Lecture 5 (Sep. 20, 2017)

5.1 The Position Operator

In the last class, we talked about operators with a continuous spectrum. A prime example is the position operator. Let's first consider a particle in $d = 1$. We define x as the position operator, with corresponding eigenstates $|x'\rangle$ satisfying

$$x|x'\rangle = x'|x'\rangle\,. \tag{5.1}$$

Here, we are using the Sakurai notation, where operators are symbols with no hats or primes, and the eigenstates are named by their eigenvalues.

We postulate that the $|x'\rangle$ form a complete set of states for the Hilbert space. This means that we can expand any state $|\psi\rangle$ as

$$|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x'\ |x'\rangle\langle x'|\psi\rangle\,. \tag{5.2}$$

In particular, the identity can be resolved as

$$\mathbb{1} = \int_{-\infty}^{\infty} \mathrm{d}x'\ |x'\rangle\langle x'|\,. \tag{5.3}$$

5.1.1 Measurement of Position

Imagine an experiment in which we measure the position of a particle, which could come in the form of a detector that registers a click when a particle enters the detector. Any physical detector will have some finite resolution, below which we cannot resolve the precise location of the particle. Assume we have a detector that detects a particle when it is between $x' - \frac{\Delta}{2}$ and $x' + \frac{\Delta}{2}$.

We will now modify our "collapse" postulate from earlier in the course. After measurement, the state of the particle will be such that a second measurement of x will yield a value between $x' - \frac{\Delta}{2}$ and $x' + \frac{\Delta}{2}$. Mathematically, this means that an initial state

$$|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x'\ |x'\rangle\langle x'|\psi\rangle \tag{5.4}$$

is sent by the measurement to a state

$$|\psi\rangle \to |\psi'\rangle = \int_{x'-\frac{\Delta}{2}}^{x'+\frac{\Delta}{2}} \mathrm{d}x''\ |x''\rangle\langle x''|\psi\rangle\,. \tag{5.5}$$

We assume that the resolution Δ is small by comparison with the length scale of variation of $\langle x''|\psi\rangle$. Then, we can approximate this function to be constant over the range $\left[x' - \frac{\Delta}{2}, x' + \frac{\Delta}{2}\right]$, in which case we find

$$\text{Prob(detection)} = |\langle x'|\psi\rangle|^2\Delta\,. \tag{5.6}$$

Taking the resolution to be infinitesimal, $\Delta \to \mathrm{d}x'$, this statement becomes

$$\text{Prob(detection)} = |\langle x'|\psi\rangle|^2\,\mathrm{d}x'\,. \tag{5.7}$$

This is the expected statement: the probability density at a point is the squared modulus of the wavefunction at that point. The total probability that the particle exists is

$$\text{Prob(particle is somewhere)} = \int_{-\infty}^{\infty} \mathrm{d}x'\ |\langle x'|\psi\rangle|^2 = 1\,, \tag{5.8}$$

which is true if $\langle\psi|\psi\rangle = 1$. The *position-space wavefunction* is defined as

$$\langle x'|\psi\rangle := \psi(x')\,. \tag{5.9}$$

5.1.2 Hilbert Spaces

We now make a brief aside about the actual definition of a Hilbert space. We generalize our notion of a vector space to the infinite-dimensional case. Consider any sequence of states in the space that has the property that for any $\epsilon > 0$, if we look sufficiently far along in the sequence, any two states in the sequence after that point will be closer together than ϵ under the metric induced by the inner product. The additional property beyond those of a vector space that a Hilbert space has, called completeness, is that all such sequences must converge to another state in the space. In practice, this means that we can approximate any given state arbitrarily well by a series expansion. For more information on Hilbert spaces, see the handwritten notes or the notes from Recitation 1.

5.1.3 Generalizing to Particles in Dimension d

So far we have talked about particles moving in only one dimension. We want to generalize this to particles moving in d dimensions for arbitrary d. In this case, there are d position operators,

$$\vec{x} = (x_1, \ldots, x_d)\,. \tag{5.10}$$

We assert that the $\{x_i\}$ are a set of compatible observables, meaning that we can simultaneously measure each of them. This allows us to know the position of a particle along all axes at the same time. (It is interesting to consider what happens if we relax this assumption, for example, if we have a particle in two dimensions where the x and y operators do not commute. We will discuss such a system later in the course.)

