Physics 221A
Fall 2010
Notes 14
Spins in Magnetic Fields

1. Introduction

A nice illustration of rotation operator methods that 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. Modern applications of the magnetic resonance technique include measurements of nuclear magnetic moments and g-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.

2. Lessons from Stern-Gerlach and Other Experiments

Earlier in the course we examined experimental and gedanken-experimental data from the Stern-Gerlach experiment, which concerned the measurement of the magnetic moment $\boldsymbol{\mu}$ of silver atoms. The three components of $\boldsymbol{\mu}$ are observables, which, according to the postulates of quantum mechanics, must be associated with Hermitian operators acting on some ket space. We found that that ket space was 2-dimensional, and that the components of magnetic moment, expressed as matrices in a basis where μ_z is diagonal with certain phase conventions, are proportional to the Pauli matrices,

$$\boldsymbol{\mu} = \text{const} \times \boldsymbol{\sigma}. \tag{1}$$

We also found that the motion of the silver atoms through the inhomogeneous magnetic field could be described by a potential

$$U(\mathbf{r}) = -\boldsymbol{\mu} \cdot \mathbf{B}(\mathbf{r}), \tag{2}$$

that is, the atoms are governed by the Hamiltonian

$$H = \frac{p^2}{2m} - \boldsymbol{\mu} \cdot \mathbf{B}. \tag{3}$$

At least this Hamiltonian is consistent with the experimental results. The quantity $-\boldsymbol{\mu}\cdot\mathbf{B}$ is the energy of orientation of a magnetic dipole in an external magnetic field in classical electromagnetic theory, so if we wanted to guess the quantum Hamiltonian for a magnetic moment in an external field, Eq. (3) would be a good place to start. Such guesses have to be tested experimentally, but the results of the Stern-Gerlach experiment suggest that this one is correct.

More recently (in Notes 12) we have learned that it is possible to define rotation operators acting on the same 2-dimensional ket space for silver atoms, and that the angular momentum (the generator of rotations) is $\mathbf{J} = (\hbar/2)\boldsymbol{\sigma}$. It follows that the magnetic moment and angular momentum vectors are proportional,

$$\boldsymbol{\mu} = \text{const} \times \mathbf{J}. \tag{4}$$

According to Notes 13, a ket space upon which rotation operators or angular momentum operators act can be broken up into a set of orthogonal irreducible subspaces, each of which is characterized by a j value and has dimension $2j+1$. In the case of the magnetic ket space of silver atoms, we see that there is one irreducible subspace with $j = \frac{1}{2}$. Other values of j do not occur, and this one occurs with multiplicity one.

In the case of silver atoms, we are really measuring the magnetic moment of the electron, that is, the one unpaired electron in the valence shell of silver. We see that the electron not only has an electric field (the monopole, Coulomb field of a point charge), but also a magnetic dipole field. The electron is a small magnet.

Experiments with the magnetic properties of other atomic and subatomic particles, both "elementary" and composite, show that in all cases the magnetic moment operator $\boldsymbol{\mu}$ acts on a ket space that consists of a single irreducible subspace under rotations, that is, it is a space associated with an angular momentum value j and has dimensionality $2j+1$. At least this is true if the magnetic field is not too strong; we will quantify this qualification later. We also find that in all these cases the magnetic moment operator is proportional to the angular momentum. In the case of elementary and not-so-elementary particles such as the electron and nuclei it is conventional to call the angular momentum "spin" and to use the notation $\mathbf{S}$ and s instead of $\mathbf{J}$ and j. Thus, the number s, said to be the "spin" of the particle, is the quantum number of the operator S^2 whose eigenvalue is $s(s+1)\hbar^2$. Likewise, the ket space is spanned by the standard angular momentum basis vectors that we can denote by $|sm\rangle$. The index γ that we used in the general notation of Notes 13 is not needed, since there is only one irreducible subspace. As for the index s, it is constant, so if it is understood we can suppress it, too, and write simply $|m\rangle$ for brevity.

These facts regarding the Hilbert spaces for spin and the Hamiltonians and other operators that act them are sufficient to start solving some problems involving spins and magnetic moments, but before we do that it will be good to address some fundamental questions raised by the cited facts. There are at least two questions. First, why is the ket space for spin a single irreducible subspace under rotations? And second, why is the magnetic moment proportional to the angular momentum? The answers to these two questions are related. We will do the best we can to answer them here,

considering where we are in the course. Some aspects will be filled in later.

3. Magnetic Moments in Classical Electromagnetic Theory

First we recall some facts about magnetic moments in classical electromagnetic theory. The magnetic moment $\boldsymbol{\mu}$ of a localized current distribution $\mathbf{J}(\mathbf{r})$ is given by

$$\boldsymbol{\mu} = \frac{1}{2c}\int d^3\mathbf{r}\,\mathbf{r}\times\mathbf{J}(\mathbf{r}). \tag{5}$$

Here $\mathbf{J}$ is the electric current (not the angular momentum). The magnetic moment characterizes and specifies the dipole component of the magnetic field produced by the current distribution. The magnetic field can be decomposed into multipole fields, the dipole, quadrupole, octupole, etc, components, of which the dipole is often the most important because it dies off most slowly with distance and so dominates at large distances. The other components are generally present, however, and are important if we come close enough to the current distribution.

If a current distribution is placed in an external magnetic field $\mathbf{B}$, it has an energy of orientation U given by Eq. (2), assuming that $\mathbf{B}$ does not change very much over the extent of the current distribution. This energy behaves as a potential energy in some respects, for example, the current distribution feels an overall force given by

$$\mathbf{F} = -\nabla U = +\nabla(\boldsymbol{\mu}\cdot\mathbf{B}). \tag{6}$$

This is the force that splits the beam in the Stern-Gerlach experiment. The current distribution also feels a torque given by

$$\mathbf{T} = \frac{d\mathbf{L}}{dt} = \boldsymbol{\mu}\times\mathbf{B}, \tag{7}$$

where $\mathbf{L}$ is the angular momentum. These are standard results discussed in all books on electromagnetism, although badly in many cases because of the difficulties of dealing with magnetic energy.

