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The Harmonic Oscillator, a Review of Classical and Elementary Quantum Mechanics

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I. SYNOPSIS

The classical harmonic oscillator is reviewed, as well as some elementary characteristics of the eigenfunctions of the quantum mechanical problem.

II. A HORIZONTALLY MOUNTED CHILD'S CART

The harmonic oscillator is best seen as a cart attached to a wall: which we can plot in Figure 1 as

which can be pulled out from the wall or pushed in towards the wall. At rest, the cart stays at a certain place, and we will often call this the origin, so that we can measure distances relative to this place. This is the place where the spring is neither compressed nor expanded, i.e., the place where there is no net force on the oscillator.

The force on the oscillator, when it is pulled a distance x from the resting position, is

$$F = -k(z - z_0) = -kx$$

where the coordinate x is defined as the relative coordinate, while the coordinate z is the one relative to the wall, i.e., z=0 means the oscillator is colliding with the wall (which corresponds to $x = -z_0$.

Before we go too far, we should note that the presence of a wall on the left hand side, to which is attached the spring, means that the domain of x is truncated on the negative x-axis (by the wall). This is not true for the positive x-axis, which extends from zero to infinity. We will ignore this complication when we conceptualize the harmonic oscillator (idealize it).

Newton's second law says the rate of change of the velocity, the acceleration, is equal to the applied force, so

$$F = -k(z - z_0) = -kx = \mu \frac{d^2x}{dt^2} = \mu \ddot{x}$$

(as $\frac{dx}{dt} = \frac{dz}{dt}$), where we will use dot notation, where each dot stands for one derivative with respect to t.

We have used μ for the mass, rather than m, since we are going to later, in the diatomic molecule case, use the reduced mass rather than the actual mass (of the molecule?).

Anyway, this is a second order differential equation, whose solution is well known. The solution has the form

$$x = A\cos\omega t + B\sin\omega t$$

where ω, A, and B are constants. We have, taking the time derivative,

$$\dot{x} = -A\omega\sin\omega t + B\omega\cos\omega t$$

and, doing it again,

$$\ddot{x} = -A\omega^2\cos\omega t - B\omega^2\sin\omega t = -\omega^2 x$$

Clearly,

$$\mu\ddot{x} = -\mu\omega^2 x = -kx$$

so

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

So, one of the three constants in the proposed solution is in fact not a unknown constant, not an arbitrary constant, but has a value set by the constants of the problem.

We re-write the solution now as

$$x(t) = A\cos\left(\sqrt{\frac{k}{\mu}}t\right) + B\sin\left(\sqrt{\frac{k}{\mu}}t\right)$$

explicitly showing the two so-called arbitrary constants, which in this case correspond to the initial conditions for this particular motion. one time derivative:

$$\dot{x}(t) = -A\omega\sin\left(\sqrt{\frac{k}{\mu}}t\right) + B\omega\cos\left(\sqrt{\frac{k}{\mu}}t\right)$$

which is an expression for the velocity (actually, the instantaneous velocity at a time t). We now form the two terms (remember, $\omega = \sqrt{k/\mu}$):

$$x^2 = A^2\cos^2\omega t + 2AB\cos\omega t\sin\omega t + B^2\sin^2\omega t$$

and

$$\dot{x}^2 = \omega^2\left(A^2\sin^2\omega t - 2AB\cos\omega t\sin\omega t + B^2\cos^2\omega t\right)$$

and add them with suitable multipliers, i.e.,

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$$\frac{1}{2}\mu\dot{x}^2 + \frac{k}{2}x^2 = \frac{1}{2}\mu\omega^2\left(A^2\sin^2\omega t - 2AB\cos\omega t\sin\omega t + B^2\cos^2\omega t\right) + \frac{k}{2}\left(A^2\cos^2\omega t + 2AB\cos\omega t\sin\omega t + B^2\sin^2\omega t\right) \tag{2.1}$$

which becomes

$$\frac{k}{2}\left(A^2 + B^2\right)$$

Clearly, this is a constant, which we normally call the energy. A and B are chosen to describe the motion, and the energy follows. Then, this energy value is maintained constant during the motion, come what may! We know further, that the potential energy for this oscillator is

$$P.E. = \frac{1}{2}kx^2$$

and the kinetic energy is

$$K.E. = \frac{1}{2}\mu\left(\frac{dx}{dt}\right)^2$$

III. THE HARMONIC OSCILLATOR, QUANTUM MECHANICALLY

The quantum mechanical equivalent of Newton's second law becomes our Schrödinger Equation:

