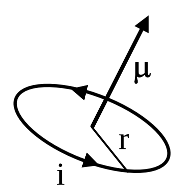
Spin ½

Recall that in the H-atom solution, we showed that the fact that the wavefunction Ψ(r) is single-valued requires that the angular momentum quantum nbr be integer: ℓ = 0, 1, 2.. However, operator algebra allowed solutions ℓ = 0, 1/2, 1, 3/2, 2…

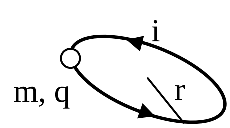
Experiment shows that the electron possesses an intrinsic angular momentum called *spin* with ℓ = ½. By convention, we use the letter s instead of ℓ for the spin angular momentum quantum number : s = ½. The existence of spin is not derivable from non-relativistic QM. It is not a form of orbital angular momentum; it cannot be derived from $\vec{L} = \vec{r} \times \vec{p}$. (The electron is a point particle with radius r = 0.)

Electrons, protons, neutrons, and quarks all possess spin s = ½. Electrons and quarks are elementary point particles (as far as we can tell) and have no internal structure. However, protons and neutrons are made of 3 quarks each. The 3 half-spins of the quarks add to produce a total spin of ½ for the composite particle (in a sense, ↑↑↓ makes a single ↑). Photons have spin 1, mesons have spin 0, the delta-particle has spin 3/2. The graviton has spin 2. (Gravitons have not been detected experimentally, so this last statement is a theoretical prediction.)

Spin and Magnetic Moment



We can detect and measure spin experimentally because the spin of a charged particle is always associated with a magnetic moment. Classically, a magnetic moment is defined as a vector **μ** associated with a loop of current. The direction of **μ** is perpendicular to the plane of the current loop (right-hand-rule), and the magnitude is $\mu = i\,A = i\,\pi r^2$. The connection between orbital angular momentum (not spin) and magnetic moment can be seen in the following classical model: Consider a particle with mass m, charge q in circular orbit of radius r, speed v, period T.



$$i = \frac{q}{T}\,, \qquad v = \frac{2\pi r}{T} \quad \Rightarrow \quad i = \frac{q v}{2\pi r} \qquad \mu = i\,A = \left(\frac{q v}{2 \cancel{\pi} \cancel{r}}\right)\left(\cancel{\pi} r^{\cancel{2}}\right) = \frac{q v r}{2}$$

| angular momentum | = L = p r = m v r , so v r = L/m , and $\mu = \frac{q v r}{2} = \frac{q}{2m} L$.

So for a classical system, the magnetic moment is proportional to the orbital angular momentum: $\boxed{\vec{\mu} = \frac{q}{2m}\vec{L} \quad \text{(orbital)}}$. The same relation holds in a quantum system.

In a magnetic field B, the energy of a magnetic moment is given by

$E = -\vec{\mu}\cdot\vec{B} = -\mu_z B$ (assuming $\vec{B} = B\hat{z}$). In QM, $L_z = \hbar m$. Writing electron mass as m_e (to avoid confusion with the magnetic quantum number m) and q = –e we have

$\mu_z = -\frac{e\hbar}{2m_e} m$, where m = $-\ell$ .. $+\ell$. The quantity $\mu_B \equiv \frac{e\hbar}{2m_e}$ is called the Bohr magneton. The possible energies of the magnetic moment in $\vec{B} = B\hat{z}$ is given by

$E_{orb} = -\mu_z B = -\mu_B B m$.

