

Spin



- Stern-Gerlach Experiment
- Spin is not quite something spinning...
- Pauli spin algebra
- Circular Orbits and the Gyromagnetic ratio
- NMR as an application of spin

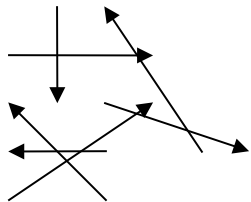
Stern-Gerlach Experiment



What they did:

Silver atoms are little magnets

Boil them out of a unmagnetized oven, they emerge with all possible spin orientations.

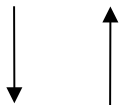


Pass them through a magnetic gradient..they get pushed by the field gradient, with a force proportional to the spin orientation.

==> Expected smeared out distribution of positions transverse to

What they actually found:

But there are only two spots...it is as if the spin was entirely up or entirely down only, the whole time!



Were they magnetized by their passage in the magnetic field gradient?
If so, why were the oppositely directed also found in roughly equal numbers?

Upshot:

- (1) Silver atoms only seem to have two possible spin states.
- (2) Possible spin along each direction either up or down only
....along any direction (!)

Spin is not quite just something spinning...



Like angular momentum mechanically;

Total angular momentum of a particle in orbit is $J = L+S$

Can take a magnet, hang it from a thread so that its North is pointing down. Then heat it up until it demagnetizes. As it demagnetizes, it will start spinning !

Not like angular momentum:

No spatial version of the wavefunction. It is not about functions in space, as was the case for the spherical harmonics.

Ex: Need to rotate 4π to get back to the same state you started

This is why spin is also sometime called “Intrinsic” rather than having to do with the wave functions look in space (which I guess we'd call “extrinsic”)

Pauli Spin Algebra



Pauli (re-)discovered a nice way to represent this spin $\frac{1}{2}$ system. Goal is to find a unitary representation of the spin algebra;

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$$

For silver (and all spin $\frac{1}{2}$ particles) we want a 2-dim representation.
We already talked about that when we talked angular momentum...

Pauli Spin Algebra



Pauli (re-)discovered a nice way to represent this spin $\frac{1}{2}$ system.

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

And let $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$

Pauli Spin Algebra



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Properties of the Pauli Spin Matrices:

$$\sigma_j \sigma_k = i \epsilon_{jkl} \sigma_l \quad i \neq j$$

$$\text{Tr}(\sigma_i) = 0$$

$$\sigma_i^2 = \mathbf{1}$$

They are Hermitean, as they must be to represent an observable.

NOTATION: it is sometimes convenient to add a fourth matrix into the mix...the identity

$$\sigma_0 = \mathbf{1}$$

Some further identities that follow from these matrices.

For any unit vector $|\vec{n}| = 1$ Note that $(\vec{n} \cdot \vec{\sigma})^2 = 1$

For any $[\sigma_i, \sigma_j]_+ = 0$ for $i \neq j$

Note that given any two vect \vec{A} and \vec{B} we have

$$\begin{aligned} & (\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) \\ &= (\vec{A} \cdot \vec{B})\sigma_0 + i(\vec{A} \times \vec{B}) \cdot \sigma \end{aligned}$$

Which, also implies the relation for the exponentiation of the generators ..thus these are the actual group elements (of the rotation group) in this 2-d complex representation.

$$e^{-i\theta\hat{\theta} \cdot \sigma} = \cos(\theta)\sigma_0 - i \sin \theta \hat{\theta} \cdot \sigma$$

$$e^{-i\theta\hat{\theta}\cdot\sigma} = \cos(\theta)\sigma_0 - i\sin\theta\hat{\theta}\cdot\sigma$$

And note that since $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, the rotation is generated by S ,

$$e^{-i\theta\hat{\theta}\cdot\vec{S}/\hbar} = \cos\left(\frac{\theta}{2}\right)\sigma_0 - i\sin\left(\frac{\theta}{2}\right)\hat{\theta}\cdot\vec{\sigma}$$

Which indicates that to get to the identity one need actually rotate 4π in order to

(Show them t'Hooft's version of the spinor made by coffee cup and arm)

