SIMPLE HARMONIC OSCILLATOR

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Oscillation

Periodic Variation

Any oscillation that can be expressed with a sinusoidal function is a harmonic oscillation.

$x(t) = x_0 \cos(\omega t + \phi)$

Where

- **x_0 is the amplitude**
- **t is the time**
- **ω is the angular frequency**
- **ϕ is the phase angle**
- **(ωt + ϕ) is the phase**

The vibrational frequency of the oscillator of mass m is given by $v = \frac{1}{2\pi}\left(\frac{k}{m}\right)^{1/2}$

For a diatomic molecule $v = \frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2}$

Where μ is the reduced mass of diatomic molecule.

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Let's understand the case…!

According to Hooke's law, the force acting on the molecule is given by

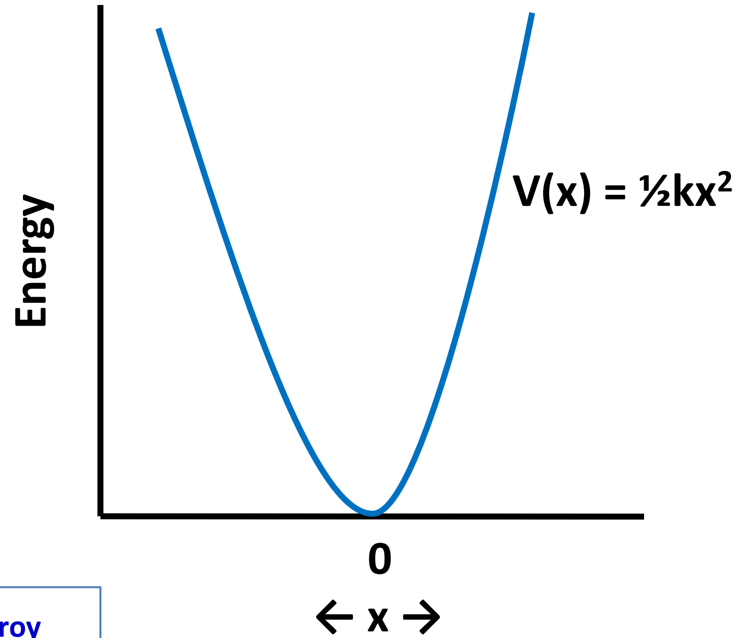
$$f = -kx$$

Where x is the displacement and k is the force constant.

The Hooke's law potential energy V(x) can be written as

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

This is the equation of parabola. Thus if we plot potential energy of a particle executing simple harmonic oscillations as a function of displacement from the equilibrium position, we get a curve like this.



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Let's solve the case…!

Using the potential energy now the Schrodinger's equation for the one dimensional simple harmonic oscillator can be represented as

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

Mathematically this equation can be rearranged as

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

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Let’s solve the case…!

The force constant in SHO is given by k = mω²

Substituting the value of k, the equation becomes

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

Defining a new variable ξ and a new parameter λ

$$\xi = \left(m\omega/\hbar\right)^{1/2} x \qquad \lambda = 2E/\hbar\omega$$

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0$$

When ξ is very large $\lambda-\xi^2 \approx -\xi^2$
So the equation becomes

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

The solutions to the above equation are

$$\psi(x) = \exp\left(\pm\,\xi^2/2\right)$$

Out of the two asymptotic solutions exp $\xi^2/2$ is not acceptable since it diverges when $|\xi| \rightarrow \infty$
Thus the exact solution can be written as

$$\psi(x) = \exp\left(-\,\xi^2/2\right).H(\xi)$$

Substituting the solution the following equation,

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

The equation becomes

$$\frac{d^2H(\xi)}{d\xi^2} - 2\xi\frac{dH(\xi)}{d\xi} + (\lambda - 1)H(\xi) = 0$$

This is the Hermite Equation and the solution will give Hermite polynomials.

$$H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$$

Substituting the above equation in previous equation

$$\sum_{k=0}^{\infty} \left[(k+1)(k+2)a_{k+2} - (2k+1-\lambda)a_k\right]\xi^k = 0$$

When the coefficient of ξ is equated to zero we obtain the recurrence relation:

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

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The unnormalized wave function of one dimensional SHO is written as

$$\psi_n(\xi) = N_n H_n(\xi) \exp\left(-\xi^2/2\right).$$

Soving this the value of normalization constant will be

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

ENERGY

The series can be terminated choosing λ in such a way that (2k+1-λ) vanishes for k = n.

