The Quantum Harmonic Oscillator

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1 Introduction

The harmonic oscillator is such an important, if not central, model in quantum mechanics to study because Max Planck showed at the turn of the twentieth century that light is composed of a "collection" of quantized harmonic oscillators, each with an energy value of some $n\hbar\omega$, where ω was the frequency of the light. The "collection" of these harmonic oscillators, from $n = 1$ to $n = \infty$, perfectly describes the blackbody emission spectrum that Planck was trying to explain. Further, Einstein used Planck's idea of a quantum of light, of energy $E = \hbar\omega$, to explain the odd results of the photoelectric effect in 1905, winning him the Nobel Prize in 1921.

Aside from the central importance in describing light, the quantum harmonic oscillator is a good toy model to introduce the beginning student to solving problems in quantum mechanics. There are two common methods for solving for the stationary states of the harmonic oscillator: the analytic method – the typical method of solving Schrödinger's equation with differential equation methods – and the operator method – a more clever method, discovered by Paul Dirac, using the Heisenberg picture of quantum mechanics. This note will focus on the operator method of Dirac. For a thorough presentation of the analytic method, see Griffiths' "An Introduction to Quantum Mechanics," for example.

Note that in order to understand the solution, you need at least a basic familiarity with quantum mechanics, most importantly the Heisenberg picture of quantum mechanics instead of the more common Schrödinger picture. The Heisenberg picture of quantum mechanics is almost completely analogous to classical Hamiltonian mechanics, and so isn't that hard to pick up. See Sakurai's "Modern Quantum Mechanics" for an excellent overview of the Heisenberg picture.

2 The Ladder Operators

We begin with the Hamiltonian for the harmonic oscillator:

$$H = \frac{1}{2m}(p^2 + m^2\omega^2 q^2) \tag{1}$$

where p is the momentum and q the position of a quantum particle, subject to the canonical condition:

$$[q, p] = i\hbar \tag{2}$$

and that satisfy the Heisenberg equations of motion[1]:

$$\begin{aligned} \dot{q} &= [q, H] = \frac{p}{m} \\ \dot{p} &= [p, H] = -m\omega^2 q \end{aligned} \tag{3}$$

[1] These are analogous to the classical Hamilton's equations.

We want to define a new operator, a, such that:

$$a = \frac{1}{\sqrt{2m\hbar\omega}}(p + im\omega q) \tag{4}$$

The first instinct is to want to call this a "ladder" operator, as is done in every textbook, and as is done in the title of this section, but as of right now we have absolutely no idea what the interpretation of this operator is, so we'll refrain from naming it for now. Note that the derivative of a is:

$$\begin{aligned}\dot{a} &= \frac{1}{\sqrt{2m\hbar\omega}}(\dot{p} + im\omega\dot{q}) \\ &= \frac{1}{\sqrt{2m\hbar\omega}}(-m\omega^2 q + i\omega p) \\ &= \frac{i\omega}{\sqrt{2m\hbar\omega}}(p + im\omega q)\end{aligned}$$

Or, that:

$$\dot{a} = i\omega a \tag{5}$$

As a side note, it wasn't mentioned explicitly in the beginning, but since we are working in the Heisenberg picture, the operators q and p are functions of time, and thus so is a (as was made obvious by the above differential equation). The time-evolution equation for a is simply the solution to the above equation, which is easy to find:

$$a(t) = a_0 e^{i\omega t} \tag{6}$$

What was the purpose of defining this operator a? Well, it turns out that we can re-write the Hamiltonian in terms of a and $a^\dagger$:

$$aa^\dagger = \frac{1}{2m\hbar\omega}(p + im\omega q)(p - im\omega q) = \frac{1}{2m\hbar\omega}(p^2 + m^2\omega^2 q^2 + i\omega(qp - pq))$$

