1 Notes and Directions on Dirac Notation

A. M. Steane, Exeter College, Oxford University

1.1 Introduction

These pages are intended to help you get a feel for the mathematics behind Quantum Mechanics. The text books will guide you through all the details. All I will do here is show the similarity between the mathematics of vectors and the mathematics of kets (or 'state vectors'). The ket can be regarded as a generalisation of the concept of a vector.

1.2 Vectors, Bases and Components

A vector is a mathematical quantity. It may be written conveniently by writing the symbol for it in bold type, for example,

$$\mathbf{a},\ \mathbf{b},\ \mathbf{r}.$$

1.2.1

In a three-dimensional 'vector space', you can write any vector in terms of just three other vectors, multiplied by certain scalars - for example

$$\begin{aligned}\mathbf{a} &= \alpha\mathbf{p} + \beta\mathbf{q} + \gamma\mathbf{r}, \\ \mathbf{a} &= a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}.\end{aligned}$$

1.2.2

Let's choose to write every vector we come across in terms of three particular vectors $\mathbf{p}$, $\mathbf{q}$, and $\mathbf{r}$. For example,

$$\begin{aligned}\mathbf{a} &= \alpha\mathbf{p} + \beta\mathbf{q} + \gamma\mathbf{r} \\ \mathbf{b} &= \alpha'\mathbf{p} + \beta'\mathbf{q} + \gamma'\mathbf{r}\end{aligned}$$

This idea is sufficiently useful that we give it a name: we say that the choice { $\mathbf{p}$, $\mathbf{q}$, $\mathbf{r}$ } is a particular *'basis'*, and the numbers α, β, γ are the *'components'* of $\mathbf{a}$ in this basis.

Now consider the vector obtained by adding $\mathbf{a}$ and $\mathbf{b}$:

$$(\mathbf{a} + \mathbf{b}) = (\alpha + \alpha')\,\mathbf{p} + (\beta + \beta')\,\mathbf{q} + (\gamma + \gamma')\,\mathbf{r}.$$

Thus, to get the components of $(\mathbf{a} + \mathbf{b})$, you just add the components of $\mathbf{a}$ to those of $\mathbf{b}$.

The *basis* is a set of *vectors*.

The *components* are simply numbers, ie scalars.

1.2.3

A useful mathematical quantity is the 'dot product' of two vectors. It is written $\mathbf{a}.\mathbf{b}$. Note two things: if $\mathbf{a}$ and $\mathbf{b}$ both have unit length, then $\mathbf{a}.\mathbf{b}$ expresses, roughly speaking, the degree to which they are pointing in the same direction. Also, $\mathbf{a}.\mathbf{b}$ may be obtained from the components of $\mathbf{a}$ and $\mathbf{b}$:

$$\mathbf{a}.\mathbf{b} = \alpha\alpha' + \beta\beta' + \gamma\gamma'.$$

This works as long as the basis vectors are orthonormal.

The dot product is a scalar, not a vector. Finally, note that if the basis vectors are orthonormal, then you can obtain each of the components of a vector by taking the dot product with the relevant basis vector:

$$\begin{aligned} \mathbf{a}.\mathbf{p} &= \alpha \\ \mathbf{a}.\mathbf{q} &= \beta \\ \mathbf{a}.\mathbf{r} &= \gamma \end{aligned}$$

This yields the important result

$$\mathbf{a} = (\mathbf{a}.\mathbf{p})\,\mathbf{p} + (\mathbf{a}.\mathbf{q})\,\mathbf{q} + (\mathbf{a}.\mathbf{r})\,\mathbf{r}.$$

1.2.4

If you choose a different basis, the components of any given vector will change. However, the value of $\mathbf{a}.\mathbf{b}$ is independant of the basis.

1.3 Kets, Bases and Wavefunctions

1.3.1

A ket is a mathematical quantity. It may be written conveniently by surrounding the symbol for it by a vertical line and an angle bracket, for example,

$$|a\rangle\,,\ |b\rangle\,,\ |c\rangle\,.$$

1.3.2

In an n-dimensional 'Hilbert space', you can write any ket in terms of just n other kets, multiplied by certain scalars - for example, in 3 dimensions,

$$\begin{aligned} |a\rangle &= \alpha\,|p\rangle + \beta\,|q\rangle + \gamma\,|r\rangle\,, \\ |a\rangle &= a_x\,|i\rangle + a_y\,|j\rangle + a_z\,|k\rangle\,. \end{aligned}$$

