Lecture 4

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1 Quantum mechanics in infinite-dimensional Hilbert spaces

So far, we have restricted our attention to the quantum mechanics in finite-dimensional Hilbert spaces. We now consider the case of infinite-dimensional Hilbert spaces. On going from finite dimensional to (uncountably) infinite-dimensional spaces, we are immediately confronted by questions of continuity and convergence of integrals that we didn't have to deal with in the finite-dimensional case. These would require rigorous mathematical treatments that are beyond the scope of our course. Here, we will instead consider the case of infinite-dimensional Hilbert spaces as a special limit for the finite-dimensional case and we will point out the main subtleties involved in taking this limit.

1.1 Position and momentum eigenbasis

The infinite-dimensional Hilbert space is best illustrated by considering a particle in one spatial dimension. Classically, the position of the particle is specified by a real number. We now want to construct a quantum mechanical description of the position of a particle. Recall in our previous lectures, we replaced a classical observable, the magnetic moment, which was described by a classical vector of fixed length by a vector in a Hilbert space whose basis span all possible values of this observable. Such basis corresponds to the eigenbasis of this observable. The analogy for the position is to consider an operator, which we denote by $\hat{x}$, whose eigenvalues are all possible positions of the particle and whose eigenkets correspond to the particle being localized at any of these positions. This is written as

$$\hat{x}|x_0\rangle = x_0|x_0\rangle \tag{1}$$

To make this more concrete, we consider a course graining of the system where the position can only be determined up to an error Δx. In other words, we think of a measurement device that measures the position of a particle but that can only detect it within a region of width Δx. We denote the state where an electron is in the interval $(x - \Delta x/2, x + \Delta x/2)$ by $|x; \Delta x\rangle$. If we also take the system size to be finite L, then everything reduces to the case of finite dimensional Hilbert space we considered earlier [1]. For a general state $|\psi\rangle$, we can write the expansion in the position basis as

$$|\psi\rangle = \sum_x |x; \Delta x\rangle\langle x; \Delta x|u\rangle \tag{2}$$

where $|\langle x; \Delta x|\psi\rangle|^2$ gives the probability of finding the particle in the interval $(x - \Delta x/2, x + \Delta x/2)$ and they satisfy the relation $\sum_x |\langle x; \Delta x|u\rangle|^2 = 1$ necessary for the probabilistic interpretation. Now for a generic state where the particle is not infinitely localized, as we make Δx smaller and smaller, we expect

[1] As we will see later, this is not something we can generally do, but it will be useful for the current purpose. We can always think that our analysis is restricted to wavefunctions which vanish outside a finite region such that $\langle x; \Delta x|\psi\rangle = 0$ for $x < 0$ or $x > L$. This will only be problematic when we consider the translation operator.

that $|\langle x;\Delta x|\psi\rangle|^2$ would also become smaller and go as $\sim \Delta x$. Thus, we can write $|\langle x;\Delta x|\psi\rangle|^2 = p_\psi(x)\Delta x$ where $p_\psi(x)$ defines a continuous probability distribution satisfying

$$\sum_x \Delta x\, p_\psi(x) \overset{\Delta x\to 0}{=} \int dx\, p_\psi(x) = 1 \tag{3}$$

Now if $|\psi\rangle$ describes a particle infinitely localized at $x = x_0$, then we have $|\langle x;\Delta x|u\rangle|^2 = \delta_{x,x_0}$ which implies that $p_u(x) = \frac{\delta_{x,x_0}}{\Delta x} \to \delta(x-x_0)$ where $\delta(x)$ is the Dirac Delta function defined by the conditions

$$\delta(x) = 0 \quad \text{for} \quad x \neq 0, \qquad \int dx\delta(x) = 1 \tag{4}$$

Note that this equation implies that $\delta(x)$ has dimension of inverse length.

