Harmonic Oscillator

For a Harmonic Oscillator potential energy V = ½ kx^2, k is the force constant, is a continuous function of the coordinate x and therefore is completely different from systems we considered so far where the potential is constant over a region.

Wave Equation

$$V = \frac{1}{2} kx^2$$

$$= \frac{1}{2} 4\pi m V_0^2 x^2$$

$$= \frac{1}{2} m\omega^2 x^2$$

The time - independent Schrödinger equation of the linear harmonic oscillator then

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - \frac{1}{2} m\omega^2 x^2) \Psi = 0 \rightarrow (1)$$

It is convenient to work with a new variable y and a new parameter λ by

$$y = (\frac{m\omega}{\hbar})^{1/2} x \text{ and } \quad \lambda = \frac{2E}{\hbar\omega}$$

In terms of these quantities schrödinger equation can be written as

$$\frac{\partial^2 \Psi}{\partial x^2} + (\lambda - y^2)\Psi = 0 \rightarrow (2)$$

Asymptotic solution

We have to find the solution when y →∞, when y is very large, $\lambda - y^2 \cong y^2$

Equation (2) becomes $\frac{\partial^2 \Psi}{\partial x^2} - y^2 \Psi = 0 \rightarrow (3)$

Its asymptotic solutions are

$$\Psi(x) = e^{\pm y^2/2}$$

$$(2) \rightarrow \quad \frac{\partial^2 \Psi}{\partial x^2} = (y^2 + 1) e^{\pm y^2/2}$$

Out of the two asymptotic solutions $e^{y^2/2}$ is not acceptable as it diverges

When $|y| \rightarrow \infty$. The exact solution can be written as

$$\Psi = e^{-y^2/2} H(y)$$

Where H(y) is a function of y and the product $e^{-y^2/2}H(y)$ tends to Zero as $|y| \rightarrow \infty$

Series Solution

Substituting the value of Ψ in (3)

$$(3) \rightarrow \frac{d^2H(y)}{dy^2} - 2y\frac{dH}{dy} + (\lambda - 1)H = 0$$

Which is known as the Hermite equation. We shall look for H(y), a series solution of the type.

$$H(y) = \sum_{n=0}^{\infty} a_n y^n \rightarrow (4)$$

Substituting the value of H(y) in equation (3)

$$\sum_{k=0}^{\infty}[(k+1)(k+2)a_{k+2} - (2k+1-\lambda)a_k]y^k = 0 \rightarrow (5)$$

For the validity of this equation, coefficient of each power of y must vanish separately. Coefficient of y^k when equated to zero gives the recurrence relation.

$$a_{k+2} = \frac{2k+1-\lambda}{(k+1)(k+2)} \rightarrow (6)$$

Equation (4) will have only odd coefficients if a_0=0 and even coefficients if a_1 = 0. Thus we have two independent solutions for H(y) and a linear combination of the two will be the most general solution. The two solutions are ;

$$H_e(y) = a_0 + a_2y^2 + a_4y^4 + ...$$

$$H_o(y) = y(a_1 + a_3y^2 + a_5y^4 + ...)$$

Energy Eigenvalues

When K → ∞ we get

$$\frac{a_{k+2}}{a_k} = \frac{2}{k}$$

Consider the Taylor series expansion of exp (y^2)

$$\exp(y^2) = \sum_{0,2,4} \frac{1}{(k/2)!} y^k \rightarrow (7)$$

The ratio of coefficients of the successive terms in equation (7) is

$$\frac{a_{k+2}}{a_k} = \frac{(k/2)!}{[(k/2)+1]!} = \frac{1}{(k/2)+1} = \frac{2}{k}$$

Where k is large. Therefore, for large values of k, Ψ = exp $\left({y^2}/{2}\right)$ tends to behave like exp $\left({y^2}/{2}\right)$, if the series is even, and y exp $\left({y^2}/{2}\right)$ if this series is odd; which is not acceptable. Substitution of λ gives

$$2n+1 - \frac{2E}{\hbar\omega} = 0$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

The energy of an oscillator based on quantum theory is

$$E_n = n\hbar\omega$$

From the two expressions, it is evident that the quantum mechanical energy value is higher than the quantum theory value by ½ħω, which is the energy possessed by the lowest state n = 0. The oscillator will have this energy even at absolute zero. This energy of ½ħω is called the zero-point energy which is a manifestation of uncertainty principle. E=0 means that both position and momentum are well defined which is a violation of uncertainty principle. It can be shown that the minimum energy of an oscillator without violating uncertainty principle ½ħω.

