8.421 AMO I Lecture Notes

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Preface

The original incarnation of these notes was developed to accompany the lectures in the MIT graduate courses in atomic physics. AMO I was created in the late 1960s as a one-term introductory course to prepare graduate students for research in atomic physics in the Physics department. Over the years Dan Kleppner and David Pritchard changed the contents of the course to reflect new directions of research, though the basic concepts remained as a constant thread. With the growth of interest in atom cooling and quantum gases, a second one-term course, AMO II, was designed by Wolfgang Ketterle in the late 1990s and presented with AMO I in alternating years. We still teach AMO I in the traditional way. These lecture notes combine the (g)olden notes of Dan and Dave. As part of the Joint Harvard/MIT Center for Ultracold Atoms summer school in Atomic Physics in 2002, John Doyle got involved and improved the notes. They have been circulated since and at some point were put into the form of an AMO Wiki. At this moment in time, I'd like to resurrect them in their traditional paper form, and only carefully add topics as I see fit.

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Chapter 1
The Two-State System: Resonance

1.1 Introduction

The cornerstone of major areas of contemporary Atomic, Molecular and Optical Physics (AMO Physics) is the study of atomic and molecular systems through their resonant interaction with applied oscillating electromagnetic fields. The thrust of these studies has evolved continuously since Rabi performed the first resonance experiments in 1938. In the decade following World War II the edifice of quantum electrodynamics was constructed largely in response to resonance measurements of unprecedented accuracy on the properties of the electron and the fine and hyperfine structure of simple atoms. At the same time, nuclear magnetic resonance and electron paramagnetic resonance were developed and quickly became essential research tools for chemists and solid state physicists. Molecular beam magnetic and electric resonance studies yielded a wealth of information on the properties of nuclei and molecules, and provided invaluable data for the nuclear physicist and physical chemist. With the advent of lasers and laser spectroscopy these studies evolved into the creation of new species, such as Rydberg atoms, to studies of matter in ultra intense fields, to fundamental studies in the symmetries of physics, to new types of metrology. With the advent of laser cooling and trapping, these techniques led to the creation of novel atomic quantum fluids, from Bose-Einstein condensates to strongly interacting Fermi gases.

Resonance techniques may be used not only to learn about the structure of a system, but also to prepare it in a precisely controlled way. Because of these two facets, resonance studies have led physicists through a fundamental change in attitude - from the passive study of atoms to the active control of their internal quantum state and their interactions with the radiation field. The chief technical legacy of the early work on resonance spectroscopy is the family of lasers which have sprung up like the brooms of the sorcerer's apprentice. The scientific applications of these devices have been prodigious. They caused the resurrection of physical optics - what we now call quantum optics - and turned it into one of the liveliest fields in physics. They have had a similar impact on atomic and molecular spectroscopy. In addition, lasers have led to new families of physical studies such as single particle spectroscopy, multiphoton excitation, cavity quantum electrodynamics, and laser cooling and trapping. This chapter is about the interactions of a two-state system with a sinusoidally oscillating field whose frequency is close to the natural resonance frequency of the system. The term "two-level" system is sometimes used, but this is less accurate than the term two-state, because the levels could be degenerate, comprising several states. However, its misusage is so widespread that we adopt it anyway. The oscillating field will be treated classically, and the linewidth of both states will be taken as zero until near the end of the chapter where relaxation will be treated phenomenologically. The organization of the material is historical because this happens to be also a logical order of presentation. The classical driven oscillator is discussed first, then the magnetic resonance of a classical spin, and then a quantized spin. The density matrix is introduced last and used to treat systems with damping - this is a useful prelude to the application of resonance ideas at optical frequencies and to the many real systems which have damping.

1.2 Resonance Studies and Q.E.D.

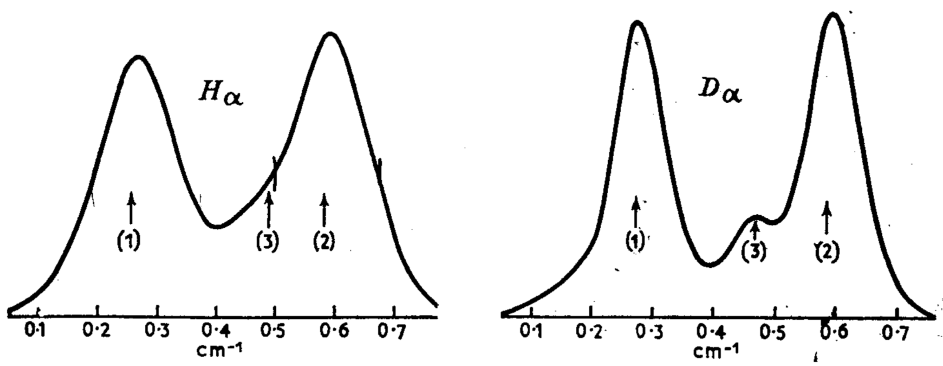

Figure 1. Spectral profile of the H_α line of atomic hydrogen by conventional absorption spectroscopy. Components 1) and 2) arise from the fine structure splitting. The possibility that a third line lies at position 3) was suggested to indicate that the Dirac theory might need to be revised. (From "The Spectrum of Atomic Hydrogen"-Advances. G.W. Series ed., World Scientific, 1988).

One characteristic of atomic resonance is that the results, if you can obtain them at all, are generally of very high accuracy, so high that the information is qualitatively different from other types. The hydrogen fine structure is a good example.

In the late 1930s there was extensive investigation of the Balmer series of hydrogen, ($n > 2 \rightarrow n = 2$). The Dirac Theory was thought to be in good shape, but some doubts were arising. Careful study of the Balmer-alpha line ($n = 3 \rightarrow n = 2$) showed that the line shape might not be given accurately by the Dirac Theory.

Pasternack, in 1939, suggested that the $2\,^2\mathrm{S}_{1/2}$ and $2\,^2\mathrm{P}_{1/2}$ states were not degenerate, but that the energy of the $2\,^2\mathrm{S}_{1/2}$ state was greater than the Dirac value by $\sim .04\,\mathrm{cm}^{-1}$ (or, in frequency, $\sim$ 1200 MHz). However, there was no rush to throw out the Dirac theory on such flimsy evidence.

In 1947, Lamb found a splitting between the $^2\mathrm{S}_{1/2}$ and $^2\mathrm{P}_{1/2}$ levels using a resonance method. The experiment is one of the classics of physics. Although his very first observa- tion was relatively crude, it was nevertheless accurate to one percent. He found

$$S_H = \frac{1}{h}\left[E(^2\mathrm{S}_{1/2}) - E(^2\mathrm{P}_{1/2})\right] = 1050(10)\,\mathrm{MHz} \tag{1.1}$$

The inadequacy of the Dirac theory was inescapably demonstrated.

The magnetic moment of the electron offers another example. In 1925, Uhlenbeck and Goudsmit suggested that the electron has intrinsic spin angular momentum $s = 1/2$ (in units of $\hbar$) and magnetic moment

$$|\mu_e| = \frac{e\hbar}{2m} = \mu_B \tag{1.2}$$

where μ_B is the Bohr magneton (and $\mu_e = -\mu_B$ is negative). The evidence was based on studies of the multiplicity of atomic lines (in particular, the Zeeman structure). The proposal was revolutionary, but the accuracy of the prediction that $|\mu_e| = \mu_B$ was poor, essentially one significant figure. According to the Dirac theory, $|\mu_e| = \mu_B$, exactly. However, our present understanding is

$$\frac{|\mu_e|}{\mu_B} - 1 = 1.1596521884(43) \times 10^{-3} \qquad \text{(experiment, U. of Washington)} \tag{1.3}$$

This result is in good agreement with theory, the limiting factor in the comparison being possible doubts about the value of the fine structure constant.

The Lamb shift and the departure of $|\mu_e|$ from μ_B resulted in the award of the 1955 Nobel prize to Lamb and Kusch, and provided the experimental basis for the theory of quantum electrodynamics for which Feynman, Schwinger and Tomonaga received the Nobel Prize in 1965.

1.2.1 The language of resonance: a classical damped system

Because the terminology of classical resonance, as well as many of its features, are carried over into quantum mechanics, we start by reviewing an elementary resonant system. Consider a harmonic oscillator composed of a series RLC circuit. The charge obeys

$$\ddot{q} + \gamma\dot{q} + \omega_0^2 q = 0 \tag{1.4}$$

where $\gamma = R/L$, $\omega_0^2 = 1/LC$. Assuming that the system is underdamped (i.e. $\gamma^2 < 4\omega_0^2$), the solution for q is a linear combination of

$$\exp\left(-\frac{\gamma}{2}\right)\exp\left(\pm i\omega' t\right) \tag{1.5}$$

where $\omega' = \omega_0\sqrt{1-\gamma^2/4\omega_0^2}$. If $\omega_0 \gg \gamma$, which is often the case, we have $\omega' \equiv \omega_0$. The energy in the circuit is

$$W = \frac{1}{2C}q^2 + \frac{1}{2}L\dot{q}^2 = W_0 e^{-\gamma t} \tag{1.6}$$

where $W_0 = W(t=0)$. The decay time of the stored energy is $\tau = \frac{1}{\gamma}$. If the circuit is driven by a voltage $E_0 e^{i\omega t}$, the steady state solution is $q_0 e^{i\omega t}$ where

$$q_0 = \frac{E_0}{2\omega_0 L}\frac{1}{(\omega_0 - \omega + i\gamma/2)}. \tag{1.7}$$

(We have made the usual resonance approximation: $\omega_0^2 - \omega^2 \approx 2\omega_0(\omega_0 - \omega)$.) The average power delivered to the circuit is

$$P = \frac{1}{2}\frac{E_0^2}{R}\frac{1}{1+\left(\frac{\omega-\omega_0}{\gamma/2}\right)^2} \tag{1.8}$$

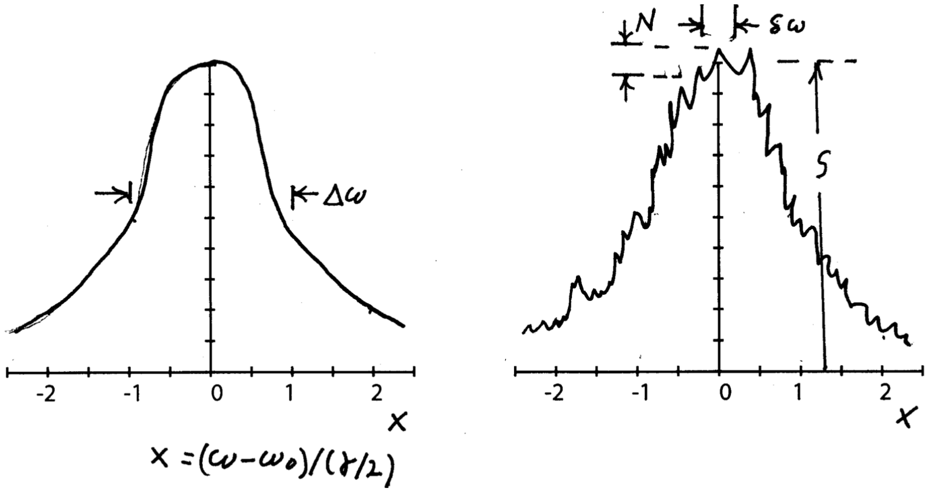

Figure 2. Sketch of a Lorentzian curve, the universal response curve for damped oscillators and for many atomic systems. The width of the curve (full width at half maximum) is $\Delta\omega = \gamma$, where γ is the decay constant. The time constant for decay is $\tau = \gamma$. In the presence of noise (right), the frequency precision with which the center can be located, $\delta\omega$, depends on the signal-to-noise ratio, S/N: $\delta\omega = \Delta\omega/(S/N)$.

The plot of P vs ω (Fig. 2) is universal resonance curve often called a “Lorentzian curve”. The full width at half maximum (“FWHM”) is $\Delta\omega = \gamma$. The quality factor of the oscillator is

$$Q = \frac{\omega_0}{\Delta\omega} \tag{1.9}$$

Note that the decay time of the free oscillator and the linewidth of the driven oscillator obey

$$\tau\Delta\omega = 1 \tag{1.10}$$

This can be regarded as an uncertainty relation. Assuming that energy and frequency are related by $E = \hbar\omega$ then the uncertainty in the energy is $\Delta E = \hbar\Delta\omega$ and

$$\tau\Delta E = \hbar \tag{1.11}$$

It is important to realize that the Uncertainty Principle merely characterizes the spread of individual measurements. Ultimate precision depends on the experimenter’s skill: the Uncertainty Principle essentially sets the scale of difficulty for his or her efforts.

