Just enough on Dirac Notation

The purpose of these brief notes is to familiarise you with the basics of Dirac notation. After reading them, you should be able to tackle the more abstract introduction to be found in many textbooks.

Basics

Dirac introduced a new notation for a quantum state, $|\alpha\rangle$. This is called a *ket*. The symbol α labels the state in some way: the most obvious label is whatever we have been calling the wavefunction, so that $|\psi\rangle$ is the state with wavefunction $\psi(x)$. If one has a set of basis functions $\phi_i(x)$, $i = 1, 2, \ldots$, (eg the eigenstates of a Hamiltonian) the corresponding kets might just be written $|i\rangle$. Or the labels might be the quantum numbers of the state, eg $|n, l, m\rangle$ for the energy eigenstates of the hydrogen atom.

To every ket $|\alpha\rangle$ there corresponds a *bra* $\langle\alpha|$ which represents the complex conjugate of the wavefunction, so that $\langle\psi|$ goes with $\psi^*(x)$.

The overlap of two states is represented by a bra and a ket (hence bra[c]ket notation!):

$$\langle\psi|\phi\rangle \equiv \int \psi^*(x)\phi(x)\mathrm{d}x\,,$$

where the integral here and everywhere subsequently is between $\pm\infty$. (I've used one dimension in these notes but the extension to two or three should be obvious).

Clearly $\langle\phi|\psi\rangle = (\langle\psi|\phi\rangle)^*$.

Just as an operator acting on a wavefunction gives another wavefunction, so an operator acting on a ket gives another ket: $\hat{Q}|\alpha\rangle = |\beta\rangle$. If the state is an eigenstate of the operator, the new state will just be a multiple of the original one: $\hat{Q}|\alpha\rangle = q|\alpha\rangle$

The expectation value of the operator $\hat{Q}$ in the state $|\psi\rangle$ is written

$$\langle Q\rangle \equiv \langle\psi|\hat{Q}|\psi\rangle \equiv \int \psi^*(x)\hat{Q}\psi(x)\mathrm{d}x$$

Similarly the matrix element of $\hat{Q}$ between two states is written

$$\langle\phi|\hat{Q}|\psi\rangle \equiv \int \phi^*(x)\hat{Q}\psi(x)\mathrm{d}x\,.$$

Analogy with vectors

If we have a complete set of orthonormal states $|i\rangle$, the overlaps will satisfy $\langle i|j\rangle = \delta_{ij}$, that is 1 if $i = j$ and 0 otherwise.

Any other state can be written as a superposition of these states: $|\psi\rangle = \sum_i a_i|i\rangle$ (or $\psi(x) = \sum_i a_i\phi_i(x)$) where the numbers a_i can be complex. The relationship between the bras will be

$\langle\psi| = \sum_i a_i^* \langle i|$. The values of the coefficients a_i can be found by taking the overlap of $|\psi\rangle$ with the appropriate state $|i\rangle$:

$$\begin{aligned}\langle i|\psi\rangle &= \langle i|\Big(\sum_j a_j|j\rangle\Big)\\ &= \sum_j a_j\langle i|j\rangle\\ &= \sum_j a_j\delta_{ij}\\ &= a_i\end{aligned}$$

This is very similar to the expansion of a general vector in terms of an orthonormal basis, where the list of coefficients $(a_1, a_2, a_3, \ldots)$ is the representation of the vector in this basis. So a ket is like a column vector, and the corresponding bra is like the row vector with elements which are the complex conjugates of the elements of the ket. (That's the Hermitian conjugate of the column vector: transpose and complex conjugate, denoted "†".) The overlap of a ket $|\alpha\rangle$ with elements a_i and a bra $\langle\beta|$ with elements b_i^* is then

$$\langle\beta|\alpha\rangle = \sum_i b_i^* a_i.$$

Note that this is just a (complex) number, not a vector – it is the scalar product of the two vectors.

