C/CS/Phys 191 Spin Algebra, Spin Eigenvalues, Pauli Matrices
9/25/03
Fall 2003 Lecture 10

Spin Algebra

"Spin" is the intrinsic angular momentum associated with fundamental particles. To understand spin, we must understand the quantum mechanical properties of angular momentum. The spin is denoted by $\vec{S}$.

In the last lecture, we established that:

$$\begin{aligned}
\vec{S} &= S_x\hat{x} + S_y\hat{y} + S_z\hat{z} \\
S^2 &= S_x^2 + S_y^2 + S_z^2 \\
[S_x, S_y] &= i\hbar S_z \\
[S_y, S_z] &= i\hbar S_x \\
[S_z, S_x] &= i\hbar S_y \\
[S^2, S_i] &= 0 \text{ for } i = x, y, z
\end{aligned}$$

Because S^2 commutes with S_z, there must exist an orthonormal basis consisting entirely of simultaneous eigenstates of S^2 and S_z. (We proved that rule in a previous lecture.)

Since each of these basis states is an eigenvector of both S^2 and S_z, they can be written with the notation $\left|a,b\right\rangle$, where a denotes the eigenvalue of S^2 and b denotes the eigenvalue of S_z.

Now, it will turn out that a and b can't be just any numbers. The word "quantum" in "quantum mechanics" refers to the fact that many operators have "quantized" eigenvalues – eigenvalues that can only take on a limited, discrete set of values.

(In the example of the position and momentum, from previous lectures, the position and momentum eigenvalues were *not* discrete or quantized in this sense; they were continuous. However, the energy of the "particle on a ring" was quantized.)

Question: What values a and b can have?

We'll give away the answer first, and most of the lecture will be spent proving this answer:

Answer:

a can equal $\hbar^2 n(n+1)$, where n is an integer or half of an integer Given that $a = \hbar^2 n(n+1), b$ can equal $\hbar(-n), \hbar(-n+1), \ldots \hbar(n-2), \hbar(n-1), \hbar n.$

Now, let's prove it.

First, define the "raising" and "lowering" operators S_+ and S_-: $S_+ \equiv S_x + iS_y$, $S_- \equiv S_x - iS_y$

Let's find the commutators of these operators:

$[S_z, S_+] = [S_z, S_x] + i[S_z, S_y] = i\hbar S_y + i(-i\hbar S_x) = \hbar(S_x + iS_y) = \hbar S_+$

Therefore $[S_z, S_+] = \hbar S_+$. Similarly, $[S_z, S_-] = -\hbar S_-$.

Now act S_+ on $|a,b\rangle$. Is the resulting state still an eigenvector of S^2? If so, does it have the same eigenvalues a and b, or does it have new ones?

First, consider S^2:

What is $S^2(S_+|a,b\rangle)$? Since $[S^2,S_+]=0$, the S^2 eigenvalue is unchanged: $S^2(S_+|a,b\rangle) = S_+(S^2|a,b\rangle) = S_+(a|s,m\rangle) = a(S_+|a,b\rangle)$. The new state is also an eigenstate of S^2 with eigenvalue a.

Now, consider S_z:

What is $S_z(S_+|a,b\rangle)$? Here, $[S_z,S_+] = \hbar S_+ (\neq 0)$. That is, $S_zS_+ - S_+S_z = \hbar S_+$. So $S_zS_+ = S_+S_z + \hbar S_+$, and:

$$
\begin{aligned}
S_z(S_+|a,b\rangle) &= (S_+S_z + \hbar S_+)|a,b\rangle \\
&= (S_+b + \hbar S_+)|a,b\rangle \\
S_z(S_+|a,b\rangle) &= (b+\hbar)S_+|a,b\rangle
\end{aligned}
$$

Therefore $S_+|a,b\rangle$ *is* an eigenstate of S_z. But S_+ raises the S_z eigenvalue of $|a,b\rangle$ by $\hbar$! S_+ *changes* the state $|a,b\rangle$ to $|a,b+\hbar\rangle$.

but S_+ raises the S_z eigenvalue of $|s,m\rangle$ by $\hbar$!

