Tricks of the quantum trade

The main reason for learning the Dirac notation is that it makes it *much easier* to do quantum mechanics. Not just because it tends to be shorter, but because it lets you make a number of 'sanity checks' on the equations you write. This document tries to spell this out, and also to highlight points where you have to take care because the notation does not help you.

Making the notation work for you

You are used to checking that all the terms in an equation have the same physical dimensions/units. You also know that every term in a vector equation must be a vector, every term in a matrix equation must be a matrix with the same number of columns and rows, etc.

In the same way, in QM, the terms in equations may be bras, kets, operators, or scalars (i.e. numbers, often complex numbers). Each side of an equation must be the same kind of thing, and only things of the same kind can be added or subtracted. Also, you shouldn't mix terms which apply to different vector spaces. Checking this avoids a lot of potential mistakes... here are some examples:

$\|a\rangle = \|b\rangle + \|d\rangle$	OK: all terms are kets, presumably in the same space
$\hat{R}\|a\rangle = \|h\rangle$	OK: operators act to the right on a ket to make a new ket
$\|d\rangle = \sum_i c_i \|a_i\rangle$	OK: scalar (here, c_i) times a ket is a ket
$\hat{T} = \hat{p}^2/2m$	OK: all terms are operators (op divided by scalar is an op)
$\hat{P}_a = \|a\rangle\langle a\|$	OK: outer products are one type of operator
$\langle b\|h\rangle = \langle b\|\hat{R}\|a\rangle = 3 + 4i$	OK: inner products are complex numbers.
$\langle b\|\hat{R} = \langle e\|$	OK: operators act to the left on a bra to make a new bra
$\|1\rangle = \|\uparrow\rangle \otimes \|\uparrow\rangle$	OK: direct products of kets are kets (but in a bigger vector space)
$\langle b\|\hat{G}\|a\rangle = \langle b\|a\rangle\hat{G}$	WRONG: LHS is a complex number, RHS is an operator
$\langle b\| + \|a\rangle - \langle b\|a\rangle = 0$	WRONG: can't add bras, kets and/or scalars to each other
$\|2\rangle = \|\uparrow\rangle \otimes \|\uparrow\rangle + \|\downarrow\rangle$	WRONG: all kets in an equation must belong to the same space
$\hat{A}\|a_0\rangle = 0$	OK: here '0' means the zero (ket) vector, not scalar zero
$\hat{M} = \hat{S_z}^2 + 2\hbar^2$	OK(ish): what is really meant is $\hat{M} = \hat{S_z}^2 + 2\hbar^2\hat{I}$ ...i.e. scalars are implicitly multiplied by the identity operator
$\hat{J} = \hat{L} + \hat{S}$	OK(ish): the operators act on three different spaces, but we mean...
$\hat{J} = \hat{L} \otimes \hat{I} + \hat{I} \otimes \hat{S}$	OK: all terms are ops acting on the $L \otimes S$ product space

A second check is that each equation should refer to just one level of description. So far we have been talking about the level of abstract vectors for which we use Dirac notation. When we pick a particular basis, we get a 'representation' of these abstract quantities as a set of numbers in a less abstract (so-called 'concrete') notation; in this course we have used matrices and wave functions. These should not be mixed, with each other or with abstract bras and kets. Here

are some examples:

Abstract	ket $\|a\rangle$	bra $\langle a\|$	operator $\hat{O}$	number $\langle a\|b\rangle$
Matrix rep	column $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$	row (a_1^*, a_2^*)	square $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(a_1^*, a_2^*)\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = a_1^* b_1 + a_2^* b_2$
Wave fn rep	$a(x)$	$a^*(x)$	$x\times\ldots,\ -i\hbar d/dx,$ etc.	$\int a^*(x)b(x)\,dx$

Here are some no-no's:

$$\langle\uparrow|\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}|\downarrow\rangle = 0$$

This mixes abstract & matrix levels, although it's pretty clear what's meant.

$$\langle p\rangle = \int \langle\psi|\frac{\hbar}{i}\frac{d}{dx}|\psi\rangle\,dx$$

This mixes abstract vectors & wave functions and is wrong in two ways. First, one of the main reasons Dirac notation is shorter & neater than using wave functions is that it *avoids* have to write out such integrals; they are implicit in expressions like $\langle\psi|\hat{p}|\psi\rangle$. Second, the differential operator for $\hat{p}$ applies to wave functions, $\psi(x) = \langle x|\psi\rangle$, not to kets $|\psi\rangle$. Notice that the momentum wave function $\psi(p)$, which is the Fourier transform of $\psi(x)$, is also encoded in $|\psi\rangle$: $\psi(p) = \langle p|\psi\rangle$. $|\psi\rangle$ is not a function of x — its value does not change as x changes, because it implicitly accounts for all values of x simultaneously:

$$|\psi\rangle = \hat{I}|\psi\rangle = \int_{-\infty}^{\infty} |x'\rangle\langle x'|\psi\rangle\,dx' = \int_{-\infty}^{\infty} |x'\rangle\psi(x')\,dx'$$

(notice that x' is a dummy variable). So you will get into trouble if you try to differentiate by x! Note that, in contrast, kets representing quantum states *are* functions of time because they do change (i.e. rotate in their abstract vector space) with time, under the control of the Schrödinger equation.