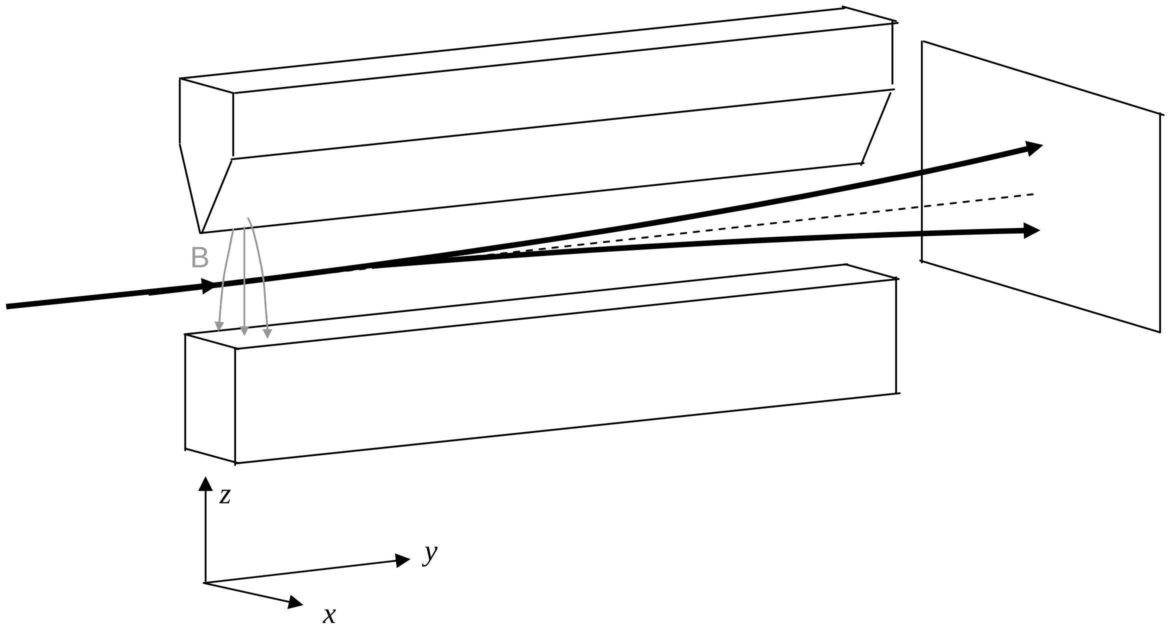
For *spin* angular momentum, it is found experimentally that the associated magnetic moment is twice as big as for the orbital case: $\boxed{\vec{\mu} = \frac{q}{m}\vec{S} \quad \text{(spin)}}$ (We use S instead of L when referring to spin angular momentum.) This can be written

$\mu_z = -\frac{e\hbar}{m_e} m = -2\mu_B m$. The energy of a spin in a field is $E_{spin} = -2\mu_B B m$ (m = ±1/2) a fact which has been verified experimentally. The existence of spin (s = ½) and the strange factor of 2 in the gyromagnetic ratio (ratio of $\vec{\mu}$ to $\vec{S}$) was first deduced from spectrographic evidence by Goudsmit and Uhlenbeck in 1925.

Another, even more direct way to experimentally determine spin is with a Stern-Gerlach device, next page

(This page from QM notes of Prof. Roger Tobin, Physics Dept, Tufts U.)

Stern-Gerlach Experiment (W. Gerlach & O. Stern, Z. Physik **9**, 349-252 (1922).



$\vec{F} = -\vec{\nabla}\left(\vec{\mu} \bullet \vec{B}\right) = -\vec{\mu} \bullet \vec{\nabla}\vec{B}$ $\qquad$ $\vec{F} = \hat{z}\left(\mu_z \frac{\partial B_z}{\partial z}\right)$

Deflection of atoms in z-direction is proportional to z-component of magnetic moment μ_z, which in turn is proportional to L_z. The fact that there are two beams is proof that ℓ = s = ½. The two beams correspond to m = +1/2 and m = –1/2. If ℓ = 1, then there would be three beams, corresponding to m = –1, 0, 1. The separation of the beams is a direct measure of μ_z, which provides proof that $\mu_z = -2\mu_B m$

The extra factor of 2 in the expression for the magnetic moment of the electron is often called the "g-factor" and the magnetic moment is often written as $\mu_z = -g\mu_B m$. As mentioned before, this cannot be deduced from non-relativistic QM; it is known from experiment and is inserted "by hand" into the theory. However, a relativistic version of QM due to Dirac (1928, the "Dirac Equation") predicts the existence of spin (s = ½) and furthermore the theory predicts the value g = 2. A later, better version of relativistic QM, called Quantum Electrodynamics (QED) predicts that g is a little larger than 2. The g-factor has been carefully measured with fantastic precision and the latest experiments give g = 2.0023193043718(±76 in the last two places). Computing g in QED requires computation of a infinite series of terms that involve progressively more messy integrals, that can only be solved with approximate numerical methods. The computed value of g is not known quite as precisely as experiment, nevertheless the agreement is good to about 12 places. QED is one of our most well-verified theories.

Spin Math

Recall that the angular momentum commutation relations

$[L^2, L_z] = 0$, $[L_i , L_j] = i\hbar L_k$ (i j k cyclic)

were derived from the definition of the orbital angular momentum operator: $\vec{L} = \vec{r} \times \vec{p}$.