Energy Eigenfunctions

When λ = 2n + 1 Eq (3) reduces to

$$\frac{d^2H_n(y)}{dx^2} - 2y\frac{dH_n(y)}{dy} + 2nH_n(y) = 0$$

The energy eigenfunctions can be expressed as

$$\Psi_n(y) = N_nH_n(y)\exp\left(-\frac{y^2}{2}\right), \qquad y^2 = \frac{m\omega}{h}x^2$$

The first - four Hermite polynomials are

$$H_0(y) = 1$$

$$H_1(y) = 2y$$

$$H_2(y) = 4y^2 - 2$$

$$H_3(y) = 8y^2 - 12y$$

The normalization condition leads to

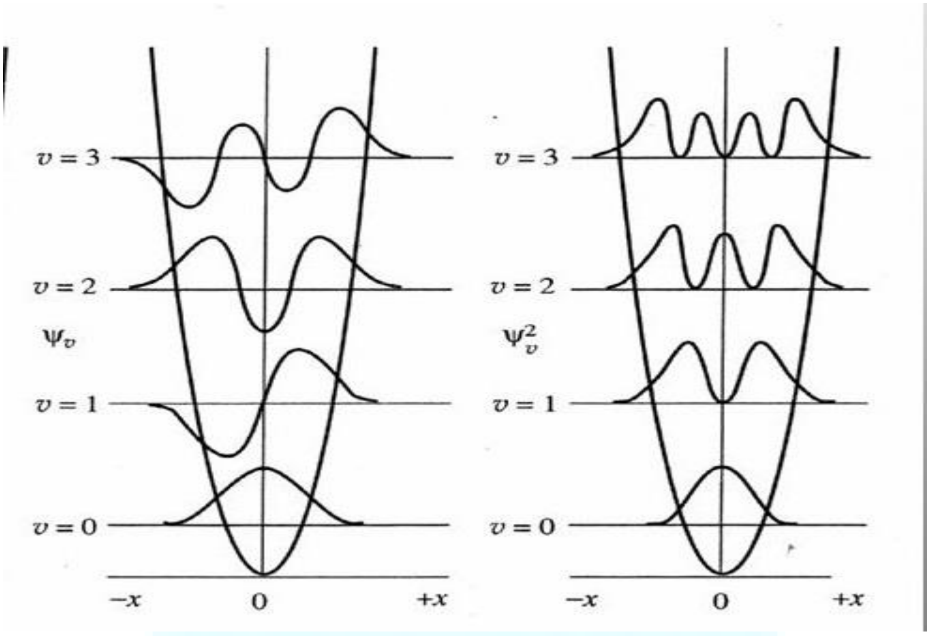
$$|N_n|^2\left(\frac{\hbar}{m\omega}\right)^{½}\int_{-\infty}^{\infty} H^2{}_n(y)exp(-y^2)\,dy = 1$$

The normalized eigenfunctions and ground state eigenfunctions are given by

$$\Psi_n(y) = \left[\frac{(m\omega)^{1/2}}{(h\pi)}\frac{1}{2^n(n)!}\right]^{1/2} H_n(y)\exp\left(-\frac{y^2}{2}\right)$$

$$\Psi_0(x) = \left(\frac{m\omega}{h\pi}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

The wave functions $\Psi_n(x)$ and the probability density $|\Psi_n(x)|^2$ of the lowest four States are illustrated below.



(a) (b)

Figure ; (a) Energy levels (E_n) and wave functions $\Psi_n(x)$ of the lowest four states of the linear harmonic oscillator. (b) probability density $|\Psi_n(x)|^2$of the lowest four states.