A Heuristic Derivation of the Linear Harmonic Oscillator Energy Levels

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In the usual flow of an undergraduate physical chemistry course on quantum mechanics, students are first introduced to the de Broglie theory of the wave properties of matter, the particle-in-a-box system, and then the harmonic oscillator (1–3). The de Broglie theory allows for an exact derivation for the particle-in-a-box energy levels by forcing the wavelength of the particle to fit exactly inside the box (2). This derivation is appealing because it involves only algebra and incorporates the most important physics in the problem, namely, that the wave function of the particle must vanish at the ends of the box.

The energy levels for the harmonic oscillator, on the other hand, are hard to derive from first principles from the exact solution of the Schrödinger equation. Consider the following direct quotes from two representative undergraduate textbooks in physical chemistry. Both quotes refer to the solution of the harmonic oscillator Schrödinger equation.

"The solution of this equation involves the use of Hermite polynomials. We will not give details but merely state the main conclusions." (4)

"The solution of the Schrödinger equation is too complicated to discuss here in detail, but when solved it is found that there are well-behaved solutions only if the harmonic oscillator has energies given by..." (5)

In both of these texts the authors then write down the energy levels for the harmonic oscillator. Thus, in presenting the harmonic oscillator to undergraduates, the instructor has two choices: (i) writing down the energy levels of the harmonic oscillator stating that these energies arise from the solution of the Schrödinger equation (which seems to be the more common approach taken by the typical undergraduate physical chemistry text), or (ii) explicitly solving the Schrödinger equation for the harmonic oscillator. Neither option is optimal. The first asks the student to take the result on faith without discussion of the important physical principles behind the quantization of the energy levels. The second involves an extremely complicated power series solution of a differential equation (2) that will leave most students in a daze, still not seeing the important reason behind the quantization of the energy levels through the haze of the chalk dust. As an alternative to these less than desirable choices, I offer here a heuristic derivation of the energy levels of a linear harmonic oscillator that involves only algebra.

Heuristic Derivation: The Harmonic Oscillator as a Particle in a Box

We consider a linear harmonic oscillator of reduced mass $\mu$ and frequency $\omega$. The classical Hamiltonian for this oscillator is given by

$$H(x,p) = \frac{p^2}{2\mu} + \frac{\mu \omega^2}{2} x^2$$

(1)

The potential energy for this system is shown below.

As indicated this figure, the turning points of the potential energy get farther apart as the potential energy increases. The distance, $a$, between the turning points can be found from solving

$$V = \frac{\mu \omega^2}{2} \left( \frac{a}{2} \right)^2$$

(2)

The distance between the turning points can then be expressed in terms of the numerical value of the potential $V$ as

$$a = \left( \frac{8V}{\mu \omega^2} \right)^{1/2}$$

(3)

The virial theorem for the harmonic oscillator can then be used to express the distance between the turning points in terms of the total energy, $E$, of the oscillator. The virial theorem for the harmonic oscillator gives $V = E/2$, which when substituted into eq 3 yields

$$a = \left( \frac{4E}{\mu \omega^2} \right)^{1/2}$$

(4)

Now we make the statement (not entirely correct, as will be discussed shortly) that the amplitude of the particle must vanish at the turning points of the potential energy. Applying these zero-boundary conditions for the wave function beyond the classically allowed region is not only justified but is, in fact, the most reasonable assumption at this point in an undergraduate quantum mechanics course. Students are told early in the quantum mechanics course that the probability of locating a particle in a particular region of space is proportional to the square of the wave function in this region. The student then, has no recourse (other than solving the Schrödinger equation) but to assume that the particle cannot be in a classically forbidden region, that is, a region where it has an imaginary momentum. This condition yields the following equation relating the distance between the turning points and the wavelength of the particle:
Substituted into eq 4 to give the following relation between the wavelength and the total oscillator energy $E$:

$$\lambda = \left(\frac{16E}{\hbar^2 \mu \omega^2}\right)^{1/2}$$  \hspace{1cm} (6)