We can then find a complete set of states that are simultaneous eigenstates of each of the position operators, which we label as

$$\vec{x}|\vec{x}'\rangle = \vec{x}'|\vec{x}'\rangle\,, \tag{5.11}$$

and then we proceed as in the $d = 1$ case.

5.2 The Momentum Operator

In the position basis, the momentum operator is given by the familiar expression

$$p_i = -i\hbar\frac{\partial}{\partial x_i}\,. \tag{5.12}$$

On the space of square-integrable functions $\psi(x)$, this operator acts as

$$p\psi(x) = -i\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}\,. \tag{5.13}$$

From this, we see that

$$[x,p]\psi = -i\hbar\left(x\frac{\mathrm{d}\psi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}(x\psi)\right) = i\hbar\psi(x)\,, \tag{5.14}$$

from which we conclude that

$$[x,p] = i\hbar\,. \tag{5.15}$$

Applying the generalized uncertainty principle,

$$\Delta A \Delta B \geq \frac{1}{2}|\langle[A,B]\rangle|\,, \tag{5.16}$$

we find the Heisenberg uncertainty principle,

$$\Delta x \Delta p \geq \frac{\hbar}{2}\,. \tag{5.17}$$

5.2.1 Momentum Basis

The momentum operator is Hermitian, and so we can find a complete set of eigenstates of the momentum operator. The momentum eigenstates $|p'\rangle$ satisfy

$$p\big|p'\big\rangle = p'\big|p'\big\rangle\,, \tag{5.18}$$

and they form an orthonormal basis with

$$\big\langle p''\big|p'\big\rangle = \delta\big(p''-p'\big)\,. \tag{5.19}$$

The identity can then be resolved as

$$\mathbb{1} = \int_{-\infty}^{\infty} \mathrm{d}p'\ \big|p'\big\rangle\big\langle p'\big|\,, \tag{5.20}$$

which allows us to decompose an arbitrary state $|\psi\rangle$ as

$$|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p'\ \big|p'\big\rangle\big\langle p'\big|\psi\big\rangle\,. \tag{5.21}$$

Analogously to the discussion of measurement of position, measurements of momentum will have

$$\mathrm{Prob}\big(\text{momentum is between } p' \text{ and } p'+\mathrm{d}p'\big) = \big|\big\langle p'\big|\psi\big\rangle\big|^2\,\mathrm{d}p'\,. \tag{5.22}$$

We similarly define the *momentum-space wavefunction* as

$$\big\langle p'\big|\psi\big\rangle := \psi\big(p'\big)\,. \tag{5.23}$$

Although we will rarely use this notation, it is worth noting that Sakurai denotes the momentum-space wavefunction as

$$\big\langle p'\big|\psi\big\rangle := \phi\big(p'\big)\,. \tag{5.24}$$

How are $|p'\rangle$ and $|x'\rangle$ related? We need to find $\langle x'|p'\rangle$. We can determine this by inserting a momentum operator:

$$-\,i\hbar\frac{\partial}{\partial x}\big\langle x'\big|p'\big\rangle = \big\langle x'\big|p\big|p'\big\rangle = p'\big\langle x'\big|p'\big\rangle\,. \tag{5.25}$$

The expression on the left-hand side is found by using the expression for the momentum operator in the position basis,since $\langle x'|p'\rangle$ is the position-space wavefunction for the state $|p'\rangle$, while the expression on the right-hand side is found by having the momentum operator act on the ket $|p'\rangle$. This solution to this differential equation is

$$\big\langle x'\big|p'\big\rangle = Ne^{ip'x'/\hbar} \tag{5.26}$$

for some normalization factor N.

To fix the normalization, we use

$$\big\langle x'\big|x''\big\rangle = \delta\big(x'-x''\big)\,, \tag{5.27}$$

which implies

$$\int_{-\infty}^{\infty} \mathrm{d}p'\ \big\langle x'\big|p'\big\rangle\big\langle p'\big|x''\big\rangle = \delta\big(x'-x''\big)\,. \tag{5.28}$$

The left-hand side of this equation is

$$\int_{-\infty}^{\infty} \mathrm{d}p' \, \langle x'|p'\rangle\langle p'|x''\rangle = |N|^2 \int_{-\infty}^{\infty} \mathrm{d}p' \, e^{ip'(x'-x'')/\hbar} = 2\pi\hbar |N|^2 \delta\big(x' - x''\big) \,, \tag{5.29}$$

which must equal the right-hand side,

$$2\pi\hbar |N|^2 \delta\big(x' - x''\big) = \delta\big(x' - x''\big) \,. \tag{5.30}$$

