Physics 221A Fall 1996 Notes 13 Spins in Magnetic Fields

A nice illustration of rotation operator methods which is also important physically is the problem of spins in magnetic fields. The earliest experiments with spins in magnetic fields were those of Stern and Gerlach, which first revealed the quantization of electron spin. Similar but later experiments by Stern and other collaborators were used to make crude measurements of the proton magnetic moment and other nuclear magnetic moments. In the late 1930's, these experiments were improved upon by Rabi, who developed the technique of spin flipping with time-dependent magnetic fields. With his new apparatus, Rabi was able to make much more accurate measurements of nuclear magnetic moments. After World War II, Bloch and Purcell developed methods for studying magnetic resonance in bulk samples (solid or liquid), by measuring microwave power absorbed at resonance or by looking at the time development and relaxation of induced magnetization. In the same period, Rabi's beam techniques were improved upon by Ramsey. In modern applications, pulsed fields are used to craft precise quantum states and to watch their time evolution. Applications of the magnetic resonance technique include measurements of nuclear magnetic moments and *q*-factors, measurements of diamagnetic shielding of external fields in molecules or solids (important in chemistry and solid state physics), the construction of sensitive magnetometers and atomic clocks, and tomography or imaging in medicine and biology.

A classical model of a particle of charge q and mass m in a circular orbit leads to a proportionality between the (orbital) angular momentum **L** of the particle and the magnetic moment μ of the current loop,

$$\boldsymbol{\mu} = \frac{q}{2mc} \mathbf{L}.$$
(13.1)

Equation (13.1) is a vectorial relation, and, in particular, if the charge is negative, the magnetic moment and angular momentum point in opposite directions. This equation is derived from a classical model, but in fact it is also valid for the quantum mechanical treatment of orbital motion of electrons in atoms. In the case of particle spins, however, it is necessary to introduce a fudge factor or g-factor, and to write

$$\boldsymbol{\mu} = g \frac{q}{2mc} \mathbf{S}.$$
(13.2)

The g-factors are measured experimentally for different particles and can sometimes be calculated theoretically (notably in the case of the leptons, especially the electron and

muon). In other cases (the hadrons such as the proton, neutron, or various atomic nuclei), current theory can provide no more than crude estimates.

Why are the magnetic moments of nuclei and particles proportional to the spin? These two vectors are certainly not proportional in all systems, because the angular momentum is determined by the mass distribution of the system and its state of motion, while the magnetic moment is determined by the charge distribution and its state of motion. In fact, for many atoms and molecules, μ is not proportional to **J** (the total angular momentum). Why then should it be so for nuclei and particles like the proton and electron?

The answer has to do with energy scales. Consider first the case of nuclei. Normal laboratory processes in atomic physics involve energies which are much smaller than the energy scales in the nucleus, which are typically of the order of MeV. Furthermore, the interaction energies of spins in typical laboratory magnetic fields are much smaller than typical atomic energy scales. Therefore if the nucleus is in its ground state, or even in an excited state with a lifetime which is long in comparison to the duration of some experiment, then the nucleus is essentially in a single energy level. That is, very little mixing between nuclear energy levels can be induced by interactions with either atomic or external fields (electric or magnetic), because of the large energy differences between nuclear levels. This can be seen in perturbation theory, where the energy denominators would be very large.

Now a single energy level of a nucleus is characterized by an angular momentum value, called the spin of the nucleus and denoted here by s. Therefore, if $s \neq 0$, this level is degenerate, since the magnetic quantum number m_s can take on the 2s + 1 values between -s and +s. This degeneracy is due to the rotational invariance of the nuclear Hamiltonian. However, nuclei have no other symmetry which leads to any further degeneracies, as we will discuss more fully later in the course. Therefore the subspace of the nuclear Hilbert space corresponding to a definite energy level consists of a single irreducible subspace under rotations, of dimensionality 2s+1, and the basis kets in this space can be taken to be $|s, m_s\rangle$. As long as we restrict consideration to a single energy level, this (2s+1)-dimensional space is the Hilbert space of the nucleus.

