DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB101J-Electromagnetic Theory, Quantum Mechanics, Waves and Optics

Module 3- Lecture-14

Concepts of classical harmonic oscillator, Quantum harmonic oscillator - Ground state wavefunction & energy quantization

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TOPICS OF TODAY'S LECTURE:-

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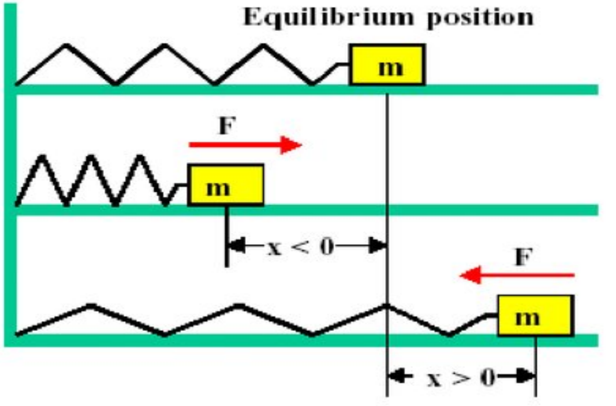
CLASSICAL HARMONIC OSCILLATOR

Simple Harmonic Motion

When a vibration or an oscillation repeats itself over and over, the motion is called periodic.

A mass on a spring is oscillating on a frictionless surface. As the mass moved from the equilibrium position there is a restoring force applied to it.



The restoring force is directly proportional to the displacement x.

$$F = -kx$$

Every system that has this force exhibits a simple harmonic motion (SHM) and is called a simple harmonic oscillator.

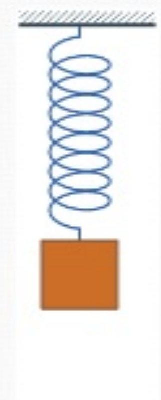
The amplitude (A) is the maximum value of its displacement on either side of the equilibrium position.

Simple Harmonic Oscillator(SHO)

Harmonic Motion:

Vibrates about an equilibrium configuration

Condition: presence of restoring force that acts to return the system to its equilibrium position when it is disturbed



For SHM:

Classical treatment :

$$F = -kx = m\frac{d^2x}{dt^2} \rightarrow \frac{d^2x}{dt^2} = -\frac{k}{m}x$$

solution $x(t) = A\sin(\omega t) + B\cos(\omega t) \quad , \quad \omega = \sqrt{\frac{k}{m}}$

Potential energy *V* is related to *F* :

$$F = -\frac{dV}{dx} \qquad V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

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Simple Harmonic Oscillator(SHO)

Quantum treatment :

$$V(x) = \frac{1}{2} m\omega^2 x^2 \qquad \hat{H}(x,\hat{p})\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

WHY TO STUDY:

This approach indentifies several problems:

1.diatomic molecule

2.an atom in a crystal lattice etc

3.explain blackbody radiation;

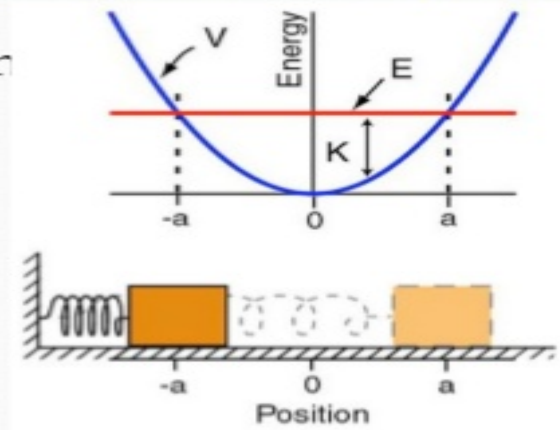
Planck postulated that the energy of a SHO is quantized.(In his model vibrating charges act as simple harmonic oscillators and emit EM radiation)

Let's write down the Schrödinger Equation for SHO

For SHO the potential energy is

$$U(x) = \frac{kx^2}{2} = \frac{m\omega^2 x^2}{2}$$

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



QUANTUM HARMONIC OSCILLATOR

Time-Independent Schroedinger Equation is

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \qquad \text{-------------------(1)}$$

Harmonic Oscillator Potential $$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad \text{-------------------(2)}$$

Schroedinger Equation with *harmonic potential is equation (3)*

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - \frac{1}{2}m\omega^2 x^2]\psi(x) = 0 \qquad \text{-------------------(3)}$$