The precision of a resonance measurement is determined by how well one can “split” the resonance line. This depends on the signal to noise ratio (S/N) (see Fig. 2). As a rule of thumb, the uncertainty $\delta\omega$ in the location of the center of the line is

$$\delta\omega = \frac{\Delta\omega}{S/N} \tag{1.12}$$

In principle, one can make $\delta\omega$ arbitrarily small by acquiring enough data to achieve the required statistical accuracy. In practice, systematic errors eventually limit the precision. Splitting a line by a factor of 10^4 is a formidable task which has only been achieved a few times, most notably in the measurement of the Lamb shift. A factor of 10^3, however, is not uncommon, and 10^2 is child's play.

1.3 Magnetic Resonance: Classical Spin in Time-Varying B-Field

1.3.1 The classical motion of spins in a static magnetic field

Note: angular momentum will always be expressed in a form such as $\hbar\boldsymbol{J}$, where the vector $\boldsymbol{J}$ is dimensionless. The interaction energy and equation of motion of a classical spin in a static magnetic field are given by

$$W = -\boldsymbol{\mu}\cdot\boldsymbol{B}, \tag{1.13}$$

$$\boldsymbol{F} = -\boldsymbol{\nabla}W = \boldsymbol{\nabla}(\boldsymbol{\mu}\cdot\boldsymbol{B}), \tag{1.14}$$

$$\text{torque} = \boldsymbol{\mu}\times\boldsymbol{B} \tag{1.15}$$

In a uniform field, $\boldsymbol{F} = 0$. The torque equation ($\mathrm{d}\hbar\boldsymbol{J}/\mathrm{d}t = \text{torque}$) gives

$$\frac{\mathrm{d}\hbar\boldsymbol{J}}{\mathrm{d}t} = \boldsymbol{\mu}\times\boldsymbol{B}. \tag{1.16}$$

Since $\boldsymbol{\mu} = \gamma\hbar\boldsymbol{J}$ (where γ is called the gyromagnetic ratio - not to be confused with the different meaning of γ in the previous section), we have

$$\frac{\mathrm{d}\boldsymbol{J}}{\mathrm{d}t} = \gamma\boldsymbol{J}\times\boldsymbol{B} = -\gamma\boldsymbol{B}\times\boldsymbol{J}. \tag{1.17}$$

To see that the motion of $\boldsymbol{J}$ is a pure precession about $\boldsymbol{B}$, imagine that $\boldsymbol{B}$ is along $\hat{\boldsymbol{z}}$ and that the spin, $\boldsymbol{J}$, is tipped at an angle θ from this axis, and then rotated at an angle $\phi(t)$ from the x-axis (i.e., θ and ϕ are the conventionally chosen angles in spherical coordinates). The torque, $-\gamma\boldsymbol{B}\times\boldsymbol{J}$, has no component along $\boldsymbol{J}$ (that is, along $\hat{\boldsymbol{r}}$), nor along $\hat{\boldsymbol{\theta}}$ (because the $\boldsymbol{J}-\boldsymbol{B}$ plane contains $\hat{\boldsymbol{\theta}}$), hence $-\gamma\boldsymbol{B}\times\boldsymbol{J} = -\gamma B|\boldsymbol{J}|\sin(\theta)\hat{\boldsymbol{\phi}}$. This implies that $\boldsymbol{J}$ maintains constant magnitude and constant tipping angle θ. Generally, for an infinitesimal change $\mathrm{d}\phi$ the component of $\mathrm{d}\boldsymbol{J}$ in the direction of $\hat{\boldsymbol{\phi}}$ is $|\boldsymbol{J}|\sin(\theta)\mathrm{d}\phi$, and so we can see that $\phi(t) = -\gamma Bt$. This solution shows that the moment precesses with angular velocity

$$\Omega_L = -\gamma B \tag{1.18}$$

where Ω_L is called the *Larmor frequency.*

For electrons, $\gamma_e = -2\pi \times 2.8\,\mathrm{MHz/G} \approx -2\mu_\mathrm{B}$, for protons, $\gamma_p = 2\pi \times 4.2\,\mathrm{kHz/G}$. Note that Planck's constant does not appear in the equation of motion: the motion is classical.

Note: G stands for gauss - it is part of the gaussian (cgs) system of units, and ubiquitous in atomic physics labs, as it is a much more typical laboratory field than the SI unit for magnetic field, 1 tesla. $10^4\,\mathrm{G} = 1\,\mathrm{T}$.

1.3.2 Rotating coordinate transformation

A second way to find the motion is to look at the problem in a rotating coordinate system. If some vector $\boldsymbol{A}$ rotates with angular velocity $\boldsymbol{\Omega}$, then

$$\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} = \boldsymbol{\Omega} \times \boldsymbol{A}. \tag{1.19}$$

If the rate of change of the vector in a system rotating at Ω is $(\mathrm{d}\boldsymbol{A}/\mathrm{d}t)_\mathrm{rot}$, then the rate of change in an inertial system is the motion *in* plus the motion *of* the rotating coordinate system.

$$\left(\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t}\right)_\mathrm{inert} = \left(\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t}\right)_\mathrm{rot} + \boldsymbol{\Omega} \times \boldsymbol{A}. \tag{1.20}$$

The operator prescription for transforming from an inertial to a rotating system is thus

$$\left(\frac{\mathrm{d}\cdot}{\mathrm{d}t}\right)_\mathrm{rot} = \left(\frac{\mathrm{d}\cdot}{\mathrm{d}t}\right)_\mathrm{inert} - \boldsymbol{\Omega} \times \cdot \tag{1.21}$$

Applying this to Eq. 1.17 gives

$$\left(\frac{\mathrm{d}\boldsymbol{J}}{\mathrm{d}t}\right)_\mathrm{rot} = \gamma \boldsymbol{J} \times \boldsymbol{B} - \boldsymbol{\Omega} \times \boldsymbol{J} = \gamma \boldsymbol{J} \times (\boldsymbol{B} + \boldsymbol{\Omega}/\gamma)\,. \tag{1.22}$$

If we let

$$\boldsymbol{B}_\mathrm{eff} = \boldsymbol{B} + \boldsymbol{\Omega}/\gamma, \tag{1.23}$$

Eq. 1.22 becomes

$$\left(\frac{\mathrm{d}\boldsymbol{J}}{\mathrm{d}t}\right)_\mathrm{rot} = \gamma \boldsymbol{J} \times \boldsymbol{B}_\mathrm{eff}. \tag{1.24}$$

If $\boldsymbol{B}_\mathrm{eff} = 0$, $\boldsymbol{J}$ is constant in the rotating system. The condition for this is

$$\boldsymbol{\Omega} = -\gamma \boldsymbol{B} \tag{1.25}$$

as we have previously found in Eq. 1.18.

1.3.3 Larmor's theorem

Treating the effects of a magnetic field on a magnetic moment by transforming to a rotating coordinate system is closely related to Larmor's theorem, which asserts that the effect of a magnetic field on a free charge can be eliminated by a suitable rotating coordinate transformation.

Consider the motion of a particle of mass m, charge q, under the influence of an applied force $\boldsymbol{F}_0$ and the Lorentz force due to a static field $\boldsymbol{B}$:

$$\boldsymbol{F} = \boldsymbol{F}_0 + q\boldsymbol{v} \times \boldsymbol{B}. \tag{1.26}$$

Now consider the motion in a rotating coordinate system. By applying Eq. 1.21 twice to $\boldsymbol{r}$, we have

$$\ddot{\boldsymbol{r}}_{\text{rot}} = \ddot{\boldsymbol{r}}_{\text{inert}} - 2\boldsymbol{\Omega} \times \boldsymbol{v}_{\text{rot}} - \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}). \tag{1.27}$$

$$\boldsymbol{F}_{\text{rot}} = \boldsymbol{F}_{\text{inert}} - 2m(\boldsymbol{\Omega} \times \boldsymbol{v}_{\text{rot}}) - m\boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}), \tag{1.28}$$

where $\boldsymbol{F}_{\text{rot}}$ is the apparent force in the rotating system, and $\boldsymbol{F}_{\text{inert}}$ is the true or inertial force. Substituting Eq. 1.26 gives

$$\boldsymbol{F}_{\text{rot}} = \boldsymbol{F}_{0,\text{inert}} + q\boldsymbol{v} \times \boldsymbol{B} + 2m\boldsymbol{v} \times \boldsymbol{\Omega} - m\boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}). \tag{1.29}$$

If we choose $\boldsymbol{\Omega} = -(q/2m)\boldsymbol{B}$, and take $\boldsymbol{B} = \hat{\boldsymbol{z}}B$, we have

$$\boldsymbol{F}_{\text{rot}} = \boldsymbol{F}_{0,\text{inert}} - m\left(\frac{qB}{2m}\right)^2 \hat{\boldsymbol{z}} \times (\hat{\boldsymbol{z}} \times \boldsymbol{r}). \tag{1.30}$$

The last term is usually small. If we drop it we have

$$\boldsymbol{F}_{\text{rot}} = \boldsymbol{F}_{0,\text{inert}} \tag{1.31}$$

The effect of the magnetic field is removed by going into a system rotating at the Larmor frequency $qB/2m$.

Although Larmor's theorem is suggestive of the rotating co-ordinate transformation, Eq. 1.22, it is important to realize that the two transformations, though identical in form, apply to fundamentally different systems. A magnetic moment is not necessarily charged- for example a neutral atom can have a net magnetic moment, and the neutron possesses a magnetic moment in spite of being neutral - and it experiences no net force in a uniform magnetic field. Furthermore, the rotating co-ordinate transformation is exact for a mag- netic moment, whereas Larmor's theorem for the motion of a charged particle is only valid when the $\propto B^2$ term is neglected.

1.3.4 Motion in a Rotating Magnetic Field

Exact resonance: Consider a moment $\boldsymbol{\mu}$ precessing about a static field $\boldsymbol{B}_0$, which we take to lie along the z axis. Its motion might be described by

$$\mu_z = \mu\ \cos\theta, \quad \mu_x = \mu\ \sin\theta\ \cos\omega_0 t, \quad \mu_y = -\mu\ \sin\theta\ \sin\omega_0 t \tag{1.32}$$

where ω_0 is the Larmor frequency, and θ is the angle the moment makes with $\boldsymbol{B}_o$.

Now suppose we introduce a magnetic field $\boldsymbol{B}_1$ which rotates in the x-y plane at the Larmor frequency $\omega_0 = -\gamma B_0$. The magnetic field is

$$\boldsymbol{B}(t) = B_1(\hat{\boldsymbol{x}}\ \cos\omega_0 t - \hat{\boldsymbol{y}}\ \sin\omega_0 t)\ +\ B_0\ \hat{\boldsymbol{z}}. \tag{1.33}$$

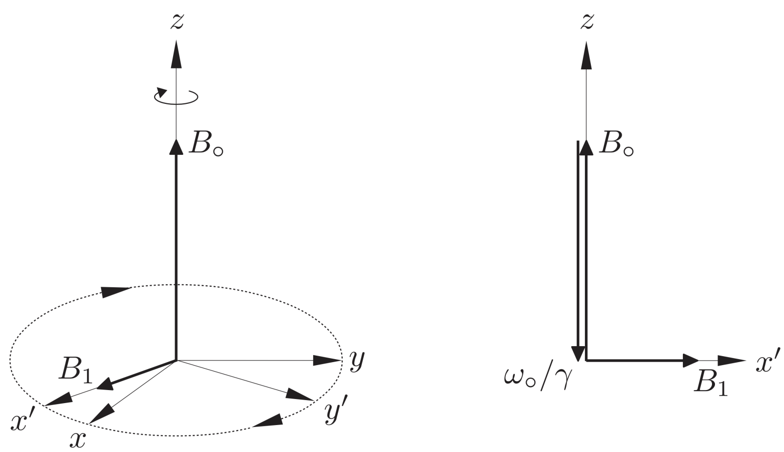

Figure 3. Rotating coordinate transformation to the primed system that is co-rotating with B_1 at ω, with x' chosen to lie along B_1. For the exact resonance case of $\omega = \omega_0$ considered here, the effective field around which the moment precesses is equal to B_1.