Similarly, $S_z(S_-|s,m\rangle) = (b-\hbar)(S_-|a,b\rangle)$ (Homework.) So S_- lowers the eigenvalue of S_z by $\hbar$.

Now, remember that $\vec{S}$ is like an angular momentum. S^2 represents the square of the magnitude of the angular momentum; and S_z represents the z-component.

But suppose you keep hitting $|s,m\rangle$ with S_+. The eigenvalue of S^2 will not change, but the eigenvalue of S_z keeps increasing. If we keep doing this enough, the eigenvalue of S_z will grow larger than the square root of the eigenvalue of S^2. That is, the z-component of the angular momentum vector will in some sense be larger than the magnitude of the angular momentum vector.

That doesn't make a lot of sense . . . perhaps we made a mistake somewhere? Or a fault assumption? What unwarranted assumption did we make?

Here's our mistake: we forgot about the ket 0, which *acts like* an eigenvector of any operator, with any eigenvalue.

I don't mean the ket $|0\rangle$; I mean the ket 0. For instance, if we were dealing with qubits, any ket could be represented as the $\alpha|0\rangle + \beta|1\rangle$. What ket do you get if you set both α and β to 0? You get the ket 0. Which is not the same as $|0\rangle$.

Remember in our proof above when we concluded that $S_z(S_+|a,b\rangle) = (b+\hbar)S_+|a,b\rangle$? Well, if $S_+|a,b\rangle = 0$, then this would be true in a trivial way. That is, $S_z \times 0 = (b+\hbar)\times 0 = 0$. But that doesn't mean that we have succesfully used S_+ to increase the eigenvalue of S_z by $\hbar$. All we've done is annihilate our ket.

So the resolution to our dilemma must be that if you keep hitting $|a,b\rangle$ with S_+, you must eventually get 0. Let $|a,b_{\text{top}}(a)\rangle$ be the last ket we get before we reach 0. ($b_{\text{top}}(a)$ is the "top" value of b that we can reach, for this value of a.) We expect that $b_{\text{top}}(a)$ is no bigger than the square root of a. Then $S_z|a,b_{\text{top}}(a)\rangle = b_{\text{top}}(a)|a,b_{\text{top}}(a)\rangle$.

Similarly, there must exist a "bottom" state $|a,b_{\text{bot}}(a)\rangle$, such that $S_-|a,b_{\text{bot}}(a)\rangle = 0$. And $S_z|a,b_{\text{bot}}(a)\rangle = b_{\text{bot}}(a)|a,b_{\text{bot}}(a)\rangle$.

Now consider the operator $S_+S_- = (S_x+iS_y)(S_x-iS_y)$. Multiplying out the terms and using the commutation relations, we get

$S_+S_- = S_x^2 + S_y^2 - i(S_xS_y - S_yS_x) = S^2 - S_z^2 + \hbar S_z$
Hence

$$S^2 = S_+S_- + S_z^2 - \hbar S_z \tag{1}$$

Similarly

$$S^2 = S_-S_+ + S_z^2 + \hbar S_z \tag{2}$$

Now act S^2 on $|a, b_{\text{top}}(a)\rangle$ and $|a, b_{\text{bot}}(a)\rangle$.

$$\begin{aligned}
S^2|a, b_{\text{top}}(a)\rangle &= (S_-S_+ + S_z^2 + \hbar S_z)|a, b_{\text{top}}(a)\rangle \text{ by (2)} \\
&= (0 + b_{\text{top}}(a)^2 + \hbar b_{\text{top}}(a))|a, b_{\text{top}}(a)\rangle \\
S^2|a, b_{\text{top}}(a)\rangle &= b_{\text{top}}(a)(b_{\text{top}}(a) + \hbar)|a, b_{\text{top}}(a)\rangle
\end{aligned}$$

