

# Chapter 8

## Operators and Eigenvectors

### 8.1 Operators

In quantum mechanics, we associate observables with *operators*. There is a position operator, an energy operator, a spin-z operator, etc. The exact form of the operators and the rules for how you work with them vary depending not only on what the operator is, but on the representation we're using for the type of states that the operator operates on. In this chapter, we're concerned with operators in general, so we're going to keep things abstract. In the next two chapters, we'll see how actually to do calculations with the operators and ket vectors that represent angular momentum states.

On the most level, an operator is just something that does something to something else. Whether you know it or not, you're already familiar with a wide variety of operators in regular mathematics. For example, the addition operator, usually denoted with the  $+$  symbol, is a *binary operator*. It takes two arguments, and returns a third argument of the same type. For example,  $3+2$  is the notation we use to apply the addition operator to the numbers 3 and 2. Our understanding of the rules for applying this operator tells us that the result is 5.

The operators we're going to use in quantum mechanics just operate on one thing, a quantum state vector. An analogy to arithmetic would be the negation operator. If you see  $-a$  written, you recognize that whatever number  $a$  represents,  $-a$  is the negative of that number. The  $-$  sign just denotes that one should apply the operator that performs this negation to the number  $a$ . Another operator you're familiar with is square root. When you see  $\sqrt{4}$ , that means that you should apply the square root operator to the number 4; the result in this case is 2.

Here, we will follow the convention of putting a “hat” on top of letters that

represent quantum operators. So,  $\hat{O}$  would be a particular operator. Operators operate on ket vectors<sup>1</sup>, and the result of the operation is another ket vector. So, if we write:

$$|\phi\rangle = \hat{O} |\psi\rangle$$

then we're saying that when you apply the  $\hat{O}$  operator to the state  $|\psi\rangle$ , the result is the state  $|\phi\rangle$ .

## 8.2 Eigenstates

An *eigenstate* is a state that corresponds to some observable having a definite value. So,  $|+z\rangle$  and  $|-z\rangle$  are eigenstates of the  $z$  component of angular momentum. Likewise,  $|+y\rangle$  and  $|-y\rangle$  are eigenstate of the  $y$  component of angular momentum. Quantum systems do not necessarily have to be in an eigenstate of anything. However, the act of measurement causes a quantum state to “collapse” to an eigenstate of the observable that was measured.

If a quantum state is an eigenstate of a given observable, then we can describe the state vector that represents that state as an *eigenvector* of the operator corresponding to that vector. For example, suppose that  $\hat{S}_z$  is the spin- $z$  operator. Then,  $|+z\rangle$  is an eigenvector of  $\hat{S}_z$ . (We will also later talk about *eigenfunctions*. This is when you are using mathematical functions as a way of representing quantum states. Before we get to that, we will use column vectors to represents  $|\psi\rangle$ , so there will be no need to invent a term beyond eigenvector.)

Eigenvectors of an operator have a special relationship with that operator. If a given vector is an eigenvector of a certain operator, then the following applies:

$$\hat{O} |\psi\rangle = v |\psi\rangle$$

where  $v$  is just a scalar constant. In other words, when an operator operates on one of its own eigenvectors, the result of that operation is the same vector that went into it, only multiplied by a constant. In quantum mechanics, there is an additional constraint: these eigenvalues must be *real* (i.e. their imaginary part must be zero). What's more, there's a very direct interpretation to them: they are the measured values that corresponds to the respective eigenstate. So, for the spin- $z$  operator:

$$\hat{S}_z |+z\rangle = \frac{\hbar}{2} |+z\rangle$$

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<sup>1</sup>They can also operate on bra vectors, but there are some wrinkles to how they work. In the standard notation, an operator always has to operate through one of the straight sides of a vector, be it bra or ket. For our present purposes, we'll only allow operators to operate to the right on ket vectors.

$$\hat{S}_z | -z \rangle = \frac{-\hbar}{2} | -z \rangle$$

This knowledge right here will allow us to do calculations with operators and ket vectors, even if we don't actually know the detailed mechanics for just what it is that the operator is doing, nor what the detailed mathematical representation we're using for our ket vectors. Just as with the probability calculations we've done before, even though we're keeping ket vectors abstract, we can still get results out of them.