The problem is to find the motion of $\boldsymbol{\mu}$. The solution is simple in a rotating coordinate system (see Fig. 3). Let system $(\hat{\boldsymbol{x}}', \hat{\boldsymbol{y}}', \hat{\boldsymbol{z}}' = \hat{\boldsymbol{z}})$ precess around the z-axis at rate $-\omega_0$. In this system the field $\boldsymbol{B}_1$ is stationary (and $\hat{\boldsymbol{x}}'$ is chosen to lie along $\boldsymbol{B}_1$), and we have

$$\boldsymbol{B}_{\text{eff}}(t) = \boldsymbol{B}(t) - (\omega_0/\gamma)\ \hat{\boldsymbol{z}} = B_1\hat{\boldsymbol{x}}' + (B_0 - \omega_0/\gamma)\hat{\boldsymbol{z}} = B_1\hat{\boldsymbol{x}}'. \tag{1.34}$$

The effective field is static and has the value of B_1. The moment precesses about the field at rate

$$\omega_R = \gamma B_1, \tag{1.35}$$

often called the *Rabi* frequency, in honor of Rabi's invention of the resonance technique.

If the moment initially lies along the z axis, then its tip traces a circle in the $\hat{\boldsymbol{y}}' - \hat{\boldsymbol{z}}$ plane. At time t it has precessed through an angle $\phi = \omega_R t$. The moment's z-component is given by

$$\mu_z(t) = \mu\ \cos\omega_R t. \tag{1.36}$$

At time $T = \pi/\omega_R$, the moment points along the negative z-axis: it has "turned over".

Off-resonant behavior: Now suppose that the field B_1 rotates at frequency $\omega \neq \omega_0$. In a coordinate frame rotating with B_1 the effective field is

$$\boldsymbol{B}_{\text{eff}} = B_1\hat{\boldsymbol{x}}' + (B_0 - \omega/\gamma)\hat{\boldsymbol{z}}. \tag{1.37}$$

The effective field lies at angle θ with the z-axis, as shown in Fig. 4. The field is static, and the moment precesses about it at rate (called the *effective*

Rabi frequency)

$$\Omega_R = \gamma B_{\text{eff}} = \gamma\sqrt{(B_0 - \omega/\gamma)^2 + B_1^2} = \sqrt{(\omega_0 - \omega)^2 + \omega_R^2} \tag{1.38}$$

where $\omega_0 = \gamma B_0, \omega_R = \gamma B_1$, as before.

Assume that $\boldsymbol{\mu}$ points initially along the +z-axis. Finding $\mu_z(t)$ is a straightforward problem in geometry. The moment precesses about B_{eff} at rate Ω_R, sweeping a circle as shown. The radius of the circle is $\mu \sin\theta$, where $\sin\theta = B_1/\sqrt{(B_0 - \omega/\gamma)^2 + B_1^2} = \omega_R/\sqrt{(\omega - \omega_0)^2 + \omega_R^2}$. In time t the tip sweeps through angle $\phi = \Omega_R t$. The z-component of the moment is $\mu_z(t) = \mu\cos\alpha$ where α is the angle between the moment and the z-axis after it has precessed through angle ϕ. As the drawing shows, $\cos\alpha$ is found from $A^2 = 2\mu^2(1 - \cos\alpha)$. Since $A = 2\mu\ \sin\theta\sin(\Omega_R t/2)$, we have $4\mu^2\ \sin^2\theta\sin^2(\Omega_R t/2) = 2\mu^2(1 - \cos\alpha)$ and

$$\begin{aligned}\mu_z(t) &= \mu\cos\alpha = \mu(1 - 2\sin^2\theta\sin^2\Omega_R t/2)\\ &= \mu\left[1 - 2\frac{\omega_R^2}{(\omega-\omega_0)^2 + \omega_R^2}\sin^2\frac{1}{2}\sqrt{(\omega-\omega_0)^2 + \Omega_R t}\right] \end{aligned}\tag{1.39}$$

$$= \mu\Big[1 - 2(\omega_R/\Omega_R)^2\sin^2(\Omega_R t/2)\Big] \tag{1.40}$$

The z-component of $\boldsymbol{\mu}$ oscillates in time, but unless $\omega = \omega_0$, the moment never completely inverts. The rate of oscillation depends on the magnitude of the rotating field; the amplitude of oscillation depends on the frequency difference, $\omega - \omega_0$, relative to ω_R. The quantum mechanical result will turn out to be identical.

1.3.5 Rapid Adiabatic Passage: Landau-Zener Crossing

Adiabatic rapid passage is a technique for inverting a spin population by sweeping the system through resonance. Either the frequency of the oscillating field or the transition frequency (e.g., by changing the applied magnetic field) is slowly varied. The principle is qualitatively simple in the rotating coordinate system.

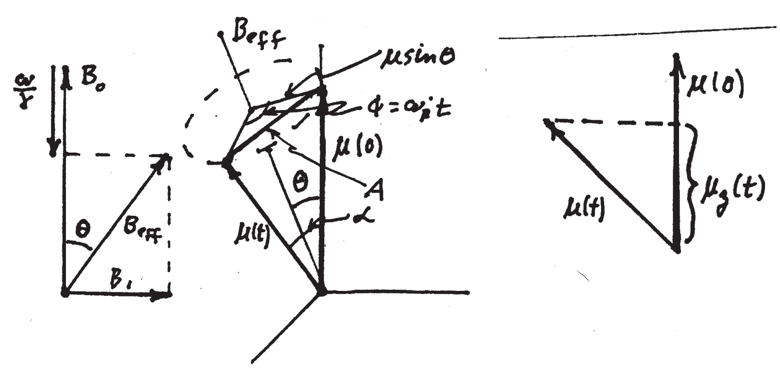

Figure 4. Constructions for viewing spin motion in a coordinate system rotating below the resonance frequency.

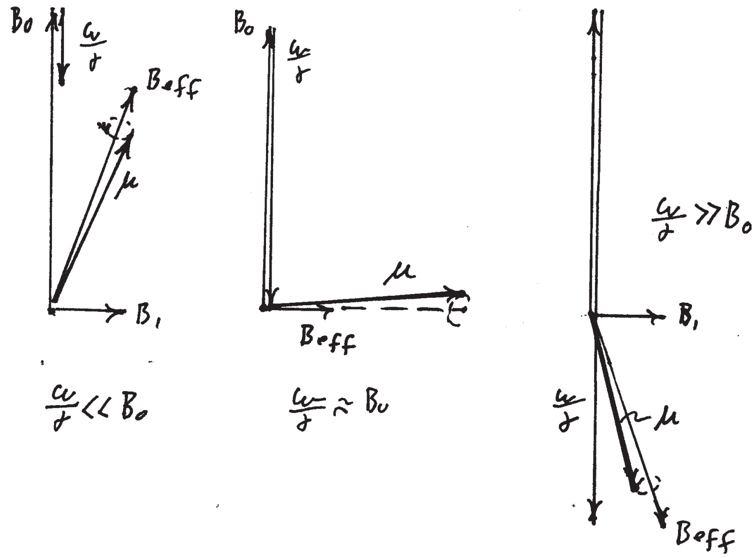

Figure 5. Motion of precessing moment in a rotating coordinate system whose frequency is swept from below resonance to above resonance.

The problem can also be solved analytically. In this section we give the qualitative argument and then, after having treated the quantum spin 1/2, we will present the analytic quantum result. The solution is of quite general interest because this physical situation arises frequently, for example in inelastic scattering, where it is called a curve crossing.

Consider a moment $\boldsymbol{\mu}$ in the presence of a static magnetic field $\boldsymbol{B}_0$ and a perpendicular field $\boldsymbol{B}_1$ rotating at some frequency ω, originally far from resonance: $\omega \ll \gamma B_0$. In the frame rotating with $\boldsymbol{B}_1$ the magnetic moment "sees" an effective field $\boldsymbol{B}_{\text{eff}}$ whose direction is nearly parallel to $\boldsymbol{B}_0$. A magnetic moment $\boldsymbol{\mu}$ initially parallel to $\boldsymbol{B}_0$ precess around $\boldsymbol{B}_{\text{eff}}$, making only a small angle with $\boldsymbol{B}_{\text{eff}}$, as shown in Fig. 5.

If ω is *slowly* swept through resonance, $\boldsymbol{\mu}$ will continue to precess tightly around $\boldsymbol{B}_{\text{eff}}$, as shown in Figs. 5b,c. and will follow its direction adiabatically. In Fig. 5 the effective field now points in the $-\hat{\boldsymbol{z}}$ direction, because $\omega \gg \gamma B_0$. Since the spin still precesses tightly around $\boldsymbol{B}_{\text{eff}}$, its direction in the laboratory system has "flipped" from $+\hat{\boldsymbol{z}}$ to $-\hat{\boldsymbol{z}}$. The laboratory field $\boldsymbol{B}_0$ remains unchanged, so this represents a transition from spin up to spin down.

The requirement for $\boldsymbol{\mu}$ to follow the effective field $\boldsymbol{B}_{\text{eff}}(t)$ is that, at all times, the magnetic moment always precesses tightly around $\boldsymbol{B}_{\text{eff}}$. That means, within one precession period $2\pi/\Omega_R$, the angle θ that $\boldsymbol{B}_{\text{eff}}$ makes with $\hat{\boldsymbol{z}}$ must not have advanced more than a few degrees, i.e.

$$\Delta\theta = \dot{\theta} \cdot \Delta t = \dot{\theta}\frac{2\pi}{\Omega_R} \ll 2\pi \tag{1.41}$$

In other words, the Larmor frequency (the generalized Rabi frequency) $\Omega_R =$

γB_{eff} must be large compared to $\dot{\theta}$, the rate at which $\boldsymbol{B}_{\text{eff}}(t)$ is changing direction.

This requirement is most severe near exact resonance where $\theta = \pi/2$.

Using $B_{z,\text{eff}}(t) = B_0 - \omega(t)/\gamma$ we have in this case (from geometry)

$$\mid \dot{\theta}_{max} \mid = \frac{1}{B_1}\frac{dB_{z,\text{eff}}(t)}{dt} = \frac{1}{B_1}\frac{1}{\gamma}\frac{d\omega}{dt} \ll \gamma B_1, \tag{1.42}$$

or using $\omega_R = \gamma B_1$,

$$\frac{d\omega}{dt} \ll \omega_R^2. \tag{1.43}$$

In this example we have shown that a slow change from $\omega \ll \gamma B_0$ to $\omega \gg \gamma B_0$ will flip the spin; the same argument shows that the reverse direction of slow change will also flip the spin.
Note that since the change of ω in one Rabi period must be much smaller than the Rabi frequency itself, and since we need to sweep the detuning $\omega - \omega_0$ from much larger than ω_R to much smaller than $-\omega_R$ to complete the inversion, it is clear that the inversion will be slower than an on-resonance π-pulse.

In the examples below (Fig. 6), we see how the magnetic moment follows the changing magnetic field $\boldsymbol{B}_{\text{eff}}$ less and less faithfully as the ramp speed $\dot{\omega}$ is increased beyond ω_R^2. We will come back to the Landau-Zener problem after having introduced the quantum spin 1/2 case.