Circular Orbits and the Gyromagnetic Ratio

To connect the spin, magnetic moment and angular momentum, consider the case of a charged particle in a circular orbit. We know that it constitutes a loop and so has some magnetic moment. Since classically,

$$\mu = IA/c$$

Putting in the current and the area of a circular orbit of radius r ,

$$\mu = \left(\frac{qv}{2\pi a} \right) (\pi a^2) / c$$

So that,

$$\mu = \gamma L$$

Where $\gamma = \frac{q}{2mc}$ is called the gyromagnetic ratio

Now, putting QM into the mix, note that the basic unit of angular momentum in QM is \hbar

This implies a smallest value for the magnetic moment of a particle, called the (electron) Bohr magneton;

$$\mu_B = \gamma L = \frac{q\hbar}{2mc}$$

Here, for m being the electron mass, we arrive at

$$\mu_B = 0.6 \times 10^{-8} \text{ eV/G}$$

Alas, this is dimensionally correct but came from a classical argument, so in reality we can measure these magnetic moments (as in the Stern-Gerlach experiment) and we find that the electron's magnetic moment is not μ_B ;

but....

It is (very nearly) twice μ_B !

We typically parameterize the magnetic moment of fundamental particles as

$$\mu = g\mu_B$$

For reasons having to do with relativity, for non-interacting, unit charge, spin- 1/2 particles one can show that $g = 2$. Of course, any unit charge particle will have interactions... keep track of how these interactions modify the magnetic moment of the particle. This is quantum field theory, and is properly the domain of your next quantum course, so more on that for now.

Suffice to say, that it is really a triumph in our understanding of nature that we can relate the electric charge and the mass of an electron to its magnetic moment to like 11 decimal places, and the fact that the theory and results of high precision experiments agree at this level...see your book Pg. 390 and 391 for more on that

Classical Precession of Spin

Note that the torque felt by a magnetic moment in a magnetic field is

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

But this relates temporal change in the angular momentum to the angular momentum itself (recall that L is parallel to the magnetic moment).

And, further, that change is perpendicular to L

THUS, the angular momentum (and so also the magnetic moment) precess around applied field B .

Even without solving the equations, but just studying them on dimensional grounds, the frequency of the precession is

$$\omega_0 = \gamma B \quad \text{Larmor frequency}$$

Quantum Spin in a Magnetic field



Our Goal is to solve; $H\Psi = i\hbar\partial_t\Psi$

With just the previous classical picture of the motion of a magnetic moment in a magnetic field, consider the quantum mechanical problem is a spin interacting with a magnetic field. In quantum we don't talk (directly) about forces and torques...instead we talk about the energy. For a classical magnetic moment in a magnetic field we would

$$H = -\vec{\mu} \cdot \vec{B}$$

We can use this as our starting point in discussing the quantum mechanical problem of a spin in a magnetic field. Just replace the magnetic moment by the gyromagnetic ratio times the angular momentum (the spin S operators).

$$H = \frac{g\mu_B}{2} \vec{\sigma} \cdot \vec{B}$$

Quantum Spin in a Magnetic field: Constant B field.



Consider the straightforward case of a constant B field. Chose that direction along the B-field to be z, then

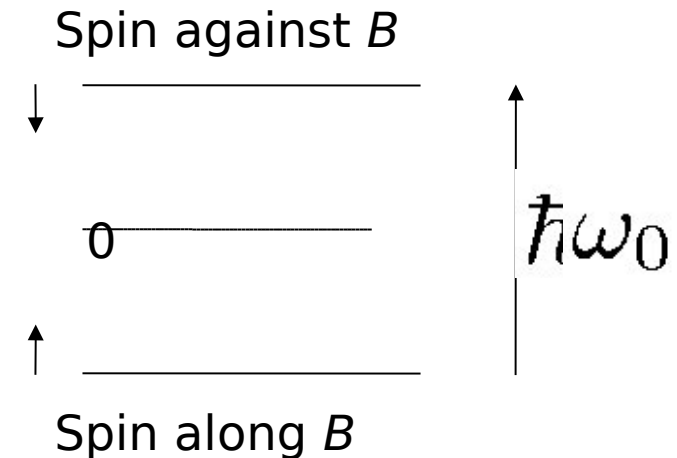
$$H\Psi = i\hbar\partial_t\Psi \quad \text{with} \quad H = -\frac{g\mu_B B}{2}\sigma_z$$

Can be solved for the eigenstates

$$H|E\rangle = E|E\rangle$$

Thus,

$$E = \pm \frac{\hbar\omega_0}{2}$$



Quantum Spin in a Magnetic field : NMR



So, from the preceding, a constant background field has created a splitting between the (originally same-energy) states of different m -quantum number.