Second term X by $2m/h^2$

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(OR), $$\frac{d^2\psi(x)}{dx^2} + \left[\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right]\psi(x) = 0$$ --------------------(4)

LET US INTRODUCE A DIMENSION-LESS VARIABLE y

$$y = ax; a = \sqrt{\frac{m\omega}{\hbar}}$$ --------------------(5)

X = y/a

$$\left[\sqrt{\frac{m\omega}{\hbar}}\right] = \left[\sqrt{\frac{M.T^{-1}}{M.L^2.T^{-1}}}\right] = \left[L^{-1}\right]$$ --------------------(6)

Hence from equation (6) we can see , y is a dimensionless variable

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\frac{dy}{dx} = a\frac{d\psi}{dy}$$ --------------------(7)

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

Substituting equation(7) and equation (8) in equation (4)

$$a^2\frac{d^2\psi}{dy^2} + \left[\frac{2mE}{\hbar^2} - a^4\frac{y^2}{a^2}\right]\psi = 0$$ ---------------------(9)

/ by a^2

$$\frac{d^2\psi}{dy^2} + \left[\frac{2mE}{a^2\hbar^2} - y^2\right]\psi = 0$$ ---------------------(10)

$$a^2 = \frac{m\omega}{\hbar}, hence, \frac{2mE}{a^2\hbar^2} = \frac{2E}{\hbar\omega}$$ ---------------------(11)

h= mw/a²

On substituting equation (11) in equation(10) we equation (12)

$$\frac{d^2\psi}{dy^2} + \left[\underbrace{\frac{2mE}{\hbar\omega}}_{=\lambda} - y^2 \right] \psi = 0 \quad \text{------------(12)}$$

(OR),

$$\frac{d^2\psi}{dy^2} + \left[\lambda - y^2 \right] \psi = 0 \quad \text{--------------------------(13)}$$

Equation (13) is like Hermite Polynomial Differential Equation

Equation (13) is like Hermite Polynomial Differential Equation and it cannot be solved in closed form. The series solution of such differential equation is studied by Hermite . It was found that the equation (13) has solution only if

$$\frac{2E}{\hbar\omega} = (2n+1) \quad \text{--------------------(14)}$$

Where n=0,1,2,3,4……….

Hence

Quantized Energy

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{--------------------(15)}$$

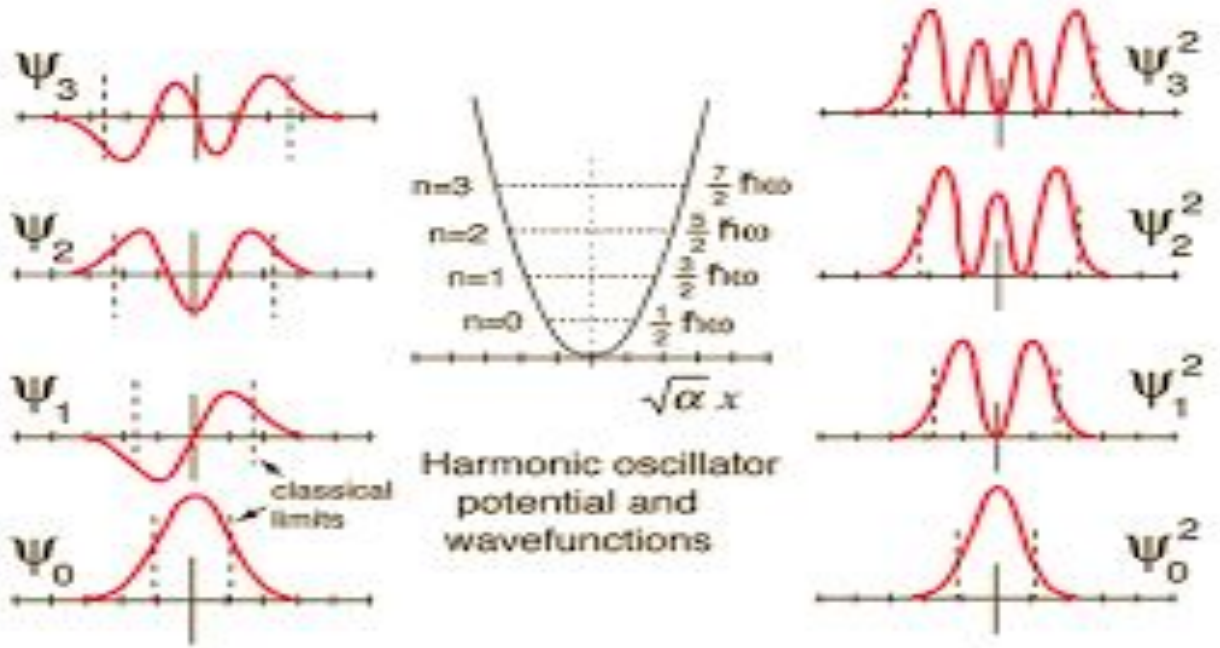
Using equation (14), equation (15) can be written as

