Spin

In classical mechanics angular motion can be decomposed into the orbital part ($\vec{L} = \vec{r} \times \vec{p}$) associated with the motion of the center of mass, and spin ($\vec{S} = I\vec{\omega}$) associated with the motion about the center of mass. Something analogues takes place in quantum mechanis. The difference, however, is this "spin" motion is intrinsic and has nothing to do with motion in space. Spin is thus an intrinsic property of all elementary particles.

The idea of spin was introduced in physics in 1925 be Uhlenbeck and Goudsmit, who came to realize about the existence of spin based on the analysis of the experimental facts. In particular, the existence of spin followed from the experiment of Stern and Gerlach, where a splitting of a beam of atoms occurs. For example, both orbital and magnetic moments of an electron in the ground state of hydrogen equal to zero. At the same time a beams of H-atoms split into two in nonhomogenеіe magnetic field, indicating two possible projections of the intrinsic magnetic moment. The experiments had shown that the absolute value of this moment is equal to μ_B:

$$\mu_B = \underbrace{\frac{e\hbar}{2m_e c}}_{\text{Gaussian units}} = \underbrace{\frac{e\hbar}{2m_e}}_{\text{SI units}}$$

The hyphotesis of spin allows to explain the experimental observations in a simple way

The algebraic theory of spin is the same as that of the orbital angular momentum and is based on the fundamental commutation relations:

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \quad \text{or more generally} \quad [\hat{S}_i, \hat{S}_j] = i\hbar \varepsilon_{ijk} \hat{S}_k$$

The eigenvectors and eigenvalues of S^2 and S_z are

$$\hat{S}^2 |sm\rangle = \hbar^2 s(s+1) |sm\rangle \qquad \hat{S}_z |sm\rangle = \hbar m |sm\rangle$$

Lastly the action of the raising/lowering operator is

$$\hat{S}_\pm |sm\rangle = \hbar \sqrt{s(s+1) - m(m\pm 1)}\; |s\,(m\pm 1)\rangle \qquad \hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$$

s may take both integer and half-integer values

While all particles posses spin ($0, \frac{1}{2}$, or something else) the most important case from practical point of view is $s = 1/2$. Many particles have $s = 1/2$. Also, this is the simplest case for the theoretical consideration. All spin operators in case $s = 1/2$ can be represented by 2×2 matrices, while the eigenstates are two-component objects called spinors.

$$\left.\begin{aligned} |s=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle &\equiv |\tfrac{1}{2}\tfrac{1}{2}\rangle \equiv |\uparrow\rangle \equiv |\alpha\rangle \\ |s=\tfrac{1}{2}, m=-\tfrac{1}{2}\rangle &= |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = |\downarrow\rangle \equiv |\beta\rangle \end{aligned}\right\} \text{ usual notations for spin eigenstates}$$

A general state, χ, can be written as

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a|\uparrow\rangle + b|\downarrow\rangle$$

For $\hat{S}^2$ matrix we have:

$$\begin{pmatrix} S^2_{11} & S^2_{12} \\ S^2_{21} & S^2_{22} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} S^2_{11} & S^2_{12} \\ S^2_{21} & S^2_{22} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Solving for S^2_{ij} yields the following

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

Similarly

$$\begin{pmatrix} S_{z_{11}} & S_{z_{12}} \\ S_{z_{21}} & S_{z_{22}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} S_{z_{11}} & S_{z_{12}} \\ S_{z_{21}} & S_{z_{22}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and

$$\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Lastly,

$$\hat{S}_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{S}_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \hat{S}_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{S}_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

and

$$\hat{S}_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \hat{S}_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Since $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ $\quad \hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$ $\quad \hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-)$ we get the explicit matrix form of $\hat{S}_x$ and $\hat{S}_y$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

For simplicity of notations Pauli spin matrices are often adopted:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

so that

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$ (which stand for $\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x$ $\hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y$ $\hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$)

For a general state $\chi = \begin{pmatrix} a \\ b \end{pmatrix}$ $|a|^2$ gives the probability of observing $m = \frac{\hbar}{2}$, while $|b|^2$ gives the probability of observing $m = -\frac{\hbar}{2}$ state. $|a|^2 + |b|^2 = 1$

Properties of the Pauli matrices.

As the operators corresponding to different components of spin obey the fundamental commutation relations,

$$[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk}\hbar \hat{S}_k$$

so do the Pauli matrices (recall that $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$):

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\varepsilon_{ijk}\hat{\sigma}_k$$

The eigenvalues of $\hat{\sigma}_i$ are ± 1. The eigenvectors of σ_z that correspond to $\pm\frac{\hbar}{2}$ projection of spin on the z-axis are

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The eigenvectors of σ_x and σ_y can be expressed as a linear combination of $|\uparrow\rangle$ and $|\downarrow\rangle$

In addition of the above commutation relations, the Pauli matrices possess some other important properties.

