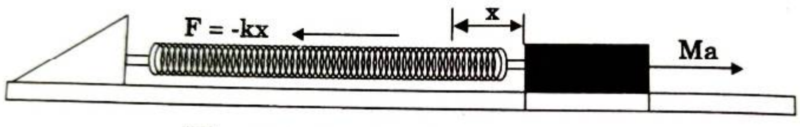


Fig. 5.1 Harmonic Oscillator

Examples.

a simple pendulum, an object floating in a liquid, a diatomic molecule and an atom in a crystal lattice.

If applied force moves the particle through $x$, then restoring force $F$ is given by

$$F \propto -x$$
$$F = -kx \text{ ---------- } (1)$$

The potential energy of the oscillator is

$$V = -\int Fdx$$
$$V = k\int xdx = \frac{1}{2}kx^2$$
$$V = \frac{1}{2}kx^2 \text{ ----------- } (2)$$

where $k$ is force constant.

In harmonic oscillator, angular frequency is given by

$$\omega = \sqrt{\frac{k}{m}}$$

Squaring on both sides

$$\omega^2 = \left(\sqrt{\frac{k}{m}}\right)^2$$
$$\omega^2 = \frac{k}{m},\ k = m\omega^2$$

where $m$ - mass of the particle

Substituting $k$ in eqn (1), we have

$$V = \frac{1}{2}m\omega^2x^2 \text{ --------- } (3)$$

Wave equations for the oscillator:

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 - - - - - - -(4)$$

where $E$ - Total energy of the particle,

$V$ - Potential energy and

$\Psi$ - Wave-function for the particle which is function of $x$ alone.

Substituting for $V$ in equation (4) we get,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2x^2\right)\psi = 0 - - - - - - - - (5)$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} - \frac{2m}{\hbar^2} \times \frac{1}{2}m\omega^2x^2\psi = 0$$

or $$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\psi = 0 - - - - - - - - - -(6)$$

This is Schrodinger wave equation for the oscillator.

Simplification of the wave equation

To simplify eqn. (6), a dimensionless independent variable $y$ is introduced. It is related to $x$ by the equation

$$y = ax - - - - - - - - - - - - - (7)$$

$$\therefore\ x = \frac{y}{a},\ \text{where } a = \sqrt{\frac{m\omega}{\hbar}}$$

Now we have

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\frac{dy}{dx} = \frac{d\psi}{dy}a$$

$$y = ax$$
$$dy = adx$$
$$\frac{dy}{dx} = a$$

Differentiating

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

and

$$\frac{d^2\psi}{dx^2} = \frac{d^2\psi}{dy^2}a^2$$

$$\frac{d^2\psi}{dx^2} = a^2\frac{d^2\psi}{dy^2} ------------(8) \qquad \frac{d^2y}{dx^2} = a^2$$

Substituting for $\frac{d^2\psi}{dx^2}$ and $x^2$ in eqn (6), we have

$$a^2\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - a^4\frac{y^2}{a^2}\right)\psi = 0 \qquad [\because{}^2) = \frac{y}{a}$$

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

Dividing through out by $a^2$, we have $\qquad a^2 = \frac{m\omega}{\hbar^2}$

$$\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{a^2\hbar^2} - y^2\right)\psi = 0 ----------- (9) \qquad a^2 = \frac{m^2\omega^2}{\hbar^2}$$

$$a^4 = \frac{m^2\omega^2}{\hbar^2}]$$

Substituting for $a^2$.

$$\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\frac{m\omega}{\hbar}\cdot\hbar^2} - y^2\right)\psi = 0 ---------(10)$$

or $$\frac{d^2\psi}{dy^2} + (\lambda - y^2)\psi = 0 -------(11)$$

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

Eigen-values of the total energy $E_n$:

The wave equation for the oscillator is satisfied only for discrete values of total energies given by

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

$$\text{(or)} \quad E_n = \frac{1}{2}(2n+1)\hbar\omega$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega \text{------}(12)$$

Substituting $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi v$, this expression has the form:

$$E_n = \left(n+\frac{1}{2}\right)hv \text{--------}(13)$$

where, $n = 0,1,2, \ldots \ldots$, and $v$ is the frequency of the classical harmonic oscillator, given by

$$v = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \left(\because (1) = \sqrt{\frac{k}{m}}\right)$$

From eqn. (13), we get the following conclusions:

1.The lowest energy of the oscillator is obtained by putting $n = 0$ in equs (12) and (13) it is,

$$E_o = \frac{1}{2}\hbar\omega = \frac{1}{2}h\text{v} \text{------}(14)$$

This is called the ground state energy or the zero point vibrational energy of the harmonic oscillator. The zero-point energy is the characteristic result of quantum mechanics. The values of $E_n$ in terms of $E_o$ are given by:

$$E_n = (2n+1)E_0 \text{----------}(15)$$

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

2. The eigen-values of the total energy depend only on one quantum number $n$. Therefore all the energy-levels of the oscillator are non-degenerate.

3. The successive energy-levels are equally spaced; the separation between two adjacent energy-levels being $\hbar\omega(h\nu)$. The energy-level diagram for the harmonic oscillator is shown in fig. 5.2.

