

Chapter 10

Pauli Spin Matrices

We can represent the eigenstates for angular momentum of a spin-1/2 particle along each of the three spatial axes with column vectors:

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

Similarly, we can use matrices to represent the various spin operators.

10.1 Spin Operators

We've been talking about three different spin observables for a spin-1/2 particle: the component of angular momentum along, respectively, the x , y , and z axes. In quantum mechanics, there is an operator that corresponds to each observable. The operators for the three components of spin are \hat{S}_x , \hat{S}_y , and \hat{S}_z . If we use the column vector representation of the various spin eigenstates above, then we can use the following representation for the spin operators:

$$\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

It is also conventional to define the three "Pauli spin matrices" σ_x , σ_y , and σ_z , which are:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Clearly, then, the spin operators can be built from the corresponding Pauli matrices just by multiplying each one by $\hbar/2$.

You can verify that this is a good representation of the spin operators by making sure that all all of the various observations about spin states are reproduced by using these operators and these vectors to predict them from the theory. For example, $|+y\rangle$ is an eigenstate for the y component of spin, so the column vector representation of $|+y\rangle$ needs to be an eigenvector of \hat{S}_y . Is it? Let's try it:

$$\begin{aligned}\hat{S}_y | +y\rangle &= \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} (0)(1/\sqrt{2}) + (-i)(i/\sqrt{2}) \\ (i)(1/\sqrt{2}) + (0)(i/\sqrt{2}) \end{bmatrix} \\ &= \frac{\hbar}{2} \begin{bmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{bmatrix} \\ &= \frac{\hbar}{2} | +y\rangle\end{aligned}$$

In at least this case, the matrix and column vector representations of \hat{S}_y and $|+y\rangle$ are working.

10.2 Expectation Values

You can also use the matrix representation of operators to figure out *expectation values*. Suppose that you have an electron in the state:

$$|\psi\rangle = \sqrt{\frac{1}{3}} | +z\rangle + \sqrt{\frac{2}{3}} | -z\rangle$$

What are the expectation values of for spin along the x -axis??

First, we construct the column vector representation of this state $|\psi\rangle$:

$$|\psi\rangle = \begin{bmatrix} \sqrt{1/3} \\ \sqrt{2/3} \end{bmatrix}$$

The corresponding bra vector is represented by a row vector:

$$\langle\psi| = [\sqrt{1/3} \quad \sqrt{2/3}]$$

To figure out the expectation value of x -spin, we sandwich the \hat{S}_x operator in between

the bra and ket vectors for this state:

$$\begin{aligned}
 \langle s_x \rangle &= \langle \psi | \hat{S}_x | \psi \rangle \\
 &= [\sqrt{1/3} \quad \sqrt{2/3}] \left(\frac{\hbar}{2} \right) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \sqrt{1/3} \\ \sqrt{2/3} \end{bmatrix} \\
 &= \left(\frac{\hbar}{2} \right) [\sqrt{1/3} \quad \sqrt{2/3}] \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \sqrt{1/3} \\ \sqrt{2/3} \end{bmatrix}
 \end{aligned}$$

(all we did between the last two lines was pull the scalar constant $\hbar/2$ out front). We've got a row vector times a matrix times a column vector. That may look intimidating, but we know how to do the matrix times the column vector, so let's do that first. That will leave us with a row vector times a column vector; we know how to work that out as well, leaving us with just a scalar. A scalar is what we need for an expectation value.

$$\begin{aligned}
 \langle s_x \rangle &= \left(\frac{\hbar}{2} \right) [\sqrt{1/3} \quad \sqrt{2/3}] \begin{bmatrix} \sqrt{2/3} \\ \sqrt{1/3} \end{bmatrix} \\
 &= \left(\frac{\hbar}{2} \right) \left(\sqrt{\frac{1}{3}} \right) \left(\sqrt{\frac{2}{3}} \right) + \left(\sqrt{\frac{2}{3}} \right) \left(\sqrt{\frac{1}{3}} \right) \\
 &= \left(\frac{\hbar}{2} \right) \frac{2\sqrt{2}}{3} \\
 &= \frac{\sqrt{2}}{3} \hbar
 \end{aligned}$$

That's a plausible expectation value. It's neither $\hbar/2$ nor $-\hbar/2$, which means that this is not a definite state for x spin. That's good, because the state is clearly not the same as $|+x\rangle$ when you write out that state in terms of $|+z\rangle$ and $| -z\rangle$. It's between those two. However, from just looking at the state, while you can fairly quickly see that $| -z\rangle$ has more amplitude than $|+z\rangle$, and thus a measurement of z spin will yield $-\hbar/2$ more often than $+\hbar/2$, it's not obvious at all just looking at the state which value of x spin would be more common, and thus whether the x expectation value should be positive or negative. In this case, you have to perform the calculation. The matrix formulation of the spin operators makes the calculations faster and easier than they would be when you explicit writing out everything in terms of the z basis states.