Similarly,

$$\begin{aligned}
S^2|a, b_{\text{bot}}(a)\rangle &= (S_+S_- + S_z^2 - \hbar S_z)|a, b_{\text{bot}}(a)\rangle \text{ by (1)} \\
&= (0 + b_{\text{bot}}(a)^2 - \hbar b_{\text{bot}}(a))|a, b_{\text{bot}}(a)\rangle \\
S^2|a, b_{\text{bot}}(a)\rangle &= \hbar b_{\text{bot}}(a)(b_{\text{bot}}(a) - \hbar)|a, b_{\text{bot}}(a)\rangle
\end{aligned}$$

So the first ket has S^2 eigenvalue $a = b_{\text{top}}(a)(b_{\text{top}}(a) + \hbar)$, and the second ket has S^2 eigenvalue $a = \hbar^2 b_{\text{bot}}(a)(b_{\text{bot}}(a) - \hbar)$.

But we know that the action of S_+ and S_- on $|a, b\rangle$ leaves the eigenvalue of S^2 unchanged. An we got from $|a, b_{\text{top}}(a)\rangle$ to $|a, b_{\text{bot}}(a)\rangle$ by applying the lowering operator many times. So the value of a is the same for the two kets.

Therefore $b_{\text{top}}(a)(b_{\text{top}}(a) + \hbar) = b_{\text{bot}}(a)(b_{\text{bot}}(a) - \hbar)$.

This equation has two solutions: $b_{\text{bot}}(a) = b_{\text{top}}(a) + \hbar$, and $b_{\text{bot}}(a) = -b_{\text{top}}(a)$.

But $b_{\text{bot}}(a)$ must be smaller than $b_{\text{top}}(a)$, so only the second solution works. Therefore $b_{\text{bot}}(a) = -b_{\text{top}}(a)$.

Hence b, which is the eigenvalue of S_z, ranges from $-b_{\text{top}}(a)$ to $b_{\text{top}}(a)$. Furthermore, since S_- lowers this value by $\hbar$ each time it is applied, these two values must differ by an integer multiple of $\hbar$. Therefore $b_{\text{top}}(a) - (-b_{\text{top}}(a)) = N\hbar$ for some N. So $b_{\text{top}}(a) = \frac{N}{2}\hbar$.

Hence $b_{\text{top}}(a)$ is an integer or half integer multiple of $\hbar$.

Now we'll define two variables called s and m, which will be very important in our notation later on.

Let's define $s \equiv \frac{b_{\text{top}}(a)}{\hbar}$. Then $s = \frac{N}{2}$, so s can be any integer or half integer.

And let's define $m \equiv \frac{b}{\hbar}$. Then m ranges from $-s$ to s. For instance, if $b_{\text{top}}(a) = frac32\hbar$, then $s = \frac{3}{2}$ and m can equal $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}$, or $\frac{3}{2}$.

Then:

$$a = \hbar^2 s(s+1) b = \hbar m$$

Since a is completely determined by s, and b is completely determined by m, we can label our kets as $|s,m\rangle$ (instead of $|a,b\rangle$) without any ambiguity. For instance, the ket $|s,m\rangle = |2,1\rangle$ is the same as the ket $|a,b\rangle = |6\hbar^2,\hbar\rangle$.

In fact, all physicists label spin kets with s and m, not with a and b. (The letters s and m are standard notation, but a and b are not.) We will use the standard $|s,m\rangle$ notation from now on.

For each value of s, there is a family of allowed values of m, as we proved. Here they are:

(table omitted for now)

<u>Fact of Nature</u>: Every fundamental particle has its own special value of "s" and can have *no other*. "m" can change, but "s" does not.

If s is an integer, than the particle is a boson. (Like photons; $s = 1$)

If s is a half-integer, then the particle is a fermion. (like electrons, $s = \frac{1}{2}$)

So, which spin s is best for qubits? Spin $\frac{1}{2}$ sounds good, because it allows for two states: $m = -\frac{1}{2}$ and $\mathbf{m} = \frac{1}{2}$.

The rest of this lecture will only concern spin-$\frac{1}{2}$ particles. (That is, particles for which $s = \frac{1}{2}$).