$$2n+1-2(E/\hbar\omega)=0$$

Since $\lambda = 2E/\hbar\omega$

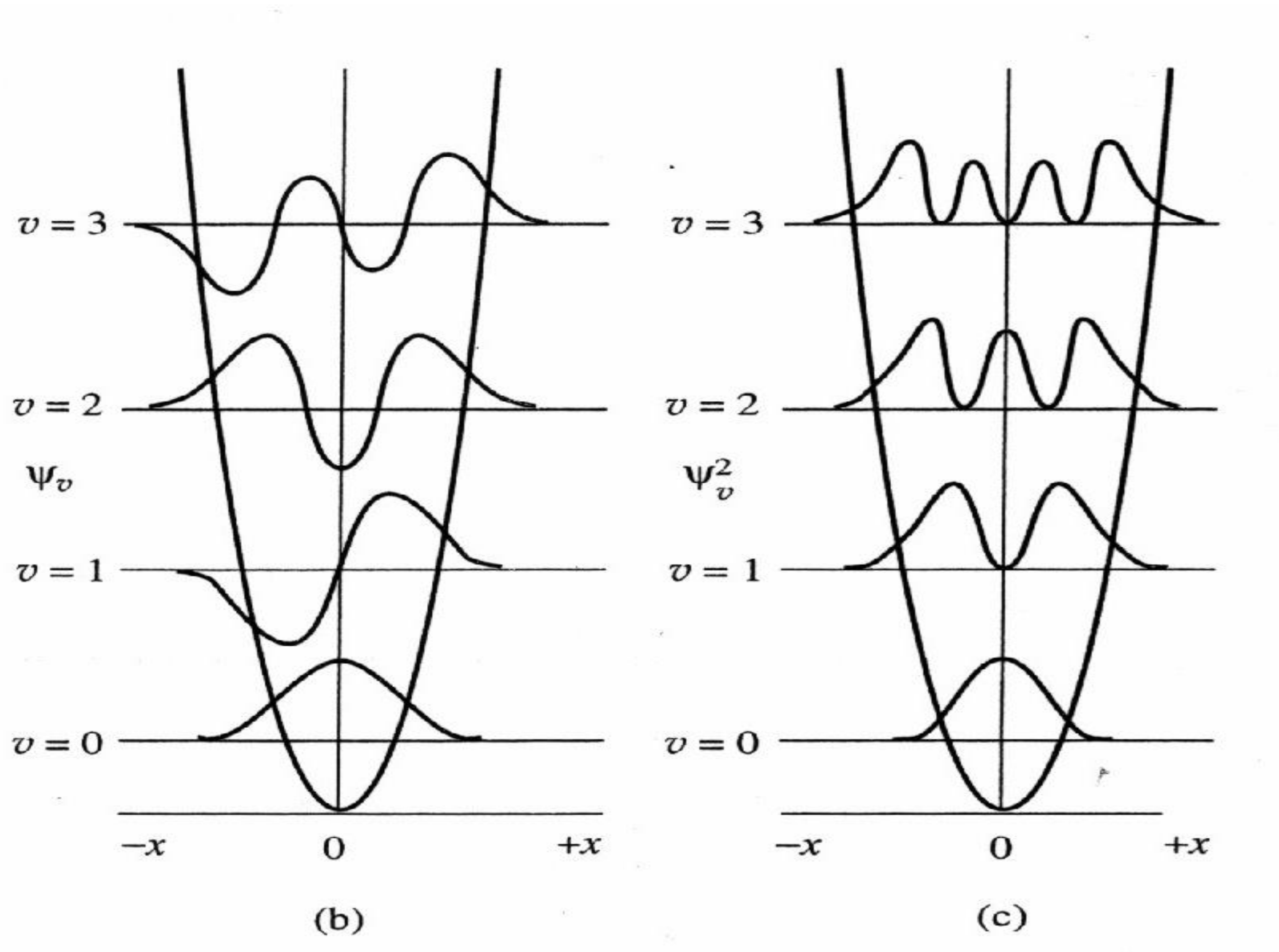
$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

