Lecture 4

Relevant sections in text: §1.2, 1.3, 1.4

The spin operators

Finally we can discuss the definition of the spin observables for a spin 1/2 system. We will do this by giving the expansion of the operators in a particular basis. We denote the basis vectors representing states in which the z component of spin is known by

$$|\pm\rangle := |S_z, \pm\rangle,$$

and define

$$S_x = \frac{\hbar}{2}\Big(|+\rangle\langle-| + |-\rangle\langle+|\Big)$$
$$S_y = i\frac{\hbar}{2}\Big(|-\rangle\langle+| - |+\rangle\langle-|\Big)$$
$$S_z = \frac{\hbar}{2}\Big(|+\rangle\langle+| - |-\rangle\langle-|\Big).$$

Note that we have picked a direction, called it z, and used the corresponding spin states for a basis. Of course, any other direction could be chosen as well. *You can now check that, with the above definition of S_z, $|\pm\rangle$ are in fact the eigenvectors of S_z with eigenvalues* $\pm\hbar/2$. Labeling matrix elements in this basis as

$$A_{ij} = \begin{pmatrix} \langle+|A|+\rangle & \langle+|A|-\rangle \\ \langle-|A|+\rangle & \langle-|A|-\rangle \end{pmatrix},$$

you can also verify the following matrix representations *in the $|\pm\rangle$ basis*:

$$(S_x)_{ij} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (S_y)_{ij} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (S_z)_{ij} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Finally, you should check that all three spin operators are self-adjoint. It will be quite a while before you get a deep understanding of why these particular operators are chosen. For now, let us just take them as given and see what we can do with them.

As a good exercise you can verify that

$$|S_x, \pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle), \quad |S_y, \pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm i|-\rangle)$$

are eigenvectors of S_x and S_y, respectively, with eigenvalues $\pm\hbar/2$. Note that these eigenvectors are normalized to have norm ("length") unity. The fact that these eigenvectors are distinct from those of S_z will be dealt with a little later. For now, just note that the three operators do not share any eigenvectors. Note also that the eigenvalues of the spin operators are all non-degenerate – exercise.

Spectral decomposition

The spin operators have the general form

$$A = \sum_{ij} A_{ij}|i\rangle\langle j|,$$

which we discussed earlier. Note, though, that S_z has an especially simple, *diagonal* form. This is because it is being represented by an expansion in a basis of its eigenvectors. It is not hard to see that this result is quite general. If $|i\rangle$ is an ON basis of eigenvectors of A with eigenvalues a_i:

$$A|i\rangle = a_i|i\rangle,$$

then the matrix elements are

$$A_{ij} = \langle i|A|j\rangle = a_j\langle i|j\rangle = a_i\delta_{ij},$$

so that (exercise)

$$A = \sum_i a_i|i\rangle\langle i|.$$

This representation of an operator is called its *spectral decomposition.* The name comes from the terminology that the set of eigenvalues forms the *spectrum* of an operator (on a finite dimensional Hilbert space). You can easily see that the definition of S_z is its spectral decomposition.

Because every self-adjoint operator admits an ON basis of eigenvectors, each such operator admits a spectral decomposition. Of course, different operators will, in general, provide a different ON basis.

Probability interpretation

We now use the third quantum mechanics postulate (relating expectation values to diagonal matrix elements) to physically interpret some elementary state vectors. Let us start with the eigenvector $|+\rangle$ of S_z. *In the state represented by this vector* we have (exercise)

$$\langle S_z\rangle = \langle +|S_z|+\rangle = \frac{\hbar}{2}, \quad \langle S_x\rangle = \langle S_y\rangle = 0.$$

This makes perfect sense since $|+\rangle \equiv |S_z, +\rangle$ is supposed to be a state where S_z is known with certainty (probability unity) to have the value $+\hbar/2$. On the other hand, we saw in the Stern-Gerlach experiment that such states have equal probability of finding $\pm\hbar/2$ for S_x and S_y whence their expectation value vanishes. You can verify as an exercise that similar comments (with appropriate permutation of x, y, and z) can be made for $|S_z, -\rangle$, $|S_x, \pm\rangle$, *etc.*

The third postulate of QM is the place where the mathematical representation of a physical system makes contact with reality. It provides the predictions that can be tested/compared with experiment. Note that the third postulate gives the physical output of QM in terms of probabilities (specifically, expectation values). In fact, as we shall see, *all* the physical predictions of quantum mechanics are intrinsically probabilistic.