1.3.6 Adiabatic Following in a Magnetic Trap

In a slight digression, an important example of adiabatic following of magnetic moments is given by the trapping of neutral atoms in magnetic traps. First, since Maxwell's equations forbid the existence of a magnetic field maximum in free space (there are no magnetic charges), we can only create magnetic field minima in free space, and therefore only trap atoms in so-called "low-field seeking" states, so for which the projection of the magnetic moment on the local magnetic field direction points opposite the field. For the atom to stay trapped, the magnetic moment must always be able to follow adiabatically the direction of the local magnetic field. Otherwise, "spin-flips", whereby the atoms flip their magnetic moments to be aligned with the field, lowering their energy and then leaving the trap (by seeking the high field right at the coils). A classic example is the quadrupole magnetic trap, formed by two parallel coils with currents running in anti-Helmholtz configuration. This results in a magnetic field zero right in the center between the coils, and a gradient field away from the zero:

$$\boldsymbol{B} = B' \begin{pmatrix} x \\ y \\ -2z \end{pmatrix}.$$

If an atom moves through the region close to the zero of magnetic field, the local Larmor frequency may become low compared to the rate of change of the field direction. For adiabatic following, the rate of change of the field angle should satisfy:

$$\dot{\theta} \ll \Omega_L$$

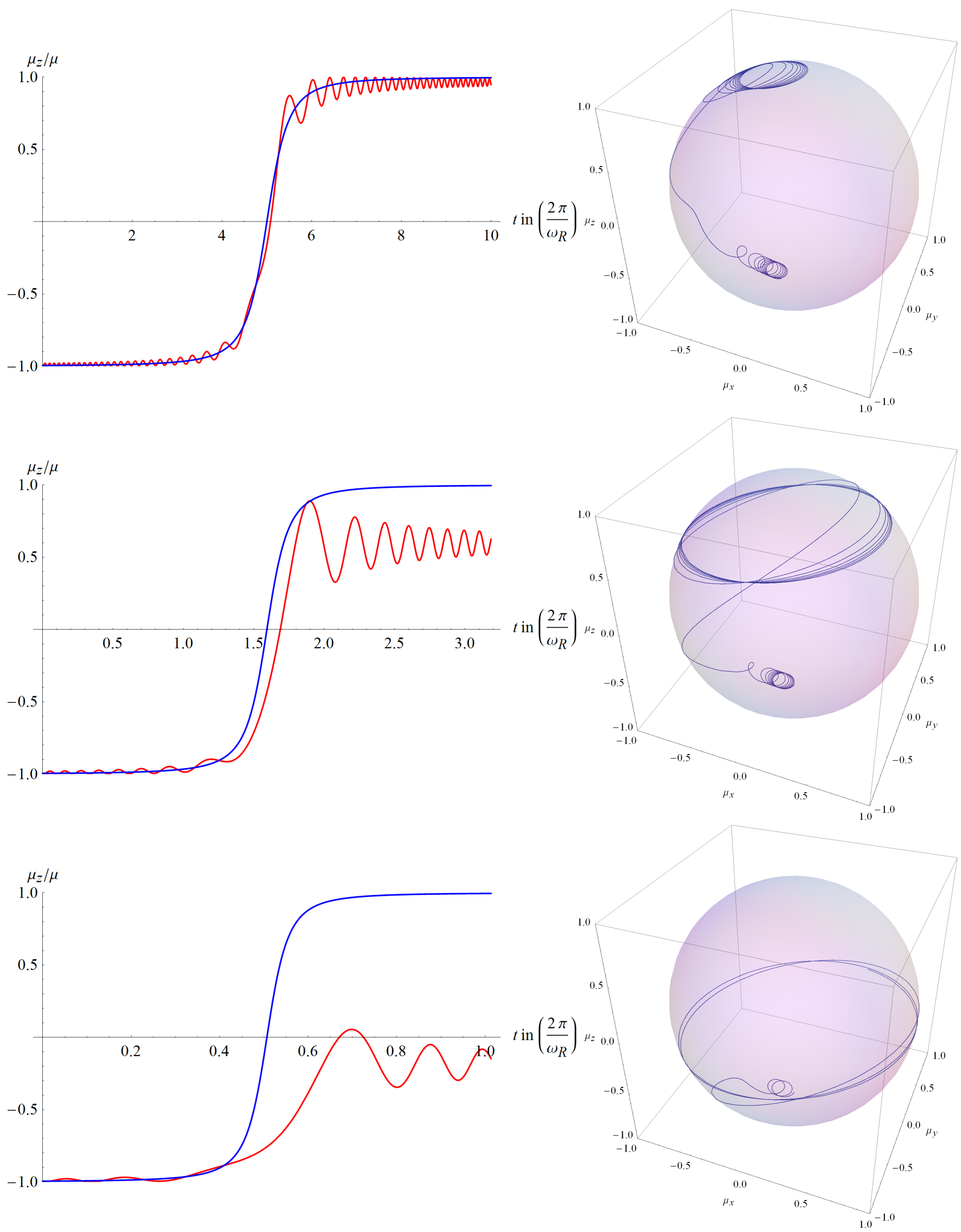

Figure 6. Top row: Adiabatic sweep. Start of sweep $\delta = -10\,\omega_R$, end of sweep $\delta = +10\,\omega_R$, sweep rate $\dot{\omega} = \frac{20\,\omega_R}{10\,\frac{2\pi}{\omega_R}} = \frac{1}{\pi}\omega_R^2$. Left: z-component of the magnetic moment versus time t measured in Rabi periods $2\pi/\omega_R$ (red curve). Blue is $\cos\theta = \frac{\delta(t)}{\sqrt{\delta(t)^2+\omega_R^2}}$, i.e. the cosine of the angle that $\boldsymbol{B}_{\text{eff}}$ makes with the z-axis. Right: Path traced out by the tip of the magnetic moment in real space (or, for a two-level system in quantum mechanics described by a pseudo-spin 1/2: the path traced out by the tip of the Bloch vector on the Bloch sphere. Middle row: sweep with imperfect adiabaticity. The sweep rate here is $\dot{\omega} = \pi\frac{20\,\omega_R}{10\,\frac{2\pi}{\omega_R}} = \omega_R^2$. Bottom row: non-adiabatic sweep. Sweep rate $\dot{\omega} = \pi^2\frac{20\,\omega_R}{10\,\frac{2\pi}{\omega_R}} = \pi\omega_R^2$.

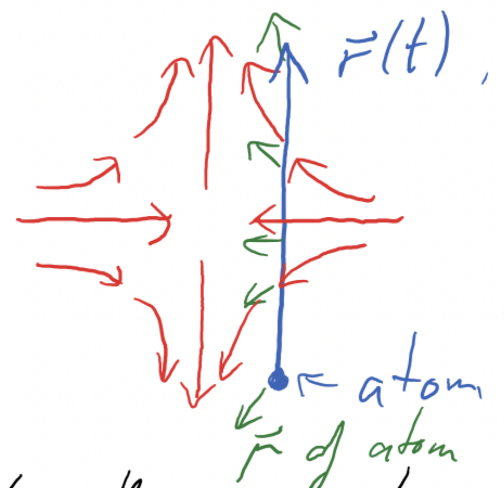

Figure 7. An atom moving in the quadrupole magnetic trap, with its magnetic moment attempting to follow the direction of the local magnetic field.

The field experienced by the atom changes as the atom is moving through space. We have (approximately, i.e. not worrying about factors on the order of two):

$$\dot{\theta} = \frac{\dot{B}}{B} = \frac{B'v}{B} = \frac{B}{r}.$$

Here, v is the atom velocity and r is the atom position. So, the adiabaticity condition is

$$\dot{\theta} \ll \Omega_L \implies \frac{v}{r} \ll \Omega_L = \gamma B = \gamma B' r.$$

So the "danger zone" where the atom may no longer be able to follow adiabatically, and therefore undergo spin flips, is the region of distances from the field zero smaller than

$$r = \sqrt{\frac{v}{\gamma B'}}.$$

This region is called the "Majorana hole". As the atom cloud is cooled (e.g. through radiofrequency evaporation), the velocity decreases like $\sqrt{T}$, the hole radius like $T^{1/4}$, but the cloud size $R \propto T/\mu B'$ decreases faster. So eventually, the cloud becomes comparable in size to the "Majorana hole" and severe losses in the number of trapped atoms are observed.

There are several solutions to this that were developed in order to keep atoms in a magnetic trap. Wolfgang Ketterle at MIT used a repulsive laser beam to "plug the hole". This is called the "plug trap". Eric Cornell at JILA added a time varying magnetic bias field that moves the magnetic field zero in a circular orbit of radius larger than the cloud size, and at a rate much faster than the atoms can follow (typically: 10 kHz, compared to the frequency of atomic motion of 100 Hz), but still much slower than the Larmor frequency (1 MHz), so that atoms stay trapped in a region of non-zero magnetic field (1 G) where their moments can adiabatically follow the rotating bias field. This was called the TOP (time orbiting potential) trap. These two completely different solutions both led to the realization of Bose-Einstein condensation.

1.4 Resonance Of Quantized Spin

1.4.1 Expectation value of magnetic moment behaves classically

Before solving the quantum mechanical problem of a magnetic moment in a time varying field, it is worthwhile demonstrating that its motion is classical. By "its motion is classical" we mean the time evolution of the expectation value of the magnetic moment operator obeys the classical equation of motion. Specifically, we shall show that

$$\frac{d}{dt}\langle\hat{\boldsymbol{\mu}}\rangle = \gamma\langle\hat{\boldsymbol{\mu}}\rangle \times \boldsymbol{B}. \tag{1.44}$$

Proof: Recall the Heisenberg equations of motion for an operator $\hat{O}$:

$$\frac{d}{dt}\hat{O} = \frac{i}{\hbar}[\hat{H}, \hat{O}] + \frac{\partial\hat{O}}{\partial t}. \tag{1.45}$$

If the operator is not explicitly time dependent the last term vanishes.

The interaction of $\hat{\boldsymbol{\mu}}$ with a static field $B_0\hat{\boldsymbol{z}}$ is

$$\hat{H} = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}_0 = -\gamma\hat{\boldsymbol{J}} \cdot \boldsymbol{B}_0 = -\gamma B_0 \hat{J}_z, \tag{1.46}$$

Note that $\hat{\boldsymbol{J}}$ has dimensions of angular momentum. Thus

$$\frac{d\hat{\boldsymbol{\mu}}}{dt} = -i\gamma B_0[\hat{J}_z, \hat{\boldsymbol{\mu}}]/\hbar. \tag{1.47}$$

Using $\hat{\boldsymbol{\mu}} = \gamma\hat{\boldsymbol{J}}$, we can rewrite this as

$$\frac{d\hat{\boldsymbol{J}}}{dt} = -i\gamma B_0\left[\hat{J}_z, \hat{\boldsymbol{J}}\right]/\hbar. \tag{1.48}$$

The commutation rules for $\hat{\boldsymbol{J}}$ are $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$, etc., or $\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}} = i\hbar\hat{\boldsymbol{J}}$ (this is a shorthand way of writing $[\hat{J}_i, \hat{J}_j] = \epsilon_{ijk}\hat{J}_k$.) Hence

$$\frac{d\hat{J}_x}{dt} = \gamma B_0 \hat{J}_y \tag{1.49}$$

$$\frac{d\hat{J}_y}{dt} = -\gamma B_0 \hat{J}_x \tag{1.50}$$

$$\frac{d\hat{J}_z}{dt} = 0 \tag{1.51}$$

These describe the uniform precession of $\hat{\boldsymbol{J}}$ about the z-axis at a rate $-\gamma B_0$. In particular, taking the expectation value, we have:

$$\frac{d}{dt}\langle\hat{\boldsymbol{J}}\rangle = \gamma\langle\hat{\boldsymbol{J}}\rangle \times \boldsymbol{B} \tag{1.52}$$

and since $\hat{\boldsymbol{\mu}} = \gamma \hat{\boldsymbol{J}}$, this directly yields Eq. 1.44:

$$\frac{d}{dt}\langle \hat{\boldsymbol{\mu}} \rangle = \gamma \langle \hat{\boldsymbol{\mu}} \rangle \times \boldsymbol{B}. \tag{1.53}$$

Thus the quantum mechanical and classical equation of motion are identical. This fact underlies the great utility of classical magnetic resonance in providing intuition about resonance in quantum spin systems.

A few comments on this result:

- the result is valid for any angular momentum operator, so also for spin 1/2...
- ... and therefore for any two-level system that can be mapped onto an effective spin 1/2.
- it is valid for the case of several angular momenta within an atom coupled to a total angular momentum $\boldsymbol{F}$ (as long as the magnetic field $\boldsymbol{B}$ is not large enough to "break" the coupling).
- it is valid also for a system of N two-level systems symmetrically coupled to an external field. In this case, we have an effective angular momentum $L = N/2$. Spin precession in this case can be understood as Dicke superradiance, the constructive interference of N "aligned" particles.

1.4.2 The Rabi transition probability

For a spin 1/2 particle we can push the classical solution further and obtain the amplitudes and probabilities for each state. Consider [1] $\langle \mu_z \rangle / \hbar = \gamma \langle J_z \rangle = \gamma m$, where m is the usual "magnetic" quantum number. For a spin 1/2 particle m has the value $+1/2$ or $-1/2$. Let the probabilities for having these values be P_+ and P_- respectively. Then

$$\langle J_z \rangle = \frac{1}{2}P_+ - \frac{1}{2}P_-, \tag{1.54}$$

or, since $P_+ + P_- = 1$,

$$\langle J_z \rangle = \frac{1}{2}(1 - 2P_-), \tag{1.55}$$

$$\langle \mu_z \rangle = \frac{1}{2}\gamma\hbar(1 - 2P_-). \tag{1.56}$$

If $\boldsymbol{\mu}$ lies along the z axis at $t = 0$, then $\mu_z(0) = \gamma\hbar/2$, and we have

$$\mu_z(t) = \mu_z(0)(1 - 2P_-). \tag{1.57}$$

In this case, P_- is the probability that a spin in state $m = +1/2$ at $t = 0$ has made a transition to $m = -1/2$ at time t, $P_{\uparrow\to\downarrow}(t)$. So for the Rabi problem, the case of a static field $\boldsymbol{B}_0 = \omega_0 \hat{\boldsymbol{z}}/\gamma$ and a rotating magnetic field $\boldsymbol{B}_1$ rotating

[1] We will in the following drop hats $\hat{}$ over operators for simplicity.

at frequency ω about the z-axis, switched on at time $t = 0$, we see immediately, comparing Eq. 1.57 with 1.39,

$$P_{\uparrow\to\downarrow}(t) = \frac{\omega_R^2}{\omega_R^2 + (\omega - \omega_0)^2} \sin^2\left(\frac{1}{2}\sqrt{\omega_R^2 + (\omega - \omega_0)^2}\, t\right) \tag{1.58}$$

$$P_{\uparrow\to\downarrow}(t) = (\omega_R/\Omega_R)^2 \sin^2(\Omega_R t/2) \tag{1.59}$$

This result is known as the *Rabi transition probability.* It is important enough to memorize. We have derived it from a classical correspondence argument, but it can also be derived quantum mechanically. In fact, such a treatment is essential for a complete understanding of the system.