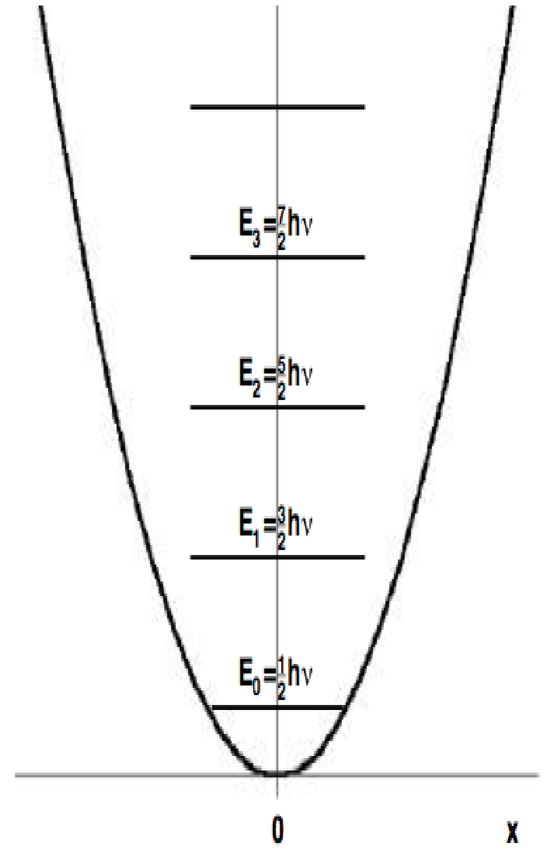
n = 0,1,2,3,4…

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

Since $\omega = 2\pi\nu$

DIAGRAMS





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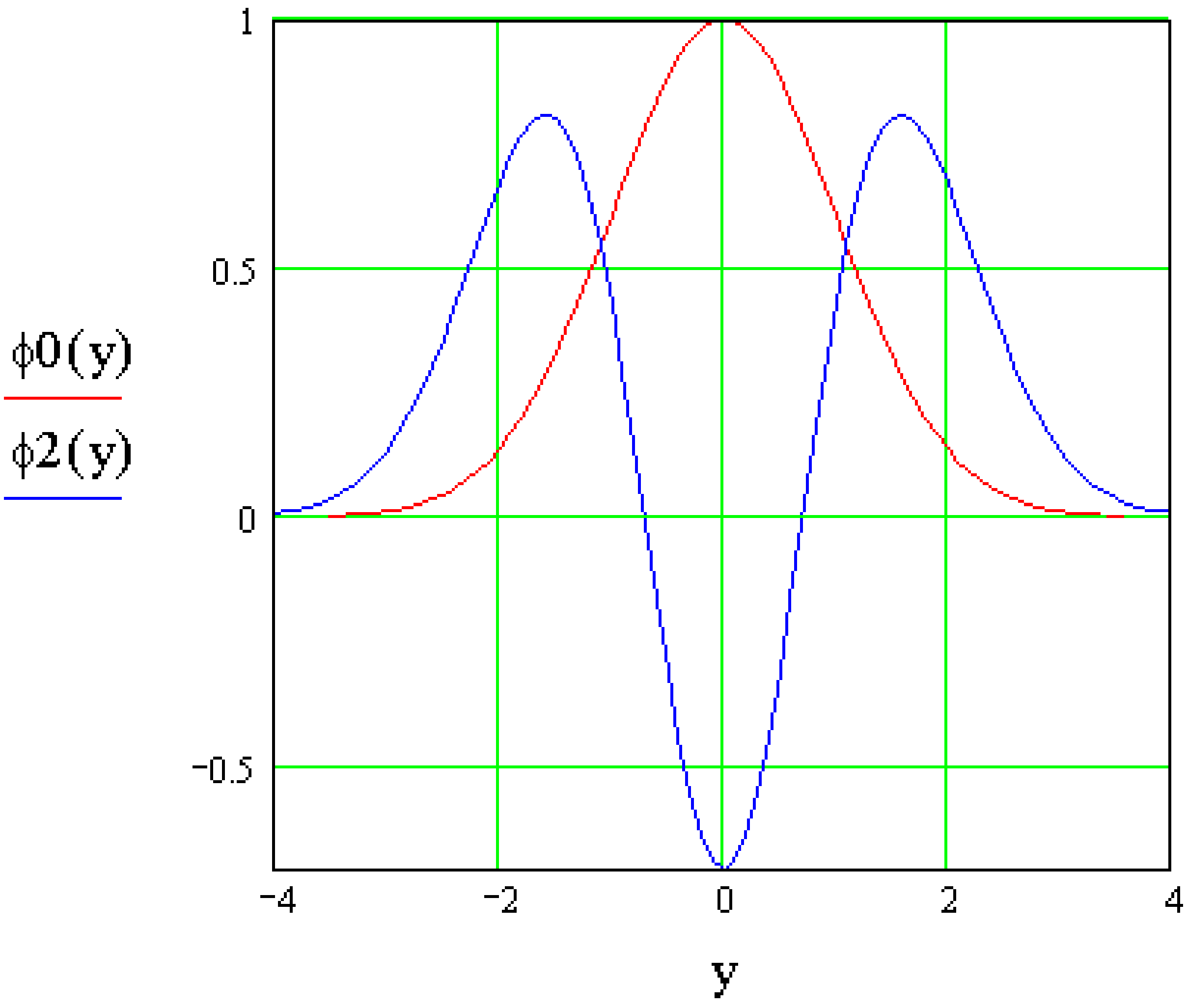

