A Brief Introduction to the Quantum Harmonic Oscillator

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Abstract

In this short paper, a very brief introduction of the quantum harmonic oscillator has been provided. The understanding of the transition from a classically damped oscillator and the quantum mechanical model of the latter is included via a clear mathematics involving simple calculus. Only the one dimensional time dependent Schrodinger's equation is being studied. This paper is intended to simply provide an analytical description of the subject, there are no advance calculations implying further suggestions in quantum theory.

The Quantum Harmonic Oscillator

The mathematical construction behind the explanation of the behavior of a quantum mechanical system may seem rather complicated at first sight. This is simply because the former deals extensively with a rather abstract of mathematics known as calculus. And the worst is that it is not one, not even two but calculus in three or more dimensions thus making use of partial differential equations. Hopefully at this level we shall be encountering only linear differential equations in one dimension then extending these to three dimensions. Understanding what is happening through the mathematical procedures described in this short introduction is poised to give us a deeper insight of the behavior of some quantum entities. And these quantum objects that I will explain here are the harmonic oscillators. Why harmonic oscillators? This is because the latter are extremely interesting from both a quantum mechanical and a classical point of view as well since they provide sets of general solutions which contribute to the modeling and understanding of many oscillatory systems. A simple example of such a system is the vibrational motion prevailing between two atoms in a diatomic molecule. Using the Lennard – Jones potential, one may have an idea of what is happening but this idea will be mostly perceived with a mechanistic point of view. This is actually a right start in order to understand oscillatory systems even at the microscopic level but the fact is that there will be observations which will be made which cannot be explained using the classical mathematical theory thus restricting our comprehension of the atom. However a complete picture is obtained by making use of quantum mechanics. Concerning the classical harmonic oscillator, I will not extend other the details as this is not topic of this discussion but if we have consider a damped (i.e: real) harmonic oscillatory system, e.g: a spring, then the general equation of motion is [1]:

$$m\ddot{x} + \beta\dot{x} + kx = \vec{G}(t) \tag{1}$$

$$\vec{x}(t) = x_0 e^{t/\tau} cos(\tilde{\omega} t + \phi) + Acos(\Omega t + \phi) \qquad (2)$$

The general solution of the above equation is rather complicated due to the large number of parameters involved, but the way of solving equation (1) is similar to the way a non - homogenous linear second order differential equation is solved, thus resulting in the general solution which is equation (2). The first part of the solution corresponds to the transient state (the envelope - due to damping) while the second part refers to the steady part of the system (the characteristic sinusoidal structure). This is the very basis of how a classical harmonic oscillator behaves, obviously these equation can be extended to produce the conditions needed for resonance to occur but this will not be discussed.

Considering now the quantum mechanical oscillator, since for the classical oscillator we have started with a general solution, it seems obvious to go through a similar procedure for a quantum oscillator. The general equation which does give a mathematical sense to this system is the Schrodinger's Equation. The latter was described by Schrodinger himself as an equation which would described the microscopic objects like the equations of Newton does in our everyday life. This is a good analogy but unlike the equations of Newton where the solutions can be predicted with much accuracy, the solutions of the Schrodinger's Equation gives us the *PROBABILITY* of finding a particle in a given quantum state in a region of space. This makes the solutions of the Schrodinger's Equations probabilistic ones while these are the equations of Newtons are deterministic ones. So it was probabilistic... and the one who inferred this idea at first was Max Born, an eminent physicist of the mid - twentieth century. This idea was then accepted by the physicist but not by Schrodinger who did refute it. Unfortunately for him it was the right interpretation.