1.4.3 The Hamiltonian of a quantized spin $\frac{1}{2}$

Let us investigate the time dependence of the wave function for a quantized spin $\frac{1}{2}$ system with moment $\boldsymbol{\mu} = \gamma\hbar \boldsymbol{S}$ that is placed in a uniform magnetic field $\boldsymbol{B}_0 = \omega_0 \hat{\boldsymbol{z}}/\gamma$ and, starting at $t = 0$, subject to a field $\boldsymbol{B}_R(t)$ which rotates in the $x-y$ plane with frequency ω. These fields are the same as the fields discussed in the preceding section on the motion of a classical spin and a time-varying field. The only difference is that now we are discussing their effect on a quantized system, so we must use Schrödinger's equation rather than the laws of classical Electricity and Magnetism to discuss the dynamics of the system.

The basis states are (using the standard column vector representation):

$$|g\rangle \equiv |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1.60}$$

$$|e\rangle \equiv |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.61}$$

with state $|1\rangle$ lower in energy.

The unperturbed Hamiltonian is (note: we will take $\omega_0 = \gamma B_0$ to be positive, and $\boldsymbol{\mu}$ is an operator)

$$\begin{aligned} H_0 &= -\boldsymbol{\mu} \cdot \boldsymbol{B}_0 = -\hbar S_z \omega_0 \\ &= -\frac{1}{2}\hbar\omega_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\frac{1}{2}\hbar\omega_0 \sigma_z \end{aligned} \tag{1.62}$$

where σ_z is a Pauli spin matrix.
The energies are

$$E_1 = -\hbar\omega_0/2; \qquad \omega_1 = -\omega_0/2$$

$$E_2 = +\hbar\omega_0/2; \qquad \omega_2 = +\omega_0/2 \tag{1.63}$$

Suppose we have a spin initially aligned along $\hat{\boldsymbol{x}}$:

$$|\psi\,(t=0)\rangle = \frac{1}{\sqrt{2}}\,(|g\rangle + |e\rangle)\,.$$

Then

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{i\omega_0 t/2}\,|g\rangle + e^{-i\omega_0 t/2}\,|e\rangle\right) = \frac{1}{\sqrt{2}}e^{i\omega_0 t/2}\left(|g\rangle + e^{-i\omega_0 t}\,|e\rangle\right).$$

This corresponds to rotation about the equator of the Bloch sphere at a rate ω_0: the state of the spin 1/2 rotates from being aligned along $\hat{\boldsymbol{x}}$ to being aligned along $-\hat{\boldsymbol{y}}$, then $-\hat{\boldsymbol{x}}$, then $\hat{\boldsymbol{y}}$ etc., so in the same sense as the classical magnetic moment.

We will now switch on the magnetic field $\boldsymbol{B}_R$ which rotates in the $x-y$ plane, with the goal of making it co-rotate with the spin when driven at $\omega = \omega_0$.

The perturbation Hamiltonian $H'(t)$ is written best in terms of $\omega_R = \gamma B_R$ where B_R is the magnetic field which rotates in the $x-y$ plane (in the magnetic resonance community the subscript R is often replaced by 1):

$$\begin{aligned} H'(t) &= -\boldsymbol{\mu}\cdot\boldsymbol{B}_R(t) \\ &= -\boldsymbol{\mu}\cdot(\omega_R/\gamma)[\hat{\boldsymbol{x}}\ \cos\ \omega t - \hat{\boldsymbol{y}}\ \sin\ \omega t] \\ &= -\omega_R[S_x\ \cos\omega t - S_y\ \sin\omega t] \\ &= -\frac{\hbar\omega_R}{2}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\cos\omega t - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\sin\omega t\right] \\ &= -\frac{\hbar\omega_R}{2}\begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \end{aligned} \tag{1.64}$$

where we used $\boldsymbol{\mu}\ \cdot\ \hat{\boldsymbol{x}} = \gamma S_x$. In the penultimate line we have replaced the operators S_x and S_y with $(\hbar/2)\ \sigma_x$ and $(\hbar/2)\ \sigma_y$ where σ_x and σ_y are Pauli spin matrices. The perturbation matrix element is just the entry $H'_{21}(t)$ in row 2 and column 1:

$$\langle 2 \mid H' \mid 1\rangle = -\frac{\hbar\omega_R}{2}\ e^{-i\omega t} \tag{1.65}$$

We have thus derived the following Hamiltonian for the spin $\frac{1}{2}$ problem:

$$H = \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & -\omega_R e^{+i\omega t} \\ -\omega_R e^{-i\omega t} & \omega_0 \end{pmatrix} \tag{1.66}$$

1.4.4 Quantum Mechanical Solution for Resonance in a Two-State System

As has been emphasized, a two-state system coupled by a periodic interaction is an archetype for large areas of atomic/optical physics. The quantum mechanical solution can be achieved by a variety of approaches, the most elegant of which is the dressed atom picture in which the atom and radiation field constitute a single quantum system and one finds its eigenstates. That approach will be introduced later. Here we follow a rather different approach, less elegant, but capable of being generalized to a variety or problems including multi-level resonance and radiative decay in the presence of oscillating fields. The starting point is the interaction representation.

1.4.5 Interaction representation

We consider a complete set of eigenstates to a Hamiltonian $H_0, \psi =\mid 1 >, \mid 2 >$ ... , such that

$$H_0 \mid j >= E_j \mid j > . \tag{1.67}$$

The problem is to find the behavior of the system under an interaction $V(t)$, i.e. to find solutions to

$$i\hbar \frac{\partial \psi(t)}{\partial t} = (H_0 + V(t))\psi(t) \tag{1.68}$$

In the interaction representation we take

$$\psi(t) = \sum_j a_j(t) \mid j > e^{-iE_j t/\hbar}. \tag{1.69}$$

Schrödinger's equation yields

$$i\hbar \dot{a}_k = \sum_j < k \mid V \mid j > a_j e^{i(E_j - E_k)t/\hbar} = \sum_j V_{kj} a_j e^{i\omega_{jk}}. \tag{1.70}$$

Given any set of initial conditions, $a_j(0), j = 1, 2, 3...$, these equations can be integrated to find $\psi(t)$. Often, this is done iteratively, following a pertubative approach. For the two-state system, with V periodic, one can obtain an exact solution.

1.4.6 Two-state problem

We consider a two-state system

$$\psi = a_1 \mid 1 > + a_2 \mid 2 >, \tag{1.71}$$

with $\mid a_1 \mid^2 + \mid a_2 \mid^2 = 1$. We assume $E_2 > E_1$, and introduce $\hbar\omega_{12} = \hbar\omega_0 = E_2 - E_1$. Without loss of generality, we let $E_1 = -\hbar\omega_0/2$; $E_2 = \hbar\omega_0/2$. We take the interaction to be of the form $V_{11} = V_{22} = 0$, and

$$V_{12} = \frac{1}{2}\hbar\omega_R \left(e^{-i\omega t}\right), \tag{1.72}$$

Eq. 1.70 gives

$$\begin{aligned} i\dot{a}_1 &= \frac{1}{2}\omega_R \Big(e^{-i\omega t}\Big) e^{+i\omega_0 t} a_2, \\ i\dot{a}_2 &= \frac{1}{2}\omega_R \Big(e^{i\omega t}\Big) e^{-i\omega_0 t} a_1. \end{aligned} \tag{1.73}$$

Introducing $\delta \equiv \omega - \omega_0$, Eqs. 1.73 becomes

$$
\begin{aligned}
i\dot{a}_1 &= \frac{1}{2}\omega_R e^{-i\delta t} a_2, \\
i\dot{a}_2 &= \frac{1}{2}\omega_R e^{i\delta t} a_1.
\end{aligned} \tag{1.74}
$$

We can eliminate the explicit time dependence by making the substitution

$$
\begin{aligned}
a_1 &= e^{-i\delta t/2} b_1, \\
a_2 &= e^{+i\delta t/2} b_2.
\end{aligned} \tag{1.75}
$$

Eqs. 1.74 become

$$
\begin{aligned}
\dot{b}_1 - i\frac{\delta}{2} b_1 &= \frac{-i}{2}\omega_R b_2, \\
\dot{b}_2 + i\frac{\delta}{2} b_2 &= \frac{-i}{2}\omega_R b_1.
\end{aligned} \tag{1.76}
$$

These equations describe periodic behavior, so that it is natural to try solutions of the form

$$
\begin{aligned}
b_1 &= \sum_j B_j e^{i\alpha_j t}, \\
b_2 &= \sum_j C_j e^{i\alpha_j t}.
\end{aligned} \tag{1.77}
$$

Substituting these in Eq. 1.76 yields

$$
\begin{aligned}
\left(\alpha_j - \frac{\delta}{2}\right) B_j + \left(\frac{\omega_R}{2}\right) C_j &= 0, \\
\left(\frac{\omega_R}{2}\right) B_j + \left(\alpha_j + \frac{\delta}{2}\right) C_j &= 0.
\end{aligned} \tag{1.78}
$$

for which the determinental equation yields two eigenfrequencies

$$
\alpha_{1,2} = \pm\frac{1}{2}\sqrt{\omega_R^2 + \delta^2} = \pm\frac{1}{2}\Omega_R, \tag{1.79}
$$

where Ω_R is the generalized Rabi frequency:

$$
\Omega_R = \sqrt{\omega_R^2 + \delta^2}. \tag{1.80}
$$

From Eqs. 1.78:

$$
C_1 = -B_1 \frac{\omega_R}{\Omega_R + \delta}, \qquad C_2 = B_2 \frac{\omega_R}{\Omega_R - \delta}. \tag{1.81}
$$

By combining this result with Eq. 1.76 and Eq. 1.77 we obtain

$$
\begin{aligned}
a_1(t) &= e^{-i(\delta-\Omega_R)t/2}B_1 + e^{-i(\delta+\Omega_R)t/2}B_2 \\
a_2(t) &= -\left(\frac{\omega_R}{\Omega_R+\delta}\right)e^{i(\delta+\Omega_R)t/2}B_1 + \left(\frac{\omega_R}{\Omega_R-\delta}\right)e^{i(\delta-\Omega_R)t/2}B_2
\end{aligned}
\tag{1.82}
$$

The solution contains two arbitrary constants, B_1 and B_2, which permit fitting the boundary condition for the two amplitudes.

If the system is in state 1 at $t=0$, then $a_1(1)=1, a_2(0)=0$, and

$$
\begin{aligned}
B_1 &= \frac{1}{2}\frac{\Omega_R+\delta}{\Omega_R}, \qquad B_2 = \frac{1}{2}\frac{\Omega_R-\delta}{\Omega_R} \\
a_2(t) &= \frac{1}{2}\frac{\omega_R}{\Omega_R}\left[-e^{i(\delta+\Omega_R)t/2} + e^{i(\delta-\Omega_R)t/2}\right] \\
&= -i\frac{\omega_R}{\Omega_R}e^{i\delta t/2}\sin\left(\Omega_R t/2\right).
\end{aligned}
\tag{1.83}
$$

The probability of being in state 2 at time t is,

$$
P_2(t) \;=\; \mid a_2(t) \mid^2 = \frac{\omega_R^2}{\Omega_R^2}\sin^2\left[\frac{1}{2}\Omega_R t\right],
\tag{1.84}
$$

which is identical to the classical result for the Rabi resonance formula, derived earlier.

