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Chapter G

The Spin 1/2 System

In this appendix we discuss the properties of a spin $1/2$ system. Since all quantum mechanical two-level systems are equivalent to the spin $1/2$ system the results derived in the following are quite general and can be transferred to other two-level systems using for the realization of quantum bits.

I Experimental Demonstration of Angular Momentum Quantization

The quantization of the components of an angular momentum has been first demonstrated by **Stern** and **Gerlach** in 1922 in the ***Stern-Gerlach experiment***, where the deflection of a beam of neutral paramagnetic atoms (silver atoms in the first experiment) in an inhomogeneous magnetic field has been studied.

Classically, the Stern-Gerlach experiment can be understood as follows: Since the used atoms are neutral, they are not subject to the Lorentz force. However, as paramagnetic atoms they possess a magnetic moment $\mathbf{m}$ and the resulting force can be derived by considering the potential energy

$$E_{\text{pot}} = -\mathbf{m}\cdot\mathbf{B} \ . \tag{I.1}$$

From the basic course in physics we know that for an atom the magnetic moment $\mathbf{m}$ and a total angular momentum $\mathbf{J}$ is caused by (i) the motion of electrons about the nucleus (orbital moment $\mathbf{L}$) and (ii) the intrinsic magnetic moment or spin of the electrons (spin moment $\mathbf{S}$). In the case of silver atoms the total angular moment is simply equal to the spin moment of the single electron in the outermost shell, since this electron is an *s*-electron with zero orbital moment and the total spin and orbital moment of other electrons forming a completely filled shell is also zero. That is, the total angular moment of the silver atom is $\mathbf{J} = \mathbf{L} + \mathbf{S} = \mathbf{S}$ with $S = 1/2$.

We further know that for a given atomic level the magnetic moment is proportional to the angular moment

$$\mathbf{m} = \gamma\mathbf{J} \tag{I.2}$$

with *gamma* the ***gyromagnetic ratio*** of the level under consideration. From (G.I.1) we immediately can derive the force exerted on the atom to

$$\mathbf{F} = \nabla(\mathbf{m}\cdot\mathbf{B}) \ , \tag{I.3}$$

which is zero if the magnetic field is homogeneous. Furthermore, the magnetic field $\mathbf{B}$ exerts a torque

$$\mathbf{D} = \mathbf{m}\times\mathbf{B} \tag{I.4}$$

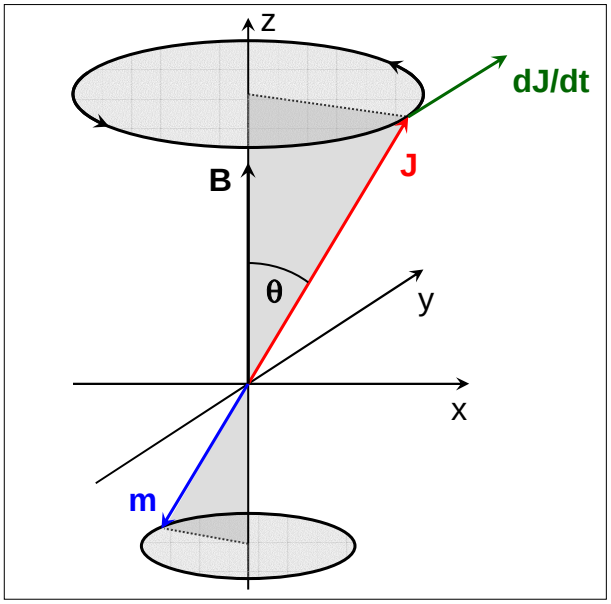

Figure G.1: In a uniform magnetic field **B** the magnetic moment **m** of an atom, which is proportional to its total angular momentum **J**, precesses around the field direction with constant angular velocity (Larmor precession).

on the magnetic moment **m**. The classical equation of motion of **J** is (angular moment theorem)

$$\frac{d\mathbf{J}}{dt} = \mathbf{D} = \gamma \mathbf{J} \times \mathbf{B} \tag{I.5}$$

or

$$\frac{d}{dt}\mathbf{m}(t) = \gamma \mathbf{m}(t) \times \mathbf{B} \tag{I.6}$$

Scalar multiplication of both sides of (G.I.6) by either $\mathbf{m}(t)$ or **B** yields

$$\frac{d}{dt}[\mathbf{m}(t)]^2 = 0 \tag{I.7}$$

$$\frac{d}{dt}[\mathbf{m}(t) \cdot \mathbf{B}] = 0 \tag{I.8}$$

That is, the magnetic moment evoles with constant modulus and maintaining a constant angle with **B**. The atom thus behaves like a gyroscope (see Fig. G.1). The time derivative $\frac{d\mathbf{J}}{dt}$ is perpendicular to **J** and **B** and the angular moment therefore turns around the magnetic field direction with the angle θ between **J** and **B** remaining constant.

