Chapter 7

$|$ket$\rangle$ and $\langle$bra$|$ notation

Introduces the bra and ket notation and gives some examples of its use.

When you change the description of the world from the inutitive and everyday classical mechanics to the more abstract quantum mechanical description, you will usually have gone from a description of a world as composed of particles to one composed of wavefunctions. Instead of describing a physical system with coordinates and momenta, x and p (Dirac called them c-numbers), the quantum mechanical description is based on *operators* x and p (q-numbers) that operate on a wavefunction ψ.

The wave function can be a function of coordinates or of momenta and yet describe the same system. Basically, the wavefunction in momentum space is the Fourier transform of the wavefunction in coordinate space, and it describes the same physical system in both cases. Likewise, one may write a wavefunction as a sum of energy eigenfunctions as long as the set of them is complete (it will be). This way we can represent a wavefunction as a vector of coefficients. In fact, the wavefunction for a specific system can be written in any number ways that can look very different but are in reality different expressions of the same state.

It must be possible to express the state of the system without explicit reference to coordinates or momenta, much the same way we can express a plane wave with a few parameters such as the wave vector, the amplitude and the phase. Once these are given we do not need to give the amplitude at all points in space explicitly to describe the wave.

Here is how we do it. The state of a system (atom, molecule, superconductor, whatever) is described by a *ket*: $|...\rangle$. The dots denote the quantities that that characterizes the state. Example: A harmonic oscillator with precisely three quanta of vibrations is described as $|3\rangle$, where it is understood that in this case we are looking at a harmonic oscillator with some given frequency ω, say.

Because the state is specified with respect to the energy we can easily find the energy by application of the Hamiltonian operator on this state,

$$H|3\rangle = (3 + 1/2)\hbar\omega|3\rangle, \tag{7.1}$$

if we chose the zero of energy equal to the classical potential energy zero.

We need to be able to write superpositions of eigenstates also. This is done in a manner very similar to superpositions of wavefunctions. Give the state a name, S for example. Then

$$|S\rangle = \sum_{j=1}^{j_{max}} c_j|q_j\rangle, \tag{7.2}$$

where $|q_j\rangle$ is the state with the jth eigenvalue of some operator Q. j_{max} is the highest of these indices. It may be infinity. Compare this expression to the expansion of a wavefunction.

$$\Psi_S(x) = \sum_{j=1}^{j_{max}} c_j\phi_j(x). \tag{7.3}$$

We need to have an expression for the things we do when we do quantum mechanics. A matrix element can be expressed in terms of wavefucntions and in the bra-ket notation as

$$\int \psi_A(x)^*\psi_B(x)d\tau = \langle A|B\rangle. \tag{7.4}$$

$d\tau$ is the symbolic representation of all volume elements one needs to integrate over, and x is the complete set of coordinates used to describe the systems A and B. The $*$ denotes complex conjugation. (We will not write $\langle A||B\rangle$. To save ink we use just one vertical bar $\langle A|B\rangle$.) Whereas it may initially be a little difficult to get an understanding of the nature of $|B\rangle$, the object $\langle A|B\rangle$ is much simpler: It is a complex number. For consistency we must require that

$$\langle A|B\rangle = \langle B|A\rangle^*. \tag{7.5}$$

This follows from a complex conjugation of Eq.(7.4).

We can understand the definition in Eq.(7.4) in terms of another definition and an application of an operator. We write $\langle A|B\rangle$ as a sum over all intermediate states. Any set of complete states can be used. Let's begin with the set of all position eigenstates. Insertion of this set is accompliced with the operator

$$1 = \sum_x |x\rangle\langle x|. \tag{7.6}$$

This is another object you will have to get used to. Insertion of this gives

$$\langle A|B\rangle = \langle A|(\sum_x |x\rangle\langle x)|B\rangle = \sum_x \langle A|x\rangle\langle x|B\rangle. \tag{7.7}$$

A sum over all x is an integral and we can write

$$\langle A|B\rangle = \int_x \langle A|x\rangle\langle x|B\rangle dx. \tag{7.8}$$

The two quantities $\langle A|x\rangle$ and $\langle x|B\rangle$ are complex numbers, and $\langle A|x\rangle = \langle x|A\rangle^*$. We can therefore identify them with the wavefunctions in coordinate space:

$$\langle x|A\rangle = \psi_A(x), \tag{7.9}$$

and similarly for B. This is precisely what Eq.(7.4) says.

