Physics 342 Lecture 16

Welcome back to week 6 (!) of quantum mechanics! Recall that a couple weeks ago we had derived (at least from the Dirac-Von Neumann axioms), the fundamental equation of quantum mechanics: the Schrödinger equation. For some wavefunction $|\psi\rangle$ on Hilbert space $\mathcal{H}$, the time dependence of that wavefunction is given by:

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle,$$ where $\hat{H}$ is the Hamiltonian,

the total energy operator of the Hilbert space. We've focused so far on states for which particles can live somewhere on a one-dimensional space, denoted by the coordinate x. In this case, the Hamiltonian $\hat{H}$ can be expressed as the sum of kinetic and potential energy operators:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x),$$ where $V(x)$ is the potential under which the particle is influenced. In this formulation, it is the potential $V(x)$ that then is responsible for completely determining properties of the state/Hilbert space and its time evolution. We considered the infinite-square well last week, for which:

$$V(x) = \begin{cases} \infty, & x<0,\ x>a \\ 0, & 0<x<a \end{cases}$$

This week we will study the ~~infinite square we~~ harmonic oscillator, which, just as in classical mechanics, will be our "canonical" quantum system, and one for which we can apply to a huge variety of systems.

The potential energy of a spring/simple harmonic oscillator is

$$U(x) = \frac{1}{2}kx^2, \qquad (*)$$

where k is the spring constant and x is the displacement from equilibrium. We can just directly "quantize" this to produce the corresponding quantum potential, but it will turn out convenient to re-write it slightly. Recall that the angular frequency ω of a spring is:

$$\omega = \sqrt{\frac{k}{m}}, \text{ or that}$$

$k = m\omega^2$. We can then express the potential energy as:

$$U(x) = \frac{1}{2}kx^2 = \frac{m}{2}\omega^2 x^2.$$

This form is more general than that of $(*)$, because it represents a harmonic oscillator of <u>any</u> kind, and not just a spring. So, it's this form that we will use in the Schrödinger equation.

Then, as an operator, the Hamiltonian of the harmonic oscillator is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2.$$

Of course, ve can replace $\hat{p}$ and $\hat{x}$ by their position-space representations, but that produces a differential equation that just isn't so fun to evaluate. Instead, we will stay in general operator land, only expressing a result in a particular basis or representation at the last possible moment.

With this strategy in mind, let's stare at this Hamiltonian and attempt to make sense of it. The first thing we note about this Hamiltonian is that it is the sum of squares. So, whenever we see such a thing, we might first want to factorize it into a product of two terms where each is linear in the two operators. If $\hat{p}$ and $\hat{x}$ were just simple numbers, this is of course easy:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2 = \left(\frac{-i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\,\hat{x}\right)\left(\frac{+i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\,\hat{x}\right)$$

However, $\hat{x}$ and $\hat{p}$ do not commute as operators, so we have to be careful. Nevertheless, let's just take this product of the complex linear combination of $\hat{x}$ and $\hat{p}$ and see what we find:

$$\left(\frac{-i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\,\hat{x}\right)\left(\frac{+i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\,\hat{x}\right)$$

$$= \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 - \frac{i\omega}{2}\hat{p}\hat{x} + \frac{i\omega}{2}\hat{x}\hat{p}$$

$$= \hat{H} + \frac{i\omega}{2}[\hat{x},\hat{p}] = \hat{H} + \frac{i\omega}{2}(i\hbar) = \hat{H} - \frac{\hbar\omega}{2}.$$

Note the appearance of the commutator! If $\hat{x}$ and $\hat{p}$ were just numbers, this of course vanishes. So, we can <u>factorize</u> the Hamiltonian at the expense of adding one remainder term:

$$\hat{H} = \left(\frac{-i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\hat{x}\right)\left(\frac{i\hat{p}}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\hat{x}\right) + \frac{\hbar\omega}{2}$$

$$= \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2.$$

It will be convenient to pull out the overall energy unit $\hbar\omega$, so that

$$\hat{H} = \hbar\omega\left[\left(-i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right)\left(i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right) + \frac{1}{2}\right]$$

Now, everything in the square brackets is <u>dimensionless</u>, as all units are covered by $\hbar\omega$. Additionally, note that this indeed has units of energy because $\hbar$ has units of energy times time, and ω has units of (radians) per time.

In doing this factorization, we have isolated the operators a and a^+ that are the linear combinations of the momentum and position operators. We call

$$a^+ \equiv -i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}, \quad a \equiv i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}$$

and so the harmonic oscillator Hamiltonian is extremely compactly written as:

$$\hat{H} = \left(a^+a + \frac{1}{2}\right)\hbar\omega.$$

Note that a and a^+ are not Hermitian; indeed

$(a)^+ = a^+$ (and vice-versa), but their product is Hermitian: $(a^\dagger a)^\dagger = (a)^\dagger (a^\dagger)^\dagger = a^\dagger a$. Of course, this final property is required as the Hamiltonian is Hermitian.

We can almost forget about the particular representation of a and $a^\dagger$ in terms of $\hat{x}$ and $\hat{p}$ with one caveat: we need to know the commutation relation of a and $a^\dagger$. Well, we can just evaluate it explicitly:

$$a^\dagger a = \left(-i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right)\left(i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right)$$

$$= \frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}\hat{x}^2 - i\frac{\hat{p}\hat{x}}{2\hbar} + i\frac{\hat{x}\hat{p}}{2\hbar}$$

Also,

$$a a^\dagger = \left(i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right)\left(-i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}\right)$$

$$= \frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}\hat{x}^2 + i\frac{\hat{p}\hat{x}}{2\hbar} - i\frac{\hat{x}\hat{p}}{2\hbar}$$

Then, we find its commutator to be:

$$[a^\dagger, a] = a^\dagger a - a a^\dagger = \frac{i}{\hbar}[\hat{x},\hat{p}] = \frac{i}{\hbar}(i\hbar) = -1$$

or that $\boxed{[a, a^\dagger] = 1}$

In going forward, to find the eigenenergies of the harmonic oscillator Hamiltonian, we will just use

$\hat{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$, with $(a)^\dagger = a^\dagger$ and $[a, a^\dagger] = 1$.