Recalling the canonical condition $qp - pq = i\hbar$, if we multiply the above by $\hbar\omega$, we can split the result into the original Hamiltonian and a constant term:

$$\hbar\omega aa^\dagger = H - \frac{1}{2}\hbar\omega \tag{7}$$

Notice that if we had performed the multiplication $a^\dagger a$ instead, we would have $(p - im\omega q)(p + im\omega q)$, which would result in a term like $-i\omega(qp - pq)$, so everything would be the same except the constant factor added to the Hamiltonian would have the opposite sign:

$$\hbar\omega a^\dagger a = H + \frac{1}{2}\hbar\omega \tag{8}$$

Without realizing it, this is our first glance as to why a and $a^\dagger$ are known as ladder operators: the difference between $aa^\dagger$ and $a^\dagger a$ is a unit of energy $\hbar\omega$, which is exactly the amount of energy one quantum of light carries. It turns out that formulating the Hamiltonian for the Harmonic oscillator in this form will allow us to begin at a state with an energy of $\hbar\omega$ and form a "ladder of higher states," each of energies $2\hbar\omega$, $3\hbar\omega$, and so on. This is why the quantum harmonic oscillator is the perfect model to describe Planck's quantum view of light.

3 Operator Algebra

The next thing to discuss is the operator algebra: how to construct the eigenstates of the operators a and $a^\dagger$, and what their eigenvalues are. The first thing to notice is that eigenstates of a or $a^\dagger$ are *not* eigenstates of each other, nor are they eigenstates of the Hamiltonian. This is easily seen by looking at the commutators for these operators.

First, let's see how a and $a^\dagger$ commute (or, rather, don't commute). Using equations (7) and (8) from the previous section:

$$aa^\dagger - a^\dagger a = \frac{1}{\hbar\omega}\left(H - \frac{1}{2}\hbar\omega\right) - \frac{1}{\hbar\omega}\left(H + \frac{1}{2}\hbar\omega\right)$$

So:

$$[a, a^\dagger] = -1 \tag{9}$$

Since they don't commute, no state can be simultaneously an eigenstate of a and $a^\dagger$.

For the Hamiltonian and the a operator, notice that we can re-write the Hamiltonain in equation (7) as

$$H = \hbar\omega aa^\dagger + \frac{1}{2}\hbar\omega$$

Then, we can find the commutation relation by first looking at aH alone:

$$aH = \hbar\omega aaa^\dagger + \frac{1}{2}\hbar\omega a$$

Recalling the above commutation relation between a and $a^\dagger$, note that $aa^\dagger = a^\dagger a - 1$, and so the above equation becomes:

$$aH = \hbar\omega aa^\dagger a - \hbar\omega a + \frac{1}{2}\hbar\omega a = \left(\hbar\omega aa^\dagger + \frac{1}{2}\hbar\omega\right)a - \hbar\omega a = Ha - \hbar\omega a$$

So, the commutator between H and a is:

$$[a, H] = -\hbar\omega a \tag{10}$$

And, once again, since these operators don't commute, they cannot have simultaneous eigenstates. Similarly to the above relation, the commutator between H and $a^\dagger$ is easily found to be:

$$[a^\dagger, H] = \hbar\omega a^\dagger \tag{11}$$

So, let's say we have a state $|\psi_j\rangle$ which is an energy eigenstate such that:

$$H|\psi_j\rangle = E_j|\psi_j\rangle \tag{12}$$

We know now that $|\psi_j\rangle$ is *not* an eigenstate of a or $a^\dagger$. But instead of simply asking what the eigenstates of a or $a^\dagger$ would be, it turns out to be much more interesting to investigate $a|\psi_j\rangle$ or $a^\dagger|\psi_j\rangle$. Let me make this more specific: is $a|\psi_j\rangle$, or $a^\dagger|\psi_j\rangle$, an eigenstate of H as well, and if so, what's it's energy? This is obviously a leading question, since if you took a random operator O such that $[O, H] \neq 0$, there's no reason to suspect that $O|\psi_j\rangle$ would be an eigenstate of H, but it turns out to be true in this case.

We can see this by exploiting the commutation relation between H and a:

$$H(a|\psi_j\rangle) = (Ha)|\psi_j\rangle = (aH + \hbar\omega a)|\psi_j\rangle = a(H|\psi_j\rangle) + \hbar\omega a|\psi_j\rangle = aE_j|\psi_j\rangle + \hbar\omega a|\psi_j\rangle$$

That is, the state $a\left|\psi_j\right\rangle$ is, in fact, an energy eigenstate, with an energy one factor of $\hbar\omega$ greater than that of $\left|\psi_j\right\rangle$:

$$H(a\left|\psi_j\right\rangle) = (E_j + \hbar\omega)(a\left|\psi_j\right\rangle) \tag{13}$$

