Spin

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Introduction

The Stern Gerlach experiment for the simplest possible atom, hydrogen in its ground state, demonstrated unambiguously that the component of the magnetic moment of the atom along the *z*-axis could only have two values. It had been well established by this time that the magnetic moment vector was along the same axis as the angular momentum. This is obviously true for the Bohr model of hydrogen, where the circulating electron is equivalent to a ring current, generating a magnetic dipole. The problem is, though, that a magnetic moment generated in this way by *orbital* angular momentum will have a *minimum* of three possible values of its *z*-component: the lowest nonzero orbital angular momentum is $l = 1,$ with allowed values of the *z*-component $m\hbar,\ m = 1, 0, -1.$

Recall, however, that in our derivation of allowed angular momentum eigenvalues from very general properties of rotation operators, we found that although for any system the allowed values of *m* form a ladder with spacing $\hbar,$ we could *not* rule out half-integral *m* values. The lowest such case, $l = 1/2,$ would in fact have just *two* allowed *m* values: $m = 1/2, -1/2.$ However, this cannot be any kind of *orbital* angular momentum because the *z*-component of the orbital wave function ψ has a factor $e^{\pm i\varphi},$ and therefore picks up a factor -1 on rotating through $2\pi,$ meaning ψ is not single-valued, which doesn't make sense for a Schrödinger wave function.

Yet the experimental result is clear. Therefore, this must be a new kind of non-orbital angular momentum. It is called "spin", the simple picture being that just as the Earth has orbital angular momentum in its yearly circle around the sun, and also spin angular momentum from its daily turning, the electron has an analogous spin. But the analogy has obvious limitations: the Earth's spin is after all made up of material orbiting around the axis through the poles, the electron's spin cannot similarly be imagined as arising from a rotating body, since *orbital* angular momenta always come in integral multiples of $\hbar.$

Fortunately, this lack of a simple quasi-mechanical picture underlying electron spin doesn't prevent us from using the general angular momentum machinery previously developed, which followed just from analyzing the effect of spatial rotation on a quantum mechanical system. Recall this led to the spacing $\hbar$ of the ladder of eigenvalues, and to values of the matrix elements of angular momentum components J_i between the eigenkets $|j,m\rangle$: enough information to construct matrix representations of the rotation operators for a system of given angular momentum. As an example, for the orbital angular momentum $j = l = 1$ state, we constructed the 3×3 matrix representation of an arbitrary rotation operator $e^{-\frac{i\vec{\theta}\cdot\vec{J}}{\hbar}}$ in the space with orthonormal basis $|1,1\rangle, |1,0\rangle, |1,-1\rangle$ (in the $|l,m\rangle$ notation). The spin $j = s = 1/2$ case can be handled in exactly the same way.

Spinors, Spin Operators, Pauli Matrices

The Hilbert space of angular momentum states for spin one-half is two dimensional. Various notations are used: $|j,m\rangle$ becomes $|s,m\rangle$ or $|s,m_s\rangle$, or even, more graphically,

$$\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle \equiv |\uparrow\rangle, \quad \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle \equiv |\downarrow\rangle.$$

Any state of the spin can be written

$$\alpha|\uparrow\rangle + \beta|\downarrow\rangle \equiv \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \text{ with } |\alpha|^2 + |\beta|^2 = 1$$

and this two-dimensional ket is called a ***spinor***.

Operators on spinors are necessarily 2×2 matrices. We shall follow the usual practice of denoting the angular momentum components J_i by S_i for spins.

From our definition of the spinor,

$$S_z = \tfrac{1}{2}\hbar\sigma_z, \text{ with } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The general formulas for raising and lowering operators

$$J_+|j,m\rangle = \sqrt{j(j+1)-m(m+1)}\hbar|j,m+1\rangle, \quad J_-|j,m\rangle = \sqrt{j(j+1)-m(m-1)}\hbar|j,m-1\rangle$$

become for $j=\tfrac{1}{2}, m=\tfrac{1}{2}$ simply

$$S_+\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = \hbar\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle, \quad S_-\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle = \hbar\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle$$

so

$$S_x + iS_y = S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_x - iS_y = S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

It follows immediately that an appropriate matrix representation for spin one-half is

$$\vec{S} = \tfrac{1}{2}\hbar\vec{\sigma}, \quad \text{where } \vec{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right).$$

These three 2×2 matrices representing the (x, y, z) spin components are called the *Pauli spin matrices*. They are hermitian, traceless, and obey

$\sigma_i^2 = I$, $\sigma_i\sigma_j = -\sigma_j\sigma_i$, and $\sigma_i\sigma_j = i\sigma_k$ for (i, j, k) a cyclic permutation of $(1,2,3)$. This can be written $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k$.