Our thinking from Modern Physics class suggests that if we shine in light of the energy (*i.e.* that matches the splitting) we can get transitions between the states.
Let's do it !

Expose the system to a type of light; here simple a time changing magnetic field.

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

B_0 Constant field

B Time-varying field...here circularly polarized light.

Quantum Spin in a Magnetic field : NMR



Aside: You could also compute the electric field impressed here...using Maxwell equations. But fuggeddaboutit for now...the electric field is parity odd and the magnetic field is parity even SO the electric field will not contribute to a transition between these states ... Think of what happens to states under parity.

ANYWAYS, we thus plug this total B field into the hamiltonian

$$H = -\vec{\mu} \cdot \vec{B}$$

And solve

$$H\Psi = i\hbar\partial_t\Psi$$

But, we do so in two steps...

Quantum Spin in a Magnetic field : NMR



We are solving

$$\begin{bmatrix} \frac{\omega_0}{2} & \frac{g\mu_B B}{2} e^{-i\omega t} \\ \frac{g\mu_B B}{2} e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix} \Psi = i\hbar \partial_t \Psi$$

Step 1: Go into the (most convenient) rotating frame; This is what that means
Use a diagonal (but time dependent) unitary re-definition of the wavefunction

$$\Psi = U \psi$$

With, for example, $U = \begin{bmatrix} e^{i\Omega t} & 0 \\ 0 & e^{-i\Omega t} \end{bmatrix}$

Quantum Spin in a Magnetic field : NMR



In this frame, the Schroedinger equation thus reads,

$$\begin{bmatrix} \frac{\omega_0}{2} - \Omega & \frac{g\mu_B B}{2} e^{-i\omega t + i2\Omega t} \\ \frac{g\mu_B B}{2} e^{i\omega t - i2\Omega t} & -\frac{\omega_0}{2} + \Omega \end{bmatrix} \psi = i\hbar \partial_t \psi$$

Thus we can see that in the frame rotating $\Omega = \frac{\omega}{2}$ the Hamiltonian becomes time independent.

$$\begin{bmatrix} \frac{\omega_0 - \omega}{2} & \frac{g\mu_B B}{2} \\ \frac{g\mu_B B}{2} & -\frac{\omega_0 - \omega}{2} \end{bmatrix} \psi = i\hbar \partial_t \psi$$

Step 2: Solve the time independent Hamiltonian the usual way, finding the energy eigenvalues and eigenvectors.

$$H\psi = \mathcal{E}\psi$$

Quantum Spin in a Magnetic field : NMR



$$H\psi = \mathcal{E}\psi$$

Where H is the time independent matrix (the hami in the rotating frame) and we use script ' \mathcal{E} ' for this energy to remind the reader that this is not quite the energy of the states...it is the energies shift Ω by

So, diagonalizing this 2x2 matrix we arrive at eigenvalues

$$\mathcal{E} = \pm\gamma\sqrt{B^2 + \left(B_0 - \frac{\omega}{\gamma}\right)^2}$$

Now we can re-assemble the full wave function of the whole problem. This means that we can, in principle, compute any observable in this system...we focus now on just a single one, the net magnetization of the state.

Quantum Spin in a Magnetic field : NMR



$$\langle \mu_z \rangle = \mu_z(0) \left[\frac{(\omega_0 - \omega)^2 + \gamma^2 B^2 \cos(\omega_r t)}{(\omega_0 - \omega)^2 + \gamma^2 B^2} \right]$$

with $\omega_r = \frac{\mathcal{E}}{\hbar}$

Note: 1) Resonance Structure...pumping at the larmor frequency greatly increases the response of the system.