Let us now define the continuous position eigenbasis as

$$|x\rangle = \lim_{\Delta x\to 0} \frac{1}{\sqrt{\Delta x}}|x;\Delta x\rangle \tag{5}$$

We then can interpret $|\langle x|u\rangle|^2 = p_\psi(x)$ as a continuous probability distribution. Recall that in wave mechanics, the norm squred of the wavefunction $|\psi(x)|^2$ played the same role as $p_\psi(x)$. Thus, we can make the identification $\psi(x) = \langle x|\psi\rangle$. With this identification, we can use the same equations we used before for the finite-dimensional case provided that we replace every sum over a complete basis by an integral and every Kronecker delta function by a Dirac delta function. Thus, our recipe to move from the finite-dimensional case to the infinite dimensional one is

	Finite dimensional	Infinite dimensional
Orthonormality	$\langle\alpha|\alpha'\rangle = \delta_{\alpha,\alpha'}$	$\langle x|x'\rangle = \delta(x-x')$
Resolution of unity	$\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1}$	$\int dx|x\rangle\langle x| = \mathbb{1}$
Wavefunction normalization	$\sum_\alpha |\langle\psi|\alpha\rangle|^2 = 1$	$\int dx|\langle\psi|x\rangle|^2 = \int dx|\psi(x)|^2 = 1$

1.2 Translation operator and momentum

Given a position basis, one very important operator we can define in addition to the position operator is the translation operator. A translation operator T_a is defined as an operator which shifts a position eigenstate localized at $x = x_0$ to a position eigenstate localized at $x = x_0 + a$. This means that it satisfies

$$\hat{x}T_a - T_a\hat{x} = aT_a \tag{6}$$

To see this, we act on the position eigenstate $|x\rangle$

$$\hat{x}T_a|x\rangle = T_a\hat{x}|x\rangle + aT_a|x\rangle = (x+a)T_a|x\rangle \tag{7}$$

This means that $T_a|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalues $|x+a\rangle$ i.e. $T_a|x\rangle = |x+a\rangle$ up to a phase. We can take this phase to be zero by simply fixing some state $|0\rangle$ and defining $|x\rangle := T_x|0\rangle$ [2]. Thus, we can simply write

$$T_a|x\rangle = |x+a\rangle \tag{8}$$

We would now like to construct an explicit representation of the translation operator based on its properties. First, we see that T_a has to preserve the norm since $1 = \langle x+a|x+a\rangle = \langle x|T_a^\dagger T_a|x\rangle$ for every $|x\rangle$ and a which means that

$$T_a^\dagger T_a = \mathbb{1} \tag{9}$$

[2] Recall that multiplication by a phase yields a different ket that describes the same physical state. This means that we can choose the ket which makes the representation of certain operators as easy as possible. This is usually referred to as a gauge choice.

Second, translating by a then b is the same as translating by $a + b$:

$$T_a T_b = T_b T_a = T_{a+b} \tag{10}$$

Third, the translation by $a = 0$ is the identity $T_0 = \mathbb{1}$. This implies that we can reverse any translation $T_a T_{-a} = T_{a-a} = \mathbb{1}$ which implies

$$T_{-a} = T_a^{-1} = T_a^\dagger \tag{11}$$

These relations imply that translations form an Abelian group.

These properties have a particularly simple form for infinitesmal translations $a = dx$. Let us write the expansion

$$T_{dx} = \mathbb{1} - idx\,\hat{k} \tag{12}$$

where $\hat{k}$ is some operator which has dimension of inverse length whose properties we will derive below. This operator is called the infinitesmal generator of translation. To satisfy (11), we write

$$\mathbb{1} + idx\,\hat{k} = \mathbb{1} + idx\,\hat{k}^\dagger \tag{13}$$

which implies that $\hat{k}$ is hermitian. Using the commutation relation (6), we find

$$\hat{x}\hat{k} - \hat{k}\hat{x} = [\hat{x}, \hat{k}] = i \tag{14}$$

To interpret the operator $\hat{k}$, let us introduce wavevector eigenbasis $|k\rangle$ related to $|x\rangle$ via the Fourier transform

$$|x\rangle = \int \frac{dk}{\sqrt{2\pi}} e^{-ikx} |k\rangle \tag{15}$$

Acting with T_a, we get

$$T_a|x\rangle = \int \frac{dk}{\sqrt{2\pi}} e^{-ikx} T_a|k\rangle = |x + a\rangle = \int \frac{dk}{\sqrt{2\pi}} e^{-ikx} e^{-ika} |k\rangle \tag{16}$$