Numbers in Quantum mechanics

In quantum mechanics, scalar numbers play several different roles, but unfortunately the notation does not help tell them apart, and many mistakes are due to getting these roles confused:

Values of observables: Operators representing physical observables have physical dimensions (usually) and therefore units. Their eigenvalues, which are the allowed values of the observables, have the same dimensions and units, for instance in the equation

$$\hat{H}|E_0\rangle = E_0|E_0\rangle,$$

the Hamiltonian $\hat{H}$ and the scalar E_0 have dimensions of energy. Eigenvalues of Hermitian operators are always real numbers. Note that, in contrast, unitary operators (such as rotations) are dimensionless, and so are their eigenvalues, which may be complex. Expectation values of operators, e.g. $\langle\psi|\hat{p}|\psi\rangle$, are averages over eigenvalues and, of course, share the same units.

Useful check: If one term in an equation involves an operator with physical dimensions, all the other terms must also have those same physical dimensions and so the numbers multiplying the dimensionless kets (or bras) in any terms lacking operators must involve values of observables, at least implicitly.

Probability amplitudes: We represent physical states, and vectors in orthonormal bases, as normalised kets, e.g. $|\psi\rangle$, where $\langle\psi|\psi\rangle = 1$. These are therefore dimensionless. If we expand such a ket in terms of a basis

$$|\psi\rangle = \sum_i c_i |a_i\rangle$$

the scalars complex numbers $c_i = \langle a_i|\psi\rangle$ must also be dimensionless, and we must also have $|c_i| \leq 1$ (NB: only if $|\psi\rangle$ *is* normalised, of course). They are often called probability amplitudes. They can be thought of as 'coordinates' for the tip of the vector $|\psi\rangle$, in the chosen basis.

Probabilities: The absolute square of a probability amplitude, e.g. $|c_1|^2 = c_1^* c_1$ gives the probability that a suitable measurement will find the system in the state given by the corresponding basis vector, here $|a_1\rangle$. Probabilities are dimensionless real numbers between 0 and 1. ("Suitable" means we measure some observable for which $|a_1\rangle$ is an eigenstate).

Useful check: you never get equations where bras, kets, or operators are multiplied by probabilities.

Probability (amplitude) densities Bases like $\{|\mathbf{x}\rangle\}$, appropriate for a wave function in N spatial dimensions, are normalised to a delta-function instead of unity, i.e. $\langle x|x'\rangle = \delta(x - x')$. Instead of probabilities we get probability densities which can be converted to probabilities by integrating over a suitable N-dimensional volume, e.g. in 1-D

$$\text{Prob}(x \leq 0) = \int_{-\infty}^{0} |\psi(x)|^2 \, dx.$$

Probability amplitude densities like $\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle$ have dimensions of length to the $(-N/2)$ power (e.g. $(\text{length})^{-1/2}$ for 1-D), so the above integral gives a dimensionless probability. Since $|\psi\rangle$ is dimensionless, $\langle\mathbf{x}|$ and $|\mathbf{x}\rangle$ must also have dimension $(\text{length})^{-N/2}$.

Many beginners confuse probability amplitudes with values of observables, since both are commonly found as multipliers of kets. The best way to tell them apart is to read carefully the words surrounding the equations, especially the ones that go "where a_i are the eigenvalues of operator $\hat{A}$" etc. Notice that sometimes you get both:

$$\hat{A}|\psi\rangle = \hat{A}\sum_i c_i|a_i\rangle = \sum_i c_i \hat{A}|a_i\rangle = \sum_i c_i a_i |a_i\rangle.$$

A last warning: mathematically, it is legitimate to write

$$c_2 a_2 |a_2\rangle = b_2 |a_2\rangle = |\Xi\rangle \quad \text{(DON'T DO THIS!)}$$

but this is horrible because b_2 is a probability amplitude (likely complex) multiplied by something physical like an energy or position, and the final ket $|\Xi\rangle$ is not dimensionless but has the same units as the eigenvalue a_2. Save yourself a lot of trouble by not writing things like this: keep the different kinds of numbers separate, and work out your own notation to help. For instance, in this document I've consistently used c_i for probability amplitudes, and deliberately not used 'C' to name any operator and hence eigenvalues.