ENGINEERING PHYSICS

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Class # 21

- Two body problem - two atoms in bonding
- Potential energy of the system
- SWE of the system
- Eigen functions and Eigen energy values of the system

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- ***Suggested Reading***

  1. *Concepts of Modern Physics, Arthur Beiser, Chapter 6*
  2. *Learning Material prepared by the Department of Physics*

- ***Reference Videos***

  1. *Video lectures : MIT 8.04 Quantum Physics I*
  2. *Engineering Physics Class #20*

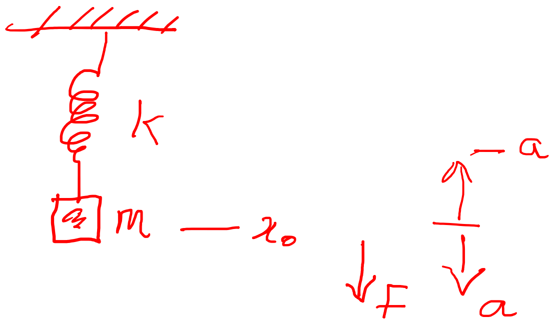
Classical Harmonic Oscillator

Classical harmonic oscillator is a bound particle of mass m subjected to oscillations about a mean position by a force

$$F = ma = m\frac{d^2x}{dt^2}$$

The amplitude of the oscillations is limited by Hooke's law

The restoring force is proportional to the displacement of the particle from a mean position $F_r = -kx$



Classical Harmonic Oscillator

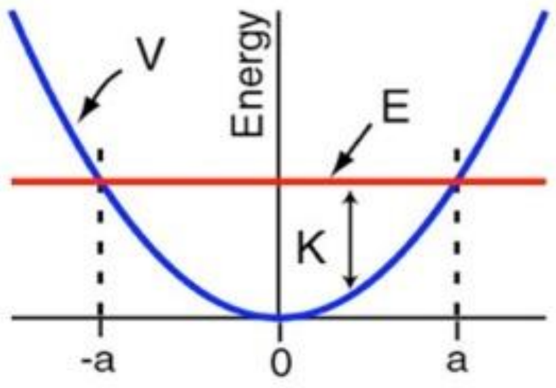
The fundamental frequency of oscillation of such a system

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

spring constant $k = m\omega^2$

The restoring force $F_r = -kx = -\frac{dV}{dx}$

The potential energy of the system $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$



Diatomic molecule

A diatomic molecule with atoms of mass m_1 and m_2

bound by a bond that is springy in nature

Analyzed as a spring mass system with spring constant k

which basically depend on the bond strength

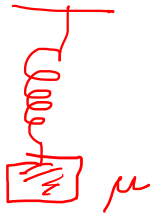
The effective mass μ of the system will decide the

frequency of oscillations of the bond $\omega = \sqrt{\frac{k}{\mu}}$

the potential energy of the system $V(x) = \frac{1}{2}\mu\omega^2x^2$.

$$\mu = \frac{m_1 m_2}{m_1+m_2}$$

$\equiv$



Solution of the Schrodinger's wave equation

The Schrodinger wave equation for the system can be written as

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

$V(x)$ is finite in this case and

$\left(E - \frac{1}{2}\,\mu\omega^2 x^2\right)$ will be positive

the eigen functions and eigen energy values of the system can be obtained

The solution can be attempted with a substitution

$\xi = \gamma x \;\; where \;\; \gamma = \sqrt{\frac{\mu\omega}{\hbar}}$ $\qquad \xi \Rightarrow "xi"$

Eigen functions of the Classical Harmonic Oscillator

The eigen functions of the system are

$$\psi_n(x) = N_n H_n(\xi) e^{-\frac{1}{2}(\xi)^2}$$

where $n = 0, 1, 2, 3, 4 \ldots$

the normalization constant $N_n = \sqrt{\left[\frac{\gamma}{2^n n! \sqrt{\pi}}\right]}$ and

$H_n(\xi)$ are the Hermite polynomials described by

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \;\; for\; n \geq 1$$

The first two terms of the Hermite polynomial are

$H_0(\xi) = 1$ and $H_1(\xi) = 2\xi$ which can be used to find the successive terms of the polynomial

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

Eigen functions of the Classical Harmonic Oscillator

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The eigen functions of the first two states of the system ..

$$n = 0 \implies N_o = \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} \text{ and } H_0(\xi)=1$$

$$\psi_0(x) = N_0 H_0(\xi) e^{-\frac{1}{2}\xi^2} = \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2}$$

$E_0 = \frac{1}{2}\hbar\omega$

$$n = 1 \implies N_1 = \sqrt{\frac{2}{\sqrt{\pi}}}.\left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} \text{ and } H_0(\xi) = 2\xi$$

$$\psi_1(x) = N_1 H_1(\xi) e^{-\frac{1}{2}\xi^2} = \sqrt{\frac{2}{\sqrt{\pi}}}.\left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{3}{4}}.x.e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2}$$

$E_1 = \frac{3}{2}\hbar\omega$

$$\frac{d^2\psi_0(x)}{dx^2} + \frac{2\mu}{\hbar^2}\left(\frac{1}{2}\hbar\omega - \frac{1}{2}\mu\omega^2 x^2\right)\psi_0(x) = 0$$