$$Since, \nu = \frac{\omega}{2\pi}; and\, \nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$ --------------------(16)

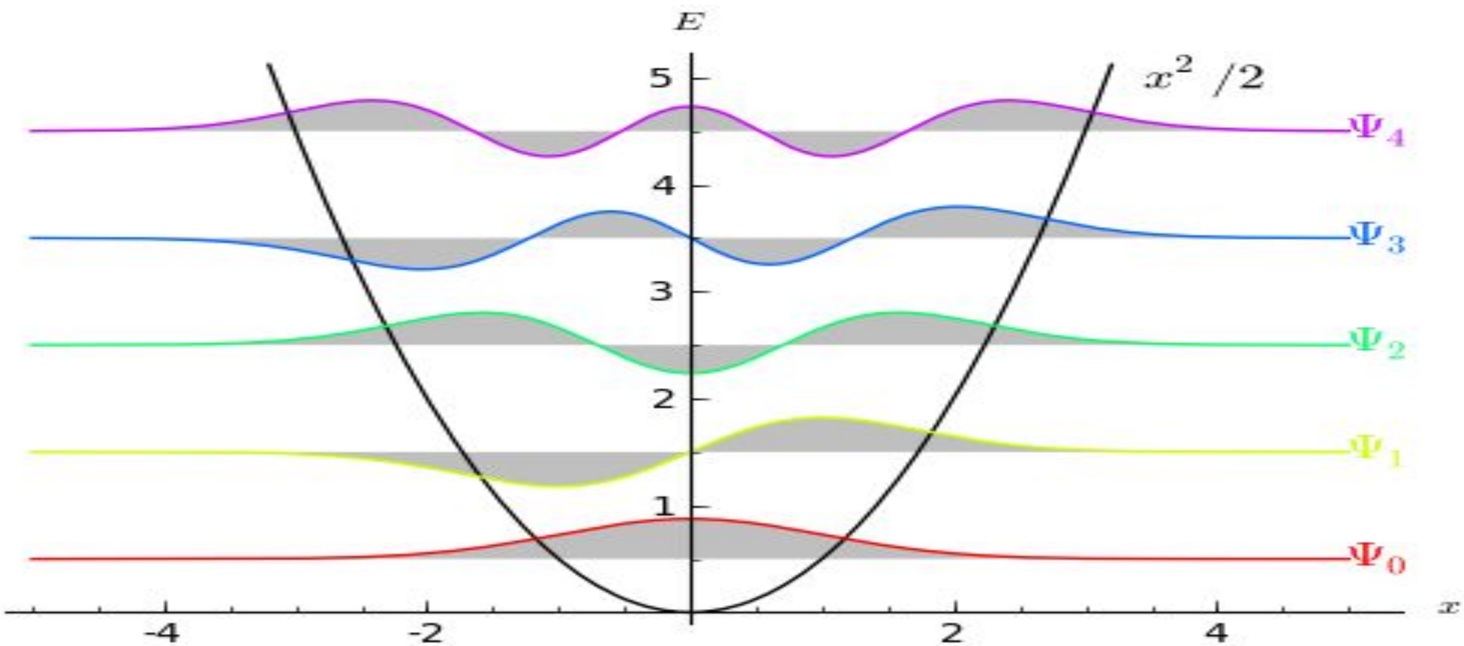
$$E_n = \left(n + \frac{1}{2}\right) h\nu$$ --------------------(17)