To calculate the force from (G.I.3) we can neglect in very good approximation the terms proportional to m_x and m_y and take m_z as constant. This can be done since the oscillation frequency due to the rotation of **m** is so high that only time-averaged values of m_x and m_y can play a role in E_{pot} and these are both zero. Then, we obtain

$$\mathbf{F} = \nabla (m_z B_z) = m_z \nabla B_z \ . \tag{I.9}$$

With $\mathbf{B} = (0,0,B_z(z))$ also the components of ∇B_z along the x- and y-direction are zero. Then, the resulting force is parallel to z and proportional to m_z. In the Stern-Gerlach experiment the deflection of

silver atoms in such magnetic field has been measured. Since the force is causing a deflection of the atoms in z-direction proportional to m_z and hence J_z, one would expect continuous distribution along z if the moments of the various atoms would be distributed homogeneously. In contrast, in the experiment only two spots have been observed showing that the moment m_z of the silver atoms can have only two distinct values $+m_z$ and $-m_z$.

II Theoretical Description

We are now going to show how quantum mechanics describes the degrees of freedom of a spin $1/2$ system. The idea is to give examples of kets and observables in order to show how physical predictions can be extracted from them and how to distinguish clearly between the various stages of an experiment (state preparation, time evolution, measurement). We know that every physical quantity must be associated with an observable, i.e. a Hermitian operator whose eigenvalues can form a basis in the state space. We therefore must define the state space and the observables corresponding to the components S_x, S_y and S_z of a spin $\mathbf{S}$ and, more generally, $S_u = \mathbf{S} \times \widehat{\mathbf{u}}$, where $\widehat{\mathbf{u}}$ is an arbitrary unit vector.

II.1 The Spin Space

From experiments it is known that with S_z we must associate an observable $\mathscr{S}_z$, which has the two eigenvalues $\pm\hbar/2$. We assume that these two eigenvalues are not degenerate. We further denote by $\uparrow\rangle$ and $\downarrow\rangle$ the corresponding orthonormal eigenvectors:

$$\mathscr{S}_z|\uparrow\rangle = +\frac{\hbar}{2}|\uparrow\rangle \tag{II.10}$$

$$\mathscr{S}_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle \ . \tag{II.11}$$

The spin state space is the two-dimensional space S^2 spanned by its eigenvectors $|\uparrow\rangle$ and $|\downarrow\rangle$. The most general normalized vector in this space is a linear superposition of $|\uparrow\rangle$ and $|\downarrow\rangle$

$$|\Psi(t)\rangle = a(t)|\uparrow\rangle + b(t)|\downarrow\rangle \tag{II.12}$$

with

$$|a(t)|^2 + |b(t)|^2 = 1 \ . \tag{II.13}$$

Note that $|\Psi\rangle$ can be viewed as a vector on the Bloch sphere S^2 (see Fig. E.1).

In the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis the matrices representing the observables $\mathscr{S}_x$, $\mathscr{S}_y$ and $\mathscr{S}_z$ are given by (we will not derive this result here)

$$\mathscr{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathscr{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix} \qquad \mathscr{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathscr{S} = \frac{\hbar}{2}\overrightarrow{\sigma} \tag{II.14}$$

with the Pauli spin matrices $\overline{\sigma} = (\mathbf{X}, \mathbf{Y}, \mathbf{Z})$. With the angles θ and φ defined in Fig. E.1 we can write the component $\mathscr{S}_u$ of $\mathscr{S}$ along the unit vector $\widehat{\mathbf{u}}$ as

$$\mathscr{S}_u = \mathscr{S} \cdot \widehat{\mathbf{u}} = \mathscr{S}_x \sin\theta\cos\varphi + \mathscr{S}_y \sin\theta\sin\varphi + \mathscr{S}_z \cos\theta \ . \tag{II.15}$$

Using (G.II.14) we easily find the matrix, which represents the corresponding observable $\mathscr{S}_u = \mathscr{S} \cdot \widehat{\mathbf{u}}$ in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis:

$$\begin{aligned} \mathscr{S}_u &= \mathscr{S}_x \sin\theta\cos\varphi + S_y \sin\theta\sin\varphi + S_z\cos\theta \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta \mathrm{e}^{-\imath\varphi} \\ \sin\theta\mathrm{e}^{+\imath\varphi} & -\cos\theta \end{pmatrix} . \end{aligned} \tag{II.16}$$

We now have to derive the eigenvalues and eigenvectors of the observables $\mathscr{S}_x$, $\mathscr{S}_y$ and $\mathscr{S}_u$. The calculation using the matrices (G.II.14) is straightforward. For $\mathscr{S}_u$ the eigenvalue equation $\mathscr{S}_u|\Psi\rangle = \lambda|\Psi\rangle$ with $|\Psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$ can be written as

$$\frac{\hbar}{2}\begin{pmatrix} \cos\theta - \lambda & \sin\theta\mathrm{e}^{-\imath\varphi} \\ \sin\theta\mathrm{e}^{+\imath\varphi} & -(\cos\theta + \lambda) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0 . \tag{II.17}$$