Comparing these classical facts to the quantum results quoted in Sec. 2, one question that arises is whether the electron has higher multipole moments than the electric monopole and magnetic dipole. Normally a classical current and charge distribution would have these higher moments. The answer is that the electron does not; the multipole expansion of its electric field ends with the monopole term, and the magnetic field ends with the dipole term. This statement is subject to a minor qualification we shall consider later, when we will justify and explain it.

4. Models of Spins and Magnetic Moments

In nonrelativistic quantum mechanics it is impossible to obtain an understanding of spins and their interactions with magnetic fields without resorting to crude models or ad hoc assumptions. The relativistic theory, on the other hand, leads to much insight into the nature of spin as well as beautiful explanations of some facts that at the nonrelativistic level just have to be taken for

granted. We will now examine a crude model concerning the relation between magnetic moment and angular momentum.

A classical particle of charge q and mass m in a circular orbit possesses an angular momentum

$$\mathbf{L} = m\mathbf{r}\times\mathbf{v}. \tag{8}$$

Also, its motion creates on average a current loop that has the magnetic moment

$$\boldsymbol{\mu} = \frac{q}{2mc}\mathbf{L}. \tag{9}$$

This is a vectorial relation, and, in particular, if the charge is negative, the magnetic moment and angular momentum point in opposite directions. In this simple model, the magnetic moment and angular momentum are proportional.

They are not proportional in all classical models of mass and charge motion, however. This is easy to see, since the angular momentum depends on the mass distribution and its state of motion, while the magnetic moment depends on the charge distribution and its state of motion. These two do not have to be the same, for example, in a wire the electrons move and the ions are stationary. Thus, in classical mechanics $\mathbf{L}$ and $\boldsymbol{\mu}$ generally point in different directions.

A question is to what extent Eq. (9) can be taken over into quantum mechanics. In fact, that equation is valid, with certain understandings, for the orbital motion of a charged particle, for example, the orbital motion of an electron in an atom. This motion approximates a current loop, whose interactions with external magnetic fields can be seen for example in the Zeeman effect.

In the case of particle spins, however, it is necessary to introduce a fudge factor or *g-factor*, and to write

$$\boldsymbol{\mu} = g\frac{q}{2mc}\mathbf{S}. \tag{10}$$

The g-factors are measured experimentally for different particles and can sometimes be calculated theoretically, notably in the case of the leptons (electron, muon and tauon). In other cases (the hadrons such as the proton, neutron, or various atomic nuclei), theory can provide rough estimates but accurate calculations are very difficult.

5. Examples of Magnetic Moments and g-factors

Let us look at some important examples of spins and magnetic moments. The data is summarized in Table 1.

For the electron, a spin-$\frac{1}{2}$ particle with $q = -e$, the relation (10) can be written

$$\boldsymbol{\mu} = -g_e\Big(\frac{e\hbar}{2m_ec}\Big)\frac{\mathbf{S}}{\hbar}, \tag{11}$$

where m_e and g_e are the electron mass and g-factor, and where we have multiplied and divided by $\hbar$ to make the factor $\mathbf{S}/\hbar = \boldsymbol{\sigma}/2$ dimensionless. The factor g_e is also dimensionless, so the quantity

Particle	charge	spin	g-factor
electron	$-e$	$\frac{1}{2}$	$2 \times 1.0011\ldots$
positron	$+e$	$\frac{1}{2}$	$2 \times 1.0011\ldots$
proton	$+e$	$\frac{1}{2}$	$5.588\ldots$
neutron	0	$\frac{1}{2}$	$-3.823\ldots$
deuteron	$+e$	1	$0.857\ldots$
α-particle	$+2e$	0	—

Table 1. Spins and g-factors for various particles and nuclei.

in the parentheses has dimensions of magnetic moment. This is the *Bohr magneton*, a basic unit of magnetic moment that can be constructed out of the physical constants shown,

$$\mu_B = \frac{e\hbar}{2m_e c}. \tag{12}$$

The Bohr magneton is a convenient unit of magnetic moment for electrons or atoms with unpaired electrons.

The electron g-factor can be written,

$$g_e = 2\Big(1 + \frac{\alpha}{2\pi} + \ldots\Big) = 2.00232, \tag{13}$$

where the series indicated is a power series in the fine structure constant,

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}. \tag{14}$$

This series is the result of a perturbation calculation in quantum electrodynamics, in which the $O(\alpha)$ correction terms and higher are known as *radiative corrections* since physically they come from the interaction of the electron with the quantized electromagnetic and electron-positron fields. The first correction term in this series, shown in Eq. (13), was calculated by Schwinger in the late 1940's, and was notable as one of the first successful applications of renormalization theory. These correction terms are small, so to a good approximation $g_e \approx 2$. The value $g_e = 2$ comes out of the Dirac equation (the equation of the electron in relativistic quantum mechanics), so it is known as the Dirac value. For a long time in the early days of atomic physics the existence of the small corrections was not known, either experimentally or theoretically, and it was believed that the g-factor was exactly 2, as predicted by the Dirac equation. The discovery of the small deviations from the Dirac value led to a theoretical push to understand radiative corrections. In more recent years (the last 50 years or so) there has been a competition between theory and experiment to determine the electron g-factor to ever higher accuracy, and it is now known to many significant digits. The purpose is to test quantum electrodynamics and to look for new physics. Approximating the g-factor by 2, the electron magnetic moment can be written,

$$\boldsymbol{\mu} = -g_e \mu_B \frac{\boldsymbol{\sigma}}{2} \approx -\mu_B \boldsymbol{\sigma}. \tag{15}$$

The minus sign in this equation means that the electron magnetic moment and angular momentum point in opposite directions.

