

SPIN ONE-HALF AND THE PAULI SPIN MATRICES

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In our introduction to spin, we saw that spin is an intrinsic, fixed quantity for each elementary particle. It doesn't really have a classical analogue, as it is not the result of any motion of the particle. Despite that, spin really *is* a form of angular momentum, as it combines with the orbital angular momentum \mathbf{L} to form a total angular momentum for a given particle. It seems that elementary particles (at least those with non-zero spin) just have an intrinsic angular momentum that is fixed, depending on the type of particle.

The lack of analogy with classical angular momentum extends to the fact that spin does not depend on spatial coordinates. As such, the eigenfunctions of the spin operators are not functions of position, so we don't need to worry about Hilbert space, or their behaviour at infinity or any of those things that make the other quantum operators so tricky (and interesting, it has to be said) to deal with.

We've seen that the eigenvalues of the square of the total spin S^2 are $\hbar^2 s(s+1)$, where s is any non-negative integer or half-integer. If $s = 0$, no spin is present and there isn't anything more to say. The simplest non-trivial case is therefore $s = \frac{1}{2}$. In this case, the eigenvalues of s_z are $\pm\frac{1}{2}$, so there are only 2 possible states. Since the spin of a particle is fixed, a particle with $s = \frac{1}{2}$ can exist *only* in a linear combination of these 2 states, no matter how much you poke it or excite it by passing electric fields through it or do anything else to it.

How does this affect the Schrödinger equation? After all, it involves derivatives with respect to both time and position, so if we're dealing with a system that makes no use of position, does that mean that the $-\hbar^2\nabla^2\Psi/2m$ is zero? If that were the case then the time derivative would also be zero, and it would seem to indicate that any particle's spin state would never change.

This isn't the case, and the reason is that we need to step back a bit in our interpretation of the Schrödinger equation. The term $-\hbar^2\nabla^2\Psi/2m$ is based on our taking the energy of the system as $p^2/2m$ and then translating the momentum into its quantum operator form. In the case of spin, we need to write the energy (or more precisely, the Hamiltonian) in terms of the spin, so the spatial derivative is replaced by a term involving the spin variables,

while the time derivative remains as it is. We'll see some examples of this in due course; for now, just be assured that the Schrödinger equation *does* still work in systems involving spin.

Returning to spin $\frac{1}{2}$, since we are allowed only 2 states, we can use a 2-dimensional vector to represent the state of a particle. These vectors form a vector space, and we can take the basis of this space to be the two stationary states, commonly called spin up and spin down. We represent these two stationary states as

$$\chi_+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \quad \chi_- = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (1)$$

We could, of course, have chosen any two independent vectors as the basis, but these two make life simpler.

With this definition, a general spin state of a spin $\frac{1}{2}$ particle is a linear combination of these two states:

$$\chi = a\chi_+ + b\chi_- = \begin{bmatrix} a \\ b \end{bmatrix} \quad (2)$$

Since the state of a particle is now a 2-dimensional vector, any operator that operates on such a vector must be a matrix. Since we want the spin operators to have eigenvalues, these matrixes must be 2×2 . We can work out the S^2 matrix since we know that its eigenvalues must both be $\hbar^2 s(s+1) = 3\hbar^2/4$ from above. By specifying the basis above, we have effectively specified the eigenvectors of S^2 , so we get

$$S^2\chi_+ = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{3\hbar^2}{4} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (3)$$

from which we get

$$s_{11} = \frac{3\hbar^2}{4} \quad (4)$$

$$s_{21} = 0 \quad (5)$$

with the other two elements undetermined, so far.

Applying the same logic to the other eigenvector gives us

$$s_{12} = 0 \quad (6)$$

$$s_{22} = \frac{3\hbar^2}{4} \quad (7)$$

Thus

$$S^2 = \frac{3\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (8)$$

Incidentally, since the eigenvalues of S^2 are degenerate (both the same), then any linear combination of the two eigenvectors that we've used above is also an eigenvector, which is just another way of saying that we could have chosen any two independent vectors to represent the two stationary states.

We can do a similar calculation for S_z , since we know that

$$S_z \chi_+ = \frac{\hbar}{2} \chi_+ \quad (9)$$

$$S_z \chi_- = -\frac{\hbar}{2} \chi_- \quad (10)$$

This gives

$$S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (11)$$

How about S_x and S_y ? Since the raising and lowering operators that we derived for orbital angular momentum depended only on the commutators, we can write similar definitions for spin. In particular

$$S_+ = S_x + iS_y \quad (12)$$

$$S_- = S_x - iS_y \quad (13)$$

The action of these operators on a stationary state is also the same as for **L**:

$$S_{\pm} |s m_s\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)} |s m_s \pm 1\rangle \quad (14)$$

We can invert the relations above and get

$$S_x = \frac{1}{2} (S_+ + S_-) \quad (15)$$

$$S_y = \frac{1}{2i} (S_+ - S_-) \quad (16)$$

Then we can apply these operators to the stationary states to get

$$S_x \left| \frac{1}{2} \frac{1}{2} \right\rangle = \frac{1}{2} (S_+ + S_-) \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (17)$$

$$S_x \left| \frac{1}{2} -\frac{1}{2} \right\rangle = \frac{1}{2} (S_+ + S_-) \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (18)$$

From this we get

$$S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (19)$$

A similar calculation gives us S_y :

$$S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad (20)$$

It is usual to extract the factor of $\hbar/2$ from these three matrixes and define $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ with

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (21)$$

These are called the *Pauli spin matrices*.

The commutation relations can be verified by direct calculation, so we give only one as an example.

$$[S_x, S_y] = \frac{\hbar^2}{4} \left[\begin{pmatrix} i0 \\ 0-i \end{pmatrix} - \begin{pmatrix} -i0 \\ 0i \end{pmatrix} \right] \quad (22)$$

$$= \frac{\hbar^2}{2} i \begin{pmatrix} 10 \\ 0-1 \end{pmatrix} \quad (23)$$

$$= i\hbar S_z \quad (24)$$

By direct calculation, we can show that

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (25)$$

Also, by direct calculation we see that

$$\sigma_j \sigma_k = i\sigma_l = -\sigma_k \sigma_j \quad (26)$$

if jkl is a forward permutation of x, y, z (that is, jkl is one of xyz, yzx or zxy). These results can be combined into the formula

$$\sigma_j \sigma_k = \delta_{jk} + i \sum_l \epsilon_{jkl} \sigma_l \quad (27)$$

where ϵ_{jkl} is the Levi-Civita symbol, which is +1 if jkl is a forward permutation of xyz , -1 if jkl is a non-forward permutation of xyz and 0 if any two of jkl are equal.

If $j \neq k$ only one term in the sum is non-zero, while if $j = k$ all terms in the sum are zero.

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