It can easily that this system is solved by $\lambda = \pm 1$ resulting in the eigenvalues $\pm\frac{\hbar}{2}$. More generally, it can be shown that $\mathscr{S}_x$, $\mathscr{S}_y$ and $\mathscr{S}_u$ have the same eigenvalues $\pm\hbar/2$ as $\mathscr{S}_z$. This result is expected, since in an experiment (e.g. a Stern-Gerlach experiment) it is always possible to make the axis defined by the magnetic field parallel to the x- and y-axis or parallel to $\widehat{\mathbf{u}}$. Since all directions of space have the same properties, the same results is expected for all directions.

As for the eigenvectors of $\mathscr{S}_x$, $\mathscr{S}_y$ and $\mathscr{S}_u$, we denote them by $|\pm\rangle_x$, $|\pm\rangle_y$ and $|\pm\rangle_u$, respectively, where the sign in the ket is that of the corresponding eigenvalue. The expansions of these eigenvectors in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis is given by

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle) \tag{II.18}$$

$$|\pm\rangle_y = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm \imath|\downarrow\rangle) \tag{II.19}$$

$$|+\rangle_u = \cos\frac{\theta}{2}\mathrm{e}^{-\imath\varphi/2}|\uparrow\rangle + \sin\frac{\theta}{2}\mathrm{e}^{+\imath\varphi/2}\downarrow\rangle \tag{II.20}$$

$$|-\rangle_u = -\sin\frac{\theta}{2}\mathrm{e}^{-\imath\varphi/2}|\uparrow\rangle + \cos\frac{\theta}{2}\mathrm{e}^{+\imath\varphi/2}\downarrow\rangle . \tag{II.21}$$

III Evolution of a Spin 1/2 Particle in a Homogeneous Magnetic Field

We consider again a silver atom in a homogeneous magnetic field $\mathbf{B}_0$ as we have done in the classical treatment in section I. The classical potential energy of the magnetic moment $\mathbf{m}$ related to the angular momentum $\mathbf{J} = \mathbf{S}$ is[1]

$$E_{\mathrm{pot}} = -\mathbf{m}\cdot\mathbf{B}_0 = -m_z B_0 = -\gamma B_0 S_z = \omega_0 S_z . \tag{III.22}$$

It is easy to be seen that the quantity $\omega_0 \equiv -\gamma B_0$ has the dimension of an inverse time, i.e. of an angular velocity.

Going to a quantum mechanical treatment we must replace S_z by the operator $\mathscr{S}_z$ and the classical energy by the Hamiltonian $\mathscr{H}$, which describes the evolution of the spin of the atom in the magnetic field $\mathbf{B}_0$:

$$\mathscr{H} = \omega_0 \mathscr{S}_z . \tag{III.23}$$

[1] Note that for an electron with spin $S = 1/2$ we have $\mathbf{m} = -g_s\frac{e}{2m_e}\mathbf{S} = \gamma\mathbf{S}$. That is, $\gamma = -g_s\frac{e}{2m_e}$ is negative with $g_s \simeq 2$ the g-factor of the electron. The potential energy then is $E_{\mathrm{pot}} = -\mathbf{m}\cdot\mathbf{B} = g_s\frac{e}{2m_e}\mathbf{S}\cdot\mathbf{B} = -\gamma S_z B_z$.

Since this operator is time independent, solving the corresponding Schrödinger equation is equivalent to solving the eigenvalue equation of $\mathscr{H}$. We immediately see that the eigenvectors of $\mathscr{H}$ are those of $\mathscr{S}_z$:

$$\mathscr{H}|\uparrow\rangle = +\frac{\hbar\omega_0}{2}|\uparrow\rangle = E_\uparrow|\uparrow\rangle \tag{III.24}$$

$$\mathscr{H}|\downarrow\rangle = -\frac{\hbar\omega_0}{2}|\downarrow\rangle = E_\downarrow|\downarrow\rangle \ . \tag{III.25}$$

There are two energy levels $E_\uparrow$ and $E_\downarrow$ separated by the energy[2]

$$\hbar\omega_0 = -\gamma\hbar B_0 \ . \tag{III.26}$$

We next discuss the ***Larmor precession*** already mentioned in the classical treatment of section I. In order to do so let us assume that at $t = 0$ the spin is in the state

$$|\Psi(0)\rangle = \cos\frac{\theta}{2}e^{-\imath\varphi/2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+\imath\varphi/2}|\downarrow\rangle \ . \tag{III.27}$$