The total spin $\vec{S}^2 = \frac{1}{4}\hbar^2\vec{\sigma}^2 = \frac{3}{4}\hbar^2$.

Any 2×2 matrix can be written in the form

$$\alpha_0 I + \sum_i \alpha_i\sigma_i .$$

Exercise: prove the above statements, then use your results to show that

(a) $\left(\hat{\vec{n}}\cdot\vec{\sigma}\right)^2 = I$ for any unit vector $\hat{\vec{n}}$

(b) $\left(\vec{\sigma}\cdot\vec{A}\right)\left(\vec{\sigma}\cdot\vec{B}\right) = \left(\vec{A}\cdot\vec{B}\right)I + \vec{\sigma}\cdot\left(\vec{A}\times\vec{B}\right)$.

Relating the Spinor to the Spin Direction

But how do α, β in $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$ relate to which way the spin's pointing? To find out, let's assume that it's pointing *up* along the unit vector $\hat{\vec{n}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, that is, in the direction (θ, φ). In other words, it's in the eigenstate of the operator $\hat{\vec{n}}\cdot\vec{\sigma}$ having eigenvalue unity:

$$\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

Evaluating, $\alpha/\beta = n_- / (1-n_z) = e^{-i\varphi}\sin\theta / (1-\cos\theta)$, using elementary trigonometric identities

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}$$

where we have multiplied by an overall phase factor $e^{i\varphi/2}$, to make it look nicer. Note that the spinor is also correctly normalized.

The physically significant parameter for spin direction is just the ratio α/β. Note that *any* complex number can be represented as $e^{-i\varphi}\cot(\theta/2)$, with $0 \le \theta < \pi$, $0 \le \varphi < 2\pi$, so for any possible spinor, there's a direction along which the spin points up with probability one.

The Spin Rotation Operator

The rotation operator for rotation through an angle θ about an axis in the direction of the unit vector $\hat{\vec{n}} = (n_x, n_y, n_z)$ is, using $\vec{J} = \vec{S} = \frac{1}{2}\hbar\vec{\sigma}$,

$$e^{-\frac{i\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}} = e^{-i(\theta/2)(\hat{\vec{n}}\cdot\vec{\sigma})}.$$

(*Warning*: we're following standard notation here, but don't confuse this θ--angle turned through—with the θ in writing $\hat{\vec{n}}$ in terms of (θ,φ)!)

Expanding the exponential,

$$e^{-i(\theta/2)(\hat{\vec{n}}\cdot\vec{\sigma})} = I + \left(\frac{-i\theta}{2}\right)(\hat{\vec{n}}\cdot\vec{\sigma}) + \frac{1}{2!}\left(\frac{-i\theta}{2}\right)^2(\hat{\vec{n}}\cdot\vec{\sigma})^2 + \frac{1}{3!}\left(\frac{-i\theta}{2}\right)^3(\hat{\vec{n}}\cdot\vec{\sigma})^3 + \dots$$

and using $(\hat{\vec{n}}\cdot\vec{\sigma})^2 = I$,

$$\begin{aligned} e^{-i(\theta/2)(\hat{\vec{n}}\cdot\vec{\sigma})} &= I + \frac{1}{2!}\left(\frac{-i\theta}{2}\right)^2 + \frac{1}{4!}\left(\frac{-i\theta}{2}\right)^4 + \dots \\ &\quad + \left(\frac{-i\theta}{2}\right)(\hat{\vec{n}}\cdot\vec{\sigma}) + \frac{1}{3!}\left(\frac{-i\theta}{2}\right)^3(\hat{\vec{n}}\cdot\vec{\sigma}) + \dots \\ &= I\cos\frac{\theta}{2} - i(\hat{\vec{n}}\cdot\vec{\sigma})\sin\frac{\theta}{2}. \end{aligned}$$