1.3.3

Let's choose to write every ket we come across in terms of three particular kets $|p\rangle$, $|q\rangle$, and $|r\rangle$. For example,

$$\begin{aligned} |a\rangle &= \alpha\,|p\rangle + \beta\,|q\rangle + \gamma\,|r\rangle \\ |b\rangle &= \alpha'\,|p\rangle + \beta'\,|q\rangle + \gamma'\,|r\rangle \end{aligned}$$

This idea is sufficiently useful that we give it a name: we say that the choice $\{\ |p\rangle,\ |q\rangle,\ |r\rangle\ \}$ is a particular *'basis'*, and the numbers α, β, γ are the *'components'* of $|a\rangle$ in this basis. These *components* are more usually referred to in quantum mechanics as *'amplitudes'*, for a reason we will see below. If the Hilbert space has an infinite number of dimensions, we get an infinite set of components or amplitudes. Such a set is called a *wavefunction.* This will be explained more fully below.

Now consider the ket obtained by adding $|a\rangle$ and $|b\rangle$:

$$(|a\rangle + |b\rangle) = (\alpha + \alpha')\,|p\rangle + (\beta + \beta')\,|q\rangle + (\gamma + \gamma')\,|r\rangle\,.$$

Thus, to get the components of $(|a\rangle + |b\rangle)$, you just add the components of $|a\rangle$ to those of $|b\rangle$.

The *basis* is a set of *kets.*

The *components* or *amplitudes* are simply complex numbers, ie scalars.

1.3.4

A useful mathematical quantity is the 'dot product' of two kets (it can also referred to as an *overlap integral*). It is written $\langle b|a\rangle$. Note two things: if $|a\rangle$ and $|b\rangle$ both have unit length, then $\langle b|a\rangle$ expresses, roughly speaking, the degree to which $|a\rangle$ is the same ket as $|b\rangle$. Also, $\langle b|a\rangle$ may be obtained from the components of $|a\rangle$ and $|b\rangle$:

$$\begin{aligned}\langle b|a\rangle &= (\alpha' \langle p| + \beta' \langle q| + \gamma' \langle r|)(\alpha |p\rangle + \beta |q\rangle + \gamma |r\rangle) \\ &= \alpha'\alpha + \beta'\beta + \gamma'\gamma\end{aligned}$$

This result is obtained as long as the basis kets are orthonormal, that is, if things like $\langle p|q\rangle = 0$ while things like $\langle p|p\rangle = 1$.

The dot product is a scalar, not a vector. Finally, note that if the basis kets are orthonormal, then you can obtain each of the components of a ket by taking the dot product with the relevant basis ket:

$$\begin{aligned}\langle p|a\rangle &= \alpha \\ \langle q|a\rangle &= \beta \\ \langle r|a\rangle &= \gamma\end{aligned}$$

This yields the important result

$$|a\rangle = |p\rangle \langle p|a\rangle + |q\rangle \langle q|a\rangle + |r\rangle \langle r|a\rangle$$

or, more generally, if the kets $|n\rangle$ form a complete orthonormal set, then for any ket $|\psi\rangle$,

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle \,.$$

1.3.5

If you choose a different basis, the components of any given vector will change. However, the value of $\langle b|a\rangle$ is independant of the basis.

1.4 Amplitudes and Quantum Mechanics

1.4.1

Why do we call things like $\langle b|a\rangle$ *amplitudes*? Here is why. First, let's think about useful choices of basis. This is like deciding how to define your axes when working with vectors. If we choose to work with a set of basis kets, it is only really useful to do so with a *complete, orthonormal* set. That is, we want to have enough kets in our basis so that we can, by adding them together in the right proportions, make up any ket whatsoever (completeness). Also, we want the basis kets to be orthonormal (ie $\langle j|i\rangle = \delta_{ij}$ where $|i\rangle$ and $|j\rangle$ are basis kets) so that the equations in the previous section work out ok. Now, it so happens that it is easy to find such sets: any group of kets which are the eigenkets of some Hermitian operator will do. That is, suppose we have a Hermitian operator Q. Then there are various kets $|q\rangle$ which satisfy the equation

$$Q\,|q\rangle = q\,|q\rangle$$

The set of solutions to such an equation forms an orthonormal set of kets. (Note that we are following the common practice that when we have an eigenket of an operator, we use the relevant eigenvalue as a label inside the ket symbol.) Now, the **Magic Law of Quantum Mechanics** states that

1. The state of a system is represented by a ket.
2. Variables such as x and p from classical mechanics are represented by Hermition operators X and P.
3. If a particle is in the state $|\psi\rangle$, measurement of the variable represented by Q will yield one of the eigenvalues q of this operator, with probability $\mathcal{P}(q) = |\langle q|\psi\rangle|^2$.