It can be shown that any spin state could be put in this form. To calculate the spin state at a time $t > 0$ we can write

$$|\Psi(t)\rangle = \cos\frac{\theta}{2}e^{-\imath\frac{\varphi}{2}}e^{-\imath E_\uparrow\frac{t}{\hbar}}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+\imath\frac{\varphi}{2}}e^{-\imath E_\downarrow\frac{t}{\hbar}}|\downarrow\rangle \ , \tag{III.28}$$

since we already have expanded $|\Psi(0)\rangle$ in terms of the eigenstates of the Hamiltonian. Using the eigenvalues $E_\uparrow$ and $E_\downarrow$ we obtain

$$|\Psi(t)\rangle = \cos\frac{\theta}{2}e^{-\imath(\varphi+\omega_0 t)/2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+\imath(\varphi+\omega_0 t)/2}|\downarrow\rangle \ . \tag{III.29}$$

We see that the presence of the magnetic field $\mathbf{B}_0$ introduces a phase shift between the coefficients of the kets $|\uparrow\rangle$ and $|\downarrow\rangle$, which is proportional to t.

Comparing (G.III.29) for $|\Psi(t)\rangle$ to the eigenket $|+\rangle_u$ of the observable $\widehat{S}\cdot\widehat{\mathbf{u}}$ (see (G.II.20)), we see that the direction $\widehat{\mathbf{u}}(t)$ along which the spin component is $+\hbar/2$ is defined by the polar angles

$$\theta(t) = \theta \tag{III.30}$$

$$\varphi(t) = \varphi + \omega_0 t \ . \tag{III.31}$$

That is, the angle θ between $\widehat{\mathbf{u}}(t)$ and the z-axis remains constant, while $\widehat{\mathbf{u}}(t)$ rotates around the z-axis at an angular velocity $d\varphi/dt = \omega_0$. Thus, the quantum mechanical treatment also gives the precession of the spin around the direction of the magnetic field, which is denoted as the ***Larmor precession***.

Form the expression (G.III.23) for the Hamiltonian it is obvious that the observable S_z is a constant of the motion. Using the expression (G.III.29) it can be shown that the probabilities for obtaining $\pm\hbar/2$ in a measurement are time independent. Since the modulus of $e^{\pm\imath(\varphi+\omega_0 t)/2}$ is equal to 1, we obtain[3]

$$\langle\Psi(t)|\mathscr{S}_z|\Psi(t)\rangle = \frac{\hbar}{2}\cos\theta \ . \tag{III.32}$$

[2]For an electron we have $gamma = -g_s\frac{e}{2m_e}$ and hence $\hbar\omega_0 = +g_s\frac{e\hbar}{2m_e}B_0 = g_s\mu_B B_0$ with the Bohr magneton $\mu_B = \frac{e\hbar}{2m_e}$.

[3]Here we have to use the equalities $\sin^2\frac{\theta}{2} = \frac{1}{2}(1-\cos\theta)$ and $\cos^2\frac{\theta}{2} = \frac{1}{2}(1+\cos\theta)$.

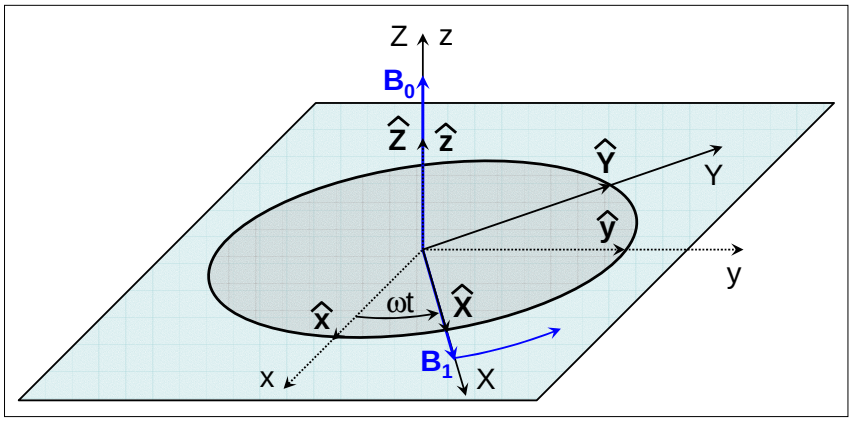

Figure G.2: The absolute reference frame (dotted lines) and the rotating reference frame (solid lines). The magnetic field $\mathbf{B}_0$ is directed along the $\hat{\mathbf{z}}$-direction. The rotating reference frame rotates about the $\hat{\mathbf{z}}$-direction at an angular velocity ω. The direction $\hat{\mathbf{X}}$ is coincides with the direction of the rotating field $\mathbf{B}_1(t)$.