The spin operator $\vec{S}$ does not exist in Euclidean space (it doesn't have a position or momentum vector associated with it), so we cannot derive its commutation relations in a similar way. Instead we boldly ***postulate*** that the same commutation relations hold for spin angular momentum:

$[S^2, S_z] = 0$, $[S_i , S_j] = i\hbar S_k$. From these, we derive, just a before, that

$$S^2 \left| s\, m_s \right\rangle = \hbar^2 s(s+1) \left| s\, m_s \right\rangle = \frac{3}{4}\hbar^2 \left| s\, m_s \right\rangle \qquad (\text{ since } s = ½)$$

$$S_z \left| s\, m_s \right\rangle = \hbar m_s \left| s\, m_s \right\rangle = \pm\frac{1}{2}\hbar \left| s\, m_s \right\rangle \qquad (\text{ since } m_s = -s ,+s = -1/2, +1/2)$$

Notation: since s = ½ always, we can drop this quantum number, and specify the eigenstates of L^2 , L_z by giving only the m_s quantum number. There are various ways to write this: $\left| s\, m_s \right\rangle = \left| m_s \right\rangle = \begin{matrix} \left|+\tfrac{1}{2}\right\rangle , \left|-\tfrac{1}{2}\right\rangle \\ \left|+\right\rangle , \left|-\right\rangle \\ \left|\uparrow\right\rangle , \left|\downarrow\right\rangle \end{matrix}$

These states exist in a 2D subset of the full Hilbert Space called *spin space*. Since these two states are eigenstates of a hermitian operator, they form a complete orthonormal set (within their part of Hilbert space) and any, arbitrary state in spin space can always be written as $|\chi\rangle = a|\uparrow\rangle + b|\downarrow\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ (Griffiths' notation is $\chi = a\chi_+ + b\chi_-$)

Matrix notation: $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Note that $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$, $\langle\uparrow|\downarrow\rangle = 0$

If we were working in the full Hilbert Space of, say, the H-atom problem, then our basis states would be $|n\ \ell\ m_\ell\ m_s\rangle$. Spin is another degree of freedom, so that the full specification of a basis state requires 4 quantum numbers. (More on the connection between spin and space parts of the state later.)

[Note on language: throughout this section I will use the symbol S_z (and S_x , etc) to refer to both the observable ("the measured value of S_z is $+\hbar/2$") and its associated operator ("the eigenvalue of S_z is $+\hbar/2$").]

The matrix form of S^2 and S_z in the $|m^{(z)}\rangle$ basis can be worked out element by element. (Recall that for any operator $\hat{A}$, $A_{mn} = \langle m|\hat{A}|n\rangle$.)

$$\langle\uparrow|S^2|\uparrow\rangle = \frac{3}{4}\hbar^2,\quad \langle\uparrow|S^2|\downarrow\rangle = 0,\ \text{etc.}\qquad \langle\uparrow|S_z|\uparrow\rangle = +\frac{1}{2}\hbar,\quad \langle\uparrow|S_z|\downarrow\rangle = 0,\ \text{etc.}$$

$$\boxed{S^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad S_z = \frac{1}{2}\hbar\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

Operator equations can be written in matrix form, for instance,

$$S_z|\uparrow\rangle = +\frac{\hbar}{2}|\uparrow\rangle \quad\Rightarrow\quad \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We are going ask what happens when we make measurements of S_z , as well as S_x and S_y , (using a Stern-Gerlach apparatus). Will need to know: What are the matrices for the operators S_x and S_y ? These are derived from the raising and lowering operators:

$$\begin{aligned} S_+ &= S_x + iS_y \\ S_- &= S_x - iS_y \end{aligned} \quad \Rightarrow \quad \begin{aligned} S_x &= \tfrac{1}{2}(S_+ + S_-) \\ S_y &= \tfrac{1}{2i}(S_+ - S_-) \end{aligned}$$

To get the matrix forms of S_+ , S_- , we need a result from the homework:

$$S_+|s,m_s\rangle = \hbar\sqrt{s(s+1)-m(m+1)}\;|s,\,m_s+1\rangle$$
$$S_-|s,m_s\rangle = \hbar\sqrt{s(s+1)-m(m-1)}\;|s,\,m_s-1\rangle$$

For the case s = ½, the square root factors are always 1 or 0. For instance, s = ½, m = –1/2 gives $s(s+1)-m(m+1) = \tfrac{1}{2}\left(\tfrac{3}{2}\right)-\left(-\tfrac{1}{2}\right)\left(\tfrac{1}{2}\right) = 1$. Consequently,

$S_+|\downarrow\rangle = \hbar|\uparrow\rangle$, $S_+|\uparrow\rangle = 0$ and $S_-|\uparrow\rangle = \hbar|\downarrow\rangle$, $S_-|\downarrow\rangle = 0$, leading to

$\langle\uparrow|S_+|\uparrow\rangle = 0$, $\langle\uparrow|S_+|\downarrow\rangle = \hbar$, etc. and

$$\boxed{S_+ = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \qquad S_- = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}}$$

Notice that S_+ , S_- are not hermitian.