If we introduce the parameter θ defined by

$$
\begin{aligned}
\cos\theta &= \left(\frac{\Omega_R+\delta}{2\Omega_R}\right)^{1/2} = \left(\frac{1}{2}(1+\frac{\delta}{\Omega_R})\right)^{1/2} \\
\sin\theta &= \left(\frac{\Omega_R-\delta}{2\Omega_R}\right)^{1/2} = \left(\frac{1}{2}(1-\frac{\delta}{\Omega_R})\right)^{1/2}
\end{aligned}
\tag{1.85}
$$

Then we have

$$
\psi(t) = a_1(t) \mid 1\rangle + a_2(t) \mid 2\rangle \tag{1.86}
$$

$$
\begin{aligned}
&= [\cos^2\theta\, e^{-i(\delta-\Omega_R)t/2} + \sin^2\theta\, e^{-i(\delta+\Omega_R)t/2}] \mid 1\rangle \\
&\quad +[\cos\theta\sin\theta][e^{i(\delta+\Omega_R)t/2} - e^{i(\delta-\Omega_R)t/2}] \mid 2\rangle \\
&= e^{-i\,\delta\,t/2}\left[\cos\left(\frac{\Omega_R t}{2}\right) + i\frac{\delta}{\Omega_R}\sin\left(\frac{\Omega_R}{2}t\right)\right]|1\rangle \\
&\quad -i\,e^{+i\,\delta\,t/2}\frac{\omega_R}{\Omega_R}\sin\left(\frac{\Omega_R}{2}t\right)|2\rangle
\end{aligned}
\tag{1.87}
$$

1.4.7 Solution via rotating frame

The preceding solution seems a bit "brute force" and required some ad hoc "tricks" like the substitution from the a to the b amplitudes. We will here see very clearly what is behind the mathematics: It is again frame rotation.

In the very same spirit of the classical solution, we want to rotate our spin 1/2 into a frame in which the magnetic fields appear stationary. In this frame the Hamiltonian will be time independent and can be solved easily. Now just like the classical angular momentum L_z generated rotation of vectors about the z-axis, the spin angular momentum operator S_z generates rotation of spinors about the z-axis. The rotation operator for rotation about $\hat{z}$ by an angle θ is thus

$$T = e^{-i\hat{S}_z\theta}.$$

We can find this result from integration of infinitesimal rotations.

To keep aligned with the rotating magnetic field, we want $\theta = -\omega t$, then we have

$$T = e^{i\omega t\sigma_z/2} = \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}.$$

Our states transform by

$$|\psi\rangle = T\left|\tilde{\psi}\right\rangle.$$

We get a new term in the Schrödinger equation according to

$$i\hbar\frac{d}{dt}|\psi\rangle = i\hbar\dot{T}\left|\tilde{\psi}\right\rangle + Ti\hbar\frac{d}{dt}\left|\tilde{\psi}\right\rangle = H|\psi\rangle = HT\left|\tilde{\psi}\right\rangle.$$

So,

$$i\hbar\frac{d}{dt}\left|\tilde{\psi}\right\rangle = \left(T^\dagger HT - i\hbar T^\dagger\dot{T}\right)\left|\tilde{\psi}\right\rangle.$$

The Hamiltonian in the rotating frame is then

$$\tilde{H} = T^\dagger\left(H - i\hbar\frac{d}{dt}\right)T.$$

H_0 and T are both diagonal, so

$$T^\dagger H_0 T = H_0.$$

For H_1, T removes the time-dependence:

$$T^\dagger H_1 T = -\frac{\hbar\omega_R}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\frac{\hbar\omega_R}{2}\sigma_x.$$

This is what we set out to do, since we chose the frame to rotate with the field. The time derivative term is

$$T^\dagger\left(-i\hbar\frac{d}{dt}T\right) = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar\omega}{2}\sigma_z.$$

We thus see the $\hat{z}$ field effectively reduced in amplitude, as occured for our classical system. The new Hamiltonian is thus

$$\tilde{H} = -\frac{\hbar}{2}\begin{pmatrix} -\delta & \omega_R \\ \omega_R & \delta \end{pmatrix} \text{ with } \delta = \omega - \omega_0.$$

We can also write

$$\tilde{H} = \frac{\hbar\delta}{2}\sigma_z - \frac{\hbar\omega_R}{2}\sigma_x = \frac{1}{2}\boldsymbol{h}\cdot\boldsymbol{\sigma} \text{ for } \boldsymbol{h} = \begin{pmatrix} -\hbar\omega_R \\ 0 \\ \hbar\delta \end{pmatrix}.$$

The Hamiltonian is now time-independent, and represents the interaction of a spin 1/2 with a static magnetic field. The eigenvectors are thus simply the two states representing the spin aligned and anti-aligned with $\boldsymbol{h}$ ($+$ and $-$). The eigenvalues are

$$E_\pm = \pm\frac{1}{2}|\boldsymbol{h}| = \pm\frac{\hbar}{2}\sqrt{\omega_R^2+\delta^2} = \pm\frac{\hbar\Omega_R}{2}.$$

We can obtain the eigenvectors from the original eigenvectors $|g\rangle \equiv |\uparrow\rangle$ and $|e\rangle \equiv |\downarrow\rangle$ which described a spin 1/2 aligned and anti-aligned with the z-axis, simply by rotating about the axis

$$\hat{\boldsymbol{z}}\times\boldsymbol{h} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} -\hbar\omega_R \\ 0 \\ \hbar\delta \end{pmatrix} = -\begin{pmatrix} 0 \\ \hbar\omega_R \\ 0 \end{pmatrix} = \hbar\omega_R\,\hat{\boldsymbol{y}}$$

by the angle ϕ satisfying

$$\cos\phi = \hat{\boldsymbol{z}}\cdot\hat{\boldsymbol{h}} = \frac{\delta}{\Omega_R}.$$

Note that

$$\tan\phi = -\frac{\omega_R}{\delta}.$$

Rotation about the y-axis is generated by S_y, again through the exponential

$$R = e^{-i\phi S_y} = e^{-i\phi\sigma_y/2}.$$

This is equivalent to

$$R = \cos\frac{\phi}{2}\mathbb{I} - i\sin\frac{\phi}{2}\sigma_y = \begin{pmatrix} \cos\frac{\phi}{2} & -\sin\frac{\phi}{2} \\ \sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}.$$

We can thus find the eigenstates, properly aligned and anti-aligned with the direction of $\boldsymbol{h}$:

$$|+\rangle_h = R|\uparrow\rangle = \begin{pmatrix} \cos\phi/2 \\ \sin\phi/2 \end{pmatrix} = \cos(\phi/2)|\uparrow\rangle + \sin(\phi/2)|\downarrow\rangle \tag{1.88}$$

$$|-\rangle_h = R|\downarrow\rangle = \begin{pmatrix} -\sin\phi/2 \\ \cos\phi/2 \end{pmatrix} = -\sin(\phi/2)|\uparrow\rangle + \cos(\phi/2)|\downarrow\rangle \tag{1.89}$$

Note that $\cos(\phi/2) = \sqrt{\frac{1+\cos\phi}{2}} = \sqrt{\frac{\Omega_R+\delta}{2\Omega_R}}$ and $\sin(\phi/2) = \sqrt{\frac{1-\cos\phi}{2}} = \sqrt{\frac{\Omega_R-\delta}{2\Omega_R}}$.

Their time-evolution is simply, since $E_+ = -\frac{\hbar\Omega_R}{2}$ and $E_- = \frac{\hbar\Omega_R}{2}$:

$$|+(t)\rangle = e^{i\Omega_R t/2}|+\rangle_h \tag{1.90}$$
$$|-(t)\rangle = e^{-i\Omega_R t/2}|-\rangle_h \tag{1.91}$$

Now say we start with $|\psi(t=0)\rangle = |\uparrow\rangle$, that is

$$|\psi(t=0)\rangle = R^T|+\rangle = \cos(\phi/2)|+\rangle - \sin(\phi/2)|-\rangle$$

We immediately obtain the time evolution

$$\begin{aligned}
|\psi(t)\rangle &= \cos\frac{\phi}{2}e^{+i\Omega_R t/2}|+\rangle - \sin\frac{\phi}{2}e^{-i\Omega_R t/2}|-\rangle \\
&= \cos\frac{\phi}{2}e^{+i\Omega_R t/2}\left(\cos(\phi/2)|\uparrow\rangle + \sin(\phi/2)|\downarrow\rangle\right) \\
&\quad - \sin\frac{\phi}{2}e^{-i\Omega_R t/2}\left(-\sin(\phi/2)|\uparrow\rangle + \cos(\phi/2)|\downarrow\rangle\right) \\
&= \cos\left(\frac{\Omega_R t}{2}\right)|\uparrow\rangle + i\sin\left(\frac{\Omega_R t}{2}\right)\cos\phi\,|\uparrow\rangle + i\sin\left(\frac{\Omega_R t}{2}\right)\sin\phi\,|\downarrow\rangle \\
&= \left(\cos\left(\frac{\Omega_R t}{2}\right) + i\frac{\delta}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\right)|\uparrow\rangle - i\frac{\omega_R}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)|\downarrow\rangle\,.
\end{aligned}$$

This is identical to what we had found before. We can also consider the time evolution operator directly

$$U(t) = e^{-i\tilde{H}t/\hbar} = \cos\left(\frac{\Omega_R t}{2}\right)\mathbb{1} + i\sin\left(\frac{\Omega_R t}{2}\right)\hat{\boldsymbol{h}}\cdot\boldsymbol{\sigma} \tag{1.92}$$
$$= \cos\left(\frac{\Omega_R t}{2}\right)\mathbb{1} + i\sin\left(\frac{\Omega_R t}{2}\right)\left(\frac{\delta}{\Omega_R}\sigma_z - \frac{\omega_R}{\Omega_R}\sigma_x\right). \tag{1.93}$$

from which the above result for $|\psi(t)\rangle = U(t)|\uparrow\rangle$ immediately follows. The probability of a spin flip is

$$p_\downarrow(t) = |\langle\downarrow|\psi(t)\rangle|^2 = \frac{\omega_R^2}{\Omega_R^2}\sin^2\left(\frac{\Omega_R t}{2}\right).$$

This is indeed just the same as the z-component of a classical magnetic moment.

1.4.8 Rapid adiabatic passage - Quantum treatment

We revisit the Landau Zener problem but now for a two-state system or equivalently a spin 1/2 system. The problem can be solved rigorously. Consider a spin 1/2 system in a magnetic field $\boldsymbol{B}_{\text{eff}}$ with energies

$$W_\pm = \pm\frac{1}{2}\hbar\gamma B_{\text{eff}}. \tag{1.94}$$

For a uniform field B_0 (with $B_1 = 0$), the effective field in the rotating frame is $B_0 - \omega/\gamma$, and

$$W_{\pm} = \pm\frac{1}{2}\hbar(\omega_0 - \omega), \tag{1.95}$$

where $\omega_0 = \gamma B_0$. As ω is swept through resonance, the two states move along their changing eigenenergies. The energies change, but the states do not. There is no coupling between the states, so a spin initially in one or the other will remain so indefinitely no matter how ω changes relative to ω_0.

In the presence of a rotating field, B_1, however, the energy levels look quite different: instead of intersecting lines they form non-intersecting hyperbolas separated by energy $\hbar\omega_R$. If the system moves along these hyperbolas, then an $\uparrow$ spin will adiabatically convert into $\downarrow$ and a $\downarrow$ spin will turn into $\uparrow$.

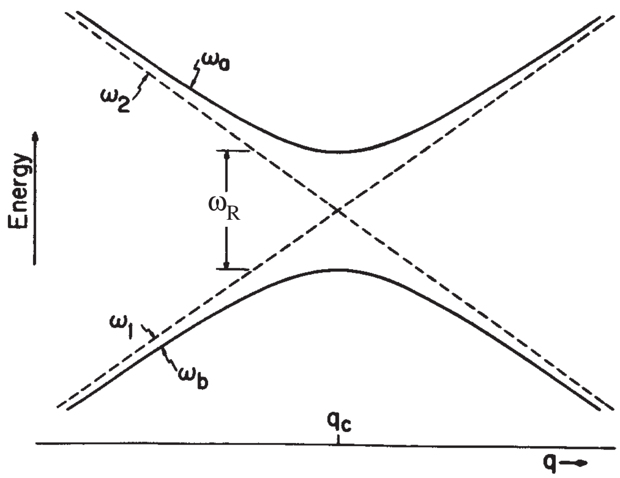

Figure 8. An avoided crossing. If the parameter q that governs the energy levels is swept slowly, the system can adiabatically change its state ("flip its spin"). If q is swept rapidly, it may instead jump across the gap and no spin flip occurs.

