Introductory Quantum Mechanics and Spectroscopy

Prof. Mangala Sunder Krishnan
Department of Chemistry
Indian Institute of Technology, Madras

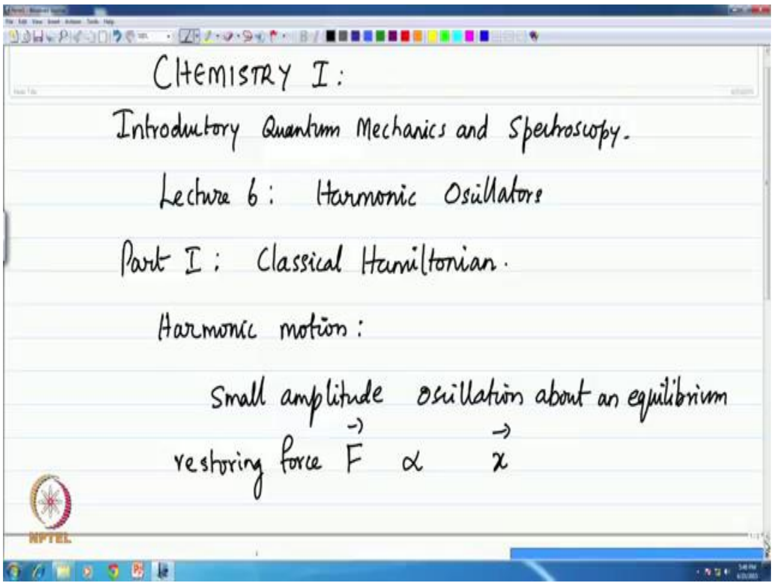
Lecture - 6
Harmonic Oscillators
Part 1: Classical Hamiltonian

Welcome back to the lectures in chemistry, the first course on elementary principles. In this series of lectures, we have been looking at introductory quantum mechanics and spectroscopy. So far we have studied a couple of model problems namely, the particle on the one-dimensional box, two-dimensional boxes, and also the electron in the hydrogen atom. Basically, we looked at the solutions and try to understand what was meant by quantization and energies and transitions between the energy levels and so on.

The other extremely important model problem, both from physics and chemistry is the problem of harmonic oscillators, which is also well known from the classical mechanics. What we would do is to study the elementary quantum mechanical aspects of harmonic oscillator using the wave function method. Later, in an advance lecture I would talk a little about the different types of rising and lowering operator formalisms of harmonic oscillator, but in this set we would look at it as a wave function method. And as has always been in the last lectures, few lectures, we start by looking at the energy of the harmonic oscillator from a classical mechanical point of view and then convert that into a quantum mechanical Hamiltonian and look at the solutions.

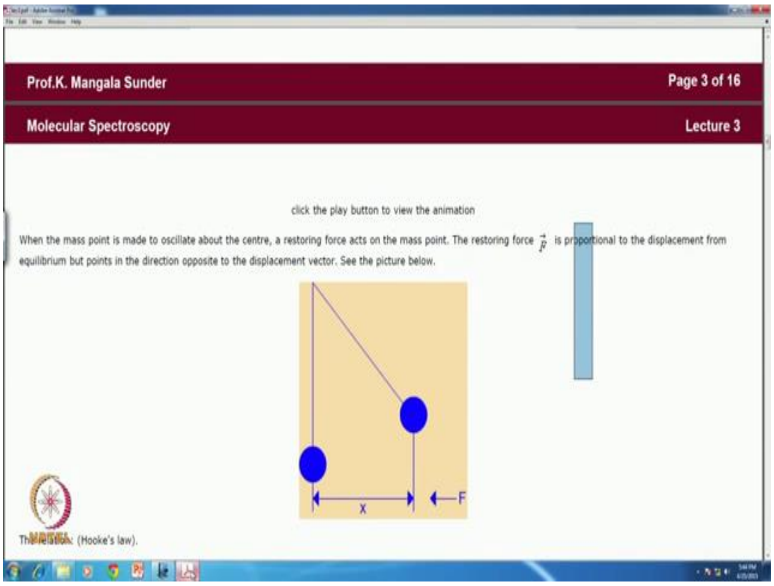
The harmonic oscillator by definition is about small amplitude oscillator emotion about an equilibrium position or periodic motion, such as motion on a circle. These things can be easily understood as cost by a restoring force, which is propositional to the displacement away from the equilibrium, but in the opposite direction.