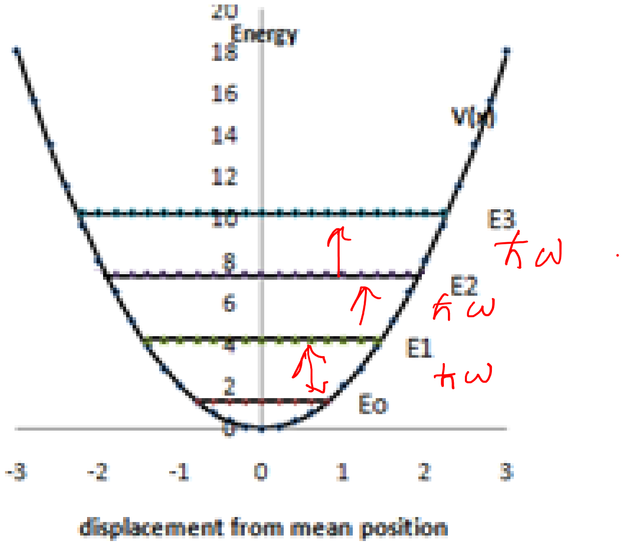
Eigen energy values of the Classical Harmonic Oscillator

The eigen values of the system

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

The energy states are $\frac{1}{2}\hbar\omega,\ \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots \ldots$

The energy states are then equally spaced with a difference of $\hbar\omega$



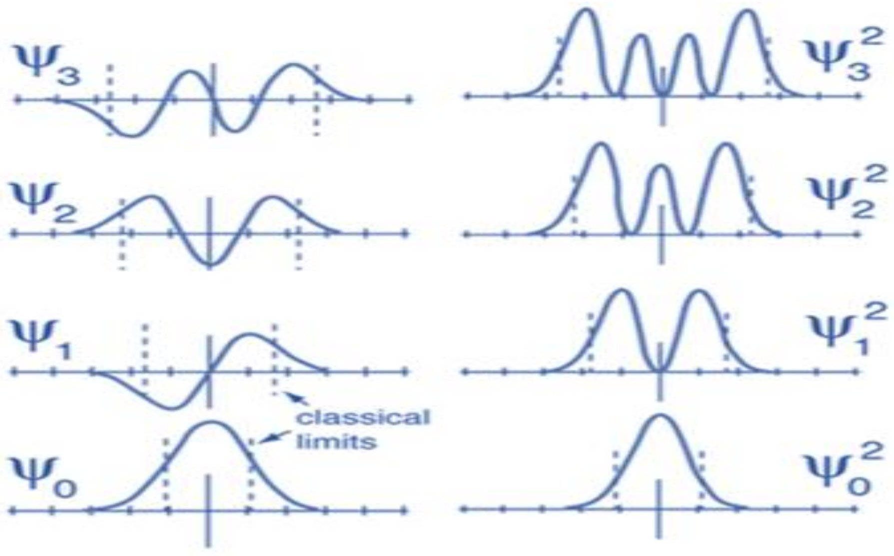
Eigen functions of the Classical Harmonic Oscillator

The wave functions of the system can be graphically inferred from the concepts of a 1D finite potential well.

The width of the well corresponds to the maximum displacement.

Each state has a increasing width and a longer decay tail

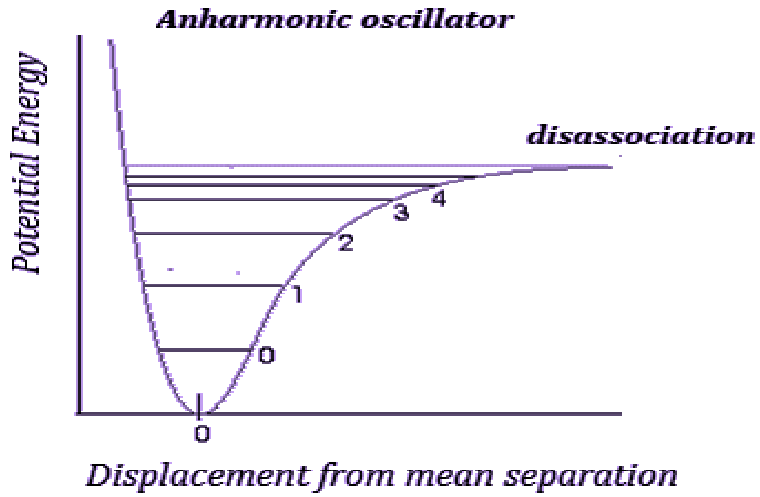
The probability distribution in the different states



Anharmonic Oscillator

Real potential energy variations deviate from the ideal parabolic potential energy curve $\propto x^2$
bonding imply exchange of electrons / sharing of electrons results in a deviation of the electrostatic interactions.
Treated as a perturbation of the harmonic oscillator potential
An additional term for the potential $\propto x^4$
Non uniform energy separation

$V_x = \frac{1}{2}kx^2 + \beta x^4 \ldots$



Class #21 …….. Quiz….

The concepts which are not true of Harmonic oscillators …

1. The harmonic oscillator potential energy is proportional to the square of the displacement from the mean position
2. In a diatomic molecule frequency of oscillation is determined by the mass of the smaller atom
3. The ground state energy of the harmonic oscillator is a zero energy state
4. The energy of the 4th excited state is $\frac{9}{2}\hbar\omega$
5. Anharmonic oscillators have the same energy separation between states

THANK YOU

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