Whether or not the system follows an energy level adiabatically depends on how rapidly the energy is changed, compared to the minimum energy separation. To cast the problem in quantum mechanical terms, imagine two non-interacting states whose energy separation, ω, depends on some parameter q which varies linearly in time, and vanishes for some value q_c. Now add a perturbation having an off-diagonal matrix element V which is independent of q, so that the energies at q_c are $\pm\, V$, as shown in Fig. 8 ($\omega_R = 2V$). The probability that the system will "jump" from one adiabatic level to the other after passing through the "avoided crossing" (i.e., the probability of non-adiabatic behavior) is

$$P_{na} = e^{-2\pi\Gamma} \tag{1.96}$$

where

$$\Gamma = \frac{\mid V \mid^2}{\hbar^2}\left[\frac{d\omega}{dt}\right]^{-1} \tag{1.97}$$

This result was originally obtained by Landau and Zener. The jumping of a system as it travels across an avoided crossing is called the Landau-Zener effect. Further description, and reference to the initial papers, can be found in [5]. Inserting the parameters for our magnetic field problem, we have

$$P_{na} = \exp\left\{-\frac{\pi}{2}\frac{\omega_R^2}{d\omega/dt}\right\} \tag{1.98}$$

Note that the factor in the exponential is related to the inequality in Eq. 1.43. When Eq. 1.43 is satisfied, the exponent is large and the probability of non-adiabatic behavior is exponentially small.

Incidentally the "rapid" in adiabatic rapid passage is something of a misnomer. The technique was originally developed in nuclear magnetic resonance in which thermal relaxation effects destroy the spin polarization if one does not invert the population sufficiently rapidly. In the absence of such relaxation processes one can take as long as one pleases to traverse the anticrossings, and the slower the crossing the less the probability of jumping.

1.4.9 Adiabatic passage - Detailed calculation

Our initial Hamiltonian in the rotating frame is (

$$H_0 = \frac{\hbar}{2}\begin{pmatrix} -\delta & 0 \\ 0 & \delta \end{pmatrix}.$$

The full Hamiltonian is

$$H = \frac{\hbar}{2}\begin{pmatrix} -\delta & \omega_R \\ \omega_R & \delta \end{pmatrix}.$$

This has eigenstates $|\pm\rangle$, which have energies separated by ω_R.

We start with $-\delta \ll \omega_R$, so the eigenstates are initially $|\uparrow\rangle$ and $|\downarrow\rangle$. If we change the system adiabatically, states connect smoothly according to the adiabatic theorem, so the system will go from $|\uparrow\rangle$ to $|\downarrow\rangle$. However, for a non-adiabatic change, the system may jump across the avoided crossing, staying in the same state. The probability of a non-adiabatic transition is

$$p_{na} = e^{-\frac{\pi}{2}\frac{\omega_R^2}{\dot{\omega}}}.$$

We thus see the previous adiabaticity criteria appear.

Now, let us derive this. Suppose we are in a perturbative limit, $p_{\text{flip}} \ll 1$.

Since the drive frequency changes, the Hamiltonian is

$$H = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_R e^{-i\phi(t)} \\ \omega_R e^{+i\phi(t)} & -\omega_0 \end{pmatrix}.$$

In the frame rotating with the drive (in a time-dependent manner),

$$\tilde{H} = \frac{\hbar}{2}\begin{pmatrix} -\delta(t) & \omega_R \\ \omega_R & \delta(t) \end{pmatrix},$$

where $\delta(t) = \dot{\phi}(t) - \omega_0$. Suppose instead we rotate the frame at ω_0. We find

$$\bar{H} = \frac{\hbar}{2}\begin{pmatrix} 0 & \omega_R e^{-i(\phi(t)-\omega_0 t)} \\ \omega_R e^{+i(\phi(t)-\omega_0 t)} & 0 \end{pmatrix}.$$

The second Hamiltonian is actually easier to deal with. We know that

$$|\psi(t)\rangle = a(t)\,|\uparrow\rangle + b(t)\,|\downarrow\rangle$$

for eigenstates of this Hamiltonian. Acting with $\bar{H}$ on this,

$$\dot{a} = -i\frac{\omega_R}{2}e^{-i(\phi(t)-\omega_0 t)}b \text{ and } \dot{b} = -i\frac{\omega_R}{2}e^{+i(\phi(t)-\omega_0 t)}a.$$

Let us use a linear sweep, $\delta(t) = \dot{\phi} - \omega_0 = \alpha t$. So, $\phi(t) = \omega_0 t + \frac{1}{2}\alpha t^2$. Then

$$\dot{a} = -i\frac{\omega_R}{2}e^{-i\alpha t^2/2}b \text{ and } \dot{b} = -i\frac{\omega_R}{2}e^{+i\alpha t^2/2}a.$$

Suppose we start in $|\downarrow\rangle$, and have weak coupling, so at all times $b \approx 1$. Then

$$\dot{a} \approx -i\frac{\omega_R}{2}e^{-i\alpha t^2/2}.$$

So, a will only grow significantly when $\alpha t^2 \leq 1$. That is, the phase needs to be fairly constant for a to accumulate. This occurs for $\Delta t \sim \frac{1}{\sqrt{\alpha}} = \frac{1}{\sqrt{\dot{\omega}}}$ around the resonance. This implies that $a \approx \omega_R \Delta t \approx \frac{\omega_R}{\sqrt{\dot{\omega}}}$. The probability of a flip is thus

$$p_{\text{flip}} = |a|^2 \sim \frac{\omega_R^2}{\dot{\omega}},$$

which is proportional to what we expect. We can do the integral exactly since the $\dot{a}$ equation is Gaussian. We find

$$a(t) = -i\omega_R \int_0^\infty dt e^{-i\alpha t^2/2} = -ie^{-i\pi/4}\omega_R\sqrt{\frac{\pi}{2\alpha}}.$$

This gives a flip probability of

$$p_{\text{flip}} = |a|^2 = \frac{\pi}{2}\frac{\omega_R^2}{\dot{\omega}},$$

which is exactly the correct limit of the Landau-Zener formula.

We can perform the calculation also fully non-perturbatively. Note in passing that we could have solved the problem of a classical spin as well, as the result will have to be identical, but it is even more difficult than the quantum case as it involves three coupled equations instead of two.

Returning to the spin-1/2 system, we start with the coupled equations

$$\dot{a} = -i\frac{\omega_R}{2}e^{-i\alpha t^2/2}b \text{ and } \dot{b} = -i\frac{\omega_R}{2}e^{+i\alpha t^2/2}a.$$

We have boundary conditiosn $a(-\infty) = 0$, $b(-\infty) = 1$. Taking another derivative of a,

$$\ddot{a} = -i\frac{\omega_R}{2}e^{-i\alpha t^2/2}\dot{b} - i\alpha t\,\dot{a}.$$

So

$$\ddot{a} = -\frac{\omega_R^2}{4}a - i\alpha t\,\dot{a}.$$

We substitute $a = e^{-i\alpha t^2/4}c$, and find

$$\ddot{c} + \left(\frac{\omega_R^2}{4} - i\frac{\alpha}{2} + \frac{\alpha^2}{4}t^2\right)c = 0.$$

This is known as the Weber solution. We make it resemble a harmonic oscillator by introducing

$$z = \sqrt{\alpha}e^{-i\pi/4}t \implies dz = \sqrt{\alpha}e^{-i\pi/4}\,dt.$$

(the same substitution was actually necessary for the gaussian integral of the perturbative calculation). From this, our equation becomes

$$\frac{d^2c}{dz^2} + \left(i\frac{\omega_R^2}{4\alpha} + \frac{1}{2} - \frac{z^2}{4}\right)c = 0.$$

This can be compared to the Schrödinger equation for the harmonic oscillator

$$-\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2x^2\psi = E\psi \implies \frac{d^2\psi}{d\tilde{x}^2} + \left(n + \frac{1}{2} - \frac{\tilde{x}^2}{4}\right)\psi = 0.$$

when expressing space in units of the harmonic oscillator length $x = \tilde{x}\sqrt{\hbar/m\omega}$, and writing energy $E = \hbar\omega(n + 1/2)$.

Here, we have $n = i\frac{\omega_R^2}{4\alpha}$. The parabolic cylinder functions are ultimately the solution, and accept complex arguments:

$$c(z) = \frac{\omega_R}{2\sqrt{\alpha}}e^{-\pi\omega_R^2/16\alpha}D_{-1-i\frac{\omega_R^2}{4\alpha}}(iz).$$

We eventually find

$$|a(\infty)|^2 = 1 - e^{-\pi\omega_R^2/2\alpha}.$$

This is exactly the spin-flip probably that we expect.

1.5 Density Matrix

1.5.1 General results

The *density matrix* provides a way of treating the time evolution of a quantized system which offers several advantages over the usual time dependent expansion,

$$| \psi(t)\rangle = \sum_n c_n(t) | \psi_n\rangle = \sum_n \langle\psi_n | \psi(t)\rangle | \psi_n\rangle \tag{1.99}$$

plus Schrödingerr equation. It provides a natural way to express coherences and to find the expectation value of operators which do not commute with the Hamiltonian, it treats *pure quantum states* and *statistical mixtures* on an equal footing, and it allows straightforward determination of the time evolution of the system even when it is affected by incoherent processes such as damping, addition or subtraction of atoms (from the system) or interactions with other quantized systems not accessible to measurement (eg. collisions).

An operator, A, with matrix elements

$$A_{\mathrm{nm}} \equiv \langle\psi_n | A | \psi_m\rangle \tag{1.100}$$

has expectation value at time t

$$\langle A\rangle_t \equiv \langle\psi(t) | A | \psi(t)\rangle \tag{1.101}$$

$$= \sum_{\mathrm{mn}} c_m^*(t) c_n(t) A_{\mathrm{nm}} (\text{using Eq.1.99}). \tag{1.102}$$

Clearly the correlation between the c_m and c_n coefficients is important - physically it reflects the coherence between the amplitude for being in states m and n. These correlations are naturally dealt with by the density operator

$$\rho(t) = \overline{| \psi(t)\rangle\langle\psi(t) |} \tag{1.103}$$

because its matrix elements are

$$\rho_{\mathrm{nm}}(t) = c_m^*(t) c_n(t) \tag{1.104}$$

The bar here indicates an ensemble average over identically (but not necessarily completely) prepared systems. An ensemble average is essential to treat probabilities (eg. only the ensemble average of spin projections of atoms from an oven is zero although each atom will have $m = +1/2$ or$-1/2$ when measured), and an ensemble average is always implicit in using a density matrix. For notational simplicity, the averaging bar will be eliminated from here on.

The density matrix permits easy evaluation of expectation values: combining Eqs. 1.99 and Eq. 1.104 gives

$$\langle A\rangle_t = \sum_{\mathrm{nm}} \rho_{\mathrm{nm}} A_{\mathrm{mn}} = Tr(\rho(t)A) \tag{1.105}$$

where Tr is the trace, i.e., the sum of the diagonal elements. Eq. 1.105

for $\langle A \rangle$ really involves two sums: the ensemble average in the preparation of the systems, and the usual quantum mechanical sum over the basis to find the expectation value.

The time evolution of the density matrix is determined by a first order differential equation which is obtained by applying Schrödingerr's equation to the time derivative of Eq. 1.103;

$$i\hbar\dot{\rho} = H\rho - \rho H \equiv [H, \rho]. \tag{1.106}$$

This reflects changes in ρ due solely to the interactions (eg. radiation, dc fields) included in the Hamiltonian - additional terms may be added to account for collisions, loss of atoms, damping, etc.

The density matrix operator also provides a convenient test for a properly normalized system (sum of all probabilities, $p_n = c_n^* c_n$, equal to unity)

$$Tr(\rho(t)) = 1, \tag{1.107}$$

and

$$Tr\rho^2 \leq Tr\rho. \tag{1.108}$$

where the equality implies a pure quantum state.

We always have in mind that ρ is to be used on a statistical ensemble of systems similarly prepared. If this preparation is sufficient to force the system into a pure state [so that Eq. 1.99 holds for each member of the ensemble], then the ensemble average is superfluous - if the preparation is insufficient, then there will be random phases between some of the $c_n's$ in Eq. 1.100 and some ensemble averages of $c_n^* c_m$ will have modulus less than $\mid c_n \mid\mid c_m \mid$. If no relative phase information is present in the ensemble the ensemble is termed a "mixture" (except it is pure if only one $\mid c_n \mid^2$ is non-zero).