This only fixes the modulus of N, but by convention we choose N to be real and positive, so that we have

$$N = \frac{1}{\sqrt{2\pi\hbar}} \,. \tag{5.31}$$

This finally gives us

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x'/\hbar} \,. \tag{5.32}$$

This allows us to relate the wavefunctions $\langle x'|\psi\rangle$ and $\langle p'|\psi\rangle$ in the position and momentum bases. By inserting the identity, we can write

$$\langle x'|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p' \, \langle x'|p'\rangle\langle p'|\psi\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}p'}{\sqrt{2\pi\hbar}} \, e^{ip'x'/\hbar} \langle p'|\psi\rangle \,. \tag{5.33}$$

Thus, we see that the momentum-space wavefunction is related to the position space wavefunction by the Fourier transform. We similarly have

$$\langle p'|\psi\rangle = \int \frac{\mathrm{d}x'}{\sqrt{2\pi\hbar}} \, e^{-ip'x'/\hbar} \langle x'|\psi\rangle \,. \tag{5.34}$$

5.3 Normalization of Position and Momentum Eigenstates

What is the wavefunction corresponding to the position eigenstate $|x'\rangle$? We have

$$\langle x''|x'\rangle = \delta\big(x'' - x'\big) \,. \tag{5.35}$$

This is not a square-integrable function, and so it is not actually an element of the Hilbert space, but we can nonetheless build all square-integrable functions out of the position states. Similarly, the momentum eigenstates are not elements of the Hilbert space, but can be used to decompose any square-integrable function.

How can we make this mathematically precise? We do this by changing the problem, and stating that our actual problem of interest is well-approximated by the new problem. The states $|x'\rangle$ and $|p'\rangle$ are not normalizable, and so we will change the problem to introduce normalizable states. We do this by assuming that our particle is moving in some finite-size space, and then take the finite size to infinity at the end of the problem.

For example, we can define momentum states by putting our particle in a large box of size L with periodic boundary conditions,

$$e^{ip'(x'+L)/\hbar} = e^{ip'x'/\hbar} \,. \tag{5.36}$$

This implies that

$$p'L = 2\pi n \,, \quad n \in \mathbb{Z} \,. \tag{5.37}$$

We now have discrete momenta, and a countable basis of momentum eigenstates. For finite L, we require that

$$\int_0^L \mathrm{d}x' \, \left|\langle x'|p'\rangle\right|^2 = 1\,, \tag{5.38}$$

which normalizes the momentum eigenstates:

$$\langle x'|p'\rangle = \frac{1}{\sqrt{L}} e^{ip'x'/\hbar}\,. \tag{5.39}$$

5.4 The Uncertainty Principle

The uncertainty relation tells us that if the position-space wavefunction $\psi(x')$ has a shape with some width ℓ, then the momentum-space wavefunction $\phi(p')$ will have a shape with some width of order $\hbar/\ell$, as seen in Figure 1.

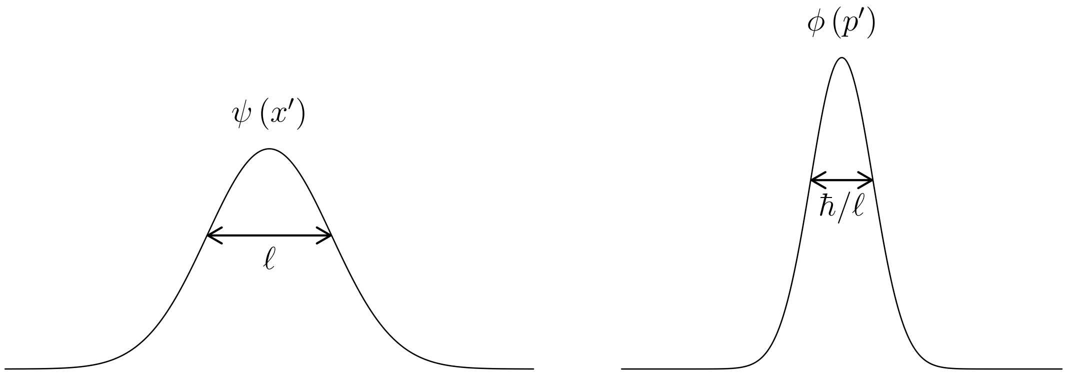

Figure 1: Example position-space and momentum-space wavefunctions that are related by the Fourier transform. The uncertainty relation tells us that their widths will be roughly reciprocal to one another.