On the other hand, $\mathscr{S}_x$ and $\mathscr{S}_y$ do not commute with $\mathscr{H}$ what can be easily shown by using the matrices in (G.II.14). We obtain

$$\langle\Psi(t)|\mathscr{S}_x|\Psi(t)\rangle = \frac{\hbar}{2}\sin\theta\cos(\varphi+\omega_0 t) \tag{III.33}$$

$$\langle\Psi(t)|\mathscr{S}_y|\Psi(t)\rangle = \frac{\hbar}{2}\sin\theta\sin(\varphi+\omega_0 t)\ . \tag{III.34}$$

We see that the mean values of the spin components behave as the components of a classical angular momentum of modulus $\hbar/2$ undergoing a Larmor precession.

IV Spin 1/2 Particle in a Rotating Magnetic Field

IV.1 Classical Treatment

We now discuss the situation, where in addition to the static magnetic field $\mathbf{B}_0$ we have an additional field $\mathbf{B}_1(t)$, which is perpendicular to $\mathbf{B}_0$ and rotates about $\mathbf{B}_0$ at constant amplitude with an angular velocity ω as shown in Fig. G.2. The field amplitude are related to the two characteristic frequencies

$$\omega_0 = -\gamma B_0 \tag{IV.35}$$

$$\omega_1 = -\gamma B_1\ . \tag{IV.36}$$

In order to analyze the behavior of a spin 1/2 system in such field we use a fixed coordinate system characterized by the unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ with the static magnetic field parallel to $\hat{\mathbf{z}}$. We further introduce a rotating reference frame characterized by the unit vectors $\hat{\mathbf{X}}$, $\hat{\mathbf{Y}}$ and $\hat{\mathbf{Z}}$, which is obtained from the fixed system by rotation through an angle ωt about $\hat{\mathbf{z}}$. The direction $\hat{\mathbf{X}}$ corresponds to the direction of the rotating field $\mathbf{B}_1(t)$.

The equation of motion of the magnetic moment $\mathbf{m}(t)$ in the presence of the total field $\mathbf{B}(t)=\mathbf{B}_0+\mathbf{B}_1(t)$ becomes (compare (G.I.6))

$$\frac{d}{dt}\mathbf{m}(t) = \gamma\mathbf{m}(t)\times[\mathbf{B}_0+\mathbf{B}_1(t)]\ . \tag{IV.37}$$

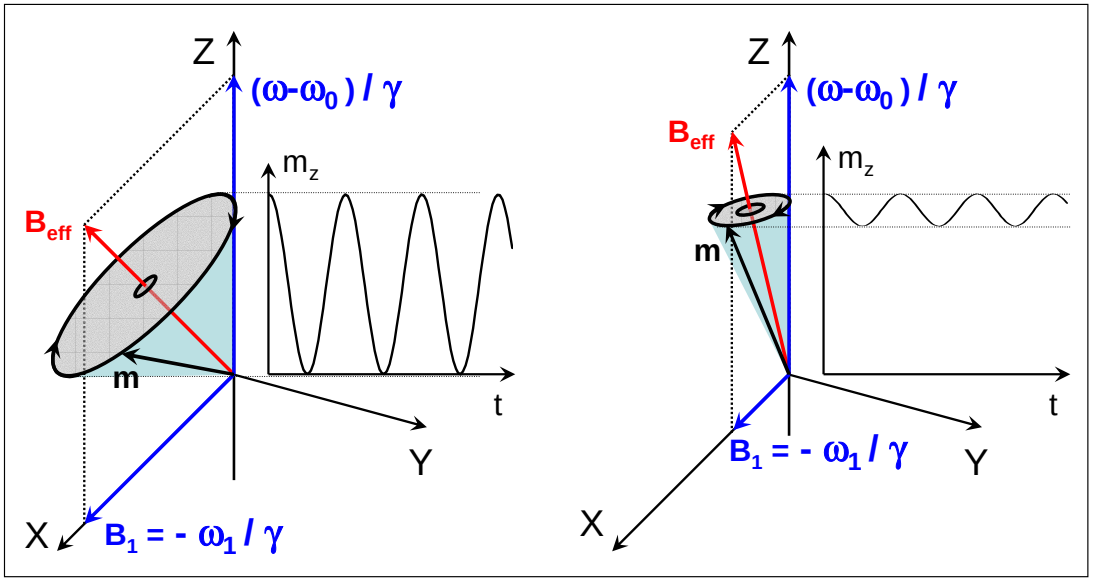

Figure G.3: In the rotating reference frame the effective magnetic field $\mathbf{B}_{\rm eff}$ has fixed direction. The magnetic moment $\mathbf{m}(t)$ rotates about the direction of $\mathbf{B}_{\rm eff}$ with constant angular velocity: precession in the rotating reference frame. Also shown is the temporal oscillation of the Z-component of the magnetic moment. Left: close to resonance case, $\Delta\omega = \omega - \omega_0 \sim \omega_1$. Right: off-resonance case, $\Delta\omega = \omega - \omega_0 \gg \omega_1$.