To extend the analogy, operators are like matrices – just as operators change states into other states, so matrices change vectors into other vectors. If we define $Q_{ij} = \langle i|\hat{Q}|j\rangle$, then the array of numbers Q_{ij} is the representation of the matrix in this basis. Hence the name "matrix element". A general matrix element can be written

$$\begin{aligned}\langle\beta|\hat{Q}|\alpha\rangle &= \Big(\sum_i b_i^*\langle i|\Big)\hat{Q}\Big(\sum_j a_j|j\rangle\Big)\\ &= \sum_i\sum_j b_i^*\langle i|\hat{Q}|j\rangle a_j\\ &= \sum_i\sum_j b_i^* Q_{ij} a_j\\ &= (b_1^*, b_2^*, b_3^*, \ldots)\begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & . & . \\ Q_{21} & Q_{22} & Q_{23} & . & . \\ Q_{31} & Q_{32} & Q_{33} & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ . \\ . \end{pmatrix}\end{aligned}$$

Actually it is more than an analogy: sets of functions can be thought of a forming a vector space, in which the vectors are more abstract than the ones you are used to in 3-D space – they are infinite dimensional, for a start, and complex. The vector space used in quantum mechanics is called a "Hilbert space". Many introductions to Dirac notation spend quite some time on the properties of this space, which are mainly rather obvious ones such as linearity of operators, $\hat{Q}(a|\alpha\rangle + b|\beta\rangle) = a\hat{Q}|\alpha\rangle + b\hat{Q}|\beta\rangle$.

More about operators

From the matrix representation above, we can see that if we have $\hat{Q}|\alpha\rangle = |\gamma\rangle$, then $\langle\gamma| = \langle\alpha|\hat{Q}^\dagger$. In quantum mechanics operators of interest are all Hermitian, ie $\hat{Q} = \hat{Q}^\dagger$, and hence their eigenvalues are real and their eigenstates orthogonal. Also, if $|i\rangle$ is an eigenket of $\hat{Q}$, so $\hat{Q}|i\rangle = q_i|i\rangle$, then $\langle i|$ is an eigenbra: $\langle i|\hat{Q} = q_i\langle i|$. In an expression such as $\langle\phi|\hat{Q}|\psi\rangle$, $\hat{Q}$ can be taken as acting backwards or forwards, that is we can interpret the expression either as $\langle\phi|(\hat{Q}|\psi\rangle)$ or as $(\langle\phi|\hat{Q})|\psi\rangle$. This freedom is useful particularly if either bra of ket is an eigenstate of $\hat{Q}$.

We can construct another sort of object from bras and kets, as follows: $|\alpha\rangle\langle\beta|$. Note the order of the ket and bra: this is not a scalar product. In fact this is an operator: when we act with it on a ket, we are left with another ket:

$$\Big(|\alpha\rangle\langle\beta|\Big)|\psi\rangle = |\alpha\rangle\Big(\langle\beta|\psi\rangle\Big),$$

which is a ket proportional to $|\alpha\rangle$. The technical term for this kind of product is a "direct product".

It is also clear that the object $\sum_{ij} Q_{ij}|i\rangle\langle j|$ is exactly equivalent to $\hat{Q}$. (Try sandwiching it between $\langle\beta|$ and $|\alpha\rangle$, both expanded in the basis $\{|i\rangle\}$, to get $\sum_{ij} b_i^* Q_{ij} a_j$ as above.)

A special operator is the following: $\sum_i |i\rangle\langle i|$. Try operating on any ket, expanded in the basis $\{|i\rangle\}$. You will see that the ket is unchanged. So this is the identity operator.

More about wavefunctions

In the above, I stopped short of saying that a ket *is* a wavefunction. Instead I say that the ket $|\psi\rangle$ is a quantum state whose wavefuntion is $\psi(x)$. It is a fairly subtle distinction, but it is rather like the difference between a physical vector (eg the velocity of a particle) and the list of its components in a particular basis. The latter is a particular representation of the former, and so it is with quantum states and wavefunctions.