Since the eigenvalues of $\hat{\sigma}_i$ are ± 1, the eigenvalues of $\hat{\sigma}_i^2$ are $+1$ (twice degenerate). In their own basis $\hat{\sigma}_i^2$ are the identity matrices

$$\hat{\sigma}_i^2 = \hat{1}$$

(recall that the identity matrix remains the identity matrix in any representation)

Indeed, this can be easily verified using the explicit matrix form:

$$\hat{\sigma}_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\sigma}_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\sigma}_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Therefore in any representation $\hat{\sigma}_i^2 = \hat{1}$.

Using the commutation relations and the fact that $\hat{\sigma}_i^2 = \hat{1}$ we can show that $\hat{\sigma}_i$ and $\hat{\sigma}_j$ anticommute:

$$\hat{\sigma}_i \hat{\sigma}_j - \hat{\sigma}_j \hat{\sigma}_i = 2i\, \varepsilon_{ijk} \hat{\sigma}_k$$

Multiplying by $\hat{\sigma}_i$ from the left/right yields:

$$\underbrace{\hat{\sigma}_i^2}_{1} \hat{\sigma}_j - \hat{\sigma}_i \hat{\sigma}_j \hat{\sigma}_i = 2i\, \varepsilon_{ijk} \hat{\sigma}_i \hat{\sigma}_k$$

$$\hat{\sigma}_i \hat{\sigma}_j \hat{\sigma}_i - \hat{\sigma}_j \underbrace{\hat{\sigma}_i^2}_{1} = 2i\, \varepsilon_{ijk} \hat{\sigma}_k \hat{\sigma}_i$$

When we add the two lines we get:

$$0 = 2i\, \varepsilon_{ijk} (\hat{\sigma}_i \hat{\sigma}_k + \hat{\sigma}_k \hat{\sigma}_i) \qquad i \neq k$$

Thus,

$$\{\hat{\sigma}_i, \hat{\sigma}_k\} \equiv \hat{\sigma}_i \hat{\sigma}_k + \hat{\sigma}_k \hat{\sigma}_i = 0 \qquad \text{when } i \neq k$$

Or, more generally,

$$\{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\, \delta_{ij} \hat{1}$$

We can also see that

$$\hat{\sigma}_i \hat{\sigma}_j = \delta_{ij} \hat{1} + i\, \varepsilon_{ijk} \hat{\sigma}_k$$

This is because

$$\hat{\sigma}_j \hat{\sigma}_i + \hat{\sigma}_i \hat{\sigma}_j = 2\delta_{ij} \hat{1}$$

$$\underbrace{\hat{\sigma}_j \hat{\sigma}_i - \hat{\sigma}_i \hat{\sigma}_j}_{-2i\, \varepsilon_{ijk} \hat{\sigma}_k} + \underbrace{\hat{\sigma}_i \hat{\sigma}_j + \hat{\sigma}_i \hat{\sigma}_j}_{2\hat{\sigma}_i \hat{\sigma}_j} = 2\delta_{ij} 1$$

$$\hat{\sigma}_i \hat{\sigma}_j = \delta_{ij} \hat{1} + i\, \varepsilon_{ijk} \hat{\sigma}_k$$

The importance of the latter formula lies in the fact that any product of $\hat{\sigma}_i$ operators, $\sigma_i \sigma_j \ldots \sigma_k$, can be linearized.

Let us note that the commutation relations $[\hat{S}_i, \hat{S}_j] = i\varepsilon_{ijk}\hat{S}_k$ hold true for any value of spin/angular momentum, while the anticommutation relations $\{\sigma_i, \sigma_k\} = 2\delta_{ik}\hat{1}$ take place for the case of $S=\frac{1}{2}$ only.

The possibility to linearize any product $\sigma_i \ldots \sigma_k$ implies that any function of $a\hat{1} + \vec{b}\cdot\vec{\sigma}$ can be written in terms of $\hat{1}$ and $\vec{b}\vec{\sigma}$, where $\vec{b}$ is an arbitrary vector. This is because any "nice" function can be expressed through its Taylor series. Thus,

$$F(a\hat{1} + \vec{b}\vec{\sigma}) = A\hat{1} + B\,\vec{n}\cdot\vec{\sigma}$$

where A and B are constants

This can also be realized if we recall that σ_i and $\hat{1}$ are 2×2 matrices. Thus, four of them form a "complete set" of matrices. Any 2×2 matrix (including any function of a 2×2 matrix) can be expressed as a linear combination of $\hat{1}$ and $\hat{\sigma}_i$'s.