Chem132A: Lecture 1

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1 Importance of Harmonic Oscillator (H.O.)

Many systems can be explained (approximately) using the H.O. equations. The H.O.is a good approximation for low energy levels (systems near equilibrium). It can represent any bound system. It is also useful in many body systems.

2 Classical Harmonic Oscillator

We will first discuss the H.O. in a classical system. Consider the potential energy function for a particle of a mass(m) moving in a potential only dependent on position (x). Where k is the spring constant.

$$V(x) = \frac{1}{2}kx^2 \tag{1}$$

We can determine an expression for Force using :

$$F_x = -\frac{\partial V}{\partial x} = -kx \tag{2}$$

We can see that the H.O. is a restoring force, and thus the the particle is attracted to x=0 [minimum of potential function V(x)]

A particles motion around x=0 is a sinusoidal of an angular frequency (ω)

$$\omega = \sqrt{\frac{k}{m}} \tag{3}$$

We can find a mathematical expression for k using the Force expression :

$$k = \frac{\partial^2 V}{\partial^2 x} \tag{4}$$

Using Newtons Second Law we can write an equation of motion for the H.O.

$$F = ma = m\frac{d^2x}{dt^2} = \frac{-dV}{dx} = -kx \tag{5}$$

Solving this differntial equation gives the general solution to describe a H.O. motion :

$$x = x_M cos(\omega t - \phi) \tag{6}$$

Where x_M and ϕ are constants and values are determined by initial conditions of the H.O.

3 Properties of QM Hamiltonian

In Quantum mechanics position and momentum are described by their respective operators X and P. Which when taking the commutator yieled the following relationsip :

$$[X, P] = i\hbar \tag{7}$$

$$[P, X] = -i\hbar \tag{8}$$

The Hamiltonian for the quantum Harmonic Oscillator is then taken from the classical representation but taking x and replacing it with the operator X.

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 X^2 \tag{9}$$

4 Eigenvalues of the Hamiltonian

4.1 $\hat{X}$ and $\hat{P}$ Operators

X and P have dimensions of legnth and momentum we want to define two new dimensionless operators. We will use S.I. units for dimensional analysis, and recall that angular frequency ω has units of inverse time,$\hbar$=Js and that a Joule is J=kg*m^{2}s^{-2}

For X :

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}X = \left(\frac{kgs^{-1}}{Js})\right)^{\frac{1}{2}} m = \left(\frac{kg}{kgm^2s^{-2}s^2}\right)^{\frac{1}{2}} m = \left(\frac{1}{m^2}\right)^{\frac{1}{2}} m = \frac{1}{m}m = 1 \tag{10}$$

For P :

$$\hat{P} = \frac{1}{\sqrt{m\hbar\omega}}P = \frac{1}{\sqrt{kg * J * s * s^{-1}}}P = \frac{1}{\sqrt{kg * kg * m^2s^{-2}}}P = \frac{1}{\sqrt{\frac{kg^2m^2}{s^2}}}P = \frac{1}{\frac{kg*m}{s}} * kg * m * s^{-1} = 1 \tag{11}$$

Thus we see that $\hat{X}$ and $\hat{P}$ are dimensionless

We now want to see the commutator relationship of our new operators.

$$[\hat{X}, \hat{P}] = \hat{X}\hat{P} - \hat{P}\hat{X} \tag{12}$$