The Quantum Harmonic Oscillator

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The Importance of the Harmonic Oscillator

The quantum harmonic oscillator holds a unique importance in quantum mechanics, as it is both one of the few problems that can really be solved in closed form, and is a very generally useful solution, both in approximations and in exact solutions of various problems.

The harmonic oscillator is characterized by the Hamiltonian:

$$\hat{H} = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2$$

This Hamiltonian appears in various applications, and in fact the approximation of the harmonic oscillator is valid near the minimum of any potential function. Expanded around a minimum point x*, any potential can then be Taylor expanded as:

$$V(x) = V_0 + (x - x^*) \frac{\partial V}{\partial x}\Big|_{x = x^*} + \frac{1}{2}(x - x^*)^2 \frac{\partial^2 V}{\partial x^2}\Big|_{x = x^*} + \cdots$$

In this case, V_0 is an arbitrary constant that can be taken to zero, and the second term is zero since the derivative is zero at critical points. If we assume that the variation around the critical point is small, then the higher order terms may be neglected, and we may readjust the variables to place the critical point at 0 and approximate it as a parabola.

The harmonic oscillator also gives the exact solution for a particle in a uniform magnetic field of a given vector potential, as that vector potential merely takes the form of a two-dimensional harmonic oscillator.

Finally, it serves as an excellent pedagogical tool. It introduces people to the methods of analytically solving the differential equations frequently encountered in quantum mechanics, and also provides a good introduction to the use of raising and lowering operators, and using the abstract vectors that are frequently used in quantum mechanics to solve problems by knowing the action of operators upon state vectors, rather than using integration to evaluate expectation values.

The Classical Oscillator: A Review

The classical harmonic oscillator is most frequently introduced as a mass on an undamped spring. The Hamiltonian for such a system is:

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2$$

and from the canonical relations we find that:

$$\frac{\partial H}{\partial p} = \dot{x} = \frac{p}{m} \qquad -\frac{\partial H}{\partial x} = \dot{p} = -kx$$

Solving this set of differential equations then gives the solution:

$$x(t) = x_0 \cos\left(\sqrt{\frac{k}{m}}\, t + \phi\right)$$

It is this solution that we should approximately get in the high energy limit solution to the quantum harmonic oscillator, and this will be our test that we have found the solution to the problem.

The Quantum Harmonic Oscillator: Analytical Solution

With the quantum harmonic oscillator we are presented with the problem of finding the eigenfunctions of the given Hamiltonian, which, in the position representation, is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

The Schrodinger equation then reads:

$$\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \psi = -i\hbar\frac{\partial \psi}{\partial t}$$

This is a second order, nonhomogeneous differential equation, for which we may apply separation of variables to turn it into the standard time independent Schrodinger equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi$$

Our first instinct in solving this problem should be to use a power series solution, as we know that the wave functions must be well behaved enough to be expressed as a power series, and the problem itself demands the use of it. First, we get the problem in unitless dimensions, doing so by making the following substitutions and dividing through by constants:

$$\epsilon = \frac{E}{\hbar\omega} \quad y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x$$

Making these substitutions, we then get a unitless differential equation:

$$\psi'' + (2\epsilon - y^2)\psi = 0$$

To find the solution to this differential equation, we first analyze its asymptotics, that is, the extreme positions of the differential equation. In this case, we look at small energy, when the y^2 term dominates. In this form, the differential equation is approximately:

$$\psi'' = y^2\psi$$

which suggests that the wave function may be a Gaussian, or something of similar form. Thus, we guess that the wave function is of the form:

$$\psi(x) = u(y)\exp\left[-y^2/2\right]$$

Plugging this into the differential equation we get:

$$u''(y)\exp\left[-y^2/2\right] - 2u'(y)y\exp\left[-y^2/2\right] + (2\epsilon - 1)u(y)\exp\left[-y^2/2\right] = 0$$