How can we see directly the probabilities for the various outcomes of a measurement of something like spin when the third postulate only gives statistical averages, *i.e.,* expectation values? We proceed as follows. Consider a function $f(x)$ that takes the value 1 at, say, $x = \hbar/2$ and vanishes otherwise.* Consider the observable, say, $f(S_x)$ – not yet viewed as an operator, but just as the experimentally accessible observable. So, $f(S_x)$ is like a detector for spin-up along the x-axis — it yields the value one when the spin along x is $\frac{\hbar}{2}$ and yields zero otherwise. If you think about repeatedly setting up an experimental state and measuring $f(S_x)$ you will see that (in the limit of an arbitrarily large number of experiments) the expectation value of $f(S_x)$ is precisely equal to the probability for finding S_x to have the value $\hbar/2$ (exercise). More generally, the probability of finding S_x to have a value in any range R of real numbers is just the expectation value of the characteristic function of the set R. Clearly we can do the same for any other component of the spin. Thus we can extract a probability by computing an expectation value, which we know how to do once we figure out how to represent $f(S_x)$. Let's see how to do this.

In general, given a Hermitian operator A with an ON basis of eigenvectors $|i\rangle$ and eigenvalues a_i, and a real-valued function $h(x)$, we can define a self-adjoint operator $h(A)$ using its spectral decomposition. We want the eigenvectors of $h(A)$ to be the same as for A, and we want the eigenvalues to be $h(a_i)$. Evidently we desire the spectral decomposition

$$h(A) = \sum_i h(a_i)|i\rangle\langle i|.$$

You can easily check that $|i\rangle$ constitute (a basis of) eigenvectors of $h(A)$ with eigenvalues $h(a_i)$. Thus we define functions of observables by their spectral decomposition. In particular, given the characteristic function f for the point $x = \hbar/2$, we *define* the *operator* $f(S_x)$ by its spectral decomposition:

$$f(S_x) = f(\frac{\hbar}{2})|S_x,+\rangle\langle S_x,+| + f(-\frac{\hbar}{2})|S_x,-\rangle\langle S_x,-| = |S_x,+\rangle\langle S_x,+|.$$

It is now easy to see, by computing expectation values of $f(S_x)$ according to the third postulate, that the following probability distributions arise (good exercise!):

State: $|S_z,\pm\rangle \longrightarrow Prob(S_x = \pm\hbar/2) = 1/2, \quad Prob(S_x = \mp\hbar/2) = 1/2$

* Such a function is called a *characteristic function* for the set $x = \frac{\hbar}{2}$.

State: $|S_x, \pm\rangle \longrightarrow Prob(S_x = \pm\hbar/2) = 1, \quad Prob(S_x = \mp\hbar/2) = 0$

State: $|S_y, \pm\rangle \longrightarrow Prob(S_x = \pm\hbar/2) = 1/2, \quad Prob(S_x = \mp\hbar/2) = 1/2.$

You can easily play similar games with other components of **S**. You can also compute the probabilities (via expectation values) in any state you like just by expanding the state in the $|\pm\rangle$ basis and computing the expectation values using the orthonormality of the basis. As a nice exercise you should be able to prove that if a state vector takes the form

$$|\psi\rangle = a|+\rangle + b|-\rangle, \quad |a|^2 + |b|^2 = 1,$$

then the probability of getting $\hbar/2$ for S_z is given by $|a|^2$ while the probability for getting $-\hbar/2$ is given by $|b|^2$. Note that the normalization condition

$$1 = \langle\psi|\psi\rangle = |a|^2 + |b|^2$$

guarantees that the probabilities add up to unity.

This implies that the probability for getting any other values for S_z must vanish. Let us prove this directly. Let $g(x)$ be a function that vanishes at $\pm\hbar/2$, that is, that vanishes at the eigenvalues of any of the spin operators. For any component of the spin, S_k, and for any state $|\psi\rangle$ we have that

$$\langle g(S_k)\rangle = \langle\psi| \left\{ g(\frac{\hbar}{2})|S_k, +\rangle\langle S_k, +| + g(-\frac{\hbar}{2})|S_k, -\rangle\langle S_k, -| \right\} |\psi\rangle = 0.$$

In particular, if you pick g to be a characteristic function of any set not including the spectrum of S_k, then the expectation value – *which is the probability for finding S_k to be in that set* – vanishes. Thus we see that *the only possible outcome of a measurement of an observable is an element of its spectrum, i.e., one of its eigenvalues.*

The foregoing results are important enough to state in all generality. The only possible outcome of a measurement of an observable represented by the self-adjoint operator A is one of the eigenvalues of A. Given a state represented by the (unit) vector $|\psi\rangle$ and given an observable (represented by) A, we can write

$$|\psi\rangle = \sum_i \langle i|\psi\rangle|i\rangle,$$

where

$$A|i\rangle = a_i|i\rangle.$$

If there is no degeneracy, the probability for getting the value a_i upon measurement of (the observable represented by) A is $|\langle i|\psi\rangle|^2$. If there is degeneracy the probability for getting a_i is given by $\sum_j |\langle j, a_i|\psi\rangle|^2$, where the sum runs over an ON basis $|j, a_i\rangle$ of the subspace associated with a_i.