The same analysis can be done with $a^\dagger$, and we would find that the state $a^\dagger\left|\psi_j\right\rangle$ is an energy eigenstate with an energy a factor of $\hbar\omega$ *lower* than E_j:

$$H\left(a^\dagger\left|\psi_j\right\rangle\right) = (E_j - \hbar\omega)\left(a^\dagger\left|\psi_j\right\rangle\right) \tag{14}$$

This is the illustration of the ladder structure of the operator algebra: if you take any energy eigenstate and apply a to it, you create a state with an energy $\hbar\omega$ "higher up" on the ladder; if you take any energy eigenstate and apply $a^\dagger$ to it, you create a state with an energy $\hbar\omega$ "lower down" the ladder. In this respect, a is knowing as the raising operator and $a^\dagger$ as the lowering operator.

Now that we know what the algebra looks like, the last thing to do is to determine exactly what the energy spectrum of the harmonic oscillator is. As far as we've shown, the ladder can go indefinitely high and indefinitely low; it turns out, however, that this isn't quite correct.

4 Energy Spectrum of the Harmonic Oscillator

Let's consider a state $\left|\psi\right\rangle$ such that:

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle$$

Using equation (7), we can compute the expectation value of $aa^\dagger$ for this state:

$$\left\langle\psi\right| aa^\dagger \left|\psi\right\rangle = \frac{1}{\hbar\omega}\left\langle\psi\right|\left(H - \frac{1}{2}\hbar\omega\right)\left|\psi\right\rangle = \frac{1}{\hbar\omega}\left\langle\psi\right|\left(E - \frac{1}{2}\hbar\omega\right)\left|\psi\right\rangle = \frac{E}{\hbar\omega} - \frac{1}{2}$$

Notice something interesting about the above expectation value, though: $\left\langle\psi\right| a$ is actually the Hermitian conjugate of $a^\dagger\left|\psi\right\rangle$, i.e. that:

$$\left(a^\dagger\left|\psi\right\rangle\right)^\dagger = \left\langle\psi\right| a$$

This means that the expectation value calculated above is equal to:

$$\left\langle\psi\right| aa^\dagger \left|\psi\right\rangle = \left|a^\dagger\left|\psi\right\rangle\right|^2 = \frac{E}{\hbar\omega} - \frac{1}{2}$$

That is, the expectation value is just the "length" of the vector $a^\dagger\left|\psi\right\rangle$ in our Hilbert space. Since any Hilbert space is an inner product space, the length of all vectors must be a positive-definite quantity, meaning:

$$\frac{E}{\hbar\omega} - \frac{1}{2} \geq 0$$

or:

$$E \geq \frac{1}{2}\hbar\omega \tag{15}$$

This means that our ladder cannot extend "downward" indefinitely, going to progressively lower and lower energies with no lower bound; the energy of any state of the harmonic oscillator must be *at least* $\frac{1}{2}\hbar\omega$. Any higher-energy state can be formed by operating on the ground state with a, which will add successive units of $\hbar\omega$ as we "climb up the ladder."

For shorthand, it's easiest to denote the energy eigenstates of the harmonic oscillator as $|n\rangle$, such that:

$$H|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle \tag{16}$$

where, in this case, I've labeled the ground state as $|0\rangle$. Then, the operation of the raising operator will be:

$$a|n\rangle = c|n+1\rangle \tag{17}$$

where c_a is a normalization constant, irrelevant to this discussion (you can look it up in any textbook). Likewise, the operation of the lowering operator will be:

$$a^{\dagger}|n\rangle = c'|n-1\rangle \tag{18}$$

where c' is another normalization constant. It's quite clear from the above that if we raise and then lower a state, or vice-versa, we should end in the same state we began with. In this respect, note that:

$$aa^{\dagger}|n\rangle = c''|n\rangle \tag{19}$$

While I don't care about the normalization constants c or c', this last normalization constant c'' is actually important to know. Luckily, it's really easy to deduce what it is. Recalling equation (7), if we compare the above equation with equation (16), it's clear by inspection that:

$$c'' = n$$

Along these lines, we typically define the operator $\hbar\omega aa^{\dagger}$ as the number operator N, such that the Hamiltonian is:

$$H = \left(N + \frac{1}{2}\right)\hbar\omega \tag{20}$$

such that, when operated on $|n\rangle$, we return equation (16):

$$H|n\rangle = \left(N + \frac{1}{2}\right)\hbar\omega|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle$$