2) Power Broadening... width of the response function (and thereby a response you can have) is proportional to the time-dependent field, B . see later that this is a consequence of stimulated emission.

3) By turning off and on the time-varying magnetic field we can rotate spin vector relative to the laboratory frame, from which it subsequent to turning off the time-varying field, results in a magnetization in the sample oscillating at the Larmor frequency...the so called free induction decay in NMR.

The two state spin $\frac{1}{2}$ system is really the gateway/testbed of much physics thinking.

$$\vec{A} \quad J = L + S \quad H\Psi = i\hbar\partial_t\Psi \quad H = \frac{g\mu_B}{2}\vec{\sigma} \cdot \vec{B}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad H = -\vec{\mu} \cdot \vec{B} \quad \pm \frac{\hbar}{2}$$

$$(\vec{n} \cdot \vec{\sigma})^2 = 1 \quad \sigma_j \sigma_k = i\epsilon_{jkl}\sigma_l$$

$$S^2 = \frac{3}{4}\hbar^2 \mathbf{1}$$

$$S^2 = S_x^2 + S_y^2 + S_z^2 \quad \vec{\tau} = \vec{\mu} \times \vec{B} \quad i \neq j$$

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \quad U = \begin{bmatrix} e^{i\Omega t} & 0 \\ 0 & e^{-i\Omega t} \end{bmatrix} \quad [\sigma_i, \sigma_j]_+ = 0$$

$$Tr(\sigma_i) = 0$$

$$\begin{bmatrix} \frac{\omega_0 - \omega}{2} & \frac{g\mu_B B}{2} \\ \frac{g\mu_B B}{2} & -\frac{\omega_0 - \omega}{2} \end{bmatrix} \psi = i\hbar\partial_t\psi \quad \sigma_0 = \mathbf{1}$$

$$\sigma_i^2 = \mathbf{1}$$

$$S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma})$$

$$= (\vec{A} \cdot \vec{B})\sigma_0 + i(\vec{A} \times \vec{B}) \cdot \sigma$$

$$\begin{aligned}
\sigma_y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} & \vec{B} & B & [S_i, S_j] &= i\hbar\epsilon_{ijk}S_k \\
\sigma_z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & \mathcal{E} & B_0 & L_z & |\vec{n}| = 1 \\
& & \gamma & \gamma = \frac{q}{2mc} & \omega_0 &= \gamma B \\
& & \hbar & \vec{L} & \omega_0 & \mu_B = \gamma L = \frac{q\hbar}{2mC} \\
\vec{B} &= B \cos(\omega t) \hat{x} & \mu_B & \mu_B &= 0.6 \times 10^{-8} \text{ eV/G} \\
& -B \sin(\omega t) \hat{y} + B_0 \hat{z} \\
e^{-i\theta \hat{\theta} \cdot \sigma} &= \cos(\theta) \sigma_0 - i \sin \theta \hat{\theta} \cdot \sigma & \Omega & \Psi &= U \psi \\
\mu &= IA/c & \vec{\mu} &= \gamma \vec{L} & H|E\rangle &= E|E\rangle & H\psi &= \mathcal{E}\psi \\
\mu &= \left(\frac{qv}{2\pi a} \right) (\pi a^2) / c & \omega & \Omega &= \frac{\omega}{2} & E &= \pm \frac{\hbar\omega_0}{2} \\
\mu &= \gamma L & \mu &= g\mu_B & E &= \hbar\omega_0 \\
\mu_z &= \left\langle \frac{g\mu_B \hbar}{2} \sigma_z \right\rangle & g &\sim 2 & \mathcal{E} &= \pm \gamma \sqrt{B^2 + \left(B_0 - \frac{\omega}{\gamma}\right)^2}
\end{aligned}$$

$$\begin{bmatrix} \frac{\omega_0}{2} - \Omega & \frac{g\mu_B B}{2} e^{-i\omega t + i2\Omega t} \\ \frac{g\mu_B B}{2} e^{i\omega t - i2\Omega t} & -\frac{\omega_0}{2} + \Omega \end{bmatrix} \psi = i\hbar \partial_t \psi$$