The positron is the antiparticle of the electron, with the same mass and g-factor but opposite charge. Its magnetic moment is therefore given by

$$\boldsymbol{\mu} = g_e \mu_B \frac{\boldsymbol{\sigma}}{2} \approx \mu_B \boldsymbol{\sigma}. \tag{16}$$

For the proton we have $q = +e$ and $s = \frac{1}{2}$, so

$$\boldsymbol{\mu} = g_p \Big(\frac{e\hbar}{2m_p c} \Big) \frac{\mathbf{S}}{\hbar}, \tag{17}$$

where the quantity in parentheses is the *nuclear magneton*,

$$\mu_N = \frac{e\hbar}{2m_p c}, \tag{18}$$

so we can write

$$\boldsymbol{\mu} = \frac{g_p}{2} \mu_N \boldsymbol{\sigma}. \tag{19}$$

The nuclear magneton is a convenient unit for the magnetic moments of the proton, neutron and other hadrons and various nuclei. It differs from the Bohr magneton by the presence of the proton mass in the denominator instead of the electron mass, and so is about 2000 times smaller than the Bohr magneton. Nuclear magnetic moments, which are of the order of a nuclear magneton, are therefore much smaller than electron magnetic moments, so they make only small corrections to the total magnetic moment of an atom with unpaired electrons. If all the electrons in an atom are paired so that their magnetic moments cancel, then the nuclear magnetic moment is all that remains. The proton g-factor $g_p \approx 5.588$ is determined experimentally.

The neutron is electrically neutral, $q = 0$, but nevertheless has a nonzero magnetic moment given by

$$\boldsymbol{\mu} = g_n \mu_N \frac{\mathbf{S}}{\hbar} = g_n \mu_N \frac{\boldsymbol{\sigma}}{2}, \tag{20}$$

where $g_n \approx -3.823$. The neutron is considered to have a negative g-factor, because $\boldsymbol{\mu}$ and $\mathbf{S}$ 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 (20). Crude models of mixtures of up and down quarks are able to explain the proton and neutron magnetic moments to within several percent, but it is very difficult to improve on these calculations. The difficulty is the usual one in hadron physics, where the strong interactions usually preclude a perturbative treatment.

The proton and neutron g-factors are sometimes said to be *anomalous*, because they differ from the Dirac value of 2. Of course, so does the electron g-factor, if we include the radiative corrections.

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

$$\boldsymbol{\mu} = g_d \mu_N \frac{\mathbf{S}}{\hbar}, \tag{21}$$

where $g_d \approx 0.857$. Notice that $\mathbf{S}/\hbar$ is the vector of 3×3 matrices for spin 1, not the Pauli matrices (see Eqs. (13.50) and (13.51)).

The magnetic moment of the deuteron can be considered as due to the magnetic moments of the constituent proton and neutron, plus some contribution due to the orbital motion of the proton. Plugging in the actual numbers gives information about the deuteron wave function, that is, the wave function of the two particle system consisting of proton and neutron. More information about this wave function comes from scattering experiments and other sources. It turns out that the interaction between the proton and neutron is not governed by a purely central force potential, but rather there are strong spin-dependent forces as well. As a result, the spatial part of the wave function is not a pure eigenstate of orbital angular momentum, but rather consists of a linear combination of an s-wave and a d-wave (with $\ell = 0$ and $\ell = 2$). The deuteron has spin 1 because the energy of the proton-neutron system is minimized when the spins are aligned. When the spins are opposite, the proton-neutron system has no bound state. In fact, deuteron has no bound excited states (there is only one bound state, the ground state).

For the α-particle, a spin-0 particle, we have $\boldsymbol{\mu} = 0$ exactly. Spin-0 particles cannot have a magnetic moment, because the spin operator vanishes (see Eqs. (13.46) and (13.47)).

6. Rotational Invariance and Energy Eigenvalues and Eigenspaces

Let us return to the question of why the ket space upon which the magnetic moment operators act is a single irreducible subspace under rotations, characterized by a single angular momentum quantum number s. This question is easiest to address in the case of composite particles such as atoms or nuclei.

In fact, let us consider a rather complicated composite particle, such as a silver atom with its many electrons or the aluminum nucleus with its many protons and neutrons. In the case of the silver atom, we have good electrostatic approximations to the interactions of the particles, so there is no trouble in writing down the Hamiltonian. It is just difficult to solve, since it involves so many particles. In the case of a nucleus, however, we do not even know how to write down the Hamiltonian, at least not very well. Nuclear forces are much more complicated than electrostatic forces, for example, they depend strongly on spin and do not add pairwise when there are more than two particles.

We consider such complicated systems to illustrate some general rules of symmetry and quantum mechanics that apply even in such cases. We consider only isolated systems (not interacting with any external fields), and we take it as physically reasonable that there are rotation operators that act on the ket spaces for these systems. We also take it as physically reasonable that the energy levels of isolated systems do not depend on the orientation. If $|\psi\rangle$ is an energy eigenstate of such a system with energy E, so that

$$H|\psi\rangle = E|\psi\rangle, \tag{22}$$

then we assume that $U(\mathsf{R})|\psi\rangle$, where U is a rotation operator parameterized by a rotation R, is an energy eigenstate of the same energy,

$$HU(\mathsf{R})|\psi\rangle = EU(\mathsf{R})|\psi\rangle. \tag{23}$$

But allowing $U(\mathsf{R})$ to act on both sides of Eq. (22), we have

$$U(\mathsf{R})H|\psi\rangle = EU(\mathsf{R})|\psi\rangle, \tag{24}$$

so the right hand sides of Eqs. (23) and (24) are the same. Since this must hold for all energy eigenstates (which form a basis in the ket space), we must have

$$U(\mathsf{R})H = HU(\mathsf{R}), \tag{25}$$

for all rotations R. We conclude that the Hamiltonian for any isolated system commutes with all rotation operators. But if H commutes with all rotations, it commutes in particular with infinitesimal rotations, and hence with the generators $\mathbf{J}$:

$$[H, \mathbf{J}] = 0. \tag{26}$$

Consequently H commutes with any function of $\mathbf{J}$.

In particular, H commutes with J^2 and J_z, which commute with each other. Thus simultaneous eigenstates of these three operators exist. Let $|\psi\rangle$ now stand for one such simultaneous eigenstate, so that

$$\begin{aligned} H|\psi\rangle &= E|\psi\rangle, \\ J^2|\psi\rangle &= j(j+1)\hbar^2|\psi\rangle, \\ J_z|\psi\rangle &= m\hbar|\psi\rangle. \end{aligned} \tag{27}$$

Let us take this state $|\psi\rangle$ and apply $J_\pm$ to it. If the state $J_\pm|\psi\rangle$ does not vanish, it is also an eigenstate of H with the same eigenvalue E, one that is linearly independent of the original state $|\psi\rangle$ because the magnetic quantum number has been raised or lowered. That is,

$$H(J_\pm|\psi\rangle) = J_\pm H|\psi\rangle = E(J_\pm|\psi\rangle). \tag{28}$$

In this manner, we see that all $2j+1$ states that can be generated from $|\psi\rangle$ by applying raising and lowering operators have the same energy, and we have at least a $(2j+1)$-fold degeneracy. In physical terms, the states created by raising and lowering the m value must have the same energy because m refers to the quantum number of J_z, the component of $\mathbf{J}$ along a particular axis, and if the system is rotationally invariant then the energy cannot depend on the choice of axes.