That's why the dot product things are called amplitudes. It's because if the bit on the right of the dot product is representing the state of your system, and if the bit on the left is an eigenket (bra) of some operator, then the dot product is a *probability amplitude*—that is, a complex number, whose modulus squared is the probability that a measurement of this particular property of the system will yield this particular eigenvalue. The eigenvalue here is of course the one associated with the eigenket on the left of the dot product.

Finally, if the left hand end of the dot product is an eigenket of the position operator with eigenvalue x, then the dot product is the amplitude that a measurement of the position of the system will yield the value x. That is,

- $\langle x|\psi\rangle =$
- (thing whose modulus squared is the probability that system will be found at x)
- = a wavefunction,
- which is a complex number which depends on x,
- which may be written $\psi(x)$.

1.4.2

I can't resist writing down some equation to do with kets, to show how neat Dirac's notation really is. I'll do it by first writing an equation using wavefunctions, which I hope will be clear to you. Then I'll write a similar equation using kets, then derive the wavefunction version from the ket version.

Here we go. Suppose a system is described by a wavefunction $\psi(x)$. Suppose that the system is not in an eigenstate of energy, but is in a superposition of two different energy eigenstates $u_1(x)$ and $u_2(x)$, (of energies E_1 and E_2), ie

$$\psi(x) = a_1 u_1(x) + a_2 u_2(x).$$

What is the probability that if we measure the energy of this state, we will get the value E_1? (so that the state becomes equal to $u_1(x)$). You should know that the answer is $|a_1|^2$.

In ket, or state vector, language, this goes as follows. Suppose a system is in a state described by the state vector $|\psi\rangle$. Any state can always be written as a superposition of energy eigenstates:

$$|\psi\rangle = \sum_n |E_n\rangle \langle E_n|\psi\rangle$$

In our particular case, only two terms in this sum are non-zero:

$$|\psi\rangle = |E_1\rangle \langle E_1|\psi\rangle + |E_2\rangle \langle E_2|\psi\rangle$$

What is the probability that if we measure the energy of this state, we will get the value E_1? (so that the state becomes equal to $|E_1\rangle$). The probability is $|\langle E_1|\psi\rangle|^2$.

Now let's see what happens when we dot the previous equation from the left with a ket $|x\rangle$ (or bra when we turn it round) which is an eigenstate of the position operator:

$$\begin{aligned} \langle x|\psi\rangle &= \langle x| \left(|E_1\rangle \langle E_1|\psi\rangle + |E_2\rangle \langle E_2|\psi\rangle\right) \\ &= \langle x|E_1\rangle \langle E_1|\psi\rangle + \langle x|E_2\rangle \langle E_2|\psi\rangle \end{aligned}$$

This is exactly our original wavefunction equation, since

$$\begin{aligned} \langle x|\psi\rangle &= \psi(x), \\ \langle x|E_1\rangle &= u_1(x) \\ \langle E_1|\psi\rangle &= a_1. \end{aligned}$$

Finally, we note that any ket can be expressed as a superposition of position eigenstates, as follows:

$$|\psi\rangle = \sum_n |x_n\rangle \langle x_n|\psi\rangle$$

Dot this equation from the left with some other ket $|\phi\rangle$:

$$\langle\phi|\psi\rangle = \sum_n \langle\phi|x_n\rangle \langle x_n|\psi\rangle$$

and let the position eigenstates tend to a continuum of states:

$$\langle\phi|\psi\rangle = \int \langle\phi|x\rangle \langle x|\psi\rangle \, dx$$

In other words,

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

which is why the amplitude can also be called an overlap integral: this integral is non-zero only when the two wavefunctions are both non-zero in the same region of space, ie when they overlap one another.

1.5 Concluding remarks

I think I should finish with apologies that this description is all rather abstract. I am aware that a lot of concrete physical examples of the use of the maths would make things a lot clearer. I recommend Shankar's book and the Feynman lectures, volume 3, as a help towards getting you to think quantum mechanically.