To solve this equation it is convenient to switch to the rotating reference frame. The velocity of the vector $\mathbf{m}(t)$ with respect to this rotating reference frame is

$$\left(\frac{d\mathbf{m}}{dt}\right)_{\rm rel} = \frac{d\mathbf{m}}{dt} - \omega\hat{\mathbf{z}}\times\mathbf{m}(t) \ . \tag{IV.38}$$

With

$$\Delta\omega = \omega - \omega_0 \tag{IV.39}$$

we obtain

$$\begin{aligned}\left(\frac{d\mathbf{m}}{dt}\right)_{\rm rel} &= \gamma\mathbf{m}(t)\times[\mathbf{B}_0 + \mathbf{B}_1(t)] - \omega\hat{\mathbf{z}}\times\mathbf{m}(t) \\ &= \mathbf{m}(t)\times[\Delta\omega\,\hat{\mathbf{Z}} - \omega_1\,\hat{\mathbf{X}}] \ .\end{aligned} \tag{IV.40}$$

This equation can be solved easier, since the coefficients on the right hand side are now no longer time dependent. Moreover, the form of (G.IV.40) is analogous to that of (G.I.6). Hence, the relative motion of the vector $\mathbf{m}(t)$ is therefore a rotation about an ***effective field*** $\mathbf{B}_{\rm eff}$, which is static with respect to the rotating reference frame and given by (see Fig. G.3)

$$\mathbf{B}_{\rm eff} = \frac{1}{\gamma}\,[\Delta\omega\,\hat{\mathbf{Z}} - \omega_1\,\hat{\mathbf{X}}] \ . \tag{IV.41}$$

In order to obtain the absolute motion of $\mathbf{m}(t)$ we have to combine the precession about $\mathbf{B}_{\rm eff}$ with the rotation about $\hat{\mathbf{z}}$ with the angular velocity ω.

We use the above discussion to understand the phenomenon of magnetic resonance. For this purpose let us consider a magnetic moment which is parallel to the field $\mathbf{B}_0$ at $t = 0$. The question is: What

happens if we switch on the rotating field $\mathbf{B}_1(t)$? We first consider the case that the rotation frequency $\omega/2\pi$ of this field is very different from the natural frequency $\omega_0/2\pi$, so that $\Delta\omega = \omega - \omega_0 \gg \omega_1$. We immediately see from Fig. G.3 that in this case the effective magnetic field is directed practically along $\widehat{\mathbf{z}}$. The precession of $\mathbf{m}(t)$ about $\mathbf{B}_{\text{eff}}$ then has a very small amplitude and hardly modifies the direction of the magnetic moment. That is, nothing happens.

The more interesting case is the resonance case, when $\omega \simeq \omega_0$ and hence $\Delta\omega = \omega - \omega_0 \ll \omega_1$. In this case the angle between $\mathbf{B}_{\text{eff}}$ and $\widehat{\mathbf{z}}$ is large and the precession of the magnetic moment then has a large amplitude. Moreover, in the case of resonance, $\Delta\omega = 0$, $\mathbf{B}_{\text{eff}}$ is directed along $\widehat{\mathbf{X}}$ and the magnetic moment can be completely flipped.

IV.2 Quantum Mechanical Treatment

With the two eigenvectors $|\uparrow\rangle$ and $|\downarrow\rangle$ of the projection $\mathscr{S}_z$ of the spin onto the $\widehat{\mathbf{z}}$-direction the state vector of the system can be written as

$$|\Psi(t)\rangle \;=\; a(t)|\uparrow\rangle + b(t)|\downarrow\rangle \;. \tag{IV.42}$$

The Hamilton operator of the system is[4]

$$\mathscr{H}(t) \;=\; -\mathscr{M}\cdot\mathbf{B}(t) \;=\; -\gamma\mathscr{S}\cdot[\mathbf{B}_0 + \mathbf{B}_1(t)] \;. \tag{IV.43}$$

With $\mathbf{B}_0$ parallel to $\mathbf{z}$ and $\mathbf{B}_1(t)$ rotating in the xy-plane with angular frequency ω we obtain

$$\mathscr{H}(t) \;=\; \omega_0\mathscr{S}_z + \omega_1[\cos\omega t\,\mathscr{S}_x + \sin\omega t\,\mathscr{S}_y] \;. \tag{IV.44}$$

With the spin matrices (G.II.14) we obtain the matrix representing $\mathscr{H}$ to

$$\mathscr{H}(t) \;=\; \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 \mathrm{e}^{-\imath\omega t} \\ \omega_1 \mathrm{e}^{+\imath\omega t} & -\omega 0 \end{pmatrix} \;. \tag{IV.45}$$