The two possible spin states $|s,m\rangle$ are then $|\frac{1}{2},\frac{1}{2}\rangle$ and $|\frac{1}{2},-\frac{1}{2}\rangle$.

Since the s quantum number doesn't change, we only care about $m = \pm\frac{1}{2}$.

Possible labels for the two states ($m = \pm\frac{1}{2}$):

$$\begin{array}{cc} |\frac{1}{2},\frac{1}{2}\rangle & |\frac{1}{2},-\frac{1}{2}\rangle \\ |+\rangle & |-\rangle \\ |0\rangle & |1\rangle \end{array}$$

All of these labels are frequently used, but let's stick with $|0\rangle, |1\rangle$, since that's the convention in this class.

<u>Remember</u>: $|0\rangle = |\uparrow\rangle =$ state representing ang. mom. w/ z-comp. up
$|1\rangle = |\downarrow\rangle =$ state representing ang. mom. w/ z-comp. down

So we have derived the eigenvectors and eigenvalues of the spin for a spin-$\frac{1}{2}$ system, like an electron or proton:

$|0\rangle$ and $|1\rangle$ are simultaneous eigenvectors of S^2 and S_z.

$$
\begin{aligned}
S^2|0\rangle &= \hbar^2 s(s+1)|0\rangle = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)|0\rangle = \frac{3}{4}\hbar^2|0\rangle \\
S^2|1\rangle &= \hbar^2 s(s+1)|1\rangle = \frac{3}{4}\hbar^2|1\rangle \\
S_z|0\rangle &= \hbar m|0\rangle = \frac{1}{2}\hbar|0\rangle \\
S_z|1\rangle &= \hbar m|1\rangle = -\frac{1}{2}\hbar|0\rangle
\end{aligned}
$$

<u>Results of measurements</u>:

$S^2 \rightarrow \frac{3}{4}\hbar^2, S_z \rightarrow +\frac{\hbar}{2}, -\frac{\hbar}{2}$

Since S_z is a Hamiltonian operator, $|0\rangle$ and $|1\rangle$ from an orthonormal basis that spans the spin-$\frac{1}{2}$ space, which is isomorphic to $\mathscr{C}^{\in}$.

So the most general spin $\frac{1}{2}$ state is $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$.

<u>Question</u>: How do we represent the spin operators (S^2, S_x, S_y, S_z) in the 2-d basis of the S_z eigenstates $|0\rangle$ and $|1\rangle$?

<u>Answer</u>: They are matrices. Since they act on a two-dimensional vectors space, they must be 2-d matrices. We must calculate their matrix elements:

$$
S^2 = \begin{matrix} s^2_{11} & s^2_{12} \\ s^2_{21} & s^2_{22} \end{matrix}, S_z = \begin{matrix} s_{z11} & s_{z12} \\ s_{z21} & s_{z22} \end{matrix}, S_x = \begin{matrix} s_{x11} & s_{x12} \\ s_{x21} & s_{x22} \end{matrix}, \text{ etc. } (S_y)
$$

<u>Calculate S^2 matrix</u>: We must sandwich S^2 between all possible combinations of basis vector. (This is the usual way to construct a matrix!)

$$
\begin{aligned}
s^2_{11} &= \langle 0|S^2|0\rangle = \langle 0|\frac{3}{4}\hbar^2|0\rangle = \frac{3}{4}\hbar^2 \\
s^2_{12} &= \langle 0|S^2|1\rangle = \langle 0|\frac{3}{4}\hbar^2|1\rangle = 0 \\
s^2_{21} &= \langle 1|S^2|0\rangle = \langle 1|\frac{3}{4}\hbar^2|0\rangle = 0 \\
s^2_{22} &= \langle 1|S^2|1\rangle = \langle 1|\frac{3}{4}\hbar^2|1\rangle = \frac{3}{4}\hbar^2
\end{aligned}
$$