To see the connection more rigorously, consider a rather unusual quantum state, namely the one where a particle is known to be exactly at a given position x_0. (Yes, the momentum will be completely unknown; that doesn't matter right now.) We will label the corresponding ket as $|x_0\rangle$. The wavefunction of this state will be $\delta(x - x_0)$, that is zero if x is anything but x_0 and non-zero if x is exactly x_0. It's an infinitely sharp spike at $x = x_0$. The value at x_0 is real, infinite, and exactly large enough that the total area under the spike is one. Now let's consider the overlap of this state with some other (more normal) state:

$$\langle x_0|\psi\rangle = \int \delta(x - x_0)\psi(x)\mathrm{d}x = \psi(x_0)$$

The last stage is obvious if you realise that, since the delta function is zero everywhere but at x_0, the value of $\psi(x)$ elsewhere is irrelevant; however the value at x_0 is just a multiplicative factor on the integral over the delta function, which is one.

Thus to be precise, the relation between the ket and the wavefunction is $\psi(x) = \langle x|\psi\rangle$. Imagine plotting these numbers for successive values of x: you would exactly map out the function $\psi(x)$. The numbers are are the coefficients of the vector $|\psi\rangle$ in the basis $\{|x\rangle\}$, so $|\psi\rangle = \int \psi(x)|x\rangle$. This is called the position-space representation. The physical interpretation of the wavefunction is that $|\psi(x)|^2\mathrm{d}x$ is the probability of finding the particle between x and $x + \mathrm{d}x$.

The state $|x\rangle$ is an eigenfunction of position with eigenvalue x: $\hat{x}|x\rangle = x|x\rangle$ (and $\langle x|\hat{x} = x\langle x|$). Thus the wavefunction corresponding to the state $\hat{x}|\psi\rangle$ is $\langle x|\hat{x}|\psi\rangle = x\langle x|\psi\rangle = x\psi(x)$. Thus we have shown that in the position-space representation, the position operator is just the function x (the extension to 3-D is obvious).

The operator $\int |x\rangle\langle x|\mathrm{d}x$ is an identity operator. To see this, act with it on $|\psi\rangle$, giving $\int |x\rangle\psi(x)\mathrm{d}x = |\psi\rangle$.

Note that states of different position are orthogonal: $\langle x|x'\rangle = \delta(x - x')$.

Momentum states

As well as defining states of definite position, we can also define states of definite momentum $|p\rangle$. These satisfy $\langle p|p'\rangle = \delta(p - p')$.

It follows that $\tilde{\psi}(p) \equiv \langle p|\psi\rangle$ is the momentum-space representation of the state $|\psi\rangle$, from which we can construct the probability $|\tilde{\psi}(p)|^2\mathrm{d}p$ of finding the particle with momentum between p and $p + \mathrm{d}p$.

By an argument exactly analogous to the one above, we can show that in the momentum representation, the momentum operator $\hat{p}$ is just the function p, so $\hat{p}\tilde{\psi}(p) = p\tilde{\psi}(p)$.

We already know that the spatial wavefunction of a state with definite momentum is just a plane wave; with the appropriate normalisation we have

$$\langle x|p\rangle \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

It can then be shown that the momentum-space wavefunction $\tilde{\psi}(p)$ is the Fourier transform of the position-space wavefunction $\psi(x)$:

$$\begin{aligned}
\tilde{\psi}(p) &= \langle p|\psi\rangle \\
&= \int \langle p|x\rangle\langle x|\psi\rangle\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar}\psi(x)\mathrm{d}x
\end{aligned}$$

In line two we've used a common trick, inserting the identity operator $\int |x\rangle\langle x|\mathrm{d}x$ between the bra and the ket.

We can also use this to deduce the form of the momentum operator in position space (and vice versa). Of course you know already what it is, but perhaps not why. We want the wavefunction corresponding to $\hat{p}|\psi\rangle$, namely $\langle x|\hat{p}|\psi\rangle$. By again using the identity-operator trick (this time with the momentum-space representation) we can show

$$\begin{aligned}
\langle x|\hat{p}|\psi\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int p\, e^{ipx/\hbar}\tilde{\psi}(p)\mathrm{d}p \\
&= \left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi(x)
\end{aligned}$$

(Question 8 asks you to fill in the missing lines for yourself.) Thus the momentum operator in position space is just $(-i\hbar\mathrm{d}/\mathrm{d}x)$. Similarly one can show that the position operator in momentum space is $(i\hbar\mathrm{d}/\mathrm{d}p)$. In either space they explicitly satisfy the commutation relation $[\hat{x}, \hat{p}] = i\hbar$.