5.4.1 Minimum Uncertainty States

For what wavefunction is the uncertainty relation $\Delta x \Delta p \geq \frac{\hbar}{2}$ saturated? The answer is a simple Gaussian,

$$\psi(x') = Ae^{-\frac{x'^2}{2w}}\,. \tag{5.40}$$

You will prove this in the homework.

5.5 Momentum and Translation

We will now use the momentum operator p to define a unitary operator

$$T(a) = e^{-iap/\hbar}\,, \quad a \in \mathbb{R}\,. \tag{5.41}$$

This operator is unitary because p is Hermitian:

$$(T(a))^\dagger = e^{iap/\hbar} = (T(a))^{-1}\,. \tag{5.42}$$

The operator exponential used here can be defined using the series expansion,

$$T(a) = e^{-iap/\hbar} = \sum_{n=0}^{\infty} \frac{(-ia/\hbar)^n p^n}{n!} \,. \tag{5.43}$$

Note that this definition can only make sense when acting on a Hilbert space.

We can see that this operator satisfies the following properties:

1. $T^{-1}(a) = T(-a)$
2. $T(a')T(a'') = T(a' + a'')$
3. $T(a)xT^{-1}(a) = x - a$

Let's prove the final property.

Proof. Define

$$F(a) = T(a)xT^{-1}(a) = e^{-ipa/\hbar} x e^{ipa/\hbar} \,. \tag{5.44}$$

The trick to the proof will be to compute the derivative of this quantity with respect to a:

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}a} &= \frac{i}{\hbar}\Big(e^{-ipa/\hbar}(-px)e^{ipa/\hbar} + e^{-ipa/\hbar} x p e^{ipa/\hbar}\Big) \\ &= \frac{i}{\hbar} e^{-ipa/\hbar} [x, p, e]^{ipa/\hbar} \\ &= \frac{i}{\hbar} e^{-ipa/\hbar} i\hbar e^{ipa/\hbar} \\ &= -1 \,. \end{aligned} \tag{5.45}$$

We can then integrate this equation to find

$$F(a) = F(0) - a \,. \tag{5.46}$$

Because $F(0) = x$, this completes the proof. □

For this reason, we will call $T(a)$ the *translation operator*. What happens to a state $|\psi\rangle$ under the action of this operator? We know that

$$T(a)xT^{-1}(a)\big|x'\big\rangle = (x - a)\big|x'\big\rangle = \big(x' - a\big)\big|x'\big\rangle \,. \tag{5.47}$$

By applying $T^{-1}(a)$ to each side of this equation, we find

$$xT^{-1}(a)|x'\rangle = \big(x' - a\big)T^{-1}(a)\big|x'\big\rangle \,, \tag{5.48}$$

from which we conclude that

$$T^{-1}(a)\big|x'\big\rangle \propto \big|x' - a\big\rangle \,. \tag{5.49}$$

This operator does not change the modulus of a state because it is unitary, so we actually have

$$T^{-1}(a)\big|x'\big\rangle = \big|x' - a\big\rangle \,. \tag{5.50}$$

The effect on the wavefunction is thus

$$\big\langle x'\big|T(a)\big|\psi\big\rangle = (T^{-1}(a)\big|x'\big\rangle, |\psi\rangle) = \big\langle x' - a\big|\psi\big\rangle = \psi\big(x' - a\big) \,. \tag{5.51}$$

We see that $T(a)|\psi\rangle$ has the shifted wavefunction $\psi(x'-a)$ if $|\psi\rangle$ has the wavefunction $\psi(x')$. This wavefunction is shifted to the right.

We have now seen that this unitary translation operator, which is a natural operator to define acting on the Hilbert space, is determined entirely be the Hermitian operator p. We could have turned this story around, by first defining the unitary translation operator and then using it to define a Hermitian operator p. In the classical limit, the operator p found in this way has the right properties to be called a momentum. Note that any unitary operator U can be written as e^{iA} for some Hermitian operator A. This is the approach we will take when we discuss angular momentum later in the course: it will be defined to be the operator that, when exponentiated, rotates the quantum mechanical system.

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