In fact, all the eigenspaces of H consist of one or more irreducible subspaces under rotations, each with its own j value. The total degeneracy is the sum of the quantities $2j+1$ for each irreducible subspace of the same energy. This applies to any isolated system, no matter how complex. As we shall now argue, however, it is extremely unlikely that we have different irreducible subspaces of the same energy. This means that the eigenspaces of H consist of precisely one irreducible subspace under rotations, they are also eigenspaces of J^2 with quantum number j, and the energy is $(2j+1)$-fold degenerate.

7. What it Takes to Make a Degeneracy

It is a basic rule in quantum mechanics that degeneracies do not occur unless there is some symmetry to make them happen. This rule is not absolute, however, and must be properly understood. If we have a Hamiltonian that depends on some parameters, then the eigenvalues also depend on those parameters. If the parameters are under experimental control, then as they are adjusted the eigenvalues move around. By adjusting enough parameters carefully enough it is possible to make one or more energy eigenvalues coincide, although it is not as easy as it sounds (one must vary more parameters than you would naively think). A degeneracy created in this way would be considered an *accidental* degeneracy, that is, due to the accidental values of some parameters. If we just use the parameters given to us by nature (the electron charge and mass, etc), then it is unlikely that there will be degeneracies, unless there are systematic symmetries that force them to happen. It is like picking two random numbers between 0 and 1; they could be equal, but the probability that they are equal is zero. Of course, eigenvalues could come very close together even in a system without symmetry, and indeed they will do so when we go to higher energies where the density of states becomes large, especially in multiparticle systems.

Symmetry sometimes forces eigenvalues to be identical. We just saw this in the case of rotational invariance, where there is always at least a $(2j+1)$-fold degeneracy of energy levels (the value of j depends on the energy level). But if the system has no other symmetry that forces additional degeneracy beyond these, then the different irreducible subspaces under rotations (each characterized by a j value) will be unlikely to have the same energy. That is, in the absence of any further symmetry beyond rotations, the $(2j+1)$-fold degeneracy caused by rotational invariance will be the only degeneracy there is, apart from accidental coincidences that occur with probability zero.

Atoms and nuclei do have other symmetries besides rotations, for example, they possess symmetry under parity and time reversal (to a high degree of approximation). But these extra symmetries do not force any extra degeneracies. Thus, in the real world, systems such as isolated atoms, molecules and nuclei possess energy levels that are characterized by an angular momentum quantum number j and that are precisely $(2j+1)$-fold degenerate.

This applies, for example, to the ground state of nuclei, the states of the nuclei we normally deal with in atoms. (Radioactive nuclei are in excited states, but the same considerations about angular momentum and degeneracy apply to them, too.) Thus, the ground state of a nucleus has an angular momentum value, which we call s instead of j, and the space of degenerate energy eigenstates is a single irreducible subspace under rotations of dimensionality $(2s+1)$. The spin of the nucleus is just the total angular momentum of the nucleus, regarded as a quantum system of protons and neutrons. Similar statements can be made about the state of an atom (ground state or excited state).

A few systems have extra symmetry beyond rotational invariance that does cause extra degeneracy, beyond that predicted on the basis of rotational invariance alone. These are not real systems, but idealized models that have more symmetry than exists in the real world. They are, however, important in practice. Examples include the multidimensional, isotropic harmonic oscillator,

the electrostatic model of the hydrogen atom, and the central field approximation in multielectron atoms. It is interesting to see how the extra degeneracy in these systems gets split as corrections are turned on and the model is made more realistic. This is a particularly interesting story in the case of hydrogen. When enough physics has been added, we always find that only the degeneracy due to rotational invariance remains.

8. Energy Scales and the Mixing of Irreducible Subspaces

In the case of a nucleus, the ground state is typically separated from the first excited state by an energy of one or two MeV. This compares to the energy of magnetic interaction $\boldsymbol{\mu} \cdot \mathbf{B}$ that is of the order of 10^{-6} eV, even in strong laboratory magnetic fields. Since this energy is so small compared to the distance to the nearest energy level, the quantum mechanics of the nucleus is well described by the $(2s+1)$-dimensional subspace of the nuclear Hilbert space which is the energy eigenspace of the ground state alone. As we say in perturbation theory, there is negligible mixing coming from the first excited state. This is why the magnetic moment operators act on a Hilbert space that is a single irreducible subspace under rotations.

As we shall see later in the course, on a single irreducible subspace, there is only one way to construct a vector operator, that is, all vector operators are proportional to one another. A vector operator is defined as one that transforms as a vector under rotations. Thus, on an irreducible subspace, all vector operators, such as the magnetic moment, are proportional to the angular momentum, a given vector operator. The fact that the angular momentum is a vector operator is a consequence of the adjoint formula, Eq. (13.66).

There is, however, the quantitative matter of how far away the neighboring energy eigenstates are, compared to the energy of magnetic interactions. While it would take an enormously large magnetic field to mix substantially the ground state of a nucleus with the first excited state (the field would be so strong that it would substantially modify the nuclear structure), in the case of atoms or in the case of the highly excited states of any multiparticle system where the density of states becomes large the distance to nearby energy levels is not so large. In such cases, there will be a more moderate magnetic field beyond which we obtain substantial mixing of different energy levels, each of which is an irreducible subspace under rotations. In this case, there would be contributions to the magnetic moment coming from more than one energy level, each with its own g-factor, and the vector sum of the magnetic moments would no longer be proportional to the vector sum of the angular momenta. This in fact occurs in the strong field limit of the Zeeman effect in atoms, as we shall see. This mixing explains why $\boldsymbol{\mu}$ and $\mathbf{L}$ need not be proportional in classical systems.