The different eigenstates of a given operator are orthogonal. This was already discussed in Section 6.4, although there we hadn't yet introduced the concept of operators. There, we said that the different states corresponding to definite states for a given observable were orthogonal. Now, we know that another way to say "the states corresponding to the definite states for a given observable" is "the eigenstates for the observable's operator". This means that if you have an operator with eigenstates  $|\phi_n\rangle$ , then

$$\langle \phi_n | \phi_m \rangle = 0 \quad \text{if } n \neq m.$$

Also, the eigenstates for a given operator need to be normalized, that is,

$$\langle \phi_n | \phi_n \rangle = 1.$$

The set of eigenstates for a given operator form a set of "basis states". If you put all of them together, you can express *any* state in terms of those basis states (as long as you're talking about the same general kind of state). So, for example, the spin- $z$  operator  $\hat{S}_z$  has two eigenstates,  $|+z\rangle$  and  $|-z\rangle$ . Those two eigenstates form a basis, and you can write *any* electron spin state as a sum of constants times those two states. (For example,  $|+x\rangle$  can be written  $\frac{1}{\sqrt{2}}|+z\rangle + \frac{1}{\sqrt{2}}|-z\rangle$ .) This is why we call the complete set of eigenstates for the operator a "basis": it's a base upon which all other states can be built. By considering different different operators from the same general type, you may be able to come up with a different basis. For example, all electron spin states could just as well be written as sums of the eigenvalues of  $\hat{S}_x$ ; in that case,  $|+x\rangle$  and  $|-x\rangle$  form a different set of basis states. By convention, we generally use  $|+z\rangle$  and  $|-z\rangle$  as the basis states for spin angular momentum, but we don't have to.

### 8.3 Linear Operators

In order to go any further, there are two properties of these operators that we have to know. These operators are what we call *linear* operators. Do not confuse this with a straight line on a graph, for when we say "linear" here we do not mean anything so concrete. Rather, to say that an operator  $\hat{O}$  is linear is to imply the following two

properties, where  $k$  is a scalar constant:

$$\begin{aligned}\hat{O} (|\psi_1\rangle + |\psi_2\rangle) &= \hat{O} |\psi_1\rangle + \hat{O} |\psi_2\rangle \\ \hat{O} (k |\psi\rangle) &= k \hat{O} |\psi\rangle\end{aligned}$$

The action of an operator on a sum of vectors is just the sum of the actions of that operator on the two vectors. Second, if a constant multiplies a vector and you want to operate on that constant times that vector, you are free to pull the constant out in front of the operator, and do the multiplication of by the constant after you perform the operation of the operator on the vector. (Notice that you can't do the multiplication by the constant first once you've pulled it out before the operator. All we've defined for using these vectors is to have one of them operate on a ket vector that is to its right. We haven't defined any way for one of these operators to interact with something to its left.)

## 8.4 Operators on Non-Eigenstates

What happens when an operator works on a ket vector that is not one of its eigenstates out? You get a different ket vector out, one that can't be expressed as a constant times the ket vector that the operator did its work on. As an example, let's figure out the result of the spin- $z$  operator on an  $x$  eigenstate:

$$|\psi\rangle = \hat{S}_z |+x\rangle$$

We don't know enough to perform the calculation on the right side of the equation. However, we can substitute for  $|+x\rangle$  in terms of the  $z$  eigenvectors:

$$|\psi\rangle = \hat{S}_z \left( \frac{1}{\sqrt{2}} |+z\rangle + \frac{1}{\sqrt{2}} |-z\rangle \right)$$

We can use the fact that  $\hat{S}_z$  is linear to make the next step:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \hat{S}_z |+z\rangle + \frac{1}{\sqrt{2}} \hat{S}_z |-z\rangle$$