Writing this in the same *D*-notation we used for orbital angular momentum earlier (the superscript refers to the *j*-value)

$$D^{(1/2)}\left(R(\theta\hat{\vec{n}})\right) = e^{-\frac{i\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}} = e^{-i(\theta/2)(\hat{\vec{n}}\cdot\vec{\sigma})} = I\cos\frac{\theta}{2} - i(\hat{\vec{n}}\cdot\vec{\sigma})\sin\frac{\theta}{2}.$$

The rotation operator $D^{(1/2)}\left(R(\theta\hat{\vec{n}})\right)$ is a 2×2 matrix operating on the ket space

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix},\quad |\alpha|^2 + |\beta|^2 = 1.$$

Explicitly, it is

$$D^{(1/2)}\left(R\left(\theta\hat{\vec{n}}\right)\right)=\begin{pmatrix}\cos(\theta/2)-in_z\sin(\theta/2) & -\left(in_x+n_y\right)\sin(\theta/2)\\ \left(-in_x+n_y\right)\sin(\theta/2) & \cos(\theta/2)+in_z\sin(\theta/2)\end{pmatrix}.$$

Notice that this matrix has the form

$$\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix}$$

with

$$|a|^2+|b|^2=1.$$

The inverse of this rotation operator is clearly given by replacing θ with $-\theta$, that is,

$$\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix}^{-1}=\begin{pmatrix}a^* & -b\\ b^* & a\end{pmatrix}.$$

These 2×2 matrices have determinant $|a|^2+|b|^2=1$, and so are *unitary*. They clearly form a group, since they represent operations of rotation on a spin. This group is called *SU*(2), the 2 refers to the dimensionality, the *U* to their being unitary, and the *S* signifying determinant +1.

Note that for rotation about the *z*-axis, $\hat{\vec{n}}=(0,0,1)$, it is more natural to replace θ with φ and the rotation operator becomes

$$D^{(1/2)}\left(R\left(\varphi\,\hat{\vec{z}}\right)\right)=\begin{pmatrix}e^{-i\varphi/2} & 0\\ 0 & e^{i\varphi/2}\end{pmatrix}.$$

In particular, the wave function is multiplied by -1 for a rotation of 2π. Since this is true for any initial wave function, it is clearly also true for rotation through 2π about any axis.

Exercise: write down the infinitesimal version of the rotation operator $e^{-\frac{i\delta\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}}$ for spin ½ , and prove that $e^{\frac{i\delta\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}}\vec{\sigma}e^{-\frac{i\delta\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}}=\vec{\sigma}+\delta\theta\,\hat{\vec{n}}\times\vec{\sigma}$, that is, $\vec{\sigma}$ is rotated in the same way as an ordinary three-vector—note particularly that the change depends on the angle rotated through, as opposed to the half-angle, so, reassuringly, there is no -1 for a complete rotation (as there cannot be—the direction of the spin is a physical observable, and cannot be changed on rotating the measuring frame through 2π).

Spin Precession in a Magnetic Field

As a warm up exercise, consider a magnetized *classical* object spinning about its center of mass, with angular momentum $\vec{L}$ and parallel magnetic moment $\vec{\mu}$, $\vec{\mu}=\gamma\vec{L}$. The constant γ is called the *gyromagnetic ratio*. Now add a magnetic field $\vec{B}$, say in the *z*-direction. This will exert a torque $\vec{T}=\vec{\mu}\times\vec{B}=\gamma\vec{L}\times\vec{B}=d\vec{L}/dt$, easily solved to find the angular momentum vector $\vec{L}$ precessing about the magnetic field direction with angular velocity of precession $\vec{\omega}_0=-\gamma\vec{B}$.

(*Proof*: from $d\vec{L}/dt=\gamma\vec{L}\times\vec{B}$, take $L_+=L_x+iL_y$, $dL_+/dt=-i\gamma BL_+$, $L_+=L_+^0e^{-i\gamma Bt}$. Of course, $dL_z/dt=0$, since $d\vec{L}/dt=\gamma\vec{L}\times\vec{B}$ is perpendicular to $\vec{B}$, which is in the *z*-direction.)

