Chapter 9

Vectors and Matrices

Up to now, we've treated each ket vector as an abstract mathematical object unto itself. In the next chapter, we will see a way in which we can represent the ket vectors for a spin-1/2 system and do calculations with them. In order do that, we first have to lay some groundwork for the mathematical objects and operations we will be using.

9.1 Column Vectors

In Section 3.1, we were introduced to the concept of vectors in 3-d space, or 3-vectors. We talked about visualizing them as an arrow in space, and we also talked about representing them as a sum of scalars (i.e. just numbers) times the three basis vectors $\vec{e}_x$, $\vec{e}_y$, and $\vec{e}_z$. Those three basis vectors are vectors with unit magnitude (so that the constants in front of them end up giving you the vector's real magnitude) that just point along the three cardinal axes.

There is a second way that we could represent a 3-vector: as a column vector. Take again our example of $\vec{v}$, the velocity of our car going due northwest, from Section 3.1. From the equation

$$\vec{v} \;=\; v_x\,\vec{e}_x \;+\; v_y\,\vec{e}_y \;+\; v_z\,\vec{e}_z$$

we see that it takes three numbers— v_x, v_y, and v_z— to represent this vector. Instead of representing it as an arrow on a drawing, and instead of writing out the equation above, we could come up with a more compact notation that just lists those three numbers. One such way to do that is to list those three numbers one above each other in a column vector, as such

$$\vec{v} \;=\; \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix}$$

In the specific example of our car, we could even numerically represent its velocity as a column vector:

$$\vec{v} = \begin{bmatrix} -35 \text{ km/h} \\ 35 \text{ km/h} \\ 0 \end{bmatrix}$$

If we're going to use this representation, we need to know how to apply the standard vector operators in this representation. For example, you can add together two vectors in order to get a third vector, $\vec{c} = \vec{a} + \vec{b}$. In the column vector representation, this is easy; you just add the individual components:

$$\begin{bmatrix} c_x \\ c_y \\ c_z \end{bmatrix} = \begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} + \begin{bmatrix} b_x \\ b_y \\ b_z \end{bmatrix} = \begin{bmatrix} a_x + b_x \\ a_y + b_y \\ a_z + b_z \end{bmatrix}$$

When you multiply a vector by a scalar, $\vec{b} = k\,\vec{a}$, you just multiply each component by that scalar:

$$\begin{bmatrix} b_x \\ b_y \\ b_z \end{bmatrix} = k \begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} = \begin{bmatrix} k\,a_x \\ k\,a_y \\ k\,a_z \end{bmatrix}$$

All of this started above when we went from writing the vector as a sum of components times the basis vector into a column listing those components. We can do the same thing for ket vectors! For the spin-1/2 system, you can write a ket vector in terms of the basis vectors; the basis vectors we're using here are $|+z\rangle$ and $|-z\rangle$. Any ket vector can be written as:

$$|\psi\rangle = a\,|+z\rangle + b\,|-z\rangle$$

where a and b are complex scalars. Just as the coefficients on the basis vectors for a 3-vector could become the elements of a column vector, we can represent a ket as a column vector. Here, there are only two basis vectors, so we can represent the ket with just a two-row column vector:

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

For instance, the column vectors corresponding to the eigenstates for angular momentum along the three axes are:

$$|+z\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |+y\rangle = \begin{bmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{bmatrix} \quad |+x\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$|-z\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad |-y\rangle = \begin{bmatrix} i/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \quad |-x\rangle = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$$

9.2 Row Vectors

If you can represent ket vectors as column vectors, how about bra vectors? Bra vectors may be represented as a row vector. In order to find the bra vector $\langle\psi|$ that corresponds to a ket vector $|\psi\rangle$, you turn the column vector into a row vector, and take a complex conjugate of each component of the vector:

$$|\psi\rangle \;=\; \begin{bmatrix} a \\ b \end{bmatrix} \qquad \langle\psi| \;=\; \begin{bmatrix} a^* & b^* \end{bmatrix}$$