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2\psi}{\partial x^2} + \frac{k}{2}x^2\psi = E\psi \tag{3.1}$$

This comes from the classic $p_{op} \rightarrow -\imath\hbar\frac{\partial}{\partial x}$ for the x-component of momentum.

We start with some guess work, i.e., we will ask, is

$$\psi_{guess} = e^{-\alpha x}$$

a possible solution to Equation 3.1? This question means, can we substitute the guess into the Schrödinger Equation, Equation 3.1, and show that some choice of α causes the equal sign to hold? It is trivial to take two derivatives of this guess function, and test the question:

$$\frac{\partial\psi_{guess}}{\partial x} = -\alpha e^{-\alpha x}$$

and

$$\frac{\partial^2\psi_{guess}}{\partial x^2} = +\alpha^2 e^{-\alpha x}$$

so,

$$-\frac{\hbar^2}{2\mu}\alpha^2 e^{-\alpha x} + \frac{k}{2}x^2 e^{-\alpha x} \stackrel{?}{=} E e^{-\alpha x} \tag{3.2}$$

which implies

$$-\frac{\hbar^2}{2\mu}\alpha^2 + \frac{k}{2}x^2 \stackrel{?}{=} E \tag{3.3}$$

if the equal sign held. But, if the equal sign held, this would be an equation *for* x! We want a solution ψ_{guess} which holds for any and all x, so this is not a solution.

IV. ANOTHER TRIAL WAVE FUNCTION

OK, the first guess was no good. Now, let's try

$$\psi_{guess} = e^{-\alpha x^2}$$

and again, substitute into the Schrödinger Equation for the Harmonic Oscillator. We have

$$\frac{\partial\psi_{guess}}{\partial x} = -2\alpha x\psi_{guess}$$

and

$$\frac{\partial^2\psi_{guess}}{\partial x^2} = -2\alpha\psi_{guess} + 4\alpha x^2\psi_{guess}$$

so, substituting, we have

$$-\frac{\hbar^2}{2\mu}\left(-2\alpha + 4\alpha^2x^2\right)\psi_{guess} + \frac{k}{2}x^2\psi_{guess} \stackrel{?}{=} E\psi_{guess} \tag{4.1}$$

which would mean

$$\frac{\hbar^2\alpha}{\mu} - E + \left(\frac{k}{2} - \frac{4\alpha^2\hbar^2}{2\mu}\right)x^2 = 0$$

if indeed the equal sign is going to hold. This means that the coefficient of x^2 must be zero, so that we do not have a function of x plus a constant equal to zero. We have

$$\frac{k}{2} - \frac{4\alpha^2\hbar^2}{2\mu} = 0$$

or

$$\alpha = \frac{\sqrt{k\mu}}{2\hbar}$$

Then

$$\frac{\hbar^2\alpha}{\mu} - E = 0 = \frac{\hbar^2\frac{\sqrt{k\mu}}{2\hbar}}{\mu} - E$$

which means that

$$E = \hbar \frac{\sqrt{\frac{k}{\mu}}}{2} = \frac{1}{2}\hbar\omega$$

which is (since $\sqrt{k/\mu} = \omega$), of course, the ground state energy of the harmonic oscillator.