We will denote the angular momentum operator of the nucleus by **S**. This operator consists of the orbital and spin contributions of all the constituent nuclei of the nucleus, and could consist of many terms. But when we restrict this operator to a single irreducible subspace corresponding to a definite energy level of the nucleus and express it as a matrix in the standard basis $|s, m_s\rangle$, this operator is represented by the standard matrices for the components of angular momentum as seen in Eq. (11.37). For example, for a nucleus of spin- $\frac{1}{2}$, meaning a definite energy level of a nucleus with spin- $\frac{1}{2}$, we will have $\mathbf{S} = (\hbar/2)\boldsymbol{\sigma}$. Furthermore, the spin operator \mathbf{S} is a vector operator, i.e., it transforms as a vector under rotations. This is the significance of the generalized adjoint formula, Eq. (11.57). It can also be shown that on a single irreducible subspace, every vector operator is proportional to the angular momentum (here \mathbf{S}), that is, the angular momentum is essentially the only vector operator there is on such a space. This kind of reasoning underlies the Wigner-Eckart theorem, which we will consider soon. Therefore, since the magnetic moment $\boldsymbol{\mu}$ is another vector operator, it must be proportional to \mathbf{S} . This would not be true if energy scales were large enough to mix together different energy levels of the nuclei, i.e., levels corresponding

to irreducible subspaces with different values of s. This is why atoms and molecules do not necessarily have μ proportional to **J**, since their energy levels are mixed substantially by low energy interactions.

The situation is similar with regard to "elementary" particles. The proton, of course, is not really elementary, but rather consists of three quarks. But otherwise, the situation is much as with a nucleus. As for the electron, as far as anyone currently knows, it is "elementary." But the point is the same as above; the internal Hilbert space of the particle consists of a single irreducible subspace under rotations (2-dimensional for the electron), and on such a space, every vector is proportional to the angular momentum.

Convenient units of magnetic moment are the Bohr magneton,

$$\mu_B = \frac{e\hbar}{2m_e c},\tag{13.3}$$

and the nuclear magneton,

$$\mu_N = \frac{e\hbar}{2m_p c},\tag{13.4}$$

where m_e and m_p are respectively the electron and proton mass. The Bohr magneton is a characteristic magnetic moment of an electron or an atom (such as silver) containing unpaired electrons. The nuclear magneton is characteristic of a nucleus or an atom in a spin 0 (singlet) electronic state. Because of the mass factor in the denominator, nuclear magnetic moments are typically of the order of 10^{-3} times smaller than electronic magnetic moments.

Here are some examples of magnetic moments. For the electron we have

$$\boldsymbol{\mu} = -g_e \mu_B \frac{\mathbf{S}}{\hbar} = -g_e \mu_B \frac{\boldsymbol{\sigma}}{2},\tag{13.5}$$

where

$$g_e = 2\left(1 + \frac{\alpha}{2\pi} + \ldots\right) = 2.00232.$$
 (13.6)

The minus sign in Eq. (13.5) comes from the fact that the charge is negative whereas μ_B is positive. The series indicated is the result of a perturbation calculation in quantum electrodynamics, in which $\alpha = e^2/\hbar c$ is the fine structure constant. The electron g-factor is very close to 2, the value predicted by the Dirac equation, as we will see later in the course. The positron has the same g-factor as the electron, but μ is in the same direction as **S** since the charge is positive.

For the proton we have

$$\boldsymbol{\mu} = g_p \mu_N \frac{\mathbf{S}}{\hbar} = g_p \mu_N \frac{\boldsymbol{\sigma}}{2},\tag{13.7}$$

where

$$g_p = 5.588,$$
 (13.8)

and for the neutron we have

$$\boldsymbol{\mu} = g_n \mu_N \frac{\mathbf{S}}{\hbar} = g_n \mu_N \frac{\boldsymbol{\sigma}}{2},\tag{13.9}$$

where

$$g_n = -3.823. \tag{13.10}$$

The neutron is considered to have a negative g-factor, because μ and **S** are in opposite directions. The usual electronic charge e is used in μ_N , even though the neutron is neutral; and by convention, the proton mass is used in μ_N , even in the neutron equation (13.9). Crude models of mixtures of up and down quarks are able to explain the proton and neutron magnetic moments to within several percent, but no one is able as yet to improve on these calculations.