We can get rid of the Gaussian terms, as they represent a general multiplying factor, thus:

$$u'' - 2yu' + (2\epsilon - 1)u = 0$$

If we assume that the equation for *u* is in the form of a power series, we make the substitution:

$$u(y) = \sum_{n=0}^{\infty} C_n y^n \;\Rightarrow\; \sum_{n=0}^{\infty} C_n\left[n(n-1)y^{n-2} - 2ny^n + (2\epsilon - 1)y^n\right] = 0$$

Analyzing the resulting series solution, we arrive at the recursion relation:

$$C_{n+2} = C_n\frac{(2n + 1 - 2\epsilon)}{(n+2)(n+1)}$$

In theory we've solved the problem, except for the normalization condition. In the limit of large *n*, we find that the ratio between the succeeding terms is *n*/2, which grows faster than the terms in the exponential. This series diverges faster than our Gaussian converges, and the only way for the series to converge, and thus for the wave function to have any physical meaning, is for the series to truncate. The best way to do this is to make the numerator zero, as any successive terms to that would be zero as well, and from this we get:

$$2\epsilon = 2n + 1 \Rightarrow \epsilon = n + \frac{1}{2} \Rightarrow E = \hbar\omega\left(n + \frac{1}{2}\right)$$

From the requirement that the power series converge, and therefore truncate, we find that the energy levels for the harmonic oscillator are quantized.

This power series solution is not complete, as the individual eigenstates of the Hamiltonian are not yet made orthogonal. When this is carried out, what results is a solution that involves the Hermite polynomials, and is of the form:

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] \exp\left(-\frac{m\omega}{2\hbar}x^2\right)}$$

The computation of expectation values with this involves knowledge of the Hermite polynomials, and involves integrals of Gaussians that become tedious and leave open the possibility for algebraic error. It also does not take much advantage of the tools of linear algebra that can be applied to quantum mechanics. An alternative method, developed by Paul A.M. Dirac, utilizes a different method, in which the Hamiltonian is "factored" into raising and lowering operators to acquire the different eigenstates of the Hamiltonian, and will be discussed now.

The Quantum Harmonic Oscillator: Energy Basis Method

The first thing to do is to generate a unitless form of the Hamiltonian, which we do by introducing a new operator:

$$H'\hbar\omega = H$$

This makes the new operator measure the energy states in terms of the characteristic energies, and removes several constants that would otherwise appear in the process of solving the problem, and such a substitution is made with a priori knowledge of the results that are to follow.

The substitution the makes the new Hamiltonian operator:

$$H' = \frac{P^2}{2m\hbar\omega} + \frac{1}{2}\frac{m\omega}{\hbar}X^2$$

We now introduce two new operators, what we will eventually recognize as the raising and lowering operators:

$$\boxed{\begin{aligned} a &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \\ a^\dagger &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \end{aligned}}$$

The new Hamiltonian operator we created can be expressed in terms of these operators as:

$$a^\dagger a = \frac{m\omega}{2\hbar}X^2 + \frac{1}{2m\omega\hbar}P^2 + \frac{i}{2\hbar}[X,\ P]$$

$$a^\dagger a = H' - \frac{1}{2} \Rightarrow H' = a^\dagger a + \frac{1}{2}$$

These operators then satisfy the commutation relations

$$[a, a^\dagger] = 1$$
$$[a, H'] = a$$
$$[a^\dagger, H'] = -a^\dagger$$

Such commutation relations we will find useful, and these relations indicate that these operators produce new eigenstates of the Hamiltonian:

$$H' a|n\rangle = (a H' - [a, H'])|n\rangle$$
$$H' a|n\rangle = (a H' - a)|n\rangle = (\epsilon_n - 1)a|n\rangle$$

The indication of this is that the operator a, which we will now refer to as the lowering operator, generates some new eigenstate for the Hamiltonian, which is one energy level below the previous, to within a normalization constant. A similar procedure can be done to show that $a^\dagger$ has a similar effect, only raising the eigenenergy of the state.

