Study Notes on Simple Harmonic Oscillator

https://byjusexamprep.com

Simple Harmonic Oscillator

One-Dimensional Simple Harmonic Oscillator:

A diatomic vibration molecule can be represented with the help of a simple model which is known as simple harmonic oscillator (S.H.O). The force that acts on the molecule is given by:

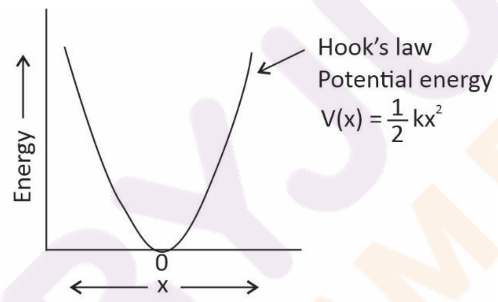
f=kx

Here, x is the displacement from the equilibrium position and k is force constant.

The expression of potential energy V(x) is given by:

$$V(x)=-\int_0^x f dx=\int_0^x kx\,dx=\frac{1}{2}kx^2 \qquad ...(1)$$

The above equation is known as the equation of a parabola. A plot of a potential energy of a particle executing simple harmonic oscillations as a function of displacement from the equilibrium position is given below:



potential energy diagram
for a simple harmonic oscillator

The vibrational frequency of the oscillator of mass m is given by:

$$\upsilon=\frac{1}{2\pi}\left(\frac{k}{m}\right)^{1/2} \qquad ...(2)$$

Vibrational frequency can be expressed more accurately as:

$$\upsilon=\frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2} \qquad ...(3)$$

Here, μ is the reduced mass of the diatomic molecule which is given by:

$$\frac{1}{\mu}=\frac{1}{m_1}+\frac{1}{m_2} \qquad ...(4)$$

Here, m_1 and m_2 are the atomic masses of the two atoms.

By using the expression of potential energy given in Equation (1), for one dimensional S.H.O., the Schrodinger equation can be represented as:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}\right)+\frac{1}{2}kx^2\right]\psi(x)=E\psi(x) \qquad ...(5)$$

Mathematically, Equation (5) may be written as:

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}kx^2\right)\psi=0 \qquad ...(6)$$

Defining α and β as $\alpha = 2mE/\hbar^2$ and $\beta = (mk)^{1/2}/\hbar$. ...(7)

Now, substitute α and β values in equation 6, it will become:

$$\frac{d^2\psi}{dx^2}+(\alpha-\beta^2x^2)\psi=0 \qquad ...(8)$$

Defining a new variable $\xi=\beta^{1/2}x$, the above equation becomes

$$\frac{d^2\psi}{d\xi^2}+\left(\frac{\alpha}{\beta}-\xi^2\right)\psi=0 \qquad ...(9)$$

Equation (9) has a solution of the form

$$\psi(\xi)=\phi(\xi)e^{-\xi^2/2} \qquad ...(10)$$

Use above solution, equation (9) will become:

$$\frac{d^2\phi}{d\xi^2}-2\xi\frac{d\phi}{d\xi}+\left(\frac{\alpha}{\beta}-1\right)\phi=0 \qquad ...(11)$$

Equation (11) is identical in form to a well-known second order differential equation, called the Hermite equation, that is:

$$\frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+2n\phi=0 \qquad ...(12)$$

The Hermite equation has solutions which depend upon the value of n.

The Hermite Polynomial having degree *n* can be defined as:

$$H_n(\xi)=(-1)^n e^{\xi^2}\left\{\frac{\partial^n\left(e^{-\xi^2}\right)}{\partial\xi^n}\right\} \qquad ...(13)$$

A few Hermite polynomials are given below:

$H_0(\xi)=1$ $\qquad$ $H_3(\xi)=8\xi^3-12\xi$

$H_1(\xi)=2\xi$ $\qquad$ $H_4(\xi)=16\xi^4-48\xi^2+12$

$H_2(\xi)=4\xi^2-2$

The normalized wave functions of the one-dimensional S.H.O. are as follows:

$$\psi_n(\xi)=\left[\frac{\beta^{1/2}}{2^n n!\sqrt{\pi}}\right]^{1/2} e^{-\xi^2/2}H_n(\xi) \qquad ...(14)$$

Here, n = 0, 1, 2, 3, …

Energy of S.H.O.: On comparing equation (11) and (12), the energy of the S.H.O. can be obtained.

It has been found out that:

$$\alpha/\beta = 2n + 1 \qquad ...(15)$$

Substituting for α and β Equation (7),

$$(2mE/\hbar^2)(mk)^{1/2}/\hbar = 2n+1 \qquad ...(16)$$

Or

$$E = \left(n+\frac{1}{2}\right)\hbar(k/m)^{1/2} \qquad ...(17)$$

From Equation (2),

$$(k/m)1/2 = 2\pi\upsilon \qquad ...(18)$$

Combining Equations (17) and (18),

$$E \equiv E_n\left(n+\frac{1}{2}\right)\hbar(2\pi\upsilon)$$

$$=\left(n+\frac{1}{2}\right)h\upsilon\text{ ; n = 0, 1, 2, 3, ...}(\hbar = h/2\pi) \qquad ...(19)$$

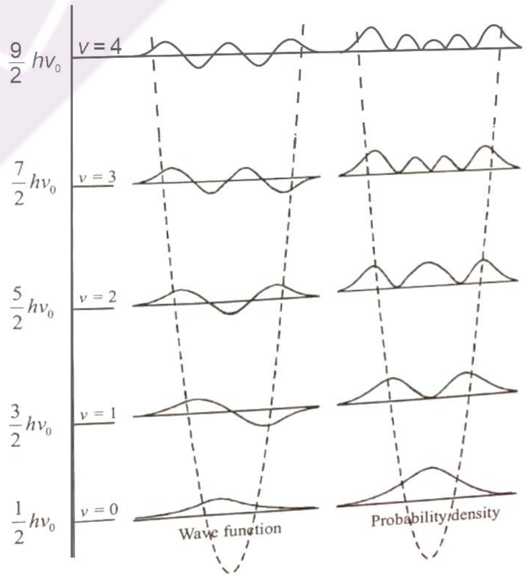
The energy state with n = 0 is the vibrational ground state. It is given by:

$$E_0 = \frac{1}{2}h\upsilon$$

This energy is called the zero-point energy of the oscillator. Classical mechanics predicts that the zero-point energy of the oscillator is zero while quantum mechanics predicts that the zero-point energy is non-zero.

The occurrence of the zero-point energy is consistent with the Heisenberg uncertainty principle.

Graph of wave function and probability:



Degeneracy for 2-D harmonic oscillator:

The energy, $E = E_x + E_y$

$$E = \left(n_x + \frac{1}{2}\right)hv + \left(n_y + \frac{1}{2}\right)hv$$

$$E = hv(n_x + n_y + 1)$$

Degeneracy for 3-D harmonic oscillator:

$$E = \left(n_x + \frac{1}{2}\right)hv + \left(n_y + \frac{1}{2}\right)hv + \left(n_z + \frac{1}{2}\right)hv$$

$$E = \left(n_x + n_y + n_z + \frac{3}{2}\right)hv$$