We could also quickly figure out what the amplitude for measuring positive x spin is with this formalism. Remember that for a particle in state $|\psi\rangle$, the amplitude for finding positive x spin is $\langle +x | \psi \rangle$. Putting together the $\langle +x |$ bra vector with the

column vector for $|\psi\rangle$ above, we get:

$$\begin{aligned}
 \langle +x | \psi \rangle &= [1/\sqrt{2} \quad 1/\sqrt{2}] \begin{bmatrix} \sqrt{1/3} \\ \sqrt{2/3} \end{bmatrix} \\
 &= \left(\sqrt{\frac{1}{2}}\right) \left(\sqrt{\frac{1}{3}}\right) + \left(\sqrt{\frac{1}{2}}\right) \left(\sqrt{\frac{2}{3}}\right) \\
 &= \sqrt{\frac{1}{6}} + \sqrt{\frac{1}{3}} \\
 &= 0.9856
 \end{aligned}$$

That's a high positive amplitude, corresponding to a probability of 0.97 that positive x spin will be measured for this state. Again, without performing the calculations, this is not at all obvious. However, this high probability for positive x spin is consistent with the fact that the x spin expectation value $\langle s_x \rangle$ is positive and only a little bit less than $\hbar/2$.

10.3 Total Angular Momentum

In 3D space, if you have three components of a vector \vec{v} , then the magnitude of that vector squared is $v^2 = v_x^2 + v_y^2 + v_z^2$. Angular momentum is a vector, and so this rule would apply to angular momentum as well. However, in quantum mechanics, we see that angular momentum behaves very differently from how it does in classical physics. In particular, if an object has a definite z component of angular momentum, then it has an *indefinite* x component of angular momentum. Does that mean that total angular momentum must also be indefinite? In order to answer this question, we must ask it in a proper quantum manner.

In quantum mechanics, we associate each observable quantity with an operator. We can then use that operator on one of its eigenstates (i.e. a state where the observable has a definite value) to pull out the value of the observable as the eigenvalue a in the equation $\hat{A}|\phi\rangle = a|\phi\rangle$. If the system is not in an eigenstate, we can figure out the “expectation value” $\langle a \rangle$ (i.e. the weighted average of all values that could be observed) using the operator in the equation

$$\langle a \rangle = \langle \psi | \hat{A} | \psi \rangle$$

What then is the operator that corresponds to total angular momentum? By analogy to classical physics, we can guess that the operator for total angular momentum squared is:

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

This begs the question as to what \hat{S}_x^2 means; we know how to square numbers and variables, but how do you square an operator? For \hat{S}^2 , we will just treat that as an operator itself, the “total spin squared” operator. We’ll not treat the superscript 2 as squaring, rather we’ll just consider it part of the name. As for the others, what really matters about an operator is what it does to a vector representing a quantum state that it’s supposed to operate on. In order to make this definition of the spin angular momentum squared operator to work, we need to interpret them as follows:

$$\hat{S}_x^2 |\psi\rangle = \hat{S}_x \hat{S}_x |\psi\rangle$$

In other words, first apply the \hat{S}_x operator to the state $|\psi\rangle$, and then apply the \hat{S}_x operator again to the vector that resulted from the first application. As an example, let’s consider the \hat{S}_x^2 operator on the state $|+z\rangle$:

$$\begin{aligned} \hat{S}_x^2 |+z\rangle &= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{aligned}$$

All we’ve done in the first step is pulled the scalar constants out front. To perform this matrix multiplication, first we must multiply the rightmost matrix by the vector, and then we can multiply the first matrix by the result.¹

$$\begin{aligned} \hat{S}_x^2 |+z\rangle &= \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= \frac{\hbar^2}{4} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \frac{\hbar^2}{4} |+z\rangle \end{aligned}$$

Interestingly, it seems that $|+z\rangle$ is in fact an eigenstate of \hat{S}_x^2 , even though it’s not an eigenstate of \hat{S}_x !

Armed with these techniques, it is possible to show that *any* properly normalized spin-1/2 state $|\psi\rangle$ is an eigenstate of \hat{S}^2 with eigenvalue $\frac{3}{4}\hbar^2$. Although it may be surprising that $|+z\rangle$ is an eigenstate of \hat{S}_x^2 , in retrospect it should not be surprising that all states are eigenstates of the total angular momentum operator. We’ve been saying all along that the *total* angular momentum of an electron is $\frac{\sqrt{3}}{2}\hbar$; what can be in an indefinite state is the components of that angular momentum along various axes.

¹If you know how to multiply 2×2 matrices, you can do the matrix multiplication first if you wish. As we will see, the commutative property does not apply to matrix multiplication, but the associative property does.