Nuclei have a variety of spins and magnetic moments. For the deuteron, a spin-one particle, we have

$$\boldsymbol{\mu} = g_d \mu_N \frac{\mathbf{S}}{\hbar},\tag{13.11}$$

where

$$g_d = 0.857,$$
 (13.12)

but for the alpha particle, a spin-0 particle, we have $\mu = 0$ exactly. Spin-0 particles cannot have a magnetic moment, because the spin operator vanishes.

Sometimes the magnetic moments of the proton and neutron are called "anomalous," since they differ from the value g = 2 predicted by the Dirac equation. Of course, the true electron magnetic moment also differs from g = 2, because of the radiative corrections seen in Eq. (13.6). But these corrections are small and can often be ignored.

The interaction of a spin with a magnetic field is governed by the Hamiltonian,

$$H = -\boldsymbol{\mu} \cdot \mathbf{B},\tag{13.13}$$

which must be added to the kinetic and potential energies if orbital degrees of freedom are important. The Hamiltonian (13.13) is the energy of interaction of a magnetic dipole with an external field in classical electromagnetic theory; its further justification for particles and nuclei calls on methods of relativisitic quantum mechanics and field theory, as we will see in Physics 221B. If only spin degrees of freedom are important, then we can work directly the Hamiltonian (13.13), in which the ket space is the (2s + 1)-dimensional vector space of spinors for the given spin s. This space always forms a single irreducible space under rotations. If we ignore the orbital degrees of freedom, then the magnetic field can be taken to be a function of time only, $\mathbf{B} = \mathbf{B}(t)$. In some cases, however, such as the Stern-Gerlach experiment, the coupling of the spin to the orbital degrees of freedom must be taken into account, due to gradients in the magnetic field. For the rest of these notes, we will ignore orbital degrees of freedom, and write Eq. (13.13) in the form,

$$H = -\gamma \mathbf{B} \cdot \mathbf{S},\tag{13.14}$$

where

$$\gamma = g \frac{q}{2mc}.\tag{13.15}$$

Consider first the general problem in which the magnetic field has an arbitrary time dependence, so that the Schrödinger equation for the time-evolution operator $U(t, t_0)$ is

$$\frac{\partial U}{\partial t} = \frac{i\gamma}{\hbar} \mathbf{B}(t) \cdot \mathbf{S}U. \tag{13.16}$$

If nothing further is said about the time dependence of \mathbf{B} , we cannot write down the solution in explicit form, but we can at least note that the time-evolution operator U is always a rotation operator. To see this, we consider the infinitesimal time advance implied by the Schrödinger equation,

$$U(t + \Delta t) = \left[1 + \frac{i\gamma\Delta t}{\hbar}\mathbf{B}(t)\cdot\mathbf{S}\right]U(t).$$
(13.17)

The factor in the square brackets is an infinitesimal rotation operator, as we can see if we compare it to

$$1 - \frac{i\Delta\theta}{\hbar} \hat{\mathbf{n}} \cdot \mathbf{S}. \tag{13.18}$$

We see that the axis of the infinitesimal rotation is given by

$$\hat{\mathbf{n}} = \hat{\mathbf{b}}(t),\tag{13.19}$$

where we write

$$\mathbf{B}(t) = B(t)\dot{\mathbf{b}}(t) \tag{13.20}$$

for the magnitude and direction of the magnetic field. The angle of the infinitesimal rotation is given by

$$\Delta \theta = -\gamma B(t) \Delta t, \tag{13.21}$$

or,

$$\omega = \frac{\Delta\theta}{\Delta t} = -\gamma B(t). \tag{13.22}$$

The angular velocity can also be written as a vector,

$$\boldsymbol{\omega} = \boldsymbol{\omega} \hat{\mathbf{n}} = -\gamma \mathbf{B}(t), \tag{13.23}$$

which is either parallel or antiparallel to **B**, depending on the sign of γ .

We see that as time proceeds, U develops by the composition of a large number of infinitesimal rotation operators; since the product of rotation operators is always a rotation operator, U itself is a rotation operator. However, the axis and rate of rotation are in general functions of time. This is very much as in classical rigid body motion, in which ω is some function of time, which in general is not constant either in magnitude or direction. In classical rigid body motion, ω is determined as a function of time by solving the Euler equations; in the quantum mechanical motion of a charged particle in a magnetic field, ω is simply given as a function of time by Eq. (13.23). In either case, once $\omega(t)$ is known, the subsequent problem of determining the time-dependent rotation is very similar.