So $S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Find the S_z matrix:

$$
\begin{aligned}
s^2_{z11} &= \langle 0|S_z|0\rangle = \langle 0| + \frac{\hbar}{2}|0\rangle = \frac{\hbar}{2} \\
s^2_{z12} &= \langle 0|S_z|1\rangle = \langle 0| - \frac{\hbar}{2}|1\rangle = 0 \\
s^2_{z21} &= \langle 1|S_z|0\rangle = \langle 1| + \frac{\hbar}{2}|0\rangle = 0 \\
s^2_{z22} &= \langle 1|S_z|1\rangle = \langle 1| - \frac{\hbar}{2}|1\rangle = -\frac{\hbar}{2}
\end{aligned}
$$

So $S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Find S_x matrix: This is more difficult

What is $S_{x11} = \langle 0|S_x|0\rangle$? $|0\rangle$ is not an eigenstate of S_z, so it's not trivial.

Use raising and lowering operators: $S_\pm = S_x \pm iS_y$

$\Rightarrow S_x = \frac{1}{2}(S_+ + S_-), S_y = \frac{1}{2i}(S_+ - S_-)$

$\Rightarrow S_{x11} = \langle 0|\frac{1}{2}(S_+ + S_-)|0\rangle \Rightarrow S_+|0\rangle = 0$, since $|0\rangle$ is the highest S_z state.

But what is $S_-|0\rangle$? Since S_- is the lowering operator, we know that $S_-|0\rangle \propto |1\rangle$. That is $S_-|0\rangle = A_-|1\rangle$ for some complex number A_- which we have yet to determine. Similarly, $S_+|1\rangle = A_+|0\rangle$.

Question: What is A_-?

(This is a homework problem.)

Answer:

$$
\begin{aligned}
A_+ &= \hbar\sqrt{s(s+1) - m(m+1)} \rightarrow S_+|s,m\rangle = A_+|s,m+1\rangle \\
A_- &= \hbar\sqrt{s(s+1) - m(m-1)} \rightarrow S_-|s,m\rangle = A_-|s,m-1\rangle
\end{aligned}
$$

So

$$
\begin{aligned}
S_+|0\rangle &= 0 \\
S_+|1\rangle &= \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1) - (-\frac{1}{2})(-\frac{1}{2}+1)}|0\rangle = \hbar|0\rangle \\
S_-|0\rangle &= \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1) - (\frac{1}{2})(\frac{1}{2}-1)}|1\rangle = \hbar|1\rangle \\
S_-|1\rangle &= 0
\end{aligned}
$$

$\Rightarrow S_{x11} = \frac{1}{2}\langle 0|(S_+ + S_-)|0\rangle = \frac{1}{2}\langle 0|[S_+|0\rangle + S_-|0\rangle]$

$$
\begin{aligned}
S_{x11} &= \frac{1}{2}\langle 0|\,[0+\hbar|1\rangle\,] = 0 \\
S_{x12} &= \langle 0|\,\frac{1}{2}(S_+ + S_-)|1\rangle = \frac{1}{2}\langle 0|\,[\hbar|0\rangle + 0] = \frac{\hbar}{2} \\
S_{x21} &= \langle 1|\,\frac{1}{2}(S_+ + S_-)|0\rangle = \frac{1}{2}\langle 1|\,[0+\hbar|1\rangle\,] = \frac{\hbar}{2} \\
S_{x22} &= \langle 1|\,\frac{1}{2}(S_+ + S_-)|1\rangle = \frac{1}{2}\langle 1|\,[\hbar|0\rangle + 0] = 0
\end{aligned}
$$

So $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Find S_y matrix: Use $S_y = \frac{1}{2i}(S_+ - S_-)$

Homework: find the $S_{y11}, S_{y12}, S_{y21}, S_{y22}$ matrix elements.

Answer: $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Define

$$
\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
$$

$S^2 = \frac{3}{4}\hbar^2\sigma_0, S_x = \frac{\hbar}{2}\sigma_1, S_y = \frac{\hbar}{2}\sigma_2, S_z = \frac{\hbar}{2}\sigma_3$

$\sigma_0, \sigma_1, \sigma_2, \sigma_3$ are called the Pauli Spin Matrices. They are very important for understanding the behavior of two-level systems.
