Dirac Notation

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Up until this point, we have (almost always!) discussed all of the states in quantum mechanics as functions of position – wavefunctions $\psi(x)$. Even when we are computing eigenvectors of other operators that *do not commute with position*, we express them as functions of position.

But we have also seen that we can describe the same objects as functions of other variables. For example, we have seen that a Fourier transform can take us from wavefunctions in position space to wavefunctions in momentum space. This transform also changes the action of operators – in position space we have $\hat{x} = x, \hat{p} = -i\hbar\frac{d}{dx}$, while in momentum space we have $\hat{p} = p, \hat{x} = i\hbar\frac{d}{dp}$.

And we have seen that writing states as functions of a continuous coordinate is not even always strictly necessary. For example, in studying the harmonic oscillator, we discuss a ground state ψ_0 that satisfies $a_-\psi_0 = 0$ and therefore also

$$\hbar\omega(a_+a_- + 1/2)\psi_0 = \frac{1}{2}\hbar\omega\psi_0$$

We learned this without *ever* writing ψ_0 as a function of x. Indeed, we could construct all the eigenvectors of $\hat{H}$ for the harmonic oscillator without *ever* talking about functions of x or of k or of anything else:

$$\psi_n = \frac{1}{\sqrt{n!}}a_+^n\psi_0$$

More generally, we can talk about eigenfunctions of an operator without ever writing them out as functions of x or k. Eigenfunctions of $\hat{H}$ are eigenfunctions of $\hat{H}$ whether we write them as a function of x or of k. Clearly, expressing states in terms of functions of x or k or anything else just amounts to a choice of some *representation* of the states, some way of writing them. We can change our choice of representations without changing the essential properties of the state.

The idea that there is some vector that we can choose to represent in different ways is familiar from finite-dimensional vector spaces. If we have a vector $\vec{a}$, we can choose to represent it in a specific basis:

$$\vec{a} = a_1\vec{e}_1 + a_2\vec{e}_2 + \dots a_n\vec{e}_n = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

But if we wanted to change basis, to say, some basis vectors $e_1', \dots e_n'$, we would have a different choice of representation for $\vec{a}$:

$$\vec{a} = a_1'\vec{e}_1{}' + a_2'\vec{e}_2{}' + \dots a_n'\vec{e}_n{}' = \begin{pmatrix} a_1' \\ a_2' \\ \vdots \\ a_n' \end{pmatrix}$$

Following in the footsteps of Dirac, we can do the same thing in our Hilbert space: label our states with an abstract label, and then compute them with respect to a specific variable if we want to. We call the abstract vector $|a\rangle$ a "ket" (which will make sense in a moment). In this notation, for example, the eigenvectors of $\hat{x}$ are denoted $|x\rangle$, such that

$$\hat{x}|x\rangle = x|x\rangle$$

where $|x\rangle$ is the eigenvector, $\hat{x}$ is the operator acting on it, and x is the eigenvalue.

Now we are accustomed to writing an inner product of two vectors $|a\rangle, |b\rangle$ as

$$\langle b|a\rangle$$

If we think of the ket $|a\rangle$ as a vector, we can think of $\langle b|$ as an object in its own right. We call it a "bra", since $\langle b|a\rangle \sim$ "bracket", so $\langle b| \sim$ "bra", $|a\rangle \sim$ "ket".

What is $\langle b|$? Properly speaking, it's not a vector. But we know what it does when it acts on a vector: $\langle b|a\rangle$ is a complex number. If $|a\rangle$ is a vector in a vector space V, we say that $\langle b|$ is an element of the *dual space* of *linear functionals* on V. Linear functionals F are just things that assign a scalar $F(\psi)$ to every vector ψ, such that $F(a\psi + b\phi) = aF(\psi) + bF(\phi)$ for scalars a, b and vectors ψ, ϕ. The set of linear functionals may itself be thought of as forming a vector space V' of its own if we define the sum of two linear functionals as $(F_1 + F_2)(\psi) = F_1(\psi) + F_2(\psi)$.