Using (G.IV.42) and (G.IV.45) we can write the Schrödinger equation as

$$\imath\frac{d}{dt}a(t) \;=\; \frac{\omega_0}{2}a(t) + \frac{\omega_1}{2}\mathrm{e}^{-\imath\omega t}b(t) \tag{IV.46}$$

$$\imath\frac{d}{dt}b(t) \;=\; \frac{\omega_1}{2}\mathrm{e}^{+\imath\omega t}a(t) - \frac{\omega_0}{2}b(t) \;. \tag{IV.47}$$

Equations (G.IV.46) and (G.IV.47) form a linear homogeneous system with time dependent coefficients. To solve this system it is convenient to switch again to the rotating reference frame. To do so, we define new functions by setting

$$\alpha(t) \;=\; \mathrm{e}^{+\imath\omega t/2}a(t) \tag{IV.48}$$

$$\beta(t) \;=\; \mathrm{e}^{-\imath\omega t/2}b(t) \;. \tag{IV.49}$$

[4]The expression $\mathscr{M}\cdot\mathbf{B}(t)$ symbolizes the scalar product $\mathscr{M}_x B_x(t) + \mathscr{M}_y B_y(t) + \mathscr{M}_z B_z(t)$, where $\mathscr{M}_x$, $\mathscr{M}_y$ and $\mathscr{M}_z$ are operators, while $B_x(t)$, $B_y(t)$ and $B_z(t)$ are numbers.

Substitution of (G.IV.48) and (G.IV.49) into (G.IV.46) and (G.IV.47) gives

$$\imath\frac{d}{dt}\alpha(t) = -\frac{\Delta\omega}{2}\alpha(t)+\frac{\omega_1}{2}\beta(t) \quad \text{(IV.50)}$$

$$\imath\frac{d}{dt}\beta(t) = +\frac{\omega_1}{2}\alpha(t)+\frac{\Delta\omega}{2}\beta(t)\ . \quad \text{(IV.51)}$$

This is equivalent to

$$\imath\hbar\frac{d}{dt}|\widetilde{\Psi}(t)\rangle = \widetilde{\mathscr{H}}|\widetilde{\Psi}(t)\rangle \quad \text{(IV.52)}$$

with

$$|\widetilde{\Psi}(t)\rangle = \alpha(t)|\uparrow\rangle+\beta(t)|\downarrow\rangle \quad \text{(IV.53)}$$

and

$$\widetilde{\mathscr{H}}(t) = \frac{\hbar}{2}\begin{pmatrix} -\Delta\omega & \omega_1 \\ \omega_1 & +\Delta\omega \end{pmatrix}\ . \quad \text{(IV.54)}$$

Thus, the transformation (G.IV.48) and (G.IV.49) has led to an equation, which is analogous to a Schrödinger equation, in which the Hamilton operator $\widetilde{\mathscr{H}}$ plays the role of a time independent Hamiltonian. Note that $\widetilde{\mathscr{H}}$ describes the interaction of a spin with a fixed field corresponding to the effective field introduced above. We therefore can conclude that the transformation (G.IV.48) and (G.IV.49) is the quantum mechanical analogue of the change from the fixed reference frame to the rotating reference frame.

Equation (G.IV.52) is simple to solve. For a given $|\widetilde{\Psi}(0)\rangle$ we can determine $|\widetilde{\Psi}(t)\rangle$ by expanding $|\widetilde{\Psi}(0)\rangle$ on the eigenvectors of $\widetilde{\mathscr{H}}$, which can be calculated exactly. Since $\widetilde{\mathscr{H}}$ does not depend explicitly on time, to find $|\Psi(t)\rangle$ at given $|\widetilde{\Psi}(0)\rangle$ we simply can multiply the coefficients of the expansion on the eigenvectors by $\mathrm{e}^{-\imath E_\pm t/\hbar}$, where $E_\pm$ are the eigenvalues of $\widetilde{\mathscr{H}}$ (for the eigenvalues compare appendix II). Finally, we go from $|\widetilde{\Psi}(t)\rangle$ to $|\Psi(t)\rangle$ by using (G.IV.48) and (G.IV.49).

IV.3 Rabi's Formula

We consider a spin residing in state $|\uparrow\rangle$ at $t=0$, i.e. $|\Psi(0)\rangle = |\uparrow\rangle$. According to (G.IV.48) and (G.IV.49) this corresponds to

$$|\widetilde{\Psi}(0)\rangle = |\uparrow\rangle\ . \quad \text{(IV.55)}$$

We are now interested in the probability $P_{\uparrow\downarrow}(t)$ of finding the spin in the state $|\downarrow\rangle$ at the tine t. This probability is given by

$$P_{\uparrow\downarrow}(t) = |\langle\downarrow|\Psi(t)\rangle|^2 = |b(t)|^2 = |\beta(t)|^2 = |\langle\downarrow|\widetilde{\Psi}(t)\rangle|^2\ . \quad \text{(IV.56)}$$

Here we have used the fact that $b(t)$ and $\beta(t)$ have the same modulus.