9. The Case of Other Particles

A similar story can be told for other composite particles, such as the proton and the neutron, which are made up of three quarks. What we call the spin of the proton and neutron can be viewed

as the total angular momentum, orbital plus spin, of the constituent quarks. This however is only a rough picture, since relativistic and field theoretic effects are important in the structure of nucleons. In any case, we have only explained the spin of composite particles (nuclei, nucleons) in terms of the spins of the constituents (nucleons, quarks). As far as quarks are concerned, as far as anyone knows they are truly elementary, and not made up out of smaller constituents. The same is true for the leptons (electron, muon, tauon). A better understanding of spin at the level of elementary particles requires methods of relativistic quantum mechanics, which we cannot pursue here. An introduction to some of these topics will be presented in Physics 221B.

10. Hamiltonian for a Spin in a Magnetic Field

Now we turn to solving some problems involving spins in magnetic fields. In these problems we will assume that the magnetic field is uniform in space, so there is no coupling to the spatial degrees of freedom (as there was, for example, in the Stern-Gerlach experiment). This is often a good approximation in practice, since laboratory magnetic fields are usually quite uniform on the atomic scale. We will, however, allow the magnetic field to be a function of time, $\mathbf{B} = \mathbf{B}(t)$, because this in fact is the principal means by which spins are controlled experimentally.

As a result, we can ignore the spatial degrees of freedom and take the Hamiltonian to be

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} = \gamma \mathbf{B} \cdot \mathbf{S}, \tag{29}$$

where

$$\gamma = -g\frac{q}{2mc}. \tag{30}$$

To be specific, in the rest of these notes we will assume $\gamma > 0$ (as it would be for an electron), but if $\gamma < 0$ then directions of precession and various other conclusions must be reversed.

11. The Time Evolution is a Rotation

Consider first the general problem in which the magnetic field has an arbitrary time dependence, $\mathbf{B} = \mathbf{B}(t)$. We denote the unitary time evolution operator by $T(t, t_0)$, reserving the symbol U for rotation operators, as in Notes 13. The Schrödinger equation for T is Eq. (5.12), which in the present case is

$$i\hbar\frac{\partial T(t,t_0)}{\partial t} = \gamma[\mathbf{B}(t)\cdot\mathbf{S}]T(t,t_0). \tag{31}$$

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 T is always a rotation operator. To see this, we consider the infinitesimal time advance implied by the Schrödinger equation,

$$T(t+\Delta t, t_0) = \Big[1 - \frac{i\gamma\Delta t}{\hbar}\mathbf{B}(t)\cdot\mathbf{S}\Big]T(t,t_0). \tag{32}$$

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

$$U(\hat{\mathbf{n}}, \Delta\theta) = 1 - \frac{i\Delta\theta}{\hbar}\hat{\mathbf{n}} \cdot \mathbf{S}, \tag{33}$$

valid when $\Delta\theta \ll 1$. We see that the axis of the infinitesimal rotation is given by

$$\hat{\mathbf{n}} = \hat{\mathbf{b}}(t), \tag{34}$$

where we write

$$\mathbf{B}(t) = B(t)\hat{\mathbf{b}}(t) \tag{35}$$

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

$$\Delta\theta = \gamma B(t)\Delta t, \tag{36}$$

or,

$$\omega = \frac{\Delta\theta}{\Delta t} = \gamma B(t). \tag{37}$$

The angular velocity can also be written as a vector,

$$\boldsymbol{\omega} = \omega\hat{\mathbf{n}} = \gamma\mathbf{B}(t), \tag{38}$$

which is parallel to $\mathbf{B}$ (antiparallel, if $\gamma < 0$).

We see that as time proceeds, T develops by the composition of a large number of infinitesimal rotation operators; since the product of rotation operators is always a rotation operator, T 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 $\boldsymbol{\omega}$ is some function of time, which in general is not constant either in magnitude or direction. In classical rigid body motion, $\boldsymbol{\omega}$ 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, $\boldsymbol{\omega}$ is simply given as a function of time by Eq. (38). In either case, once $\boldsymbol{\omega}(t)$ is known, the subsequent problem of determining the time-dependent rotation is very similar.

12. Constant Magnetic Field

We turn now to some cases in which Eq. (31) can be solved explicitly. The simplest one is that of a spin in a constant magnetic field,

$$\mathbf{B} = B\hat{\mathbf{b}} = \text{const.} \tag{39}$$

The Hamiltonian is now time-independent, so T only depends on the elapsed time t. We borrow notation from Sec. 11, writing,

$$\boldsymbol{\omega} = \gamma\mathbf{B} = \omega\hat{\mathbf{b}}, \tag{40}$$

and

$$\omega = \gamma B, \tag{41}$$

where now $\boldsymbol{\omega}$ and its magnitude ω are time-independent. Thus the Schrödinger equation for T is

$$i\hbar\frac{\partial T(t)}{\partial t} = (\boldsymbol{\omega}\cdot\mathbf{S})T(t). \tag{42}$$

This can be immediately integrated, giving

$$T(t) = \exp\Big[-\frac{i}{\hbar}(\boldsymbol{\omega}\cdot\mathbf{S})t\Big] = U(\hat{\mathbf{b}},\omega t). \tag{43}$$

The time evolution consists of a rotation about the axis $\hat{\mathbf{b}}$ with frequency ω.

In the case of the electron, the frequency of spin precession is

$$\omega = \frac{g_e}{2}\frac{eB}{mc}, \tag{44}$$

which, in the approximation $g_e \approx 2$, is equal to the nonrelativistic frequency of orbital motion of the electron in the uniform magnetic field. Certain so-called $g-2$ experiments exploit this near equality to measure the small difference between the two frequencies, which provides a direct measurement of the radiative corrections in Eq. (13).

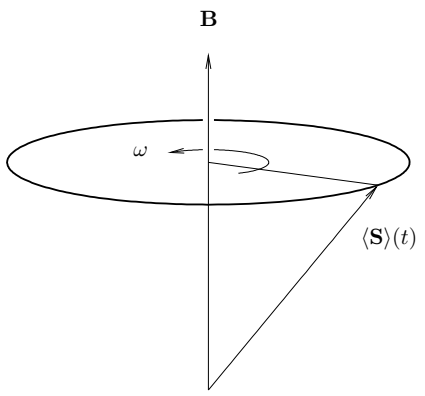

Fig. 1. In a constant magnetic field, $\langle\mathbf{S}\rangle$ precesses about the field direction at frequency $\omega = \gamma B$.