We turn now to some cases in which Eq. (13.16) can be solved explicitly. The simplest one is that of a spin in a constant magnetic field,

$$\mathbf{B} = B\hat{\mathbf{b}} = \text{const},\tag{13.24}$$

so that the Schrödinger equation for the time evolution operator U(t) is

$$\frac{\partial U}{\partial t} = \frac{i\gamma}{\hbar} B \hat{\mathbf{b}} \cdot \mathbf{S} U. \tag{13.25}$$

This equation can be immediately integrated. Previously we have been using the symbol U for rotation operators, but now we switch to D to avoid confusion with the time-evolution operator. Then we have,

$$U(t) = \exp\left[\frac{i}{\hbar}\omega t(\hat{\mathbf{b}}\cdot\mathbf{S})\right] = D(\hat{\mathbf{b}}, -\omega t), \qquad (13.26)$$

where

$$\omega = \gamma B = g \frac{qB}{2mc}.\tag{13.27}$$

If $g \approx 2$, as in the case of electrons, this frequency (spin precession frequency) is very close to the classical orbital frequency qB/mc of the particle in the given magnetic field. Certain so-called g - 2 experiments exploit this fact to measure the small difference between the two frequencies.





Fig. 13.1. In a constant magnetic field, $\langle \mathbf{S} \rangle$ precesses about the field direction at frequency $\omega = \gamma B$.

Fig. 13.2. The field in magnetic resonance experiments consists of a constant field \mathbf{B}_0 plus a timedependent field $\mathbf{B}_1(t)$ which is perpendicular to \mathbf{B}_0 and which rotates about \mathbf{B}_0 at frequency ω_1 .

Given U(t), it is straightforward to find the time evolution of the expectation value of the spin. We have

$$\langle \mathbf{S} \rangle(t) = \langle \psi(t) | \mathbf{S} | \psi(t) \rangle = \langle \psi_0 | D(\hat{\mathbf{b}}, -\omega t)^{\dagger} \mathbf{S} D(\hat{\mathbf{b}}, -\omega t) | \psi_0 \rangle$$

= $\mathsf{R}(\hat{\mathbf{b}}, -\omega t) \langle \psi_0 | \mathbf{S} | \psi_0 \rangle = \mathsf{R}(\hat{\mathbf{b}}, -\omega t) \langle \mathbf{S} \rangle(0),$ (13.28)

where we have used the adjoint formula (11.57). We see that the expectation value of **S** rotates clockwise (for $\omega > 0$) about the direction of the magnetic field, sweeping out a cone. This is illustrated in Fig. 13.1.

A more interesting case occurs in magnetic resonance experiments. Here the magnetic field consists of a constant field $\mathbf{B}_0 = B_0 \hat{\mathbf{b}}_0$, plus a time-dependent field $\mathbf{B}_1(t)$ which is perpendicular to \mathbf{B}_0 and which rotates clockwise in the perpendicular plane at some frequency ω_1 . These fields are illustrated in Fig. 13.2. We express the time-dependence of \mathbf{B}_1 by writing,

$$\mathbf{B}_1(t) = \mathsf{R}_1(t)\mathbf{B}_{10},\tag{13.29}$$

where \mathbf{B}_{10} is a constant vector [the initial value of $\mathbf{B}_1(t)$] perpendicular to \mathbf{B}_0 , and where $\mathsf{R}_1(t)$ is a time-dependent rotation about the direction of \mathbf{B}_0 ,

$$\mathsf{R}_1(t) = \mathsf{R}(\mathbf{\dot{b}}_0, -\omega_1 t). \tag{13.30}$$

The purpose of the time-dependent field is to induce flips in the spins of particles which are precessing in the constant field \mathbf{B}_0 . As would be expected, the flipping is most efficient

 $\omega_0 = \gamma B_0$ of precession in the constant field. Notice that ω_0 depends on the strength of the constant field \mathbf{B}_0 , whereas ω_1 is the frequency of the time-dependent field, and is independent of its magnitude.