It is worth noting parenthetically that the idea of an energy-dependent de Broglie wavelength in a nonconstant potential is not so farfetched. In fact, the idea of a generalized de Broglie wavelength, $\lambda(x) = \mu(x)/\hbar$ is a fundamental idea behind the extremely useful semiclassical WKB approximation in quantum mechanics (6). Here $\mu(x) = 2m[E - V(x)]^{1/2}$ and is the coordinate-dependent momentum, where $E$ is the total energy of the system and $V(x)$ is (in general) the nonconstant potential energy of the system. Students do not have to be told about such generalized de Broglie wavelengths, but their existence should make the instructor feel a little more secure about this portion of the heuristic derivation.

The total energy of the oscillator can also be expressed in terms of the wavelength $\lambda$. To do this we again exploit the virial theorem for the harmonic oscillator, this time using the relation between the total energy, $E$, and the kinetic energy, $T$ ($T = E/2$). This yields the following relation between the momentum and the total energy:

$$E = \frac{p^2}{2\mu}$$  \hspace{1cm} (7)

If one substitutes the de Broglie relation between the momentum of a particle and its wavelength (i.e., $p = h/\lambda$) into eq 7, the following relation between the total energy and the wavelength results:

$$E = \frac{\hbar^2 \omega^2}{16}$$  \hspace{1cm} (9)

Substituting eq 6 for the wavelength $\lambda$ into eq 8 yields

$$E = \frac{\hbar^2 \omega^2}{16E}$$  \hspace{1cm} (10)

Multiplying both sides of eq 9 by the total energy, $E$, results in the following:

$$E^2 = \frac{\hbar^2 \omega^2}{16}$$  \hspace{1cm} (11)

Taking the square root of both sides of eq 10 yields the following result for the energy of the harmonic oscillator:

$$E = \frac{n \hbar \omega}{4}$$  \hspace{1cm} (12)

Comparing eqs 11 and 12 shows that the above derivation does not correctly predict either the zero-point energy or the spacings between adjacent energy levels.

Even though the above derivation does not give quantitative results for the energy levels of a harmonic oscillator, it does reproduce two of the most important qualitative characteristics of the harmonic oscillator energy levels: the vibrational frequency and the linear scaling of the energy levels with the quantum number. The major flaw in the derivation is that the true wave function for the harmonic oscillator does not vanish at the classical turning points on the potential energy surface. The above derivation makes the assumption that the harmonic oscillator wave functions do vanish at the classical turning points by forcing the wavelength of the particle to exactly fit between the classical turning points. This flaw in the derivation does in fact contain positive pedagogical value, since it can lead to a discussion of the importance of tunneling in quantum mechanics. In this case, the tunneling is the wave function penetrating into the classical forbidden regions beyond the classical turning points on the potential energy surface.

**Student Response**

Some discussion is now in order on the student response to the heuristic derivation for the energy levels of the harmonic oscillator and how it compared to the student response to the exact solution of the Schrödinger equation of the harmonic oscillator. Thus far I have taught quantum mechanics to undergraduates three times. The first year I solved the Schrödinger equation for the harmonic oscillator exactly, the second year (mainly owing to the poor results of the first year) I just wrote down the energy solutions of the Schrödinger equation and discussed them, and the third year around I used the heuristic derivation presented above.

Solving the Schrödinger equation for the harmonic oscillator exactly took approximately two 50-minute lecture periods. I found the experience less than satisfying and the students easily found stronger words than these to describe the experience. It is very difficult to keep the chemistry in the quantum mechanics course, and students found these two lectures mainly of a gratuitous mathematical nature and lacking in chemistry. Their performance on exam questions was also less than satisfying. Many students were unable to answer exam questions about the important behavior of the harmonic oscillator energies, such as how the spacing between adjacent levels behaves, how vibrational energy spacings depend on molecular reduced mass, and the zero-point energy of the harmonic oscillator. Further, many students were unable to qualitatively describe the wave functions of the harmonic oscillator on an exam. Interestingly, when asked to sketch the lowest harmonic oscillator energy level inside the harmonic oscillator potential energy function, many students show the wave function exactly vanishing at the classical turning points. My conclusion was that the pedagogical value...
of exactly solving the harmonic oscillator Schrödinger equation at the undergraduate level is very low. Students tune out the lectures and when the most important aspects of the derivation finally arrive, such as the harmonic oscillator energy level structure, they are no longer paying attention and thus do not take home even the most basic knowledge of the harmonic oscillator energies and wave functions.