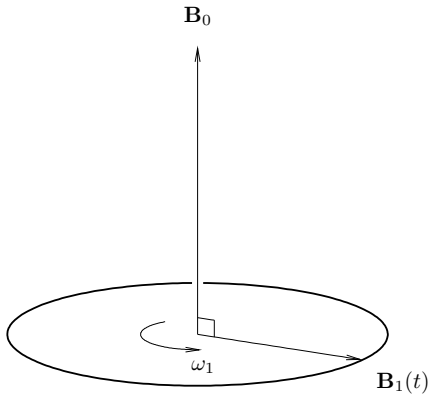

Fig. 2. The field in magnetic resonance experiments consists of a constant field $\mathbf{B}_0$ plus a time-dependent field $\mathbf{B}_1(t)$ that is perpendicular to $\mathbf{B}_0$ and that rotates about $\mathbf{B}_0$ at frequency ω_1.

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

$$\begin{aligned}\langle\mathbf{S}\rangle(t) &= \langle\psi(t)|\mathbf{S}|\psi(t)\rangle = \langle\psi_0|U(\hat{\mathbf{b}},\omega t)^\dagger\mathbf{S}U(\hat{\mathbf{b}},\omega t)|\psi_0\rangle \\ &= \mathsf{R}(\hat{\mathbf{b}},\omega t)\langle\psi_0|\mathbf{S}|\psi_0\rangle = \mathsf{R}(\hat{\mathbf{b}},\omega t)\langle\mathbf{S}\rangle(0),\end{aligned} \tag{45}$$

where we have used the adjoint formula (13.66). We see that the expectation value of $\mathbf{S}$ rotates counterclockwise (for $\gamma > 0$) about the direction of the magnetic field, sweeping out a cone. This is illustrated in Fig. 1.

13. Magnetic Resonance Experiments

A more interesting case occurs in magnetic resonance experiments. Here the magnetic field consists of a constant, background field $\mathbf{B}_0 = B_0\hat{\mathbf{b}}_0$, plus a time-dependent $\mathbf{B}_1(t)$ that is perpendicular to $\mathbf{B}_0$ and oscillating with some frequency ω_1. In the absence of $\mathbf{B}_1$, the spin would evolve according to a time-dependent rotation with angular velocity,

$$\boldsymbol{\omega}_0 = \omega_0\hat{\mathbf{b}}_0, \tag{46}$$

whose magnitude is

$$\omega_0 = \gamma B_0. \tag{47}$$

The time-dependent field $\mathbf{B}_1(t)$ is used to induce spin flips. To do this its magnitude need not be large, but its frequency ω_1 should be at or near resonance with the precession frequency ω_0 in the background field. Thus, the interesting case is $|\mathbf{B}_1| \ll B_0$ and $\omega_1 \approx \omega_0$. Notice that ω_0 is determined by the magnitude of the background field $\mathbf{B}_0$, but ω_1 is the frequency of the time-dependence of $\mathbf{B}_1(t)$, and is independent of its magnitude.

We will consider the case that $\mathbf{B}_1(t)$ rotates in a counterclockwise direction (clockwise, if $\gamma < 0$) at frequency ω_1 in the plane perpendicular to $\mathbf{B}_0$, as illustrated in Fig. 2. This case has the advantage that the Schrödinger equation can be solved exactly in terms of rotation operators. We assume the magnitude of $\mathbf{B}_1$ is constant, so the vector $\mathbf{B}_1(t)$ traces out a circle in the perpendicular plane. The time-dependence of $\mathbf{B}_1$ can be expressed in terms of a classical rotation about the axis $\hat{\mathbf{b}}_0$,

$$\mathbf{B}_1(t) = \mathsf{R}_1(t)\mathbf{B}_{10}, \tag{48}$$

where $\mathbf{B}_{10}$ is a constant vector (the initial value of $\mathbf{B}_1(t)$) perpendicular to $\mathbf{B}_0$, and where

$$\mathsf{R}_1(t) = \mathsf{R}(\hat{\mathbf{b}}_0, \omega_1 t). \tag{49}$$

Another possibility for the time-dependence of $\mathbf{B}_1$ will be mentioned below.

The Schrödinger equation can now be written,

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \gamma\{[\mathbf{B}_0 + \mathsf{R}_1(t)\mathbf{B}_{10}]\cdot\mathbf{S}\}|\psi(t)\rangle. \tag{50}$$

We solve this by effectively going over to a frame rotating with frequency ω_1 about the axis $\mathbf{b}_0$. This cancels out the rotation of the field $\mathbf{B}_1(t)$, giving a constant magnetic field $\mathbf{B}_0 + \mathbf{B}_{10}$ in the rotating frame. However, as is well known, Coriolis effects in a rotating frame reproduce the effects of a magnetic field, and can be used to enhance or cancel out the effects of a true magnetic field. In the present case, in the rotating frame the effects of $\mathbf{B}_0$ are partially or totally cancelled, resulting in an effective magnetic field $\mathbf{B}_{\text{eff}}$ that is the sum of a reduced magnetic field in the direction $\hat{\mathbf{b}}_0$ plus the constant field $\mathbf{B}_{10}$ in the perpendicular direction.