Expectation values are taken by sandwiching the ket with a bra, to give us a bra-ket (which is the origin of the name, if you didn't already notice this). The expectation value of some operator Q for state A is

$$\langle A|Q|A\rangle = \langle Q\rangle. \tag{7.10}$$

If $|A\rangle$ is an eigenstate of Q with eigenvalue a

$$Q|A\rangle = a|A\rangle, \tag{7.11}$$

the expectation value is

$$\langle A|Q|A\rangle = \langle A|a|A\rangle. \tag{7.12}$$

Because a is just a number we can take it outside the bra-ket and we get (the state is normalized, $\langle A|A\rangle = 1$),

$$\langle A|Q|A\rangle = a. \tag{7.13}$$

This can be generalized to states that are not eigenstates of Q. Write the state as a superposition of the eigenstates of Q;

$$|A\rangle = \sum_j c_j|q_j\rangle, \tag{7.14}$$

where the c_j's are complex numbers that obey the normalization condition

$$\sum_j |c_j|^2 = 1. \tag{7.15}$$

Inserting Eq.(7.14) into the definition of expectation values gives

$$\langle A|Q|A\rangle = \sum_k \langle q_k|c_k^* Q \sum_j c_j|q_j\rangle. \tag{7.16}$$

Note the complex conjugation of the coefficients on the bras. The Q operating on the kets can be calculated because the states are eigenstates of Q:

$$Q\sum_j c_j|q_j\rangle = \sum_j c_j q_j|q_j\rangle. \tag{7.17}$$

Inserting this into Eq.(7.16) we therefore get

$$\langle A|Q|A\rangle = \sum_k \langle q_k|c_k^* \sum_j c_j q_j |q_j\rangle. \tag{7.18}$$

The eigenstates of Q are orthogonal and normalized. This means that $\langle q_k|q_j\rangle = \delta_{j,k}$ (= 1 if $j = k$ and zero otherwise, the Kronecker delta). The double sum therefore reduces to a single sum

$$\langle A|Q|A\rangle = \sum_j \langle q_j|c_j^* c_j q_j|q_j\rangle = \sum_j \langle q_j||c_j|^2 q_j|q_j\rangle. \tag{7.19}$$

Here $|c_j|^2 q_j$ are just numbers, not operators, and can e taken outside the bra-ket. Because the states are normalized we finally get

$$\langle A|Q|A\rangle = \sum_j |c_j|^2 q_j. \tag{7.20}$$

Apart from the fact that the left hand side is written differently from what you may be used to, this is precisely what you have already learned in quantum mechanics about expectation values.

A complete set does not have to be spanned by coordinates. It can be every complete set, as the momentum states. The overlap $\langle A|B\rangle$ can be calculated as

$$\langle A|B\rangle = \sum_{\overline{p}} \langle A|\overline{p}\rangle\langle\overline{p}|B\rangle = \int \tilde{\psi}_A^*(\overline{p})\tilde{\psi}_B(\overline{p})d\overline{p}, \tag{7.21}$$

where the tilde indicates that it is the wavefunction in momentum space.

The use of bra's and ket's does not do anything to the fundamental equations of quantum mechanics. But they have two advantages; they provide an easier way to handle the equations, and they remind us that the world is not made out of wavefunctions that move around in space but of vectors that move around in Hilbert spaces.

A few examples. The inner product $\langle x|p\rangle$ is the wavefunction of the momentum eigenstate p (in one dimension),

$$\langle x|p\rangle \propto e^{ipx/\hbar}. \tag{7.22}$$

We may or may not include the time in this expression. The proportionality sign indicates that plane waves are non-trivial to normalize because they are infinite in extension. The inner product $\langle p_1|p_2\rangle$ is calculated to

$$\langle p_1|p_2\rangle = \int dx\langle p_1|x\rangle\langle x|p_2\rangle \propto \int dx e^{-ip_1 x/\hbar} e^{ip_2 x/\hbar} = 2\pi\hbar\delta(p_2 - p_1), \tag{7.23}$$

where δ is the Dirac deltafunction.

We can also use the formalism to find out how we convert from the coordinate representation of the wavefunction, $\langle x|A\rangle$, to the momentum representation,

$\langle p|A\rangle$. We do it by inserting a complete set:

$$\tilde{\psi}_A(p) = \langle p|A\rangle = \langle p| \sum_x |x\rangle\langle x|A\rangle = \int_x dx \langle x|p\rangle^* \langle x|A\rangle \propto \int_x dx e^{-ipx/\hbar} \psi_A(x). \tag{7.24}$$

The momentum space wavefunction is a Fourier transform of the coordinate space wavefunction, as you may know already.