Harmonic Oscillator

Seppo Nurmi, 2007

Preface

This is an elementary introduction to quantum mechanics taking the road from classical harmonic oscillator to quantum mechanical one. It is a simple enough physical object not to obscure the basic ideas, and it has been for me most helpful in understanding the transition from classical to quantum physics. I have tried to make the presentation easy to follow by also showing the most obvious of the intermediate steps. It is mainly purposed as a first look into the subject, and maybe above all, for refreshing of old and forgotten knowledge (the reason why I wrote it was in refreshing my own memory). The presentation here also takes up some elementary parts of classical theoretical physics.

1: Classical Harmonic Oscillator

1.1 Introduction

Typically consider a harmonic oscillator as two masses bound together by a linearly distance-dependent force. One could think a simple construction like two metal balls joined with a spiral spring (hanging freely in the air in a somewhat idealized case). The frequency of such an oscillation will only depend on two consttant values: a constant k describing the force's dependecy of the separation between the masses, and an other constant m called the reduced mass describing the arrangement of masses as they act totally. We write the frequency in units of angular velocity ω, which is simply 2π times the frequency ν.

$$\omega = 2\pi\nu = \sqrt{\frac{k}{m}} \tag{1.1}$$

The force between the masses due to the string has the form of the Hooke's law, a simple mathematical relation involving the displacement x and a constant k. The displacement x is the separation from the balanced position where the force F from the string is zero. The sign before the string-constant (bond force constant) k is negative because the force from the string acts in opposite direction to the displacement.

$$F(x) = -k\ x \tag{1.2}$$

We are going to compare the classical oscillator with a quantum mechanical one. Therefore consider an oscillator in a smaller scale, like a diatomic molecule, with oscillation of the two atoms in the molecule in respect to each other (one-dimensional oscillation, only depending of the separation between them this simplified case). Still the Hooke's law above is a good approximation to the intermolecular force, in case of low energies and small oscillations.

The other constant m in (1.1) is called the reduced mass m , which often turns up in classical mechanics. It is the effective mass term for a mechanical system, in this case the oscillator, with the two masses as a whole expressed as seen from the mass-center of the system. If m_1 and m_2 are the masses of the molecules (or the metal balls or whatever they are) the reduced mass m is

$$m = \frac{m_1\, m_2}{m_1 + m_2} \tag{1.3}$$

1.2. The Oscillation Formulas

Below follows a short treatment how we end into the frequency (1.1), and also how we get the time dependent swinging of the oscillator. Force is differential of the potential energy V(x):

$$F(x) = \frac{d}{dx} V(x) \tag{1.4}$$

Because we now know the differential, we get the potential by integration:

$$V(x) = \int_0^x F(x)\, dx = - \int_0^x (-k\, x)\, dx = \frac{1}{2}\, k\, x^2 \tag{1.5}$$

Kinetic energy T of the oscillator in any position of the oscillation period depends only of the reduced mass m and the momentary velocity v (which varies with time)

$$T = \frac{1}{2}\, m\, v^2 \tag{1.6}$$

Total energy E is constant, due to the energy law, an can be expressed as the sum of the kinetic and potential energies. This is the total Newtonian energy:

$$E = T + V = \frac{1}{2}\, m\, v^2 + V \tag{1.7}$$

The potential V varies with the distance, and with time, and we need to find out the time variation. Solving out the velocity v, which is a time derivative of the displacement we get:

$$v = \frac{dx}{dt} = \sqrt{\frac{2}{m}\,(E - V(x))} \tag{1.8}$$

Because energy E is constant the formula (1.8) now tells how the velocity depends on the displacement x. An as velocity is a time differential we can get the time dependency of displacement by integration of (1.8). First we write

$$dt = \frac{\sqrt{\frac{m}{2}}}{\sqrt{E - V(x)}}\,dx \tag{1.9}$$

and the integrate both sides (and we don't care to mark the integration variables, only we understand what is going on this is no problem)

$$\int_{t_0}^{t} 1\,dt = \int_{x_0}^{x} \frac{\sqrt{\frac{m}{2}}}{\sqrt{E - V(x)}}\,dx \tag{1.10}$$

This is a general expression for any potential. There is a freedom of choosing the potential expression, only it is done so that the total energy is constant of time. We then assume, for simplicity, that at the time $t_0 = 0$ the potential $V(x) = 0$. This is also case in the potential (1.5).

Equation (1.8) is a differential equation, and what is done above is more generally called setting of the initial conditions. It must be done because integration always comes with the freedom of choosing an arbitrary constant of integration. In effect one chooses the constant so that matches the actual physical situation. Now putting in to (1.10) the potential (1.5) we get

$$t = \sqrt{\frac{m}{2}} \int_{x_0}^{x} \frac{1}{\sqrt{E - \frac{k}{2}x^2}}\,d(x') \tag{1.11}$$

The integral expression (1.11) can be solved by a suitable substitution of a variable. Consider a substitution of where x is

$$x = \sqrt{\frac{2\,E}{k}}\,\sin\theta \tag{1.12}$$

and its differential is

$$dx = \sqrt{\frac{2\,E}{k}}\,\cos\theta\,\,d\theta \tag{1.13}$$

After substitution of the equation (1.11) becomes

$$t = \sqrt{\frac{m}{2}}\int_{\theta_0}^{\theta} \frac{1}{\sqrt{E\left(1 - \sin^2\theta\right)}}\left(\sqrt{\frac{2\,E}{k}}\,\cos\theta\right)d\theta \tag{2.14}$$