We obtain the effect of going to a rotating frame by stripping off the time dependence

$$U_1(t) = U(\hat{\mathbf{b}}_0, \omega_1 t) \tag{51}$$

from the state vector $|\psi(t)\rangle$, that is, by setting

$$|\psi(t)\rangle = U_1(t)|\phi(t)\rangle, \tag{52}$$

where $|\phi(t)\rangle$ is a new state vector. Notice that $U_1(t)$ has the same axis and angle as $R_1(t)$, defined in Eq. (49). Differentiating Eq. (52), we obtain

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = U_1\Big[\omega_1(\hat{\mathbf{b}}_0\cdot\mathbf{S}) + i\hbar\frac{\partial}{\partial t}\Big]|\phi(t)\rangle. \tag{53}$$

On the other hand, with the substitution (52) the Schrödinger equation (50) becomes

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \gamma[(\mathbf{B}_0 + \mathsf{R}_1\mathbf{B}_{10})\cdot\mathbf{S}]U_1|\phi(t)\rangle. \tag{54}$$

Now we equate the right hand sides of Eqs. (53) and (54) and multiply through by $U_1^\dagger$, to obtain

$$\omega_1(\hat{\mathbf{b}}_0\cdot\mathbf{S})|\phi(t)\rangle + i\hbar\frac{\partial}{\partial t}|\phi(t)\rangle = \gamma(\mathbf{B}_0 + \mathsf{R}_1\mathbf{B}_{10})\cdot(U_1^\dagger\mathbf{S}U_1)|\phi(t)\rangle. \tag{55}$$

Here we have pulled the $U_1^\dagger$ through the constant γ, the vectors $\mathbf{B}_0$ and $\mathbf{B}_{10}$ and the matrix R_1, because these are just numbers or matrices and vectors composed of numbers, while $U_1^\dagger$, $\mathbf{S}$ and U_1 are operators that act on kets. Now we use the adjoint formula (13.66), with $\mathbf{J}$ replaced by $\mathbf{S}$, U replaced by $U_1^\dagger$, and R replaced by R_1^{-1}. This gives

$$U_1^\dagger\mathbf{S}U_1 = \mathsf{R}_1\mathbf{S}, \tag{56}$$

so the dot product on the right hand side of Eq. (55) becomes

$$(\mathbf{B}_0 + \mathsf{R}_1\mathbf{B}_{10})\cdot(\mathsf{R}_1\mathbf{S}). \tag{57}$$

But if $\mathbf{X}$ and $\mathbf{Y}$ are any vectors and R is any rotation, then

$$\mathbf{X}\cdot(\mathsf{R}\mathbf{Y}) = (\mathsf{R}^{-1}\mathbf{X})\cdot\mathbf{Y}, \tag{58}$$

since the dot product is invariant under rotations. Thus the dot product (57) can be written

$$[\mathsf{R}_1^{-1}(\mathbf{B}_0 + \mathsf{R}_1\mathbf{B}_{10})]\cdot\mathbf{S} = (\mathbf{B}_0 + \mathbf{B}_{10})\cdot\mathbf{S}, \tag{59}$$

so Eq. (55) becomes

$$\omega_1(\hat{\mathbf{b}}_0\cdot\mathbf{S})|\phi(t)\rangle + i\hbar\frac{\partial}{\partial t}|\phi(t)\rangle = \gamma(\mathbf{B}_0 + \mathbf{B}_{10})\cdot\mathbf{S}|\phi(t)\rangle, = (\omega_0\hat{\mathbf{b}}_0 + \gamma\mathbf{B}_{10})\cdot\mathbf{S}|\phi(t)\rangle. \tag{60}$$

Rearranging this, we can write the effective Schrödinger equation for $|\phi(t)\rangle$ in the form

$$i\hbar\frac{\partial|\phi(t)\rangle}{\partial t} = \{[(\omega_0 - \omega_1)\hat{\mathbf{b}}_0 + \gamma\mathbf{B}_{10}]\cdot\mathbf{S}\}|\phi(t)\rangle = \gamma(\mathbf{B}_{\rm eff}\cdot\mathbf{S})|\phi(t)\rangle, \tag{61}$$

where

$$\gamma\mathbf{B}_{\rm eff} = (\omega_0 - \omega_1)\hat{\mathbf{b}}_0 + \gamma\mathbf{B}_{10}, \tag{62}$$

or,

$$\mathbf{B}_{\text{eff}} = \Big(B_0 - \frac{\omega_1}{\gamma}\Big)\hat{\mathbf{b}}_0 + \mathbf{B}_{10}. \tag{63}$$

This is the effective magnetic field in the rotating frame. We break it up into its magnitude and direction,

$$\mathbf{B}_{\text{eff}} = B_{\text{eff}}\hat{\mathbf{b}}_{\text{eff}}, \tag{64}$$

so that

$$B_{\text{eff}} = \sqrt{\Big(B_0 - \frac{\omega_1}{\gamma}\Big)^2 + B_{10}^2}. \tag{65}$$

We also define

$$\Omega = \gamma B_{\text{eff}} = \sqrt{(\omega_0 - \omega_1)^2 + \gamma^2 B_{10}^2}, \tag{66}$$

called the *Rabi flopping frequency*. Notice that if $B_{10} \ll B_0$ and $\omega_1 \approx \omega_0$, then $\Omega \ll \omega_0$ (the flopping frequency is much less than the precession frequency). We will also denote the angle between $\hat{\mathbf{b}}_0$ and $\hat{\mathbf{b}}_{\text{eff}}$ by θ, so that

$$\sin\theta = \frac{B_{10}}{B_{\text{eff}}}, \tag{67}$$

as illustrated in Fig. 3.

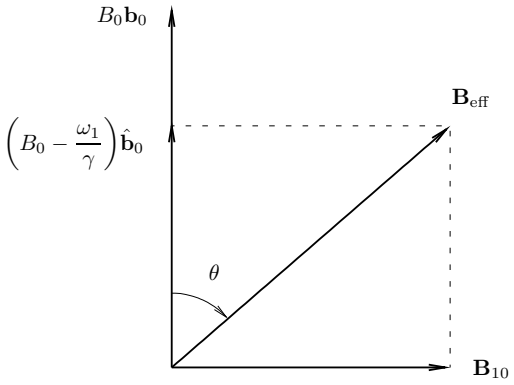

Fig. 3. In the rotating frame, the field $\mathbf{B}_1 = \mathbf{B}_{10}$ is stationary, and $\mathbf{B}_0$ is reduced in magnitude by ω_1/γ. The resulting field is $\mathbf{B}_{\text{eff}}$, which is constant in the rotating frame.

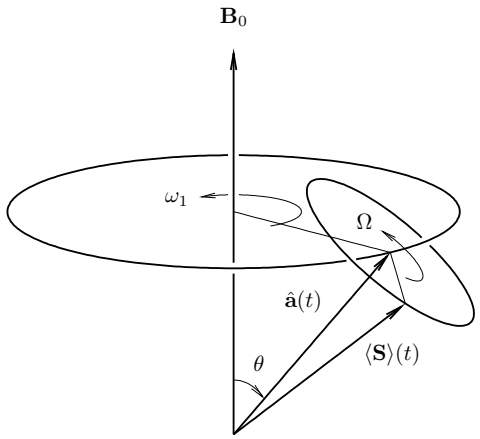

Fig. 4. The expectation value of the spin $\mathbf{S}$ precesses about the axis $\hat{\mathbf{a}}(t)$ with frequency Ω, while that axis itself precesses about $\mathbf{B}_0$ with frequency ω_1.