Now, we have the  $\hat{S}_z$  operator just operating on its own eigenstates, and we know how to handle that! We can replace  $\hat{S}_z |+z\rangle$  with  $(\hbar/2) |+z\rangle$ , because  $\hbar/2$  is the eigenvalue that goes together with the  $|+z\rangle$  eigenstate of  $\hat{S}_z$ . We can do the equivalent thing with  $|-z\rangle$ . Performing these substitutions:

$$\begin{aligned}|\psi\rangle &= \frac{1}{\sqrt{2}} \left( \frac{\hbar}{2} \right) |+z\rangle + \frac{1}{\sqrt{2}} \left( -\frac{\hbar}{2} \right) |-z\rangle \\ &= \frac{\hbar}{2} \left( \frac{1}{\sqrt{2}} |+z\rangle - \frac{1}{\sqrt{2}} |-z\rangle \right)\end{aligned}$$

You may recognize the thing in parentheses here as  $| -x \rangle$ . That means that

$$|\psi\rangle = \frac{\hbar}{2} | -x \rangle$$

which is the operation of  $\hat{S}_z$  on the state  $| +x \rangle$ :

$$\hat{S}_z | +x \rangle = \frac{\hbar}{2} | -x \rangle$$

Clearly,  $| +x \rangle$  is not an eigenstate of  $\hat{S}_z$ , as the operation of  $\hat{S}_z$  on that state doesn't return the same state, but a different state. We expected this; if eigenstates correspond to states that have definite values for the observable of a given operator, then states that *don't* have definite values for that observable can't be eigenstates for that operator. And, we've seen before that  $| +x \rangle$  doesn't have a definite value for  $z$ -spin.

## 8.5 The Hamiltonian

There is one operator in quantum mechanics that is so important it has its own name, and the eigenvalue equation for it in turn has its own name. That is the operator corresponding to energy. Energy is an observable for a quantum particle or a quantum system; it is something that you could measure. The operator that corresponds to the observable energy is called the *Hamiltonian*, and is usually denoted with the symbol  $\hat{H}$ . If a state  $|\psi\rangle$  is an energy eigenstate, then the usual eigenvalue equation applies

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

where  $E$  is the eigenvalue that corresponds to the eigenvector  $|\psi\rangle$ . This equation only works if  $|\psi\rangle$  is in fact an eigenvector for the Hamiltonian! That means that it is a state that has definite energy, and  $E$  is the value of that energy. This equation is called the time-independent Schrödinger equation.

The eigenstates for the Hamiltonian are usually expressed as functions of position. Thus, we might write

$$\hat{H} \psi(x) = E \psi(x)$$

and call that the one-dimensional time-independent Schrödinger equation. The function  $\psi(x)$  is a “wave function”, and is a representation of a quantum state that we have previously been calling  $|\psi\rangle$ . It is important to remember that both are just representations, and are quite abstract. The wave function or wave vector is an abstract mathematical object, to which you can do things to in order to make predictions about the system that the theory is modeling. The wave function is not a function like  $\vec{v}(t)$ , the velocity of a particle as a function of time. If you have a full expression for  $\vec{v}(t)$ , you can interpret it fairly directly; just plug in a time  $t$ , work out what the

function is, and you've got the velocity at that time. Not so for the wave function  $\psi(x)$ . Even if you do have the functional form, the interpretation is not so direct. One thing that you can do to it in order to get something physical out is operate the Hamiltonian on it. If you do that, you get back a constant times the function; that constant is the energy that corresponds to the state represented by the function. In later chapters, we will see ways to pull out other physical interpretations of the wave function.

Despite being called "the" Hamiltonian, it is actually not just one operator. Remember that the energy of a particle can come in two forms: kinetic energy and potential energy. The Hamiltonian operator has two parts to it, one for kinetic energy and one for potential energy. Unfortunately, we won't be able to look in detail into how we represent the Hamiltonian operator, because to do so would require calculus. However, even though kinetic energy for a given particle is only a function of its speed, potential energy can be entirely different depending on the environment that the particle is interacting with. For instance, if your particle is at the end of something that behaves just like a spring, then the potential energy for that particle (which is just a function of position) would be the simple harmonic oscillator potential. For an electron orbiting an atomic nucleus, the interaction is the electrostatic interaction and the potential is what we call the Coulomb potential. The Hamiltonians that are built from different potentials will, of course, have different eigenfunctions. We call those eigenfunctions the "solutions" of the Schrödinger equation.