(Refer Slide Time: 02:31)

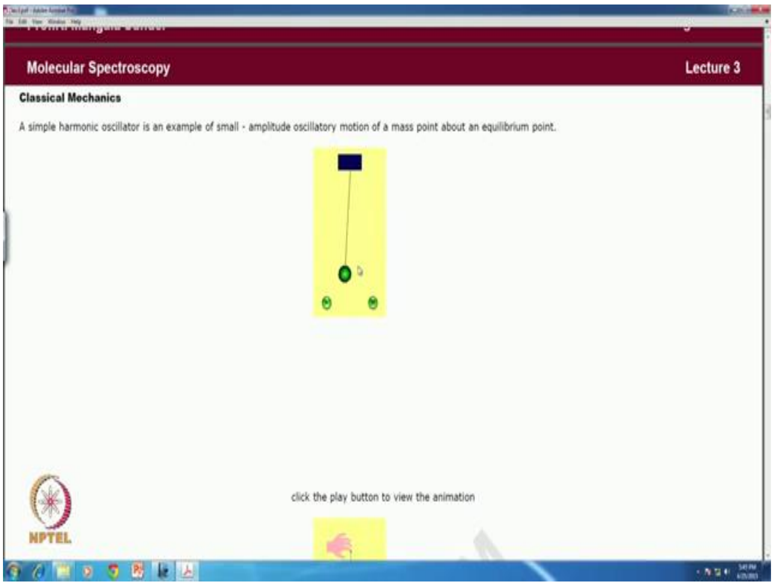


So, let me write down. Harmonic motion, small amplitude, oscillation about equilibrium, an equilibrium. If you want to visualize that here are some simple pictures.

(Refer Slide Time: 02:58)

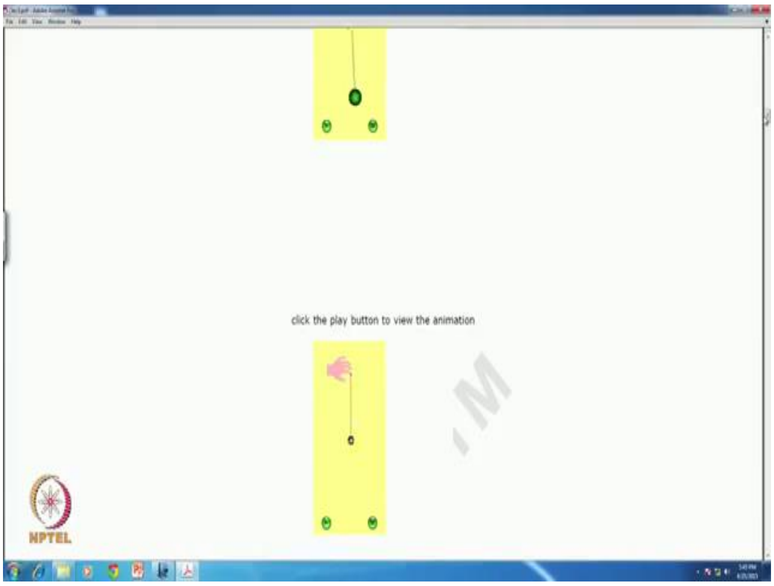


(Refer Slide Time: 03:09)



So, the equilibrium position in the first picture is the vertical distance, and you can see that the ball oscillates between two extremes rather with the small amplitude.