This makes it straightforward to write out the bra vectors corresponding to the angular momentum eigenstates along the three axes:

$$\langle +z| \;=\; \begin{bmatrix} 1 & 0 \end{bmatrix} \quad \langle +y| \;=\; \begin{bmatrix} 1/\sqrt{2} & -i/\sqrt{2} \end{bmatrix} \quad \langle +x| \;=\; \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$$\langle -z| \;=\; \begin{bmatrix} 0 & 1 \end{bmatrix} \quad \langle -y| \;=\; \begin{bmatrix} -i/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \quad \langle -x| \;=\; \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

One thing to be careful about with row vectors: remember that it's a sequence of numbers, each in a different column of the row. Don't multiply them together! They're in different spots in the row vector.

9.2.1 The Inner Product

We know we can take the inner product of a bra vector and a ket vector, $\langle\phi\,|\,\psi\rangle$. How do you do this with this column and row vector representation we're building? Let's do an example. First, define a couple of bra vectors:

$$|\phi\rangle \;=\; \begin{bmatrix} a \\ b \end{bmatrix} \qquad |\psi\rangle \;=\; \begin{bmatrix} c \\ d \end{bmatrix}$$

The inner product is only defined between a bra vector and a ket vector, so we need to get the ket vector that corresponds to $|\phi\rangle$:

$$\langle\phi| \;=\; \begin{bmatrix} a^* & b^* \end{bmatrix}$$

Now, to do the inner product, we put the two together:

$$\langle\phi\,|\,\psi\rangle \;=\; \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$

To evaluate this, you multiply the first column of the row vector by the first row of the column vector, and then add to that the second column of the row vector times the second row of the column vector:

$$\begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} \;=\; a^*c \;+\; b^*d$$

You can multiply a row vector with n rows by a column vector with the same number (n) of rows. You just multiply each component of the first with the corresponding component of the second, and add all of those products together to get the overall result. That overall result is just a scalar. You can *not* multiply a row vector by a column vector unless both have exactly the same number of components.

When you multiply a row vector by a column vector, it's standard always to write the row vector first. It's not a defined operation to multiply a column vector by a row vector if you write the column vector first (at least, as far as we are going to go for our present purposes).[1] This matches the inner product of a bra vector and a ket vector; you always write the bra vector first, as that's the way that you can make the flat sides of each vector fit together.

9.2.2 Nothing is New!

While this is a new formalism for calculations, in fact the addition of column vectors, and multiplying a row vector by a column vector, does exactly the same operations you have already performed previously just by writing out a ket vector in terms of the basis vectors $|+z\rangle$ and $|-z\rangle$. The column vector formalism makes it faster to perform certain calculations. For example, if you wanted to calculate $\langle +y\,|\,+x\rangle$, you would have to write out both vectors in terms of the z basis vectors, turn the y into a ket, and then work through the algebra. With row and column vectors, you can just start with:

$$\langle +y\,|\,+x\rangle \;=\; \begin{bmatrix}1/\sqrt{2} & -i/\sqrt{2}\end{bmatrix}\begin{bmatrix}1/\sqrt{2}\\ 1/\sqrt{2}\end{bmatrix}$$

Calculating this out, you get

$$\begin{aligned}\langle +y\,|\,+x\rangle &= \left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right) + \left(\frac{-i}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)\\ &= \frac{1-i}{2}\end{aligned}$$

If you take the absolute square of this, you get $\frac{1}{2}$, which is what we know is the probability for an electron in the $|+x\rangle$ state to subsequently be measured to have y spin along the positive y axis. This amplitude is exactly what you would get writing out the two vectors in terms of the z basis, and the ultimate calculation would be the same. By using this formalism, you get to skip writing out a bunch of terms involving $\langle +z\,|\,+z\rangle$, $\langle -z\,|\,+z\rangle$, and the like. You only end up multiplying together the terms

[1] In fact, you *can* multiply a column vector by a row vector with the column vector first. However, the result is not a scalar, but a 2×2 matrix! This operation is equivalent to the putting a ket vector and bra vector together in the order $|\phi\rangle\,\langle\psi|$. While such constructions do have their uses in more advanced quantum mechanics, we will not be using them here.

that won't go away due to the orthogonality of the z basis states, and you get fairly quickly to the calculations you need to do.