But that's exactly the property of the bras $\langle b|$: if I act on $|a\rangle$ with $\langle b|$, I can either think of this as meaning "take the inner product of two vectors $|a\rangle$ and $|b\rangle$", or I can think of it as meaning "$\langle b|$ is a linear functional that takes the vector $|a\rangle$ to the complex number $\langle b|a\rangle$."

You might worry that these things are inequivalent – maybe not every inner product of two vectors in a Hilbert space can be written as a linear functional acting on a vector. But there is a beautiful theorem, called *Riesz's Theorem*, which says there is a one-to-one correspondence between linear functionals F in V' and vectors f in V, such that all linear functionals have the form

$$F(\psi) = \langle f|\psi\rangle$$

where f is a fixed vector associated with F, and ψ is any old vector in V. For our purposes, the vector space V and the dual space V' are isomorphic.

If you are feeling lost, as always, it's a good idea to think about finite-dimensional examples. If we represent a vector as a column of numbers,

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

we know we can write the dot product of $|a\rangle$ with another vector $|b\rangle$ as multiplication of a row vector and a column vector,

$$\langle b|a\rangle = \begin{pmatrix} b_1^* & b_2^* & \dots & b_n^* \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

so we can identify the "bra" $\langle b|$ as

$$\langle b| = \begin{pmatrix} b_1^* & b_2^* & \dots & b_n^* \end{pmatrix} = (|b\rangle)^\dagger$$

i.e., the hermitian conjugate (complex conjugate & transpose) of the vector $|b\rangle$.

Formally speaking, in an infinite-dimensional vector space the hermitian conjugate is only well-defined on operators, but heuristically speaking you can still think of bras in the dual space as being related to kets in the vector space by hermitian conjugation. Clearly there is a bra for every ket, so we can think of the vector space and dual space as being isomorphic.

Now that we have given separate identities to bras and kets, we can also usefully construct another object called the *outer product*:

$$|a\rangle\langle b|$$

What is this? Well, it's an operator. That is to say, if we have some other vector $|c\rangle$, then we can compose the outer product with the vector to get

$$|a\rangle\langle b|c\rangle = \langle b|c\rangle|a\rangle$$

i.e., the outer product acting on a vector is another vector, which is what we call an operator.

Again, it helps to think of finite-dimensional cases. If we multiply N-component column vectors by N-component row vectors, we get $N \times N$ matrices:

$$|a\rangle\langle b| = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \begin{pmatrix} b_1^* & b_2^* & \dots & b_n^* \end{pmatrix} = \begin{pmatrix} a_1 b_1^* & a_1 b_2 * & \dots & a_1 b_n^* \\ a_2 b_1^* & \dots & \dots & a_2 b_n^* \\ \vdots & \ddots & \ddots & \vdots \\ a_n b_1^* & \dots & \dots & a_n b_n^* \end{pmatrix}$$

Now what does this buy us? Consider now a state $|\Psi\rangle$ in our Hilbert space. In general, we are interested in the properties of this state with respect to some operator $\hat{Q}$. In general we don't know what $\hat{Q}$ does to $|\Psi\rangle$, so to understand it better, we want to write it as a linear combination of eigenstates of $\hat{Q}$ – call them $|\psi_n\rangle$. We've done this all the time; in bra-ket notation, it's just

$$|\Psi\rangle = \sum_n c_n|\psi_n\rangle = \sum_n \langle\psi_n|\Psi\rangle|\psi_n\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\Psi\rangle$$

where in the middle step we use Fourier's trick, and in the last step I have just used the fact that $\langle\psi_n|\Psi\rangle$ is just a number. The fact that I can write any $|\Psi\rangle$ this way is a statement that the $|\psi_n\rangle$ are complete.