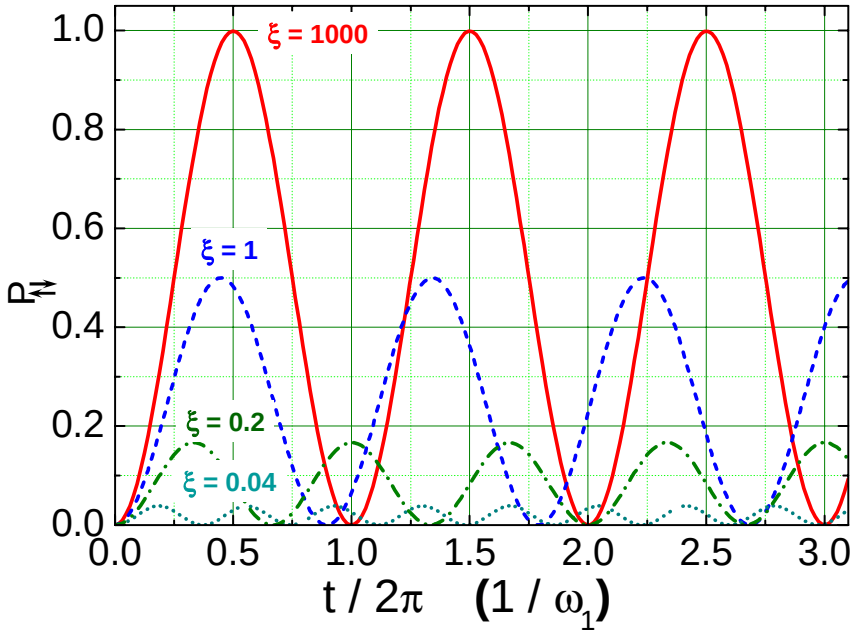

Figure G.4: Variation of the probability $P_{\uparrow\downarrow}$ of finding s spin 1/2 system in the state $|\downarrow\rangle$ at time t, when it was in state $|\uparrow\rangle$ at $t=0$. $P_{\uparrow\downarrow}(t)$ is shown for three different values of the parameter $\xi = \omega_1^2/(\Delta\omega)^2$. In resonance, $\Delta\omega \to 0$ and hence $\xi \to \infty$.

We see that we have to determined $|\langle\downarrow|\widetilde{\Psi}(t)\rangle|^2$, where $|\widehat{\Psi}(t)\rangle$ is the solution of (G.IV.52) under the initial condition (G.IV.55). This problem has already been solved in section III. To use the results derived there we have to use the following correspondences:

$$\begin{aligned} |\phi_1\rangle &\doteq |\uparrow\rangle \qquad |\phi_2\rangle \doteq |\downarrow\rangle \\ E_1 &\doteq -\frac{\hbar}{2}\Delta\omega \qquad E_2 \doteq +\frac{\hbar}{2}\Delta\omega \qquad W_{12} \doteq +\frac{\hbar}{2}\omega_1 \ . \end{aligned} \tag{IV.57}$$

With these replacements Rabi's formula (III.43) becomes

$$P_{\uparrow\downarrow}(t) = \frac{\omega_1^2}{\omega_1^2+(\Delta\omega)^2}\,\sin^2\left[\sqrt{\omega_1^2+(\Delta\omega)^2}\,\frac{t}{2}\right] \ . \tag{IV.58}$$

The probability is of course zero at $t=0$ and then varies sinusoidally with time between the minimum value zero and the maximum value $\frac{\omega_1^2}{\omega_1^2+(\Delta\omega)^2}$. We see, that for $|\omega_1| \ll |\Delta\omega|$ (this corresponds to the weak coupling case $|W_{12}| \ll E_1 - E_2$ in section III), $P_{\uparrow\downarrow}(t)$ remains almost zero as shown in Fig. G.4. However, near resonance, i.e. for $\Delta\omega \simeq 0$, the oscillation amplitude of $P_{\uparrow\downarrow}(t)$ is large and becomes exactly 1 for $\Delta\omega = 0$ at the moments $t = (2n+1)\pi/\omega_1$ (see Fig. G.4). This is in agreement with the result of our classical treatment. We find that at resonance a very weak rotating field is able to reverse the direction of the spin. We further note that the angular frequency of the oscillation of $P_{\uparrow\downarrow}(t)$ is $\sqrt{\omega_1^2+(\Delta\omega)^2} = |\gamma\mathbf{B}_{\rm eff}|$. In the rotating reference frame this oscillation corresponds to the projection of the precession of the magnetic moment about the effective field and is usually called ***Rabi precession*** or ***Rabi oscillation***. We also would $P_{\uparrow\downarrow}(t)$ is $\sqrt{\omega_1^2+(\Delta\omega)^2} \simeq \omega_1 \propto B_1$. That is, the oscillation frequency increases linearly with the amplitude of the rotating field.