From which we deduce

$$T_a|k\rangle = e^{-ika}|k\rangle \tag{17}$$

Thus, $|k\rangle$ are eigenvectors of the translation operator. Taking the infinitesmal limit, $a = \Delta x$, we find

$$\hat{k}|k\rangle = k|k\rangle \tag{18}$$

Thus, the operator $\hat{k}$ which is the generator of translation is the wavevector operator. To make the connection with momentum, we have to invoke another relation which relates the momentum of a quantum particle to the wavelength of the associated wave. This is called the De-Broglie wavelength and is given by $\lambda = h/p$. Writing this as a wavenumber $k = 2\pi/\lambda$, we get the relation $p = \hbar k$. Thus, we can identify the quantum mechanical momentum operator by the generator of infinitesmal translation times $\hbar$. Substituting in (14), we get the famous Heisenberg commutation relations

$$[\hat{x}, \hat{p}] = i\hbar \tag{19}$$

Using the general uncertainty relation derived last lecture, we can derive the Heisenberg uncertainty relation

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle \geq \frac{\hbar^2}{4} \tag{20}$$

We note something very peculiar about the commutation relation (19). Unlike the commutation relation for spin components which had a non-trivial operator on the right-hand-side. Here, the right-hand-side is proportional to the identity. To see why this is strange, let us imagine, we can represent $\hat{x}$ and $\hat{p}$ with matrices in a course grained description and take the trace of both sides. The trace of a commutation always vanishes since $\mathrm{tr}AB = \mathrm{tr}BA$, thus the trace of the left-hand-side is zero. The trace of the right-hand-side on the other hand is equal to the dimension of the space. This tells us that the relation (19) can only be realized by operators on an infinite dimensional space. In particular, $\hat{x}$ and $\hat{p}$ both have an unbounded spectrum from above and below. This means that truncating the system will introduce large error.

From the previous discussion, we see that we can write the momentum operator as

$$\hat{p} = i\hbar \lim_{\Delta x \to 0} \frac{T_{\Delta x} - \mathbb{1}}{\Delta x} \tag{21}$$

To connect with the familiar expression from wave mechanics, note that

$$\begin{aligned} T_{\Delta x}|\psi\rangle &= T_{\Delta x} \int dx |x\rangle\langle x|\psi\rangle = \int dx |x + \Delta x\rangle \psi(x) = \int dx |x\rangle \psi(x - \Delta x) \\ &= \int dx |x\rangle \psi(x) - \Delta x \int dx |x\rangle \frac{d}{dx}\psi(x) \end{aligned} \tag{22}$$

This yields the expression

$$\hat{p}|\psi\rangle = \int dx |x\rangle \left(-i\hbar \frac{d}{dx}\right) \psi(x) \tag{23}$$

which is the expression we get in wave mechanics. Notice that this is a Hermitian operator since

$$\langle\phi|\hat{p}\psi\rangle = -i\hbar \int dx \phi^*(x) \frac{d}{dx}\psi(x) = i\hbar \int dx (\frac{d}{dx}\phi^*(x))\psi(x) = \int dx (-i\hbar \frac{d}{dx}\phi(x))^* \psi(x) = \langle\hat{p}\phi|\psi\rangle \tag{24}$$

Here, we have integrated by parts and assumed that the function $\phi(x)$ and $\psi(x)$ vanish at infinity (which is always the case for normalized wavefunctions).

The generalization for multi-spatial dimensions is straightforwards since, unlike the different components of spin, the operators associated with the different spatial components, x, y, and z, commute with each other [3]. Thus, we can choose simultaneous eigenbasis for $\hat{x}$, $\hat{y}$, and $\hat{z}$:

$$\hat{x}|x_0, y_0, z_0\rangle = x_0|x_0, y_0, z_0\rangle, \qquad \hat{y}|x_0, y_0, z_0\rangle = y_0|x_0, y_0, z_0\rangle, \qquad \hat{z}|x_0, y_0, z_0\rangle = z_0|x_0, y_0, z_0\rangle \tag{25}$$

Similarly, the generators for translations in the x, y, and z commute with each other. Also, the generators of translations along one direction, let's say x, commute with the position operator along a perpendicular direction, let's say y or z. This leads to the more general commutation relation

$$[x_i, x_j] = [p_i, p_j] = 0, \qquad [x_i, p_j] = i\hbar\delta_{i,j} \tag{26}$$

The action of the momentum operator on the wavefunction $\psi(\vec{x})$ becomes $-i\hbar\vec{\nabla}\psi(\vec{x})$.

[3] Ultimately, this is due to the fact the different translations and boosts (translations in momentum) commute with each other but different rotations do not