Chemistry Atomic Structure and Chemical Bonding
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Lecture – 15
Simple Harmonic Oscillator: Classic Hamiltonian

Welcome back to the lectures in chemistry. So, far we have studied a couple of model problems namely the particle in the one dimensional box, 2 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 will do is to study the elementary quantum mechanical aspects of Harmonic oscillator, using the wave function method later in an advanced lecture I would talk a little bit about the different types of raising 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 a 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 oscillatory motion about an equilibrium position or periodic motion such as motion on a circle. These things can be easily understood as caused by a restoring force, which is proportional to the displacement away from the equilibrium, but in the opposite direction.

So, let me write down Harmonic motion; small amplitude oscillation about equilibrium.

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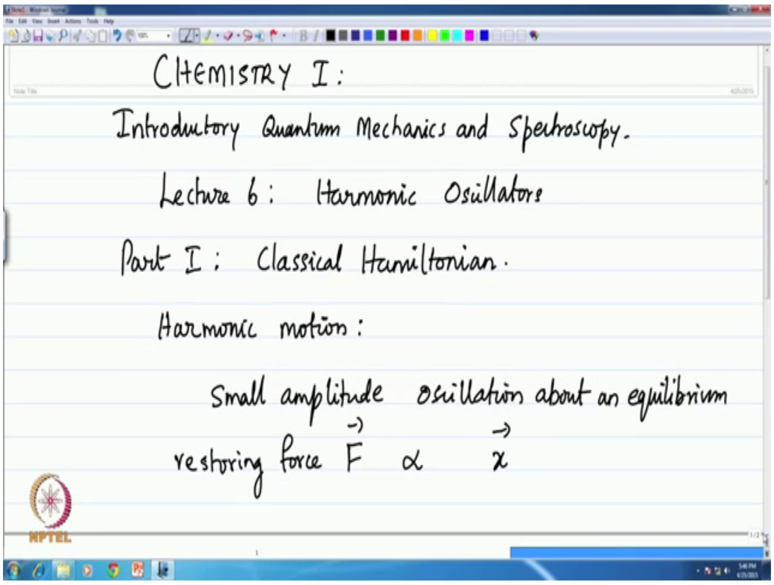

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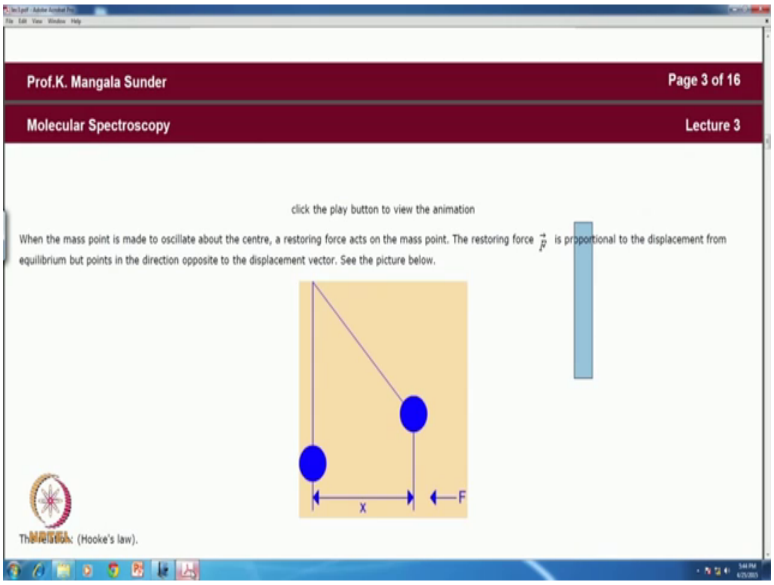

If you want to visualize that here are some simple pictures.

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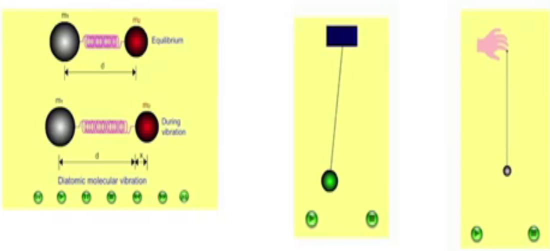

So, these are some examples of what is meant by a small amplitude vibration or oscillation about an equilibrium position. Now the restoring force if you write that it is proportional to the displacement vector from the equilibrium and the mathematics is that the proportionality constant is a constant.

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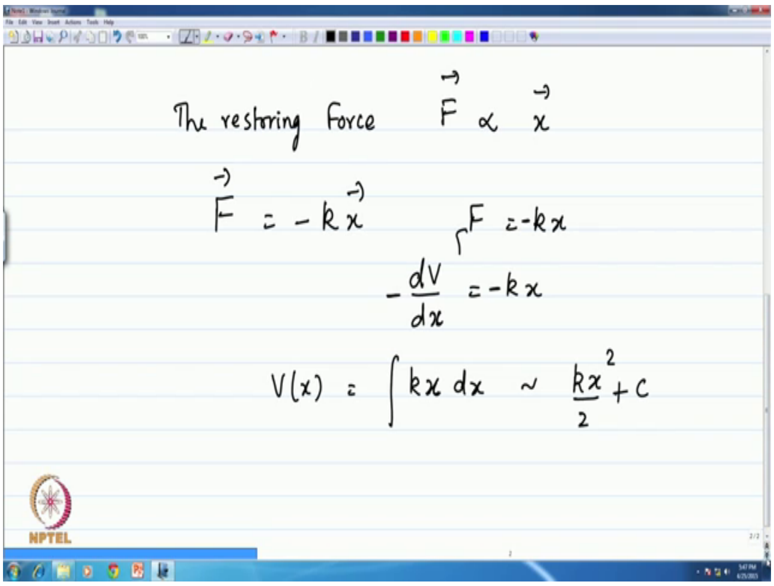

And since it is in the opposite direction, it is minus k x. We would assume that the force is in a direction opposite to that of the displacement.