Schrodinger's equation [1] is actually a postulate that is something that exists simply because the observations made by scientists are coherent with the equation and nothing more. That solving this equation provides us with an object which has no physical significance even though the mathematics may be fully consistent; this is the wave-function. Actually the wave-function is a useless object from a physical point view, it is the square of the modulus of the latter which is known as the Born Interpretation which gives the probability of finding a particle with a given amount of energy to exist in a given region of space, which is sensical. However what was making sense in the microscopic world was not at all coherent with our real macroscopic world and this idea really confused physicists, and the one which has difficulties in viewing this probabilistic version of our reality was Albert Einstein himself. This is actually seen in one of his famous phrases: *"God does not play dice"*. However today physicists know that God does play dice! The weird behavior of discretionary that does prevail in the quantum theory of matter was not completely understood by many scientist because in the real world energy is continuous but it is discrete in the microscopic world, that is not all the solutions of the wave-functions and those of energy when solving the Schrodinger's equation are accepted. This bizarre picture of the behavior of quantum particles is today accepted and understood by all physicists on the planet. The Schrodinger's equation is something which is rather easy to treat with, its derivation is also not complicated and there are many ways of doing. I derived it starting with the quantum mechanical operators and obtained the final equation by doing some algebraic manipulations. Another way of deriving the Schrodinger equation is to start from the de Broglie wave-function. In a first case, the time derivative is taken and both sides of the equation are multiplied by $ih/2\pi$ .Then the wave-function is differentiated twice and both sides of the equation are multiplied by $h^2/8m$. Equation (3) is the de Broglie wave-function and (4) is the time dependent Schrodinger's equation in one dimension.

$$\psi(x,t) = e^{ikx - i\omega t} \tag{3}$$

$$\left[-\frac{h^2}{8m\pi^2}\frac{d^2}{dx^2}\psi(x,t) + V(x)\right]\psi(x,t) = \; i\frac{h}{2\pi}\frac{d}{dt}\psi(x,t) \tag{4}$$

The quantity in the square bracket is known as the Hamiltonian operator [2],$\widehat{H}$. The latter is the sum of the kinetic energy operator and the potential of a particle. And there are many other ways of doing so, for example one may start with the wave equation, all these methods are interlinked. OK now that we have encountered Schrodinger's equation, things will get a bit more rigorous, the latter shall be used as a template to model the system of the harmonic oscillator. (Note: The above equation can easily be transformed for a 3 dimensional system but I will not deal with now, the calculations would become too long.) The detailed mathematical proofs are long and tedious to write using computer programs and they would rapidly make the discussion uninteresting, for this reason I will concentrate on the final results and equations. The harmonic oscillator is defined by the potential *V(x)*, where *V(x)* is the elastic potential just like it is done with a spring. The latter is then inserted in the time independent Schrodinger's equation. This is given below:

$$\frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2 \tag{5}$$

Thus the Schrodinger's equation becomes:

$$\left[\frac{h^2}{8m\pi^2}\frac{d^2}{dx^2} + \;\frac{1}{2}m\omega^2x^2\right]\varphi(x) = E\varphi(x) \tag{6}$$

As one can notice, if we want the wave-function and energies for a quantum harmonic oscillator, using the above equation as it is would be rather inappropriate and complicated. Thus to make things simpler, some new operators [Equations (7)] are introduced along with coordinate transformation shown in (8):

$$\hat{b^+} = \frac{1}{\sqrt{2}}(-\frac{d}{d\xi} + \xi)$$

(7)

$$\hat{b} = \frac{1}{\sqrt{2}}(\frac{d}{d\xi} + \xi)$$

$$\xi = \sqrt{\frac{2m\omega\pi}{h}}x$$

(8)

Equation (7) and (8) are substituted in (6) leading to equation (9) shown below:

$$\frac{h\omega}{2\pi}\left[-\frac{h^2}{8m\omega\pi^2}\frac{d^2}{dx^2} + \frac{1}{2}\left(\frac{2m\omega\pi}{h}\right)x^2\right]\phi = E\phi \quad (9)$$