So here we have a mechanism for determining all future eigenstates of the Hamiltonian given only one of them. Theoretically we have the capacity to generate an infinite number of energy states just by

repeatedly applying these raising and lowering operators, but we require that the energies be positive just because of our choice of potential and the fact that the state vector must be zero below the minimum potential energy. Therefore, we conclude that for some eigenstate of the Hamiltonian:

$$a|0\rangle = 0$$

The next question to ask is what the minimum energy of this eigenstate is. We can do this simply by exploiting the linearity of the raising and lowering operators:

$$\boxed{\begin{aligned} a|0\rangle = 0 &\Rightarrow a^\dagger a|0\rangle = 0 \\ a^\dagger a = H' - \frac{1}{2} &\Rightarrow (H' - \frac{1}{2})|0\rangle = 0 \\ H'|0\rangle = \frac{1}{2}|0\rangle &\Rightarrow H|0\rangle = \frac{1}{2}\hbar\omega|0\rangle \end{aligned}}$$

The minimum energy of the harmonic oscillator is $1/2\hbar\omega$, which is exactly what we predicted using the power series method to solving the oscillator. Now we need to find the energy level of the n[th] eigenstate for the Hamiltonian. To do this, we use the fact that any eigenstate can be represented as the ground state acted upon n times by the raising operator. Doing so, we find that the energy difference between any two energy eigenstates is $\hbar\omega$ which then gives us that the energy levels are $E_n = (n+1/2)\hbar\omega$, which is exactly the result we gained using the power series method, but without the messy algebra.

Now all that is left for using the raising and lowering operators is to find the normalization constant sitting in front of the newly created eigenstates generated by the raising and lowering operators. First, we consider the equation

$$a|n\rangle = C_n|n-1\rangle$$

and its complex conjugate:

$$\langle n|a^\dagger = \langle n-1|C_n^*$$

We combine these two equations to get:

$$\langle n|a^\dagger a|n\rangle = \langle n-1|n-1\rangle C_n^* C_n$$

$$\langle n|H' - \frac{1}{2}|n\rangle = C_n^* C_n$$

$$\langle n|n|n\rangle = |C_n|^2$$

$$|C_n|^2 = n$$

$$C_n = n^{1/2} e^{i\phi}$$

where the φ in the above equation is an undetermined phase constant usually taken as zero by convention, as it is an unobservable rotation in the energy eigenspace. A similar procedure gives us that

$$a^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle$$

From all this we can then find that any eigenstate of our Hamiltonian can be expressed as:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

To recap what we have done so far, we can express everything about the energy of the eigenstates of the harmonic oscillator as follows:

$$\boxed{\begin{aligned} H|n\rangle &= (n+\frac{1}{2})\hbar\omega|n\rangle \\ a|n\rangle &= n^{1/2}|n-1\rangle \\ a^\dagger|n\rangle &= (n+1)^{1/2}|n+1\rangle \end{aligned}}$$

We then have a nice mechanism for computing the eigenstates of the Hamiltonian, but we can also express expectation values using the raising and lowering operators. By simply making the substitutions:

$$X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^{\dagger})$$
$$P = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^{\dagger}-a)$$

we can compute any arbitrary expectation values that depend upon these quantities, merely by knowing the effects of the raising and lowering operators upon the eigenstates of the Hamiltonian.

Remarks on the Oscillator

There are several items of note that should be verified by the reader. First of all, the ground state wave function of the harmonic oscillator represents the minimum uncertainty state, for which the Heisenberg uncertainty inequality for momentum and position

$$\Delta x \Delta p \geqslant \frac{\hbar}{2}$$

is minimized, that is, the above expression is a strict equality rather than an inequality. This can be easily confirmed using the raising and lowering operators to find that

$$\langle x \rangle = 0 \quad \langle p \rangle = 0$$
$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \quad \langle p^2 \rangle = \frac{m\omega\hbar}{2}$$

The harmonic oscillator also has its uses in a uniform magnetic field, in which the vector potential and revised Hamiltonian can be written:

$$\vec{A} = \frac{B_0}{2}(-y\,\hat{x} + x\,\hat{y})$$
$$\hat{H} = \frac{1}{2m}\left(\vec{p} - q\,\vec{A}\right)^2$$

When the new Hamiltonian is expanded, you get a two dimensional harmonic oscillator in the x-y coordinates and a free particle in the z coordinates.