1.5.2 Density matrix for two level system

The density matrix for a two level system is

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \text{ with } \rho_{12}^* = \rho_{21}^* \tag{1.109}$$

We shall consider a two level system in which $E_1 = \hbar\omega_0/2$ and $E_2 = -\hbar\omega_0/2$ where ω_0 is constant, and we shall subject it to an off-diagonal perturbation of arbitrary strength and time dependence: $\langle 1 \mid H' \mid 2 \rangle = (V_1 - iV_2)/2$. Thus

$$H_0 = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix} = \frac{\hbar\omega_0}{2}\sigma_z \tag{1.110}$$

and

$$H' = \frac{1}{2}\begin{pmatrix} 0 & V_1 - iV_2 \\ V_1 + iV_2 & 0 \end{pmatrix} = \frac{V_1}{2}\sigma_x + \frac{V_2}{2}\sigma_y \tag{1.111}$$

so

$$H = \frac{1}{2}\begin{pmatrix} \hbar\omega_0 & V_1 - iV_2 \\ V_1 + iV_2 & \hbar\omega_0 \end{pmatrix} = \frac{1}{2}[V_1\sigma_x + V_2\sigma_y + \hbar\omega_0\sigma_z] \tag{1.112}$$

is the full Hamiltonian (the σ's are Pauli spin matrices). This is a general enough system to encompass most two-level systems which are encountered in resonance physics.

Before solving for $\dot{\rho}$ (which we could do by grinding away using Eq. 1.106) we shall change variables in the density matrix:

$$\rho = \frac{1}{2}\begin{pmatrix} r_0 + r_3 & r_1 - ir_2 \\ r_1 + ir_2 & r_0 - r_3 \end{pmatrix} = \frac{1}{2}[r_0 I + r_1\sigma_x + r_2\sigma_y + r_3\sigma_z] \tag{1.113}$$

There is no loss of generality in this substitution (it has 4 independent quantities just as ρ does), and it makes the physical constraints on ρ manifest, e.g.

$$Tr(\rho) = r_0 = 1 \tag{1.114}$$

and $\rho_{12} = \rho_{21}^*$ obviously.

Now we have expressed both H and ρ in terms of Pauli spin matrices. We can now solve the equation of motion for $\rho(t)$,

$$i\hbar\dot{\rho} = [H, \rho], \tag{1.115}$$

by using the cyclic commutation relations $[\sigma_j, \sigma_{j+1}] = 2i\sigma_{j+2}$ and then equating the coefficients of σ_x, σ_y, and σ_z, (rather than having to grind out the matrix products term by term):

$$\sigma_x : \dot{r}_1 = \frac{1}{\hbar}V_2 r_3 - \omega_0 r_2$$

$$\sigma_y : \dot{r}_2 = \omega_0 r_1 - \frac{1}{\hbar}V_1 r_3$$

$$\sigma_z : \dot{r}_3 = \frac{1}{\hbar}V_1 r_2 - \frac{1}{\hbar}V_2 r_1 \tag{1.116}$$

These final results can be summerized by using the vector representation due [1]. Define

$$\boldsymbol{\omega} = \frac{1}{\hbar}V_1\hat{\boldsymbol{x}} + \frac{1}{\hbar}V_2\hat{\boldsymbol{y}} + \omega_0\hat{\boldsymbol{z}} \quad \text{and} \quad \hat{\boldsymbol{r}} = r_1\hat{\boldsymbol{x}} + r_2\hat{\boldsymbol{y}} + r_3\hat{\boldsymbol{z}} \tag{1.117}$$

Using these definitions it is easy to see that Eq. 1.116,1.116, 1.116 become

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{\omega} \times \boldsymbol{r} \tag{1.118}$$

1.118 proves that the time evolution of the density matrix for our very general 2-level system is isomorphic to the behavior of a classic magnetic moment in a magnetic field which points along $\boldsymbol{\omega}$ (**??**. Our previous discussion showing that the quantum mechanical spin obeyed this equation also is therefore superfluous for spin 1/2 systems.)

One consequence of 1.118 is that $\boldsymbol{r}$ is always perpendicular to $\dot{\boldsymbol{r}}$ so that $|\ \boldsymbol{r}\ |$ does not change with time. This implies that if ρ is initially a pure state, ρ remains forever in a pure state no matter how violently $\boldsymbol{\omega}$ is gyrated, because

(recall $\sigma_i^2 = I$)

$$Tr\rho^2 = \frac{1}{2}(r_0^2 + r_1^2 + r_2^2 + r_3^2) = \frac{1}{2}(\mid \boldsymbol{r} \mid^2 + r_0^2) \tag{1.119}$$

1.119 will be satisfied for all time since $\mid \boldsymbol{r} \mid^2$ doesn't change and, the state will remain pure. In general it is not possible to decrease the purity (coherence) of a system with a Hamiltonian like the one in 1.112. Since real coherences do, in fact die out, we shall have to add relaxation processes to our description in order to approach reality. The density matrix formulation makes this easy to do, and this development will be done in the next part of the section.

1.5.3 Phenomological treatment of relaxation: Bloch equations

Statistical mechanics tells us the form which the density matrix will ultimately take, but it does not tell us how the system will get there or how long it will take. All we know is that ultimately the density matrix will thermalize to

$$\rho^T = \frac{1}{Z} e^{-H_0/kT}, \tag{1.120}$$

where Z is the partition function.

Since the interactions which ultimately bring thermal equilibrium are incoherent processes, the density matrix formulation seems like a natural way to treat them. Unfortunately in most cases these interactions are sufficiently complex that this is done phenomenologically. For example, the equation of motion for the density matrix 1.116 might be modified by the addition of a damping term:

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] - (\rho - \rho^T)/T_e \tag{1.121}$$

which would (in the absence of a source of non-equilibrium interactions) drive the system to equilibrium with time constant T_e.

This equation is not sufficiently general to describe the behavior of most systems studied in resonance physics, which exhibit different decay times for the energy and phase coherence, called T_1 and T_2 respectively.

- T_1 - decay time for population differences between non- degenerate levels, eg. for r_3 (also called the energy decay time)

- T_2 - decay time for coherences (between either degenerate or non-degenerate states), i.e. for r_1 or r_2.

The reason is that, in general, it requires a weaker interaction to destroy coherence (the relative phase of the coefficients of different states) than to destroy the population difference, so some relaxation processes will relax only the phase, resulting in $T_2 < T_1$. (caution: certain types of collisions violate this generality.)

The effects of thermal relaxation with the two decay times described above are easily incorporated into the vector model for the 2-level system since the z-component of the population vector $\boldsymbol{r}$ 1.117 represents the population difference and r_x and r_y represent coherences (i.e. off-diagonal matrix elements of ρ): The results (which modify 1.119) are

$$\dot{\boldsymbol{r}}_z = \frac{1}{\hbar}(\boldsymbol{\omega} \times \boldsymbol{r})_2 - \left(r_z - r_z^T\right)/T_1 \tag{1.122}$$

$$\dot{\boldsymbol{r}}_{x,y} = \frac{1}{\hbar}(\boldsymbol{\omega} \times \boldsymbol{r})_{x,y} - \left(r_{x,y} - r_{x,y}^T\right)/T_2 \tag{1.123}$$

(r_z^T is determined from 1.120). For a magnetic spin system $\boldsymbol{r}$ corresponds directly to the magnetic moment $\boldsymbol{\mu}$. The above equations were first introduced by Bloch [4] in this context and are known as the Bloch equations.

The addition of phenomenological decay times does not generalize the density matrix enough to cover situations where atoms (possibly state-selected) are added or lost to a system. This situation can be covered by the addition of further terms to $\dot{\rho}$. Thus a calculation on a resonance experiment in which state-selected atoms are added to a two-level system through a tube which also permits atoms to leave (eg. a hydrogen maser) might look like:

$$\begin{aligned}\dot{\rho} = {} & \frac{1}{i\hbar}[\rho, H] - \begin{pmatrix} (\rho_{11} - \rho_{11T})/T_1 & \rho_{12}/T_2 \\ \rho_{21}/T_2 & (\rho_{22} - \rho_{22T})/T_1 \end{pmatrix} \\ & + R\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - \rho/T_{\text{escape}} - \rho/T_{\text{collision}}\end{aligned} \tag{1.124}$$

R is the rate of addition of state-selected atoms

The last two terms express effects of atom escape from the system and of collisions (e.g. spin exchange) that can't easily be incorporated in T_1 and T_2.

The terms representing addition or loss of atoms will not have zero trace, and consequently will not maintain $\mathrm{Tr}(\rho) = 1$. Physically this is reasonable for systems which gain or lose atoms; the application of the density matrix to this case shows its power to deal with complicated situations. In most applications of the above equation, one looks for a steady state solution (with $\dot{\rho} = 0$), so this does not cause problems.

1.5.4 Introduction: Electrons, Protons, and Nuclei

The two-level system is basic to atomic physics because it approximates accurately many physical systems, particularly systems involving resonance phenomena. All two-level systems obey the same dynamical equations: thus to know one is to know all. The archetype two level system is a spin-1/2 particle such as an electron, proton or neutron. The spin motion of an electron or a proton in a magnetic field, for instance, displays the total range of phenomena in a two level system. To slightly generalize the subject, however, we shall also include the motion of atomic nuclei. Here is a summary of their properties.

MASS		
	electron	$m = 0.91 \times 10^{-31} kg$
	proton	$M_p = 1.67 \times 10^{-27}$ kg
	neutron	M_p
	nuclei	$M = AM_p$
		$A = N + Z =$ mass number
		Z = atomic number
		N = neutron number
CHARGE		
	electron	-e $\quad e = 1.60 \times 10^{-19}$ C
	proton	+e
	neutron	0
	nucleus	Ze
ANGULAR MOMENTUM		
	electron	S = $\hbar/2$
	proton	I = $\hbar/2$
	neutron	I = $\hbar/2$
	nuclei	even A:I/$\hbar$ = 0, 1, 2, . . .
		odd A: I/$\hbar$ = 1/2, 3/2, . . .
STATISTICS		
	electrons	Fermi-Dirac
	nuclei:	even A, Bose-Einstein
		odd A, Fermi-Dirac
ELECTRON MAGNETIC MOMENT		

$\mu_e = \gamma_e S = -g_s \mu_B S/\hbar$
$\gamma_e =$ gyromagnetic ratio $= e/m = 2\pi \times 2.80 \times 10^4$MHzT^{-1}
$g_s =$ free electron g-factor = 2 (Dirac Theory)
$\mu_B =$Bohr magneton $= e\hbar/2m = 0.93 \times 10^{-24}$JT^{-1} (erg/gauss)

(Note that μ_e is negative. We show this explicitly by taking g_s to be positive, and writing $\mu_e = -g_s \mu_B S$)

NUCLEAR MAGNETIC MOMENTS

$$\mu_{nuc} = \gamma_{nuc}\hbar I = g_{nuc}\mu_N I/\hbar$$

γ_I = gyromagnetic ratio of the nucleus

μ_N = nuclear magneton = $e\hbar/2Mc = \mu_B(m/M_p)$

proton $g_p = 5.6, \gamma_p = 2\pi \times 42.6$ MHz T^{-1}

neutron $g_n = -3.7$

References

[1] R.P. Feyman, F.L. Vernon, and R.W. Hellwarth, J. Appl. **28** 49 (1957).

[2] N.F. Ramsey, Phys. Rev. **76** 996 (1949).

[3] S.R. Lundeen and F.M. Pipkin, Phys. Rev. Lett. **34** , 1368 (1975).

[4] F. Bloch, Phys. Rev. **70** 460 (1946).

[5] Rubbermark et al., Phys. Rev. A **23**, 3107 (1981).

[6] A.H. Autler and C.H. Townes, Phys. Rev. **100**, 703, 1955.

[7] B.R. Mollow, Phys. Rev. A ??, 1522.

[8] B.R. Mollow, Phys. Rev. A **5**, 2217, 1972.

[9] R.E. Grove, F.Y. Wu, S. Ezekiel, Phys. Rev. A **15**, 227.

[10] R.M. Whitley and C.R. Stroud, Phys. Rev. A **14**, 1498.

[11] C. Delsart and J.C. Keller, J. Phys. B **9**, 2769.

[12] J.L. Picque and J. Pinard, J. Phys. B **9**, L77.

[13] F.Y. Wu, S. Ezekiel, M. Ducloy, B.R. Mollow, Phys. Rev. Lett. **38**, 1077.