Now the wave-function is also changed:

$$\varphi_n \rightarrow \phi_n$$

After expanding and factorizing the terms with the operators, one is able to obtain the final Schrodinger equation for a harmonic oscillator and the latter reads:

$$\frac{h\omega}{2\pi}\left(\hat{b^+}\hat{b} + \frac{1}{2}\right)\phi_n = E_n\phi_n$$

(10)

The operators used known as the annihilation and creation operator (the one with the +). This is because when applied to the wave-function with quantum number n, the effect is that *b - cap* decreases the quantum number to *n - 1*, thus destroying a quantum hence its name annihilation. The other operator *b - cap - plus* does the opposite by actually increasing the quantum number to *n + 1*, creating one quantum. We shall use these to obtain the expression for the wave-function of the oscillator. Let's consider the action of *b - cap* on wave-function with quantum number *0*. Obviously:

$$\hat{b}\phi_0 = 0 \tag{11}$$

$$\phi_0 \left(\frac{d}{d\xi} + \xi \right) = 0 \tag{12}$$

From equation (12) one can easily formed a first order linear separable differential equation, very easy to solve for the wave-function.

$$\frac{d\phi_0}{\phi_0} = -\xi d\xi \tag{13}$$

Thus the wave-function is given as:

$$\phi_0 = A_0 e^{-\frac{\xi^2}{2}} \tag{14}$$

The value of the constant of integration is determined using normalization of the wave-function shown below:

$$\int_a^b |\phi_0|^2 \, d\xi = \int_a^b A_0^2 e^{-\xi^2} d\xi = 1 \tag{15}$$

The limits *a* and *b* corresponds to negative and positive infinity respectively. Now one can found the value of the integration constant. However I want to make one point, the integral here is non-intuitive. If one tries to do this integral using the usual analytical method it would become too long and complex. This is a Gaussian integral and the best methodology is to make use of the multiple integrals methods to solve it. It is then easier after a transformation of coordinates form Cartesian to polar. Finally, the full equation for the wave-function with quantum number 0 is given as:

$$\phi_0 = \pi^{-\frac{1}{4}} e^{-\frac{\xi^2}{2}} \tag{16}$$

In a similar way using the Schrodinger's equation, the state energy eigenvalue can be evaluated and is given as:

$$E_0 = \frac{h\omega}{2\pi} \tag{17}$$

Now we have to generalize the above results, this is the easiest part as it is almost purely mathematical. So, we want to find the wave-function of the first excited state, thus we have to use to creation operator applied onto the wave-function of the ground state. In fact if we want to find the wave-function with a given quantum number *n*, we have to apply the creation operator raised to the power of *n* on the Eigen function with quantum number *0*.

$$\phi_1 = \hat{b^+} \phi_0 \tag{18}$$

$$\phi_2 = (\hat{b^+})^2 \phi_0 \tag{19}$$

$$\phi_3 = (\hat{b^+})^3 \phi_0 \tag{20}$$

These calculations may be not difficult to understand but are rather long, there are many parameters with many change of sign occurring, I have thus stopped at quantum number *n = 3* but for those interested you may continue if you have access to some computer programs. This would be quite easy if you use FORTRAN, you will get the values for the different quantum numbers but it would be difficult to figure the general final solution since the solutions would all be numerical.

Finally, the general solution for the wave-functions and the energies of the quantum harmonic oscillator at different quantum numbers is given as:

$$\phi_n = \frac{(-1)^n}{\sqrt{2^n}} e^{\xi^2} \frac{de^{-\frac{\xi^n}{2}}}{d\xi^n} \frac{1}{\sqrt{n!\sqrt{\pi}}} \tag{21}$$