Since \mathbf{B}_0 is an axis of the rotation $\mathsf{R}_1(t)$, we have $\mathbf{B}_0 = \mathsf{R}_1(t)\mathbf{B}_0$, so that the overall magnetic field can be written,

$$\mathbf{B}(t) = \mathsf{R}_1(t)(\mathbf{B}_0 + \mathbf{B}_{10}). \tag{13.31}$$

This allows us to transform the Schrödinger equation as follows:

$$\frac{\partial U}{\partial t} = \frac{i\gamma}{\hbar} \left[\mathsf{R}_1(\mathbf{B}_0 + \mathbf{B}_{10}) \right] \cdot \mathbf{S} U = \frac{i\gamma}{\hbar} (\mathbf{B}_0 + \mathbf{B}_{10}) \cdot \left(\mathsf{R}_1^{-1} \mathbf{S} \right) U$$

$$= \frac{i\gamma}{\hbar} (\mathbf{B}_0 + \mathbf{B}_{10}) \cdot (D_1 \mathbf{S} D_1^{\dagger}) U,$$
(13.32)

where we use the adjoint formula (11.57) in the final step, and where the operator D_1 is the time-dependent spinor rotation corresponding to R_1 ,

$$D_1 = D(\hat{\mathbf{b}}_0, -\omega_1 t) = \exp\left[\frac{i}{\hbar}\omega_1 t(\hat{\mathbf{b}}_0 \cdot \mathbf{S})\right].$$
 (13.33)

We now multiply Eq. (13.32) through by D_1^{\dagger} , to obtain

$$D_{1}^{\dagger} \frac{\partial U}{\partial t} = \frac{\partial (D_{1}^{\dagger} U)}{\partial t} - \frac{\partial D_{1}^{\dagger}}{\partial t} U = \frac{\partial (D_{1}^{\dagger} U)}{\partial t} + \frac{i}{\hbar} \omega_{1} (\hat{\mathbf{b}}_{0} \cdot \mathbf{S}) (D_{1}^{\dagger} U)$$
$$= \frac{i\gamma}{\hbar} (\mathbf{B}_{0} + \mathbf{B}_{10}) \cdot \mathbf{S} (D_{1}^{\dagger} U), \qquad (13.34)$$

or,

$$\frac{\partial (D_1^{\dagger}U)}{\partial t} = \frac{i\gamma}{\hbar} (\mathbf{B}_{\text{eff}} \cdot \mathbf{S}) (D_1^{\dagger}U), \qquad (13.35)$$

where

$$\mathbf{B}_{\text{eff}} = \left(B_0 - \frac{\omega_1}{\gamma}\right)\hat{\mathbf{b}}_0 + \mathbf{B}_{10}.$$
 (13.36)

We will write this effective magnetic field in the form,

$$\mathbf{B}_{\rm eff} = B_{\rm eff} \hat{\mathbf{b}}_{\rm eff},\tag{13.37}$$

where

$$B_{\rm eff} = \sqrt{\left(B_0 - \frac{\omega_1}{\gamma}\right)^2 + B_{10}^2}.$$
 (13.38)

We will also denote the angle between \mathbf{b}_0 and \mathbf{b}_{eff} by θ , so that

$$\sin \theta = \frac{B_{10}}{B_{\text{eff}}}.$$
(13.39)



Fig. 13.3. In the rotating frame, the field $\mathbf{B}_1 = \mathbf{B}_{10}$ is stationary, and \mathbf{B}_0 is reduced in magnitude by ω_1/γ . The resulting field is \mathbf{B}_{eff} , which is constant in the rotating frame.

Fig. 13.4. The expectation value of the spin **S** precesses about the axis $\hat{\mathbf{a}}$ with frequency Ω , while that axis itself precesses about \mathbf{B}_0 with frequency ω_1 .

The physics of these transformations is that we have effectively gone over to a frame rotating at frequency ω_1 . In this frame, the field \mathbf{B}_1 is stationary (and is represented by the vector \mathbf{B}_{10}), while the constant field \mathbf{B}_0 is reduced in magnitude by ω_1/γ by the effects of the rotation. As is well known, inertial effects in a rotating frame can be used to simulate (or cancel) the effects of a magnetic field; this is known as Larmor's theorem. In the present case, the net field in the rotating frame is \mathbf{B}_{eff} , which is constant.