But now we see that we can think of $|\Psi\rangle$ as a vector and $|\psi_n\rangle\langle\psi_n|$ as operators. For this to hold, it must be the case that we can identify

$$\sum_n |\psi_n\rangle\langle\psi_n| = 1$$

This is an equivalent way (at the level of operators made out of bras and kets) of saying that the ψ_n form a complete basis; this is just a *completeness relation*. This was the form appropriate for a discrete set of eigenfunctions; if instead we want to use a continuous set of eigenfunctions, it's going to be

$$|\Psi\rangle = \int c(n)|\psi(n)\rangle\, dn = \int |\psi(n)\rangle\langle\psi(n)|\Psi\rangle\, dn$$

and completeness amounts to

$$\int |\psi(n)\rangle\langle\psi(n)|\, dn = 1$$

Now for the question you are undoubtedly asking yourself at this point: What is the relationship between the abstract state vector $|\Psi\rangle$ and the position-space wavefunction $\Psi(x)$? The answer: the position-space wavefunction is the inner product of $|\Psi\rangle$ with definite-position states $|x\rangle$:

$$\Psi(x) \equiv \langle x|\Psi\rangle$$

You can see that this is a sensible relationship by first inserting a complete set of position states,

$$|\Psi\rangle = \int_{-\infty}^{\infty} |x'\rangle\langle x'|\Psi\rangle dx'$$

Then if I dot in $\langle x|$ on both sides,

$$\langle x|\Psi\rangle = \int_{-\infty}^{\infty} \langle x|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} \delta(x-x')\langle x'|\Psi\rangle dx'$$

using Dirac orthogonality of the eigenfunctions of $\hat{x}$. But this is just the statement that

$$\Psi(x) = \int \delta(x-x')\Psi(x')dx'$$

That is what the position-space wavefunction is – the state $|\Psi\rangle$ in terms of the eigenfunctions of the $\hat{x}$ operator.

The following added by CC.
A slightly different way of seeing what is going on. Write

$$|\Psi\rangle = \int_{-\infty}^{\infty} c(x')|x'\rangle dx'$$

. Then $|c(x')|^2$ is the probability of finding the particle between x' and $x' + dx'$, i.e., $c(x')$ is what we called **the wavefunction**, $c(x') = \Psi(x')$. Now dot in $\langle x|$ on both sides:

$$\langle x|\Psi\rangle = \int_{-\infty}^{\infty} c(x')\langle x|x'\rangle dx' = \int_{-\infty}^{\infty} c(x')\delta(x - x')dx' = c(x) = \Psi(x)$$

. Also, the expectation value of x is:

$$\langle x\rangle = \langle\Psi|\hat{x}|\Psi\rangle$$

inserting a complete set of states "in the middle":

$$\langle x\rangle = \int_{-\infty}^{\infty} \langle\Psi|\hat{x}|x'\rangle\langle x'|\Psi\rangle dx'$$

since $\hat{x}|x'\rangle = x'|x'\rangle$:

$$\langle x\rangle = \int_{-\infty}^{\infty} x'\langle\Psi|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} x'\Psi^*(x')\Psi(x')dx' = \int_{-\infty}^{\infty} x'|\Psi(x')|^2 dx'$$

which is what we expected
End of addition by CC.

What about the momentum-space wavefunction? Your natural guess is the correct one: the momentum-space wavefunction is

$$\Phi(k) = \langle k|\Psi\rangle$$

Again, this makes sense if we use the completeness relation for eigenstates of $\hat{p}$:

$$|\Psi\rangle = \int_{-\infty}^{\infty} |k'\rangle\langle k'|\Psi\rangle dk'$$

and if I dot in $\langle k|$ on both sides,

$$\langle k|\Psi\rangle = \int_{-\infty}^{\infty} \delta(k - k')\langle k'|\Psi\rangle dk'$$

What about the inner product of two states? Consider the norm-squared of an abstract state $|\Psi\rangle$ and insert a complete set of position eigenvectors,

$$\langle\Psi|\Psi\rangle = \int \langle\Psi|x\rangle\langle x|\Psi\rangle dx = \int \Psi(x)^*\Psi(x)dx$$

The LHS is just the abstract inner product for two vectors, but the RHS we recognize as our usual L_2 norm on wavefunctions in position space. The same goes for writing the inner product in momentum space,

$$\langle\Psi|\Psi\rangle = \int \langle\Psi|k\rangle\langle k|\Psi\rangle dk = \int \Phi(k)^*\Phi(k)dk$$