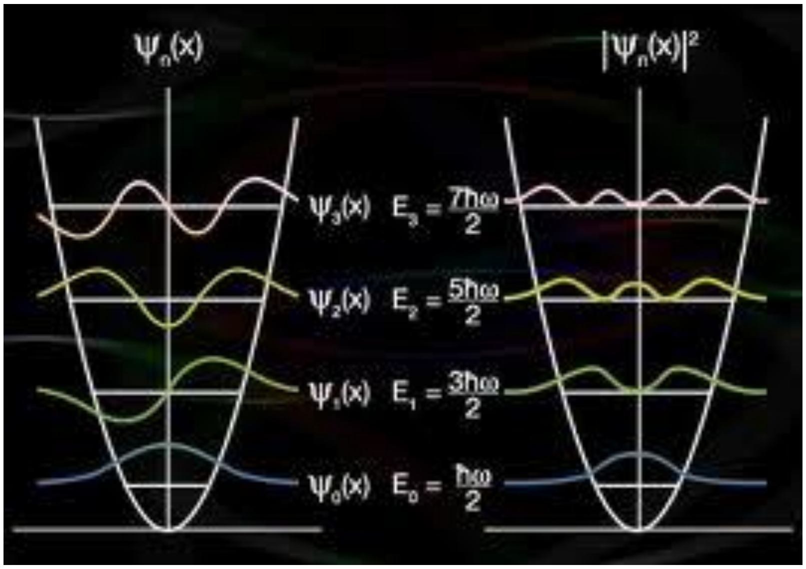
The above equation may look scary but believe me it is not. The equation can be used to describe molecular vibration thus giving a more accurate perception on the behavior of molecular models. This equation is accurate for a diatomic molecule. A simpler way of expressing it given below:

$$\phi_n = \frac{1}{\sqrt{n!}} (\hat{b}^+)^n \phi_0 = e^{-\frac{\xi^2}{2}} H_n(\xi) \tag{22}$$

The right hand side of the equation is known as the Hermite polynomial. The final general equation for the energies is given:

$$E_n = (n + \frac{1}{2}) \frac{h\omega}{2\pi} \tag{23}$$

After we have derived these equations which are rather impressive at first sight; let’s go through their implications. Below is a plot of the various wave-functions with different quantum numbers at different energies based on equation (22) and (23).



This is what we get after all this mathematical analysis; the results are rather interesting even surprising I should say! I said above the wave-function itself is not physically interesting but what does the plot on the left hand side tell us is that the energy of a quantum system is not zero like it can be in classical mechanics. The energies are also distributed in a discrete manner and are indeed not continuous as indicated in our calculations. But it is the second graphical plot which is interesting. If we observe carefully the plot we can see that it is the square of the modulus of the wave-function, and the latter as said above gives us the probability of finding a particle with a given quantum of energy in a region of space. Thus one may argue that since we have started with the potential of a spring, then why are then wave-function not contained within that potential (i.e: the parabola in the plots) in the graph. Actually this is the beauty of quantum physics; our equations are telling us that a quantum particle has the potentiality to exist in classically forbidden regions! Particles with lower energy states have the possibility to traverse a barrier with higher energy. This is an absurd idea and we all this is not possible but the fact is that the equations do indicate a non - vanishing probability possessed by quantum entities in a quantum system. Particles have the possibility to Quantum Tunnel through a barrier with higher energy than they possess the wave-function of the particle then propagate normally after it passed through the barrier! This part of quantum physics has opened new doors and it is only in the 21st century that physicists are trying to fully understand and exploit this phenomenon. The thing is that quantum tunneling has been existing well before us; it is actually because of this phenomenon that we are able to live on this planet. How? This is because it is occurring on the sun, the latter does not possess enough energy to make a large number of protons to undergo fusion, thus when the latter came close to each other they can quantum tunnel thus overcoming the highly repulsive forces due to like charges and fuse. Hence for sure quantum mechanics have enhanced our comprehension of the atom allowing us to understand how the microscopic world behaves and why does it differ so much with our known version of the macroscopic reality.

References

[1] R. Gautreau, W. Savin *“Schaum Outline of Modern Physics, 1999*” McGraw Hill.

[2] P.A.M. Dirac “Principle of Quantum Mechanics, 2001” Dover Publications Inc., Mineola New York.