(Refer Slide Time: 03:25)

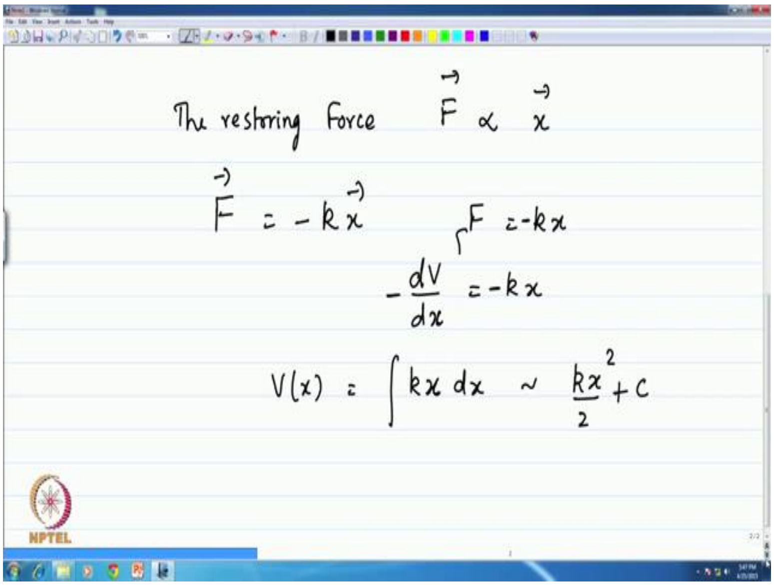


Another example is the usual play, that you have with the spring ball and the motion of the spring ball is also harmonic.

(Refer Slide Time: 03:33)

From the point view of chemistry if you look at the diatomic molecular motion at very low temperatures is very nearly harmonic, and the amplitudes of vibration of a fairly stable bond that is about the equilibrium distances. They are also modeled using harmonic motion. So, these are some examples of what is meant by a small amplitude vibration or oscillation about an equilibrium position.

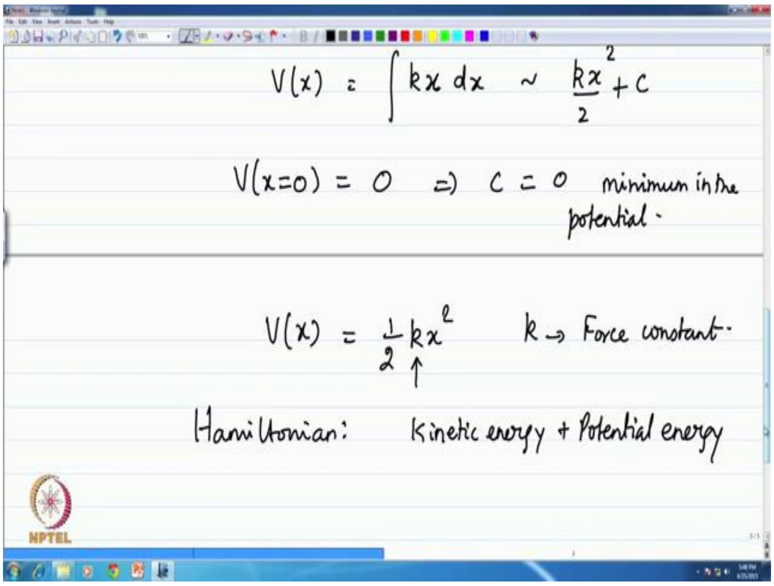
(Refer Slide Time: 04:34)



Now, the restoring force F, if you write that, it is propositional to the displacement vector from the equilibrium. And the mathematics is that the proportionality constant is a constant, and since it is in the opposite direction, it is minus kx and in one dimension we would assume that the force is in a direction opposite to that of the displacements. So, we no need to worry about the vector arrow here.

But knowing that the force is the negative derivative of potential with respect to the distance or with respect to the position coordinate, this is equal to kx, and you can see therefore the potential energy V of x is with minus kx and the minus kx, therefore V of x is the integral kx dx, which gives you kx square by 2 plus a constant.