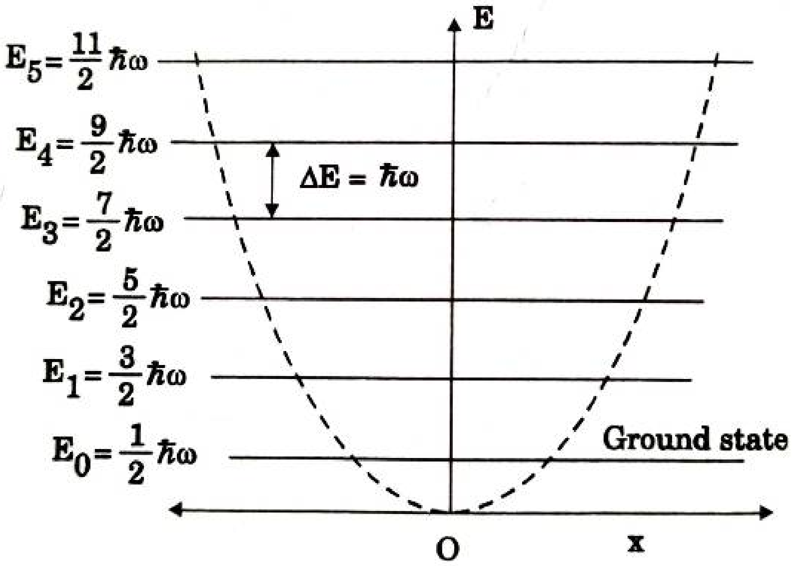


Fig. 5.2 Energy levels allowed for a harmonic oscillator.

**Wave functions of the harmonic oscillator**

For each value of the parameter $\lambda = \frac{2E}{\hbar_{(S)}} = 2n + 1$, there is a different wave function $\psi_n$ which consists of:

(i) the normalization constant $N_n$ given by:

$$N_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (2^n n!)^{-1/2}$$

(ii) the exponential factor $e^{-y^2/2}$ and

(iii) a polynomial $H_n(y)$, called Hermite polynomial in either odd or even powers of $y$.

Thus the general formula for the $n^{\text{th}}$ wave function is:

$$\Psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (2^n n!)^{-1/2} e^{-y^2/2} H_n(y)$$

The first six Hermite polynomials are given in the following table:

| $n$ | $\lambda = 2n + 1$ | $E_n$ | $H_n(y)$ |
|---|---|---|---|
| 0 | 1 | $\frac{1}{2}\hbar\omega$ | $H_0(y) = 1$ |
| 1 | 3 | $\frac{3}{2}\hbar\omega$ | $H_1(y) = 2y$ |
| 2 | 5 | $\frac{5}{2}\hbar\omega$ | $H_2(y) = 4y^2 - 1$ |
| 3 | 7 | $\frac{7}{2}\hbar\omega$ | $H_3(y) = 8y^3 - 12y$ |
| 4 | 9 | $\frac{9}{2}\hbar\omega$ | $H_4(y) = 16y^4 - 48y^2 + 12$ |
| 5 | 11 | $\frac{11}{2}\hbar\omega$ | $H_6(y) = 32y^5 - 160y^3 + 120y$ |

The first six wave functions are shown in fig.

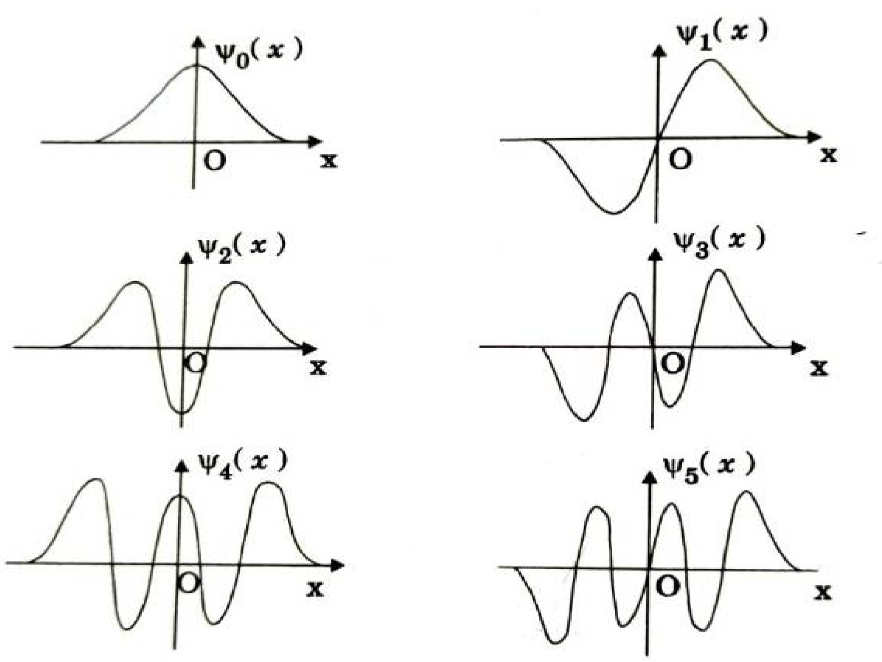

Fig. 5.3 Wave functions for Harmonic Oscillator

**Significances of zero point energy**

For lowest (ground) state, $n = 0$

$$E_0 = \frac{1}{2}hv$$

This is the lowest value of energy, called zero point energy. Even it the temperature reduces to absolute zero, the oscillator would still have an amount of energy $\frac{1}{2}hv$.

In old quantum mechanics, the energy of $n^{\text{th}}$ level.

$$E_n = nhv$$

whereas in wave mechanics

$$E_n = \left(n + \frac{1}{2}\right)hv$$

A comparison of two results shows that the only difference in old quantum mechanics and wave mechanics is that all the equally spaced energy levels are shifted upward by an amount equal to half the separation of energy levels

i.e., $\frac{1}{2}hv$ (equal to zero point zero).