Einstein utilized the 3N uncoupled harmonic oscillators to approximate the heat capacity of a crystal lattice, and approximation far more accurate than the classical one but corrected upon by Debye to deal with the fact that all the oscillators are actually coupled, and provides a good solution for low temperatures.

These last two examples can be worked out on your own without much difficulty; the magnetic field example can be done by simply plugging into the new Hamiltonian, whereas the heat capacity problem is an example that can be found in several textbooks.

The Three Dimensional Oscillator

For a three dimensional oscillator, the solutions are the same as three one-dimensional oscillators added together. Each raising and lowering operator has to be specified to coordinates, and the eigenstates are given by

$$\hat{H}\left|n_x n_y n_z\right\rangle = (n_x + n_y + n_z + 3/2)\hbar\omega\left|n_x n_y n_z\right\rangle$$

for an isotropic oscillator. This oscillator experiences various degeneracies on the level of the number of solutions to

$$n_x + n_y + n_z = k$$

which is given by the formula

$$D_k = \binom{k+3-1}{k}$$

Such degeneracies require a study in identical particles to resolve further.

Like the one-dimensional harmonic oscillator, we have raising and lowering operators, but these

operators act specifically on the different spatial coordinates, thus, we have the raising and lowering operators

$$a_x, a_x^\dagger, a_y, a_y^\dagger, a_z, a_z^\dagger$$

so that their individual actions on an eigenstate are given by

$$a_i \left| n_i\ n_j\ n_k \right\rangle = n_i^{1/2} \left| n_i - 1\ n_j\ n_k \right\rangle$$
$$a_i^\dagger \left| n_i\ n_j\ n_k \right\rangle = (n_i + 1)^{1/2} \left| n_i + 1\ n_j\ n_k \right\rangle$$
$$a_i^\dagger a_i \left| n_i\ n_j\ n_k \right\rangle = n_i \left| n_i\ n_j\ n_k \right\rangle$$

while the individual operators satisfy their own commutation relations for the same spatial coordinate, but commute with the operators of different coordinates:

$$[a_i, a_j^\dagger] = \delta_{i,j}$$

This three dimensional quantum oscillator was used by Albert Einstein in 1907 when he provided a very primitive and crude explaination of the heat capacity of crystalline solids from the viewpoint of each solid being held in place as a quantum harmonic oscillator. Although this description lacks the sophistication required to provide a legitimate theory explaining the phenomena (it neglects the fact that all the oscillators are coupled), it still provided a qualitative approach which Debye followed with greater success.

The Harmonic Oscillator Approximation for the Minima of Potentials

As mentioned, in the introduction, the quantum harmonic oscillator is useful as it provides an approximation of the minima of any potential well. To illustrate this, we will analyze the quantum states given by the Hamiltonian

$$\hat{H} = \frac{p^2}{2m} + V_0 \cosh x/a$$

Our first job is to find the critical point of the potential

$$\frac{\partial}{\partial x} V_0 \cosh x/a = \frac{V_0}{a} \sinh x/a = 0 \Rightarrow x = 0$$

Now we have to Taylor expand the potential function about zero, and use zero to find the approximate value for ω. The Taylor expansion is given by:

$$V_0 \cosh x/a = V_0 (1 + \sinh 0\, x + \frac{1}{2}\frac{1}{a^2} \cosh 0\, x^2 + O(x^3))$$

The first constant can be disregarded as a scaling factor that can be taken into account with the energy states, finding the total energy by adding back one V_0. Therefore we find that the Hamiltonian can be approximately expressed as:

$$\hat{H} \approx \frac{p^2}{2m} + \frac{1}{2}\left(\frac{V_0}{a^2}\right) x^2 + V_0$$

From this and keeping in mind that the scalar in front of the potential Taylor expansion gives:

$$E_n \approx \left(n + \frac{1}{2}\right) \hbar \sqrt{\frac{V_0}{m a^2}} + V_0$$

Keeping this in mind, we therefore see that we can use the harmonic oscillator to give a partial approximation to the first few energy states for more esoteric potentials for which we have no hope of finding a closed form solution for.