The *exact same result* comes from the *quantum* mechanics of an electron spin in a magnetic field. The electron has magnetic dipole moment $\vec{\mu}=\gamma\vec{S}$, where $\gamma=g\left(-e/2mc\right)$ and *g* (known as the Landé *g*-factor) is very close to 2. (This *g*-factor terminology is used more widely: the magnetic moment of an atom is written $\mu=g\mu_B$, where $\mu_B=e\hbar/2mc$ is the *Bohr magneton*, and *g* depends on the total orbital angular momentum and total spin of the particular atom.)

The Hamiltonian for the interaction of the electron's dipole moment with the magnetic field is $H=-\vec{\mu}\cdot\vec{B}=-\gamma\vec{S}\cdot\vec{B}$, hence the time development is

$$\left|\psi(t)\right\rangle=U(t)\left|\psi(0)\right\rangle$$

with the propagator

$$U(t)=e^{-iHt/\hbar}=e^{i\gamma\vec{\sigma}\cdot\vec{B}t/2}$$

but this is exactly the *rotation* operator (as shown earlier) through an angle $-\gamma Bt$ about $\vec{B}$!

For an arbitrary initial spin orientation

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix}=\begin{pmatrix}e^{-i\varphi/2}\cos(\theta/2)\\ e^{i\varphi/2}\sin(\theta/2)\end{pmatrix},$$

the propagator for a magnetic field in the *z*-direction

$$U(t)=e^{i\gamma\vec{\sigma}\cdot\vec{B}t/2}=\begin{pmatrix}e^{-i\omega_0t/2} & 0\\ 0 & e^{i\omega_0t/2}\end{pmatrix},$$

so the time-dependent spinor is

$$\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix}=\begin{pmatrix}e^{-i(\varphi+\omega_0t)/2}\cos(\theta/2)\\ e^{i(\varphi+\omega_0t)/2}\sin(\theta/2)\end{pmatrix}.$$

The angle θ between the spin and the field stays constant, the azimuthal angle around the field increases as $\varphi = \varphi_0 + \omega_0 t$, *exactly as in the classical case*.

Exercise: for a spin initially pointing along the *x*-axis, prove that $\langle S_x(t)\rangle = (\hbar/2)\cos\omega_0 t$.

Paramagnetic Resonance

We have shown that the spin precession frequency is independent of the angle of the spin to the field. Consider how all this looks in a frame of reference which is *itself* rotating with angular velocity ω about the *z*-axis. Let's call the magnetic field $\vec{B}_0 = B_0\hat{\vec{z}}$, because we'll soon be adding another one.

In the rotating frame, the observed precession frequency is $\vec{\omega}_r = -\gamma\left(\vec{B}_0 + \vec{\omega}/\gamma\right)$, so there is a different effective field $\vec{B}_0 + \vec{\omega}/\gamma$ in the rotating frame. Obviously, if the frame rotates exactly at the precession frequency, $\vec{\omega} = \vec{\omega}_0 = -\gamma\vec{B}_0$, spins pointing in any direction will remain *at rest* in that frame—there's no effective field at all.

Suppose now we add a small rotating magnetic field with angular frequency ω in the *x*,*y* plane, so the total magnetic field

$$\vec{B} = B_0\hat{\vec{z}} + B_1\left(\hat{\vec{x}}\cos\omega t - \hat{\vec{y}}\sin\omega t\right).$$

The effective magnetic field in the frame rotating with the same frequency ω as the small added field is

$$\vec{B}_r = \left(B_0 + \omega/\gamma\right)\hat{\vec{z}} + B_1\hat{\vec{x}}.$$

Now, if we tune the angular frequency of the small rotating field so that it exactly matches the precession frequency in the original static magnetic field, $\vec{\omega} = \vec{\omega}_0 = -\gamma\vec{B}_0$, all the magnetic moment will see in the rotating frame is the small field in the *x*-direction! It will therefore precess about the *x*-direction at the slow angular speed γB_1. This matching of the small field rotation frequency with the large field spin precession frequency is the "resonance".

If the spins are lined up preferentially in the *z*-direction by the static field, and the small resonant oscillating field is switched on for a time such that $\gamma B_1 t = \pi/2$, the spins will be preferentially in the *y*-direction in the rotating frame, so in the lab they will be rotating in the *x*,*y* plane, and a coil will pick up an ac signal from the induced emf.