We see that Eq. (13.35) has the same form as Eq. (13.25), the Schrödinger equation in a constant field, with U replaced by $D_1^{\dagger}U$ and **B** replaced by \mathbf{B}_{eff} . The solution is immediate; it is

$$U(t) = D(\hat{\mathbf{b}}_0, -\omega_1 t) D(\hat{\mathbf{b}}_{\text{eff}}, -\Omega t), \qquad (13.40)$$

where

$$\Omega = \gamma B_{\text{eff}} = \sqrt{(\omega_0 - \omega_1)^2 + \gamma^2 B_{10}^2}.$$
(13.41)

The frequency Ω is the *Rabi flopping frequency*.

As before, we can use the solution (13.40) to find the evolution of the expectation value of the spin. We find,

$$\langle \mathbf{S} \rangle(t) = \mathsf{R}(\hat{\mathbf{b}}_0, -\omega_1 t) \mathsf{R}(\hat{\mathbf{b}}_{\text{eff}}, -\Omega t) \langle \mathbf{S} \rangle(0).$$
(13.42)

Thus, $\langle \mathbf{S} \rangle$ sweeps out a cone at frequency Ω about an axis $\hat{\mathbf{a}}$ which makes an angle θ with the direction $\hat{\mathbf{b}}_0$, while this axis itself sweeps out a cone about $\hat{\mathbf{b}}_0$ at frequency ω_1 . This

is illustrated in Fig. 13.4. The direction $\hat{\mathbf{b}}_{\text{eff}}$ is the initial direction of the axis at t = 0, so that

$$\hat{\mathbf{a}}(t) = \mathsf{R}(\hat{\mathbf{b}}_0, -\omega_1 t)\hat{\mathbf{b}}_{\text{eff}}.$$
(13.43)

Equation (13.42) can be expressed explicitly in terms of the time-dependent axis $\hat{\mathbf{a}}(t)$ by use of the exponentiated adjoint formula, Eq. (9.33):

$$\langle \mathbf{S} \rangle(t) = \mathsf{R}(\hat{\mathbf{a}}(t), -\Omega t) \mathsf{R}(\hat{\mathbf{b}}_0, -\omega_1 t) \langle \mathbf{S} \rangle(0), \qquad (13.44)$$

which provides another way of visualizing the time evolution of $\langle \mathbf{S} \rangle$.

As a sample calculation, suppose we have a spin- $\frac{1}{2}$ particle, initially in an up state, $|\psi_0\rangle = |+\rangle$, and suppose we ask for the probability at a later time of finding the spin in the down state $|-\rangle$. We take the direction \mathbf{B}_0 to lie along the z-axis, and we place the vectors \mathbf{B}_{10} and $\hat{\mathbf{b}}_{\text{eff}}$ in the *x*-*z* plane. To compute the probability amplitude for the $\frac{1}{2} \rightarrow -\frac{1}{2}$ transition, we use Eq. (13.40) to obtain

$$\langle -|U(t)|+\rangle = \langle -|D(\hat{\mathbf{z}}, -\omega_1 t)D(\hat{\mathbf{b}}_{\text{eff}}, -\Omega t)|+\rangle = e^{-i\omega_1 t/2} \langle -|D(\hat{\mathbf{b}}_{\text{eff}}, -\Omega t)|+\rangle.$$
(13.45)

But since

$$\hat{\mathbf{b}}_{\text{eff}} = \hat{\mathbf{z}}\cos\theta + \hat{\mathbf{x}}\sin\theta, \qquad (13.46)$$

we have

$$\langle -|U(t)|+\rangle = ie^{-i\omega_1 t/2} \sin\theta \sin\frac{\Omega t}{2}.$$
(13.47)

Thus, the transition probability is

$$P_{\frac{1}{2} \to -\frac{1}{2}} = \sin^2 \theta \sin^2 \frac{\Omega t}{2}.$$
 (13.48)

In the resonant case, $\omega_1 = \omega_0$, we have $B_{\text{eff}} = B_{10}$ and $\theta = \pi/2$, so that the axis of the rotating cone lies in the *x-y* plane. In this case, the transition probability (13.48) reaches a maximum value of unity when $t = \pi/\Omega$.