Using $S_x = \tfrac{1}{2}(S_+ + S_-)$ and $S_y = \tfrac{1}{2i}(S_+ - S_-)$ yields

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

These are hermitian, of course.

Often written: $\vec{S} = \dfrac{\hbar}{2}\vec{\sigma}$, where $\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ are called the *Pauli spin matrices*.

Now let's make some measurements on the state $|\chi\rangle = a|\uparrow\rangle + b|\downarrow\rangle = \begin{pmatrix}a\\ b\end{pmatrix}$.

Normalization: $\langle\chi|\chi\rangle = 1 \;\Rightarrow\; |a|^2 + |b|^2 = 1$.

Suppose we measure S_z on a system in some state $|\chi\rangle = \begin{pmatrix}a\\ b\end{pmatrix}$. Postulate 2 says that the possible results of this measurement are one of the S_z eigenvalues: $+\hbar/2$ or $-\hbar/2$.

Postulate 3 says the probability of finding, say $-\hbar/2$, is

Prob(find $-\hbar/2$) $= \left|\langle\downarrow|\chi\rangle\right|^2 = \left|\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}\right|^2 = |b|^2$. Postulate 4 says that, as a result of this measurement, which found $-\hbar/2$, the initial state $|\chi\rangle$ collapses to $|\downarrow\rangle$.

But suppose we measure S_x? (Which we can do by rotating the SG apparatus.) What will we find? Answer: one of the eigenvalues of S_x, which we show below are the same as the eigenvalues of S_z: $+\hbar/2$ or $-\hbar/2$. (Not surprising, since there is nothing special about the z-axis.) What is the probability that we find, say, $S_x = +\hbar/2$? To answer this we need to know the eigenstates of the S_x operator. Let's call these (so far unknown) eigenstates $|\uparrow^{(x)}\rangle$ and $|\downarrow^{(x)}\rangle$ (Griffiths calls them $|\chi_+^{(x)}\rangle$ and $|\chi_-^{(x)}\rangle$). How do we find these? We must solve the eigenvalue equation:

$S_x|\chi\rangle = \lambda|\chi\rangle$, where λ are the unknown eigenvalues. In matrix form this is,

$\begin{pmatrix}0 & \hbar/2\\ \hbar/2 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \lambda\begin{pmatrix}a\\ b\end{pmatrix}$ which can be rewritten $\begin{pmatrix}-\lambda & \hbar/2\\ \hbar/2 & -\lambda\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = 0$. In linear algebra, this last equation is called the characteristic equation.

This system of linear equations only has a solution if

$$\mathrm{Det}\begin{pmatrix}-\lambda & \hbar/2\\ \hbar/2 & -\lambda\end{pmatrix} = \begin{vmatrix}-\lambda & \hbar/2\\ \hbar/2 & -\lambda\end{vmatrix} = 0.\ \text{ So } \lambda^2 - (\hbar/2)^2 = 0 \quad \Rightarrow \quad \lambda = \pm\hbar/2$$

As expected, the eigenvalues of S_x are the same as those of S_z (or S_y).

Now we can plug in each eigenvalue and solve for the eigenstates:

$$\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}a\\ b\end{pmatrix} \Rightarrow a = b \quad ; \quad \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}a\\ b\end{pmatrix} \Rightarrow a = -b.$$

So we have $|\uparrow^{(x)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$ and $|\downarrow^{(x)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$

Now back to our question: Suppose the system in the state $\left|\uparrow^{(z)}\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and we measure S_x. What is the probability that we find, say, $S_x = +\hbar/2$? Postulate 3 gives the recipe for the answer:

$$\text{Prob(find } S_x = +\hbar/2) = \left|\left\langle \uparrow^{(x)} \middle| \uparrow^{(z)} \right\rangle\right|^2 = \left|\tfrac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right|^2 = \left|\tfrac{1}{\sqrt{2}}\right|^2 = 1/2$$

Question for the student: Suppose the initial state is an arbitrary state $\left|\chi\right\rangle = \begin{pmatrix}a\\b\end{pmatrix}$ and we measure S_x. What are the probabilities that we find $S_x = +\hbar/2$ and $-\hbar/2$?

Let's review the strangeness of Quantum Mechanics.

Suppose an electron is in the $S_x = +\hbar/2$ eigenstate $\left|\uparrow^{(x)}\right\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$. If we ask: What is the value of S_x? Then there is a definite answer: $+\hbar/2$. But if we ask: What is the value of S_z , then this is no answer. The system *does not possess* a value of S_z. If we measure S_z, then the act of measurement will produce a definite result and will force the state of the system to collapse into an eigenstate of S_z, but that very act of measurement will destroy the definiteness of the value of S_x. The system can be in an eigenstate of either S_x or S_z, but not both.