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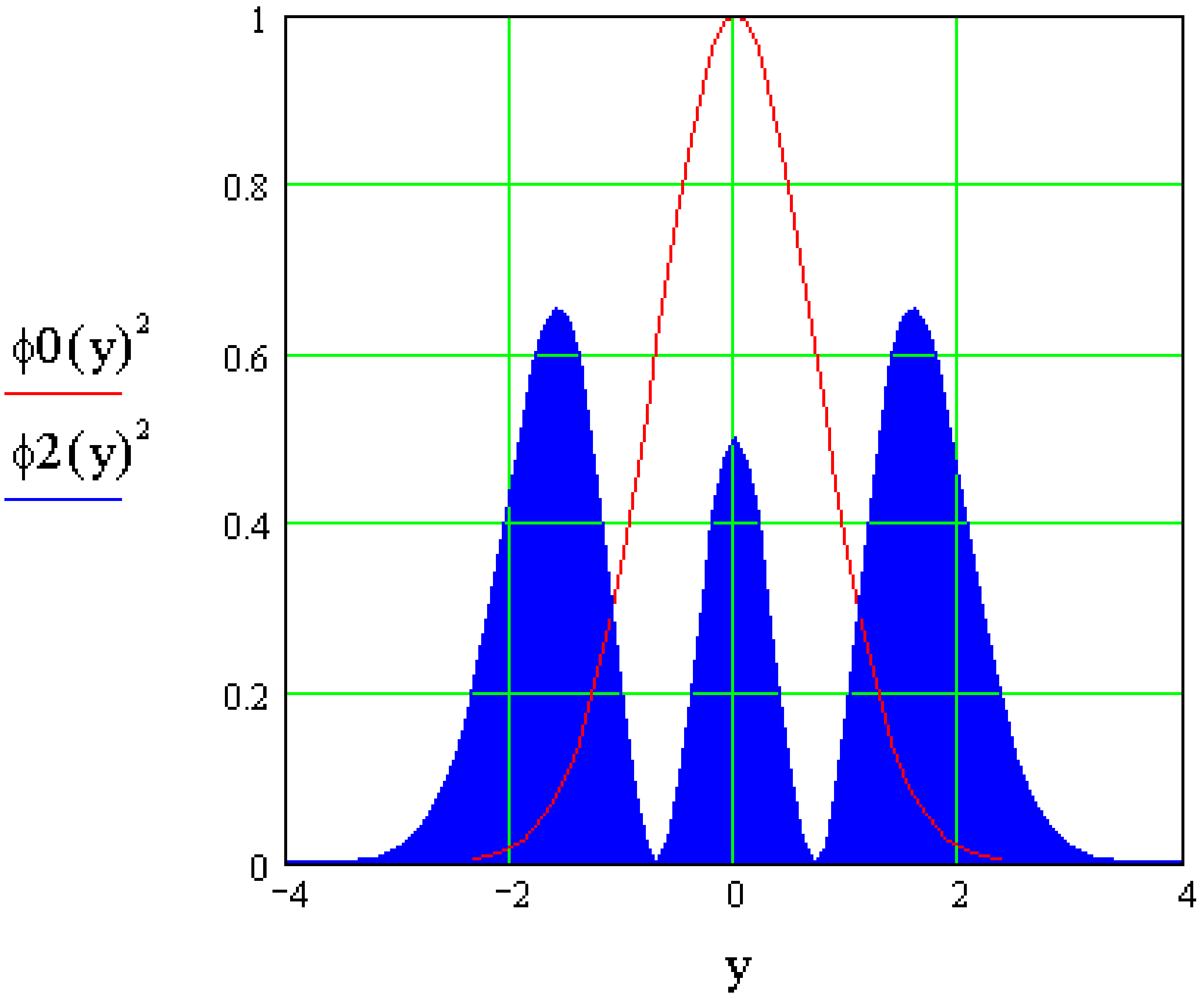

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