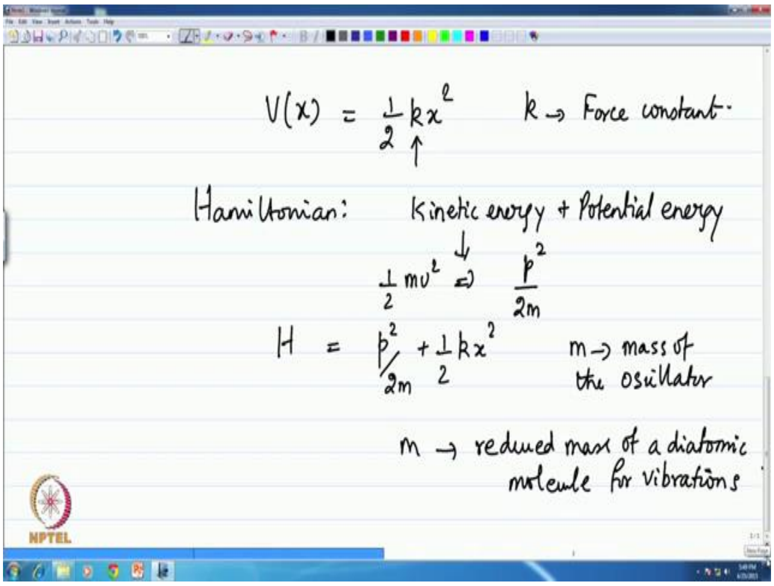
(Refer Slide Time: 05:41)



We can always choose that the potential about the equilibrium, that is ((Refer Time: 05:50)) equilibrium x is equal to 0, is 0, which means, that the constant can be chosen to be 0. This is the minimum or what is known as the minimum in the potential. And therefore, the potential energy for a harmonic oscillator as a function of the displacement from equilibrium is given by half kx square.

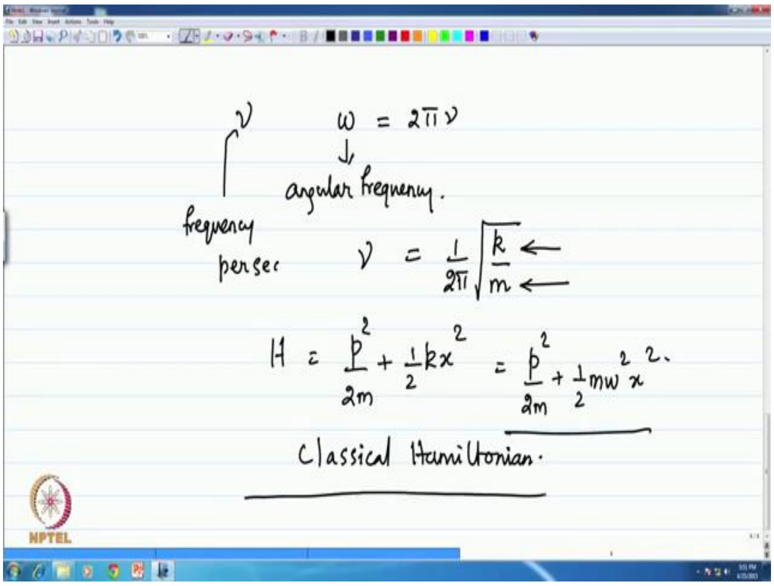
And k, you know is the force constant or the spring constant, if you are talking about spring's force constant. And you know the dimension of k, kx square is energy. So, it is very clear what k should be. And the Hamiltonian if you have to write or the harmonic oscillator is obviously the kinetic energy plus the potential energy of the harmonic oscillator.

(Refer Slide Time: 06:59)



And the potential energy is already given here. The kinetic energy is half m v square or if you want to write it using momenta, it is p square by 2m. And therefore, the Hamiltonian in a classical sense is p square by 2 m plus half k x square, where m is the mass of the oscillator. If you are worried about the diatomic molecule or vibration of a diatonic species, then m is replaced by the reduced mass of the diatomic molecular system for vibrations.

(Refer Slide Time: 08:11)



Also please remember, the harmonic oscillator is associated with a frequency nu or an angular frequency omega, which is 2 pi times nu. This is the angular frequency in radians per second. This is the frequency linear per second, the frequency of a harmonic oscillator in a classical form is something that you all know, it is 1 by 2 pi square root of the force constant by the mass.

You see that the two physical parameters for the harmonic oscillator or the extent of stiffness are the harmonicity given by k and the mass of the harmonic oscillator m and these are the only two parameters, that go in the classical Hamiltonian, namely p square by 2 m plus half k x square. And p, of course is, as you know, it is this mass times the velocity, therefore it is the parameter for the harmonic oscillator are only the m and k. And if you want to write it using the angular frequency, you can write this by writing p square by 2 m plus half m omega square x square. So, this is the classical Hamiltonian.