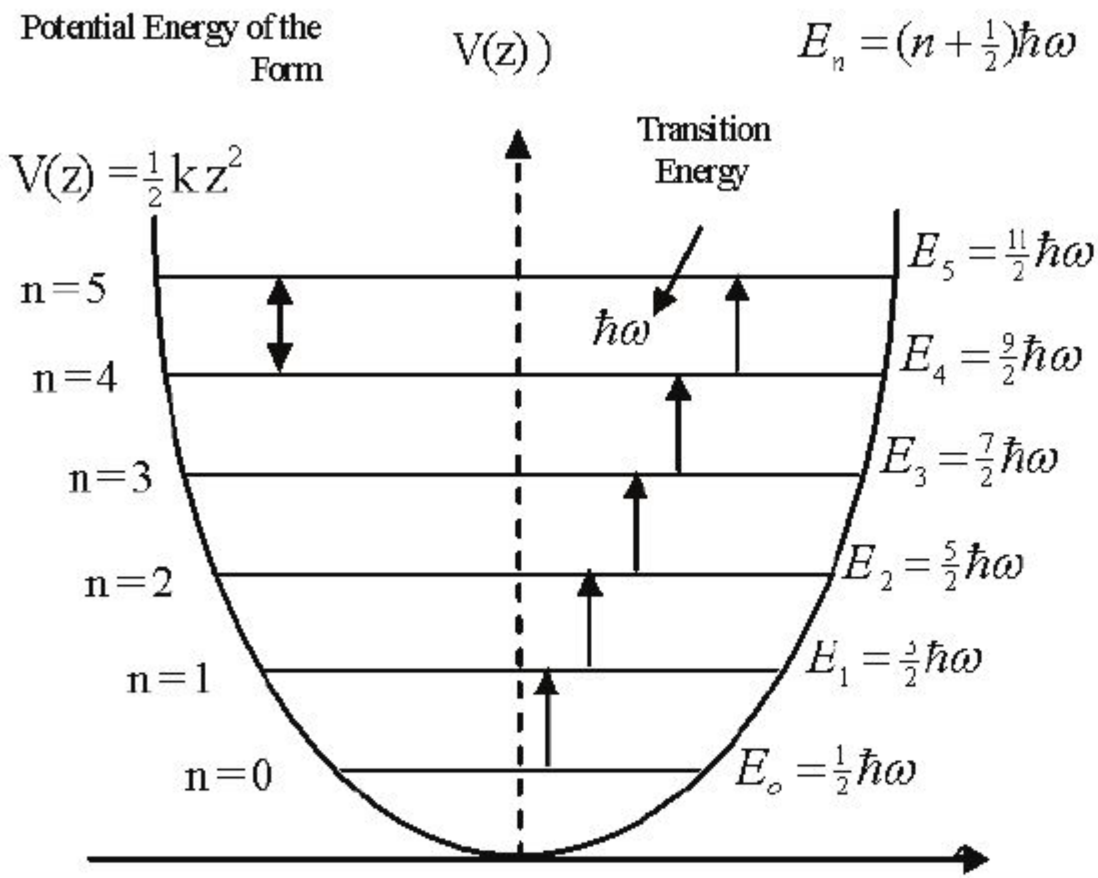
n=0-GRUND STATE

$$E_0 = \frac{1}{2}\hbar\omega;\ hence,\ E_n = (2n+1)E_0$$ --------------------(18)



Ψ_3
Ψ_2
Ψ_1
Ψ_0
classical limits
n=3
n=2
n=1
n=0
$\frac{7}{2}\hbar\omega$
$\frac{5}{2}\hbar\omega$
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
$\sqrt{\alpha}\,x$
Harmonic oscillator potential and wavefunctions
Ψ_3^2
Ψ_2^2
Ψ_1^2
Ψ_0^2


E
5
4
3
2
1
$x^2/2$
Ψ_4
Ψ_3
Ψ_2
Ψ_1
Ψ_0
-4
-2
2
4
x



Potential Energy of the Form
V(z))
$E_n = (n + \frac{1}{2})\hbar\omega$
Transition Energy
$V(z) = \frac{1}{2}kz^2$
n = 5
n = 4
n = 3
n = 2
n = 1
n = 0
$\hbar\omega$
$E_5 = \frac{11}{2}\hbar\omega$
$E_4 = \frac{9}{2}\hbar\omega$
$E_3 = \frac{7}{2}\hbar\omega$
$E_2 = \frac{5}{2}\hbar\omega$
$E_1 = \frac{3}{2}\hbar\omega$
$E_o = \frac{1}{2}\hbar\omega$