The second year I presented the quantum harmonic oscillator to undergraduates by writing down the energy levels and stating that they arise from the solution of the harmonic oscillator Schrödinger equation (the typical physical chemistry textbook approach). This approach was superior to the exact solution of the harmonic oscillator Schrödinger equation in nearly all ways. Because most of the lecture time was focused on the behavior of the harmonic oscillator energy levels, the students gained a better understanding of how the harmonic oscillator energy levels behave with respect to vibrational frequency, quantum number, and molecular reduced mass, and this increased understanding was reflected in performance on exams. There were two major disadvantages of simply writing down the energy levels for the harmonic oscillator with no explanation. First, some students were not able to sketch wave functions for the harmonic oscillator or for other symmetric bound potentials correctly; they depicted the wave functions as vanishing at the classical turning points. Second, the better students become frustrated when too many results are presented without explanation in quantum chemistry. Typically the only set of energy levels that are derived are the particle-in-a-box energy levels. The harmonic oscillator, rigid rotor, and atomic energy levels are written down with no detailed physical explanation and the better students begin to feel frustrated that so many important results must be taken on faith.

Recently I used the heuristic derivation described above to present the harmonic oscillator energy levels in the undergraduate lecture. I found that this approach to teaching the energy levels of the harmonic oscillator was superior to the two other approaches described. First, the students were able to follow the entire derivation, which lasted approximately 15 minutes. The lecture was given by asking the students to answer questions as the derivation proceeded. When asked what should happen to the wave function at the classical turning points in the harmonic oscillator potential, the students understandably responded that the wave function should vanish. This was not surprising, because I have found that most students mistakenly think this is the case from their experience with the particle-in-a-box problem. Finding the distance between the turning points is just an algebraic exercise, as is the rest of the derivation, and the students were able to answer questions as the derivation progressed. The students performed well on exam questions dealing with the harmonic oscillator. They were able to answer questions based on the energy-level structure of the harmonic oscillator as well as questions dealing with the topology of the harmonic oscillator wave functions. Most importantly, they were able to correctly sketch wave functions for the harmonic oscillator that tunneled past the classical turning points. They seemed to remember that the reason for the incorrect result of the heuristic derivation can be traced to the incorrect assumption that the harmonic oscillator wave function must exactly vanish exactly at the classical turning points, and that the correct harmonic oscillator wave functions must tunnel into the classically forbidden region. Further, students seemed to be more satisfied that the energy levels for the harmonic oscillator were written down with some explanation about their origin. I am also finding that the better students are less frustrated now when the rigid rotor energy levels are presented without derivation, since these were the first set of energy levels that were presented without derivation.

Conclusion

I have presented a heuristic derivation for the energy levels of a linear harmonic oscillator that involves only algebra. It offers the instructor a way to rationalize the energy-level spectrum of a harmonic oscillator without having to solve the complicated differential equation prescribed by the Schrödinger equation for the harmonic oscillator. It treats the harmonic oscillator as a quasiparticle in a box, yielding qualitative results (the correct scaling of the energy with quantum number and vibrational frequency) but not the exact result. The derivation does not yield quantitatively correct results because it relies on the incorrect assumption that the harmonic oscillator wave functions must vanish at the classical turning points. This deficiency in the derivation actually had positive pedagogical results, because students seem to remember that this flaw led to quantitatively incorrect results and that the harmonic oscillator wave function actually tunnels past the classical turning points.

Literature Cited