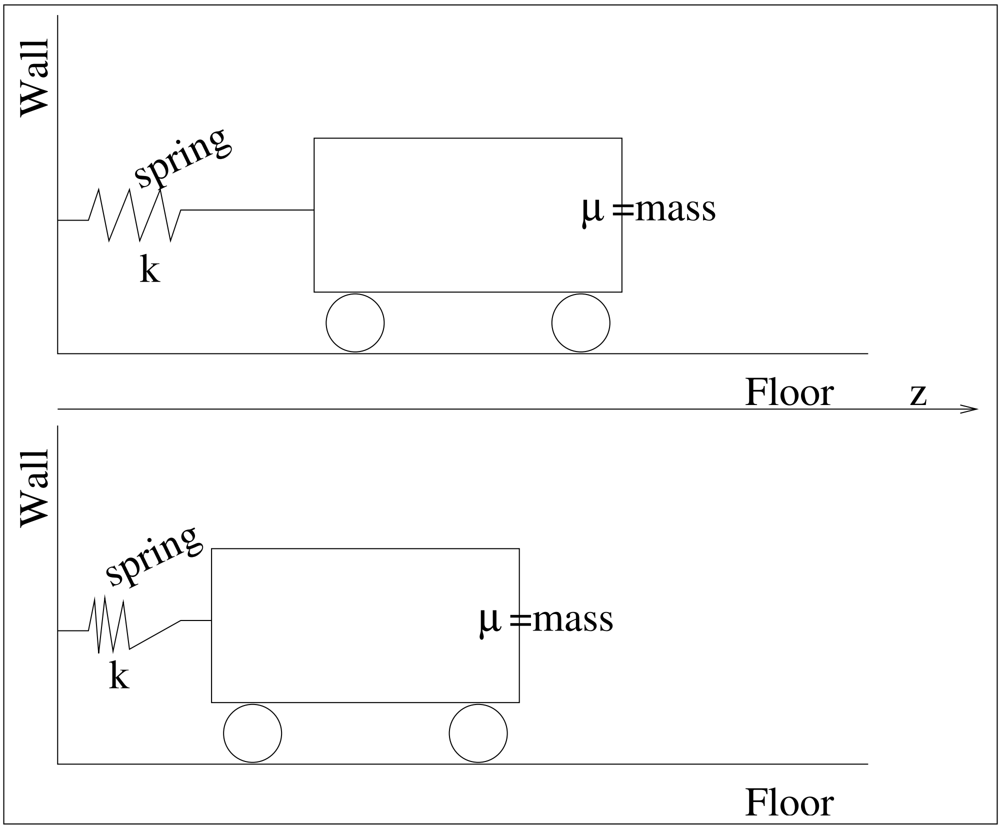

FIG. 1: The cart moves from left to right and back again depending on initial conditions.

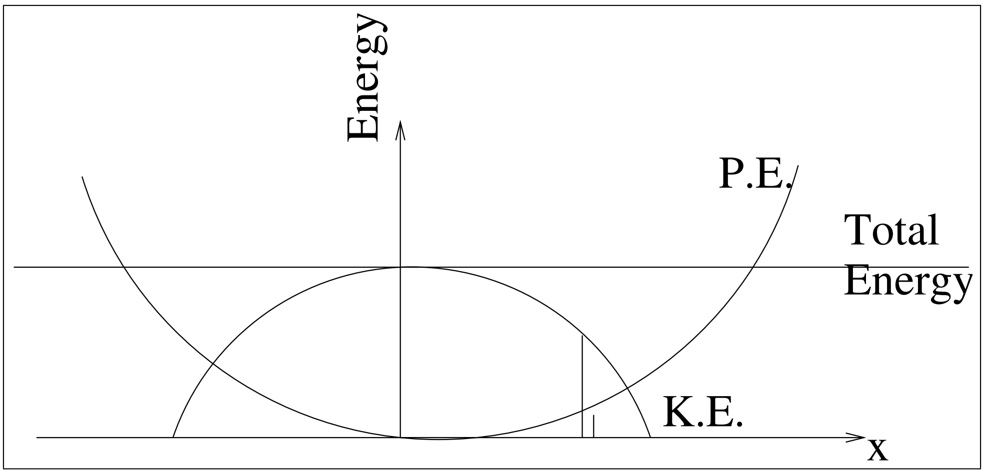

FIG. 2: The instantaneous sum of the kinetic energy (K.E.) and the potential energy (P.E.) is the constant total energy.