

Second Year Quantum Mechanics - Lecture 19

Representations and ladder operators

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1 Representations

What we have done in the previous two lectures make x and p look more and more symmetric in how they are handled. The expansion of a wavefunction in terms of momentum eigenstates is

$$\psi(x) = \int a(p) \phi(p, x) dp = \frac{1}{\sqrt{2\pi\hbar}} \int a(p) e^{ipx/\hbar} dp$$

and the overlap integral gives the inverse

$$a(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) e^{-ipx/\hbar} dx$$

These are just Fourier transforms of each other. As always, the probability density for an x measurement is $|\psi(x)|^2$ and for a p measurement is $|a(p)|^2$. Hence, there seems to be a complete symmetry between x and p with regard to how they are handled.

It turns out we could do the whole of quantum mechanics using p as the variable we are working with, rather than x , and hence would express all our operators in terms of p and d/dp . The function $a(p)$ can be thought of as the wavefunction of the state, but in momentum, rather than position, space; specifically, we could write $a(p) = \Psi(p)$. We could then calculate an expansion of $\Psi(p)$ in position eigenstates and the overlap integral would give us $\psi(x)$. Again squaring $\Psi(p)$ gives the momentum probability density while squaring $\psi(x)$ gives the position probability density. Working with a wavefunction which is a function of p rather than x is called working in the “momentum representation”, rather than the “position representation” (sometimes called the “Schrödinger representation”) which we have used in the rest of the course. Changing between representations is analogous to changing between sets of coordinate axes for normal vectors; this can make a calculation more convenient but the results you get should be independent of which set you use.

In the momentum representation, then we take $\hat{p} = p$, the variable, but what do we take for $\hat{x}$? It turns out that commutators are the same in any representation. In particular, the expression

$$[\hat{x}, \hat{p}] = i\hbar$$

is always true. This allows us to find $\hat{x}$ easily; it must be

$$\hat{x} = i\hbar \frac{d}{dp}$$

Note the positive sign here, as the commutator depends on order. To check the form of $\hat{x}$, then

$$[\hat{x}, \hat{p}]\Psi(p) = i\hbar \frac{d}{dp}(p\Psi) - pi\hbar \frac{d}{dp}(\Psi) = i\hbar a + i\hbar \frac{d}{dp}(\Psi) - pi\hbar \frac{d}{dp}(\Psi) = i\hbar \Psi$$

so that

$$[\hat{x}, \hat{p}] = i\hbar$$

as required. Hence, in the momentum representation, then the momentum eigenstates are

$$\delta(p_m - p)$$

and the position eigenstates are

$$\frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

This is why we have been writing $\hat{x}$ rather than just x in the rest of the course; while they are the same in the position representation, this is not true in other representations so we do sometimes need to specify that we mean the operator.

To check this is all consistent, then we can calculate the position probability density from the overlap of these position eigenstates with the wavefunction $\Psi(p)$, which gives

$$a(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \Psi(p) e^{ipx/\hbar} dp = \psi(x)$$

i.e. the same expression as we started with.

Dirac notation is actually more than just a shorthand; the kets stand for the states themselves, meaning they are independent of any particular representation. A physical state is clearly the same no matter how we choose to write it mathematically. E.g. if the ground state is $u_0(x)$ then this can be written as $|u_0\rangle$ or even $|0\rangle$, which does not specify whether it is a function of x or p or any other variable. To get the position amplitudes, we need to do the overlap integral, which in Dirac notation is

$$\psi(x) = \langle x|0\rangle$$

where $|x\rangle$ are the x eigenstates. Similarly

$$\Psi(p) = \langle p|0\rangle$$

These give the right expressions irrespective of whether the actual calculation is done in the position or the momentum representation so they are also representation independent.

Finally, we would need other operators, such as the Hamiltonian, if we want to work in the momentum representation. This would formally be

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x}) = \frac{p^2}{2m} + \hat{V}\left(i\hbar \frac{d}{dp}\right)$$

For example, the SHO potential would give

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 = \frac{p^2}{2m} - \frac{1}{2}m\hbar^2\omega_0^2\frac{d^2}{dp^2}$$

which is mathematically very similar to the position representation.

2 SHO ladder operators

Let's now look at the SHO again but in a way which is independent of the representation. It would seem that this would be not very useful as we cannot have specific forms for any operators. However, it turns out we can get a long way with these methods.

We saw the Hamiltonian for the harmonic oscillator was

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2\hat{x}^2}{2} = \frac{1}{2} \left(\frac{\hat{p}^2}{m} + m\omega_0^2\hat{x}^2 \right) = \hbar\omega_0 \left(\frac{1}{2m\hbar\omega_0}\hat{p}^2 + \frac{m\omega_0}{2\hbar}\hat{x}^2 \right)$$

and we found the energy eigenvalues were

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega_0$$

with the ground state being

$$u_0 \propto e^{-m\omega_0 x^2/2\hbar}$$

Consider the operators

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\hbar\omega_0}}\hat{p}, \quad \hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\hbar\omega_0}}\hat{p}$$

Note, these are not Hermitian and so do not correspond to observables; the particle has no “a-like” quantity which we can measure. It doesn’t mean they aren’t useful as mathematical tools though, as we shall see. Consider

$$\hat{a}\hat{a}^\dagger = \frac{m\omega_0}{2\hbar}\hat{x}^2 + \frac{1}{2m\hbar\omega_0}\hat{p}^2 - \frac{i}{2\hbar}\hat{x}\hat{p} + \frac{i}{2\hbar}\hat{p}\hat{x} = \frac{1}{\hbar\omega_0}\hat{H} - \frac{i}{2\hbar}[\hat{x}, \hat{p}] = \frac{\hat{H}}{\hbar\omega_0} + \frac{1}{2}$$