Further simplify, using the trigonometrical formula $1 - \sin^2\theta = \cos^2\theta$ and we are left with the simple equation

$$t = \sqrt{\frac{m}{k}}\int_{\theta_0}^{\theta} 1\,d\theta \tag{1.15}$$

then we perform the integration, taking care of the initial conditions, which means that at the lower end θ_0 of the integration interval the integration yields zero, and so $t_0 = 0$.

$$t = t - t_0 = \sqrt{\frac{m}{k}}\left(\theta - \theta_0\right) \tag{1.16}$$

and we can solve out the dependency of θ, that we identify as the phase angle of the oscillator, of the time t

$$\theta = \sqrt{\frac{k}{m}}\,t + \theta_0 \tag{1.17}$$

and we identify the angular velocity ω as the root term

$$\omega = \sqrt{\frac{k}{m}} \qquad (1.18)$$

so that we can write

$$\theta = \omega t + \theta_0 \qquad (1.19)$$

We will eliminate k from the equations (in case of molecular size oscillators we can not directly measure it anyway). From (1.18) we have

$$k = \omega^2 m \qquad (1.20)$$

Substitution of (1.19) to (1.12) gives

$$x = \frac{1}{\omega} \sqrt{\frac{2E}{m}} \, \sin\left(\omega t + \theta_0\right) \qquad (1.21)$$

From initial conditions at t_0

$$\qquad (1.22)$$
$$x_0 = \frac{1}{\omega} \sqrt{\frac{2E}{m}} \, \sin\theta_0$$

Here θ_0 is initial phase angle, telling in which phase we start the oscillator.

A macroscopic oscillator of weights on a string may be started from maximum displacement, the initial phase is then 90 degrees off, or it can be started at displacement zero with a push and then the initial phase is zero. For a molecular oscillator, however it starts oscillating, we can for simplicity choose the initial phase angle as zero at zero displacement, $\theta_0 = 0$ when $x_0 = 0$. Then we get

$$x = \frac{1}{\omega} \sqrt{\frac{2E}{m}} \, \sin\left(\omega t\right) \qquad (1.23)$$

The sinusoidal oscillation is also called a "harmonic oscillation", thereof the name of the oscillator. The amplitude A of the oscillator is the multiplier before the sinus:

$$A = \frac{1}{\omega} \sqrt{\frac{2E}{m}} \qquad (1.24)$$

which means that we can write the energy for a given amplitude

$$E = \frac{1}{2} A^2 \omega^2 m \qquad (1.25)$$

telling that the oscillation energy increases in square with increasing amplitude and frequency.

1.3. The Lagrangian and Hamiltonian Functions

What follows here is a bit theoretical part. This part is a general theory, also valid for quantum physics, at least as a limiting case, and it is maybe helpful for understanding some of the basics of the quantum theory.

We need a concise mathematical expression for the characteristics of physical system . Historically oldest of such an expressions is the Lagrangian function, named after the French mathematician and physicist Joseph-Louis Lagrange (1736-1813). The Lagrangian is defined as kinetic energy minus the potential: $\mathcal{L} = T - V$

It is a formal function of coordinates and velocities (and possibly also of the time t), and gives the amount of "physical action" in a system. It rises historically from the problem called the "principle of least action", the search of shortest, or most effective path, because it was realized that nature prefers such paths. It is a generalized form of the principle of least time or Fermat's principle, after the French mathematician Pierre de Fermat (1601 - 1665). This principle is historically older than the the energy law (which tells that nature prefers the lowest energy), but it is nearly related.

In the case of the one-dimensional oscillator the Lagrangian is a function only of one coordinate, x, and the velocity v.

$$\mathcal{L}(x,v) = T - V = \frac{1}{2} m v^2 - \frac{1}{2} k x^2 \qquad (1.26)$$

The Hamiltonian function is defined: $\mathcal{H} = T + V$, and named after the English mathematician and physicist Sir William Rowan Hamilton (1805-1865). It is a formal function of coordinates and moments (and more generally also of the time t) , and expresses the total energy. Note that energy is a value, whereas the Hamiltonian is a function with that value. Knowing the Hamiltonian we can calculate the dynamical behavior of the physical system. Here we get

$$\mathcal{H}(x,p) = \frac{p^2}{2 m} - \frac{1}{2} k x^2 \qquad (1.27)$$

There are two important equations involving the Hamiltonian function, called Hamilton's equations, that give formally the velocity and the force. In the actual case of the harmonic oscillator we get:

$$\frac{d\,x}{d\,t} = v \qquad\qquad v = \frac{\partial\,\mathcal{H}}{\partial\,p} = \frac{p}{m} = \frac{m\,v}{m} \qquad\qquad (1.28)$$

$$\frac{d\,p}{d\,t} = F \qquad\qquad F = -\frac{\partial\,\mathcal{H}}{\partial\,x} = -k\,x \qquad\qquad (1.29)$$

Note that the partial derivation symbol ∂ is needed because the Hamiltonian has more than one argument. This theoretical formulation was developed for one purpose: how to set up conditions from where the movements in a dynamical system always can be calculated. An equation that expresses such conditions is called the "equation of motion". The Hamiltonian formulation is the most important method, because we know that the Hamiltonian function expresses the total energy of the system, which in many cases is constant and known (if the system does not loose energy).

Thus one can set up an equation of motion as soon as one has worked out the form of the Hamiltonian function. In cases when energy is not preserved the Lagrangian method still can be used, by establishing a condition based on the minimum action. In matter of fact the Hamilton's equations are valid also in that case. Thus in the Lagrangian and Hamiltonian formulation we have the most general framework for theoretical physics. It is in major parts applicable also in non-classical theories, so also in general relativity and quantum theory. But of course, there are certain differences in details.

(The treatment is continued in the next chapter, which is of the quantum oscillator.)

- o -