This will demonstrate the power of the operator formalism of quantum mechanics.

The first thing we note is that eigenstates of the Hamiltonian are eigenstates of just $a^{\dagger}a$ individually. So let's see if we can understand this reduced operator's properties; i.e., its eigenvalues. As a Hermitian operator, the eigenvalues of $a^{\dagger}a$ are necessarily real. Can we learn anything about their sign? Well, let's assume that $|\psi\rangle$ is an eigenstate of $a^{\dagger}a$ with eigenvalue λ. Further, let's assume that $\lambda < 0$. What are its consequences?

As an eigenstate $|\psi\rangle$ satisfies:

$$a^{\dagger}a|\psi\rangle = \lambda|\psi\rangle.$$

Let's now act with a on both sides of this equation. Then,

$$a a^{\dagger}a|\psi\rangle = \lambda a|\psi\rangle = \left(a a^{\dagger} - a^{\dagger}a + a^{\dagger}a\right)a|\psi\rangle$$

$$= \left(a^{\dagger}a + [a,a^{\dagger}]\right)a|\psi\rangle$$

All I've done is add and subtract $a^{\dagger}a$ to the left side. Now, recall the commutator is:

$[a,a^{\dagger}] = 1$, so we have

$(a^{\dagger}a + 1)\,a|\psi\rangle = \lambda\, a|\psi\rangle$, or, in a more suggestive way,

$$a^{\dagger}a\left(a|\psi\rangle\right) = (\lambda - 1)\,a|\psi\rangle.$$

That is, if $|\psi\rangle$ is an eigenstate with eigenvalue $\lambda<0$, then, necessarily $a^\dagger a$ has another eigenstate $a|\psi\rangle$ with eigenvalue $\lambda-1<\lambda<0$. Now, you might see the problem. By acting on $|\psi\rangle$ with a we can decrease its eigenvalue arbitrarily, unbounded negatively. In particular, consider the state

$$a^n|\psi\rangle = \underbrace{aa\cdots a}_{n}|\psi\rangle$$; what is its eigenvalue?

We act with $a^\dagger a$ on it:

$$a^\dagger a\, a^n|\psi\rangle = a^\dagger a^n a|\psi\rangle.$$

Now, let's commute $a^\dagger$ past a^n: To evaluate $[a^\dagger, a^n]$, we will use induction. Note that if $n=1$, we had

$[a^\dagger, a] = -1$. Now consider $n=2$:

$$[a^\dagger, a^2] = a^\dagger aa - aaa^\dagger = aa^\dagger a + [a^\dagger, a]a - aaa^\dagger$$

$$= aaa^\dagger + a[a^\dagger, a] + [a^\dagger, a]a - aaa^\dagger = -2a.$$

This suggests the general result:

$$[a^\dagger, a^n] = -na^{n-1}.$$

Let's prove it. Using induction, we note that it is true for $n=1$. Assuming it true for n, let's calculate $n+1$:

$$[a^\dagger, a^{n+1}] = a^\dagger a^{n+1} - a^{n+1}a^\dagger = a^\dagger a^n a - a^{n+1}a^\dagger$$
$$= a^n a^\dagger a + ([a^\dagger, a^n]a) - a^{n+1}a^\dagger$$

$$= a^n a^\dagger a - n a^n - a^{n+1} a^\dagger = \cancel{a^{n+1} a^\dagger} + a^n [a^\dagger, a] - n a^n - \cancel{a^{n+1} a^\dagger}$$

$$= -(n+1) a^n \text{, exactly as assumed.}$$

Thus, connecting back to the eigenstates of $a^\dagger a$, we find:

$$a^\dagger a\, a^n |\psi\rangle = \left(a^n a^\dagger a + [a^\dagger, a^n] a\right) |\psi\rangle$$

$$= \left(a^n \lambda - n a^{n-1} a\right) |\psi\rangle = (\lambda - n)\, a^n |\psi\rangle$$

Thus, we can decrease the eigenvalue as far as we want!

What is the problem with this? Well, the Hamiltonian encodes the energies of our system, and apparently if there is one eigenstate with negative energy, there are an infinite number of them! Further, these energies are unbounded from below; there is no smallest energy or no ground state. Thus, we must use some physics insight to proceed. A system with no minimum energy is very sick: it can lose an arbitrary amount of energy, and because it can and it is energetically favorable to do so, everything does. To forbid this pathology, we must therefore enforce that there are no negative eigenvalues of $\hat{H}$ or $a^\dagger a$. This is very sensible: recall that the Hamiltonian was the sum of squares of ~~Hermitian~~ Hermitian operators:

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$, which would naturally seem to be exclusively non-negative, in a basis-independent sense.

So, with that constraint, we will look for eigenstates $|\psi\rangle$ with eigenvalue λ such that $\lambda \geq 0$ and

$$\hat{H}|\psi\rangle = \lambda|\psi\rangle = \hbar\omega\left(a^{+}a + \tfrac{1}{2}\right)|\psi\rangle.$$

What are these states and eigenvalues? More next time...