So, we do not need to worry about the vector arrow here, but 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 k x dx which gives you k x square by 2 plus a constant..

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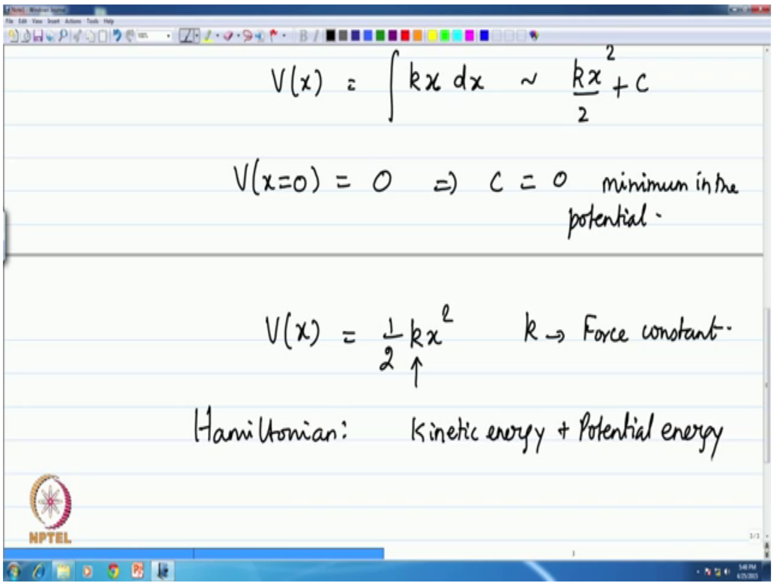

We can always choose that the potential about the equilibrium that is or at equilibrium x is equal to 0 is 0, which means that the constant can be chosen to be 0 this is the minimum or what is known as the minimum in the potential. And therefore, the potential energy for a Harmonic oscillator as a function 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 springs 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 for the Harmonic oscillator is obviously, the kinetic energy plus the potential energy of the Harmonic oscillator, and the potential energy is already given here the kinetic energy is half mv square.

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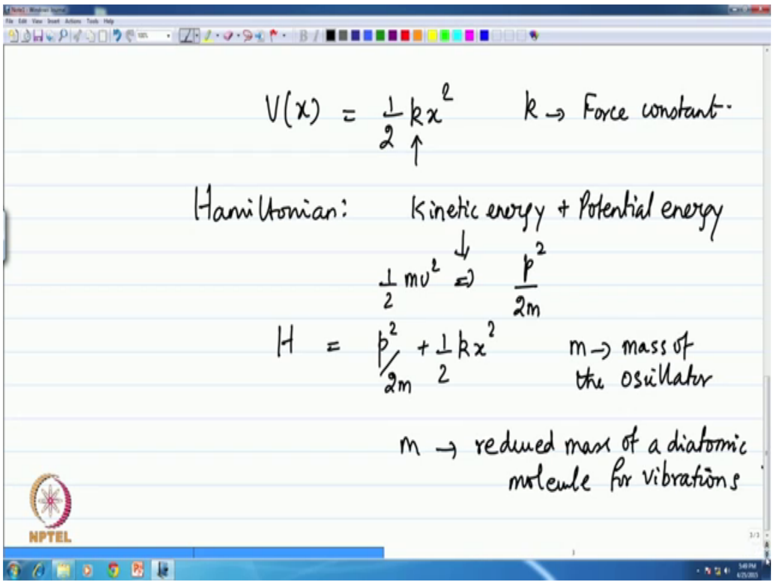

Or if you want to write it using momenta it is p square by 2 m and therefore, the Hamiltonian in a classical sense is p square by 2 m plus half k x square where m is the mass of the oscillator. I you are worried about a diatomic molecule or vibration of a diatomic species, then m is replaced by the reduced mass of the diatomic molecular system for vibrations.

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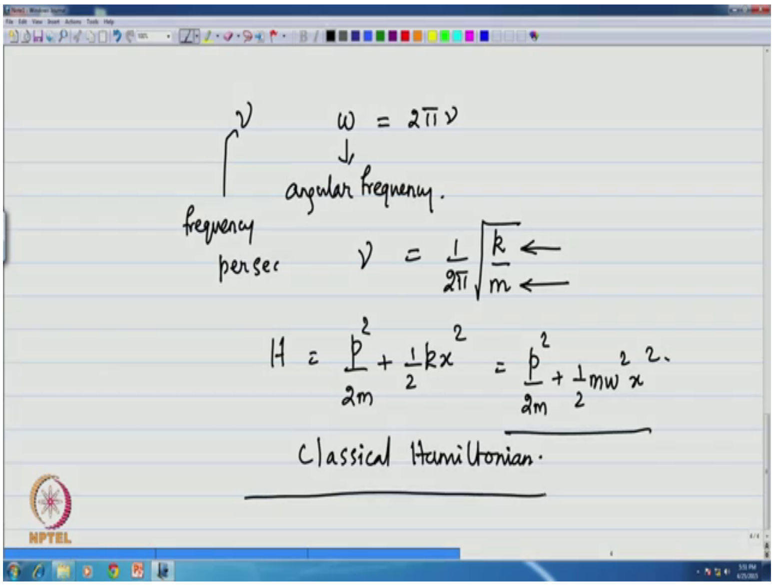

Also please remember the Harmonic oscillator is associated with a frequency nu or an angular frequency omega, which is 2 pi times nu this is the angular frequency in radians per second. This is the frequency linear per second; the frequency of a Harmonic oscillator in a classical form is something that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

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