9.3 Matrices

There is one final bit of mathematical formalism we need to learn before we can get back to the business of applying this formalism to figuring out what will happen in quantum systems. A *matrix* is an extension of column and row vectors. Whereas a column vector has one column and multiple rows, and a row vector is the other way around, a matrix can have multiple columns *and* multiple rows. For our purposes, we need only concern ourselves with square matrices. In the case of the spin-1/2 system, these matrices will be 2×2 matrices. You could write out such a matrix M as:

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

Whereas a row vector or column vector only has two components, a matrix has four components.

What are matrices for? They can be used to represent operators. Remember that an operator, when applied to a ket vector, returns another ket vector. Thus, we need to have a way to apply a 2×2 matrix to a 2-element column vector, which is what we are using to represent a ket vector.

9.3.1 Linear Operations on Matrices

Just like column vectors, you can add together two matrices of the same size. To figure out the result, just add together the components:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \end{bmatrix}$$

For example:

$$\begin{bmatrix} 2 & i \\ i & 2 \end{bmatrix} + \begin{bmatrix} 1 & 3 \\ 3 & -1 \end{bmatrix} = \begin{bmatrix} 3 & 3+i \\ 3+i & 1 \end{bmatrix}$$

Just as column vectors may be multiplied by a scalar, you may also multiply a matrix by a scalar. As before, the result is a matrix with each component multiplied by the same scalar:

$$k \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} = \begin{bmatrix} k\,M_{11} & k\,M_{12} \\ k\,M_{21} & k\,M_{22} \end{bmatrix}$$

9.3.2 Multiplying a Matrix and a Column Vector

When using a matrix as an operator that operates on a column vector, the mathematical term for what you are doing is "matrix multiplication". In fact, this is a special case of matrix multiplication; you can learn more general matrix multiplication in a linear algebra course. Multiplying a matrix by a column vector is like repeatedly multiplying row vectors by column vectors. You start with the top row of the matrix. Treat that top row as a row vector, and multiply it by the column vector. That gives you the top row of the answer (which, remember, is itself a column vector). Then go down to the second row of the matrix, and treat that row as a row vector. Multiply it by the column vector. That gives you the second row of the answer. Thus, the result would be:

$$\hat{M}\,|\psi\rangle \;=\; \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \;=\; \begin{bmatrix} M_{11}\psi_1 \,+\, M_{12}\,\psi_2 \\ M_{21}\psi_1 \,+\, M_{22}\,\psi_2 \end{bmatrix}$$

Notice that the result is *not* a 2×2 matrix. Rather, it's just a column vector!

As an example, we will see in the next chapter that the z angular momentum operator can be represented by the matrix:

$$\hat{S}_z \;=\; \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

We can verify that $|+z\rangle$ is in fact an eigenvector of $\hat{S}_z$ with the right eigenvalue by trying it out with this representation:

$$\begin{aligned} \hat{S}_z\;|+z\rangle \;&=\; \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &=\; \frac{\hbar}{2} \begin{bmatrix} (1)(1) + (0)(0) \\ (0)(1) + (-1)(0) \end{bmatrix} \\ &=\; \frac{\hbar}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &=\; \frac{\hbar}{2}\;|+z\rangle \end{aligned}$$

Sure enough, we get the answer that we expected. We get back exactly the same vector, multiplied by the measure of the z-spin corresponding to a system in the state represented by this vector.

9.3.3 The Identity Matrix

There is one special matrix called the identity matrix. If you multiply this matrix by any column vector, the result is exactly the same column vector. In a sense, the number 1 is the 1×1 identity matrix! Hopefully, you are very familiar with the notion that multiplying a number by 1 returns the same number that you started with. The 2×2 identity matrix is:

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Use of this matrix would correspond to the "identity operator" in quantum mechanics, which is not terribly useful. It doesn't really correspond to any observable, and *every* state is an eigenstate of this operator with an eigenvalue of 1! All it does is keep states exactly the way they began.