The Schrödinger equation for $|\phi(t)\rangle$, Eq. (61), is the case of a spin in a constant magnetic field, so the solution is

$$|\phi(t)\rangle = U(\hat{\mathbf{b}}_{\text{eff}}, \Omega t)|\phi(0)\rangle. \tag{68}$$

Combining this with Eq. (52), we obtain the time evolution operator for the original Schrödinger equation (50),

$$T(t) = U(\hat{\mathbf{b}}_0, \omega_1 t)U(\hat{\mathbf{b}}_{\text{eff}}, \Omega t). \tag{69}$$

As before, we can use the solution (69) to find the evolution of the expectation value of the spin. We find,

$$\langle \mathbf{S} \rangle(t) = \mathsf{R}(\hat{\mathbf{b}}_0, \omega_1 t)\mathsf{R}(\hat{\mathbf{b}}_{\rm eff}, \Omega t)\langle \mathbf{S} \rangle(0). \tag{70}$$

Thus, $\langle \mathbf{S} \rangle$ sweeps out a cone at frequency Ω about an axis $\hat{\mathbf{a}}$ that 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. 4. The direction $\hat{\mathbf{b}}_{\rm eff}$ is the initial direction of the axis at $t = 0$, so that

$$\hat{\mathbf{a}}(t) = \mathsf{R}(\hat{\mathbf{b}}_0, \omega_1 t)\hat{\mathbf{b}}_{\rm eff}. \tag{71}$$

Equation (70) can be expressed explicitly in terms of the time-dependent axis $\hat{\mathbf{a}}(t)$ by use of the exponentiated adjoint formula, Eq. (11.48):

$$\langle \mathbf{S} \rangle(t) = \mathsf{R}\big(\hat{\mathbf{a}}(t), \Omega t\big)\mathsf{R}(\hat{\mathbf{b}}_0, \omega_1 t)\langle \mathbf{S} \rangle(0), \tag{72}$$

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

We remark that in practice it is easier to use a different time-dependent field $\mathbf{B}_1$, given by

$$\mathbf{B}_1(t) = 2B_{10}\hat{\mathbf{x}}\cos\omega_1 t, \tag{73}$$

where we put $\mathbf{B}_0$ along the z-axis. This field is the sum of two counter-rotating fields,

$$\begin{aligned}\mathbf{B}_1(t) = {} & B_{10}(\hat{\mathbf{x}}\cos\omega_1 t + \hat{\mathbf{y}}\sin\omega_1 t) \\ & + B_{10}(\hat{\mathbf{x}}\cos\omega_1 t - \hat{\mathbf{y}}\sin\omega_1 t),\end{aligned} \tag{74}$$

so that if we go into the rotating frame as above then one of these fields becomes constant while the other is rotating in the opposite direction at a frequency $2\omega_1$. This is much higher than Ω under the conditions we have posited, so the oppositely rotating field causes only small changes in the solution we have given. High frequency perturbations generally have only a small effect on a system because before the effect has a chance to build up, the perturbation changes sign and starts working in the opposite direction.

14. 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 $\hat{\mathbf{b}}_{\rm eff}$ in the x-z plane. To compute the probability amplitude for the $\frac{1}{2} \to -\frac{1}{2}$ transition, we use Eq. (69) to obtain

$$\langle -|T(t)|+\rangle = \langle -|U(\hat{\mathbf{z}}, \omega_1 t)U(\hat{\mathbf{b}}_{\rm eff}, \Omega t)|+\rangle = e^{i\omega_1 t/2}\,\langle -|U(\hat{\mathbf{b}}_{\rm eff}, \Omega t)|+\rangle. \tag{75}$$

But since

$$\hat{\mathbf{b}}_{\rm eff} = \hat{\mathbf{z}}\cos\theta + \hat{\mathbf{x}}\sin\theta, \tag{76}$$

we have

$$\langle -|T(t)|+\rangle = -ie^{i\omega_1 t/2}\,\sin\theta\sin\frac{\Omega t}{2}. \tag{77}$$

Thus, the transition probability is

$$P_{\frac{1}{2}\to-\frac{1}{2}} = \sin^2\theta \sin^2\frac{\Omega t}{2}. \tag{78}$$

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 (78) reaches a maximum value of unity when $t = \pi/\Omega$.

Problems

1. Consider a particle of spin 1 and magnetic moment $\boldsymbol{\mu} = -\gamma\mathbf{S}$ in the magnetic field,

$$\mathbf{B} = B_0\hat{\mathbf{z}} + B_{10}(\hat{\mathbf{x}}\cos\omega_1 t + \hat{\mathbf{y}}\sin\omega_1 t), \tag{79}$$

employed in magnetic resonance experiments (assume $\gamma > 0$). If at $t = 0$, the particle is in state $m = 0$, find the transition probabilities $P(0 \to \pm 1)$ as a function of time.

2. If we combine Eq. (31) with (38), we obtain

$$\frac{\partial U}{\partial t} = -\frac{i}{\hbar}\boldsymbol{\omega}(t)\cdot\mathbf{S}\,U, \tag{80}$$

where we write U instead of T for the time evolution operator, which we know is a rotation. Let U be parameterized by its Euler angles, $U = U(\alpha, \beta, \gamma)$. Find equations of motion for the Euler angles, assuming $\boldsymbol{\omega}(t)$ is given. Your answer will be identical to the equations of motion of the Euler angles in classical rigid body theory (for given $\boldsymbol{\omega}(t)$).

3. Consider a biological sample at 300K in a magnetic field of 6T (for example, you in an MRI device). After a certain relaxation time, the nuclear spins will reach thermal equilibrium with their environment (a heat bath). Calculate the fractional magnetization of protons under such circumstances (the magnetization compared to the maximum we would have at 0K). Finally, for a sample of water under the conditions indicated, compute the magnetization due to protons in Gauss.