Similarly

$$\hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega_0} - \frac{1}{2}$$

Hence, subtracting and adding gives

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad \{\hat{a}, \hat{a}^\dagger\} = \frac{2\hat{H}}{\hbar\omega_0}$$

Note, we can write the Hamiltonian in one of three forms

$$\hat{H} = \hbar\omega_0 \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right) = \hbar\omega_0 \left(\hat{a}\hat{a}^\dagger - \frac{1}{2} \right) = \frac{\hbar\omega_0}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)$$

Now, consider the commutator of $\hat{a}$ with $\hat{H}$ where $\hat{H}$ is expressed using the first of the above three forms

$$[\hat{H}, \hat{a}] = \hbar\omega_0[\hat{a}^\dagger\hat{a}, \hat{a}] + \frac{1}{2}\hbar\omega_0[1, \hat{a}] = \hbar\omega_0(\hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a}) + 0 = \hbar\omega_0[\hat{a}^\dagger, \hat{a}]\hat{a} = -\hbar\omega_0\hat{a}$$

Similarly

$$[\hat{H}, \hat{a}^\dagger] = \hbar\omega_0\hat{a}^\dagger$$

This now allows us to get from one eigenstate to the next. Let’s say we have some eigenstate u_n

$$\hat{H}u_n = E_n u_n$$

Consider

$$-\hbar\omega_0(\hat{a}u_n) = [\hat{H}, \hat{a}]u_n = \hat{H}\hat{a}u_n - \hat{a}\hat{H}u_n = \hat{H}(\hat{a}u_n) - E_n(\hat{a}u_n)$$

so

$$\hat{H}(\hat{a}u_n) = (E_n - \hbar\omega_0)(\hat{a}u_n)$$

Hence, we have shown that $\hat{a}u_n$ is an eigenstate of $\hat{H}$ with an energy eigenvalue $E_n - \hbar\omega_0$. Hence, applying the $\hat{a}$ operator has converted u_n to u_{n-1} . The operator $\hat{a}$ is called a *lowering operator*. A similar calculation shows

$$\hat{H}(\hat{a}^\dagger u_n) = (E_n + \hbar\omega_0)(\hat{a}^\dagger u_n)$$

so $\hat{a}^\dagger$ converts u_n to u_{n+1} and is called a *raising operator*. The two operators are generically referred to as *ladder operators*, as they step up or down the “ladder” of energy eigenvalues.

We know the states cannot continue downwards for ever as there is a lowest energy state. This means for the lowest state that applying the lowering operator must fail; specifically, it must give zero

$$\hat{a}u_0 = 0$$

However, we can apply $\hat{a}^\dagger$ to this equation to give

$$0 = \hat{a}^\dagger \hat{a} u_0 = \left(\frac{\hat{H}}{\hbar\omega_0} - \frac{1}{2} \right) u_0 = \left(\frac{E_0}{\hbar\omega_0} - \frac{1}{2} \right) u_0$$

For this to hold, then

$$\frac{E_0}{\hbar\omega_0} - \frac{1}{2} = 0$$

so

$$E_0 = \frac{\hbar\omega_0}{2}$$

which we indeed know is the ground state energy. Hence as each energy is increased using $\hat{a}^\dagger$ by $\hbar\omega_0$, we have shown the energy spectrum is

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega_0$$

Note that the whole of the derivation of the energy eigenvalues above only used the commutation properties and we did not have to use $\hat{p} = -i\hbar d/dx$ or write down a wavefunction explicitly at all. Since commutators are the same in any representation, this means the derivation above is representation independent. It is of course always better to prove things as generally as possible, and this is a specific example of doing this.

Because we can convert from one state to the next, this means that if we can solve for any one of the eigenstates, we can calculate all of the others by repeated application of $\hat{a}$ or $\hat{a}^\dagger$. To find explicit eigenstates, we have to work in a specific representation, of course, so in the usual coordinate representation, then consider the equation above

$$0 = \hat{a} u_0 = \left(\sqrt{\frac{m\omega_0}{2\hbar}} \hat{x} + i \sqrt{\frac{1}{2m\hbar\omega_0}} \hat{p} \right) u_0 = \sqrt{\frac{m\omega_0}{2\hbar}} x u_0 + \sqrt{\frac{\hbar}{2m\omega_0}} \frac{du_0}{dx}$$

This is easy to solve; rearranging gives

$$\frac{du_0}{dx} = -\frac{m\omega_0}{\hbar} x u_0$$

so

$$\frac{du_0}{u_0} = -\frac{m\omega_0}{\hbar} x dx$$

for which

$$\ln u_0 = -\frac{m\omega_0}{2\hbar} x^2 + C$$

and so

$$u_0 = e^C e^{-m\omega_0 x^2 / 2\hbar}$$

where the e^C becomes the normalisation factor. This is what we found previously. We can get higher states by applying $\hat{a}^\dagger$ multiple times to u_0 , e.g. $u_1 \propto \hat{a}^\dagger u_0$, but note the ladder operators do not give normalised eigenstates; they have to be normalised afterwards.