Exercises

In all cases, assume $\{|i\rangle\}$ is a complete orthonormal basis, ie $\langle i|j\rangle = \delta_{ij}$ and $\sum_i |i\rangle\langle i|$ is an identity operator.

1. Verify that if $|\psi\rangle = \sum_i a_i|i\rangle$, taking the corresponding bra to be $\langle\psi| = \sum_i a_i^*\langle i|$ gives $\langle\psi|\psi\rangle = \sum_i a_i^* a_i$, and that the same result is obtained from $\int \psi^*(x)\psi(x)\mathrm{d}x$.

2. By expanding in the basis $\{|i\rangle\}$, verify that if $\hat{Q}|\alpha\rangle = |\gamma\rangle$, then $\langle\gamma| = \langle\alpha|\hat{Q}^\dagger$.

3. Verify that $Q_{ij}|i\rangle\langle j|$ is equivalent to $\hat{Q}$ if $Q_{ij} = \langle i|\hat{Q}|j\rangle$.

4. Verify that $(\sum_i |i\rangle\langle i|)$ acting on $|\alpha\rangle$ gives $|\alpha\rangle$ (don't just assume that it is an identity operator here!)

5. Verify that if we expand $|\psi\rangle$ as $\int \psi(x)|x\rangle$ and similarly for $|\phi\rangle$, $\langle\phi|\psi\rangle = \int \phi^*(x)\psi(x)\mathrm{d}x$. (Hint: you will need to use a different integration variable, say x', in the expansion of $|\phi\rangle$.)

6. Verify that $\int |p'\rangle\langle p'|\mathrm{d}p'$ is the p-space representation of the identity operator by acting with it on an arbitrary state $|\psi\rangle$.

7. Show that $\psi(x)$ is the inverse Fourier transform of $\tilde{\psi}(p)$.

8. Fill in the missing lines of the derivation of the momentum operator $-i\hbar\mathrm{d}/\mathrm{d}x$. (Hint: there comes a point when a factor of "p" prevents us treating the integral as an inverse Fourier transform. It can be replaced by $(-i\hbar\mathrm{d}/\mathrm{d}x)$ which, acting on the exponential, just pulls down p. As the differential operator doesn't itself contain p, it can be taken out of the integral.)

For many particles, it is not enough to specify the spatial wavefunction, the spin wavefunction must also be considered. For a spin-half particle the two independent spin states are spin-up and spin-down along some specified axis, and states with are linear superpositions of both are also allowed.

In the subsequent examples, we will ignore the spatial wavefunction and concentrate on the 2-dimensional space of spin states, which we will denote $|+\rangle$ and $|-\rangle$ for spin-up and spin-down along the z axis. The three spin operators have the following actions:
$S_z|+\rangle = \frac{1}{2}\hbar|+\rangle$, $S_z|-\rangle = -\frac{1}{2}\hbar|-\rangle$,
$S_x|+\rangle = \frac{1}{2}\hbar|-\rangle$, $S_x|-\rangle = \frac{1}{2}\hbar|+\rangle$,
$S_y|+\rangle = i\frac{1}{2}\hbar|-\rangle$, $S_x|-\rangle = -i\frac{1}{2}\hbar|+\rangle$.

9. Construct the matrices corresponding to the three spin operators in this basis and show that they obey the commutation relations of angular momenta. (Hint: $|+\rangle$ and $|-\rangle$ are represented by the column vectors $(1,0)$ and $(0,1)$ respectively. These are abstract vectors, though, nothing to do with vectors in the xy-plane.)

10. Find the eigenstates and eigenvalues of S_x.

11. Show that $S_x^2 + S_y^2 + S_z^2$ is $3\hbar^2/4$ times the unit matrix, and explain why that would have been expected.