

Chapter 14

Spin Qubits for Quantum Information Processing

In this chapter we will review the basic principles of manipulating spin qubits for quantum information processing. The history of spin manipulation (magnetic resonance) techniques for nuclear spins and electron spins in solids and liquids was dated back to early 1940s [1]. The first nuclear magnetic resonance (NMR) experiments were performed independently by E.M. Purcell's group at Harvard [2] and by F. Bloch's group at Stanford [3] in 1946. The first electron spin resonance (ESR) experiment was performed by E. Zavoisky in 1945 [4]. After those breakthrough experiments, people quickly recognized that the newly developed experimental techniques provide an indispensable ultra-small probe inside solids and liquids. Today, magnetic resonance techniques have many application areas in physics, chemistry, biology, medicine and engineering [5]. More recently, a single electron spin or a single nuclear spin is expected to play as a robust qubit for quantum computing. This is because the quantum state of a spin is relatively stable against external perturbations, compared to other degrees of freedom such as an electric charge.

In particular, an electron spin is suitable for a qubit in quantum processor, because an electron spin can be manipulated and also can be coupled to other electron spins with a much shorter time scale than a nuclear spin. On the other hand, a nuclear spin is suitable for a qubit in quantum memory, because a nuclear spin has a much longer coherence time than an electron spin. We will describe in this chapter how to manipulate a single electron spin and nuclear spin with an alternating magnetic field and also how to interface an electron spin and a nuclear spin, i.e. transferring a qubit of information between the two, using a hyperfine coupling.

14.1 Simple magnetic resonance theory

A nucleus (or electron) possesses a magnetic moment (vector operator),

$$\hat{\mu} = \hbar\gamma\hat{I} \quad , \quad (14.1)$$

where γ is a gyromagnetic ratio and \hat{I} is a dimension-less angular momentum operator ($\hat{J} = \hbar\hat{I}$ is a standard angular momentum operator).

A magnetic interaction Hamiltonian for a spin in a *dc* magnetic field H_0 (along z-axis) is

$$\hat{\mathcal{H}} = -\hat{\mu} \cdot \vec{k} H_0 = -\hbar\gamma H_0 \hat{I}_z \quad , \quad (14.2)$$

where \vec{k} is a unit vector along z-axis.

The squared total angular momentum \hat{I}^2 and the z-component of the total angular momentum \hat{I}_z commute [6]:

$$[\hat{I}^2, \hat{I}_z] = 0 \quad . \quad (14.3)$$

Therefore, a simultaneous eigenstate of \hat{I}^2 and \hat{I}_z exists and can be defined by

$$\hat{I}^2 |I, m\rangle = I(I+1) |I, m\rangle \quad , \quad (14.4)$$

$$\hat{I}_z |I, m\rangle = m |I, m\rangle \quad . \quad (14.5)$$

The eigenvalues take $I = \frac{1}{2}, 1, \frac{3}{2}, \dots$ and $m = I, I-1, \dots, -I$, respectively. The eigen-energies corresponding to (14.2) for such eigenstates are given by

$$E = -\hbar\gamma H_0 m \quad . \quad (14.6)$$

Figure 14.1 shows the Zeeman spectrum of the eigen-energies for an electron spin with $I = 1/2$ and *Cu* nuclear spin with $I = \frac{3}{2}$. The gyromagnetic ratio γ for an electron spin is negative so that $m = -1/2$ state is the ground state as shown in (a), while that of a *Cu* nuclear spin is positive so that $m = 3/2$ state is the ground state as shown in (b).

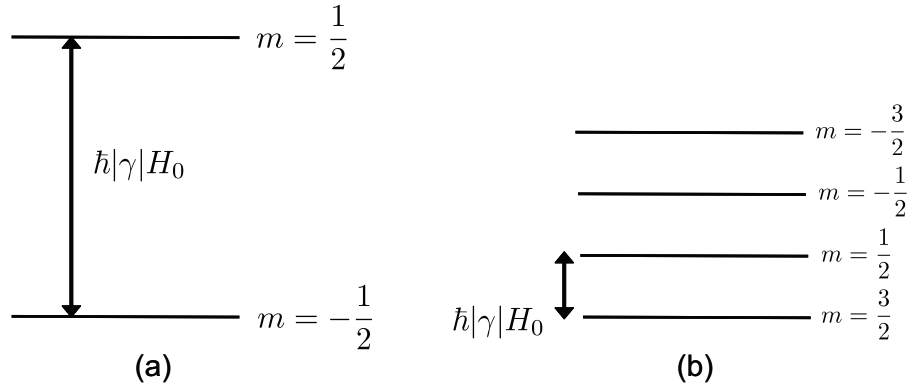


Figure 14.1: The eigen-energies of an electron spin (a) and a *Cu* nuclear spin (b).

If we apply an alternating magnetic field $H_1 \cos \omega t$ along a perpendicular direction, for instance *x*-axis, in addition to the static field H_0 , the new Hamiltonian is

$$\hat{\mathcal{H}}_I = -\hbar\gamma H_1 \cos \omega t \hat{I}_x \quad . \quad (14.7)$$

The *x*-component \hat{I}_x of the angular momentum operator is expressed as

$$\hat{I}_x = \frac{1}{2} (\hat{I}_+ + \hat{I}_-) \quad , \quad (14.8)$$

where \hat{I}_+ and \hat{I}_- are called a raising and lowering operator because of the following recursion relation:

$$\hat{I}_+ |I, m\rangle = \sqrt{I(I+1) - m(m+1)} |I, m+1\rangle \quad , \quad (14.9)$$

$$\hat{I}_-|I, m\rangle = \sqrt{I(I+1) - m(m-1)}|I, m-1\rangle \quad . \quad (14.10)$$

From the above argument, we understand the transverse ac magnetic field $H_1 \cos \omega t$ has the capability to change the eigenvalue m , if the frequency ω is close to the resonance with the Zeeman splitting,

$$\omega \simeq |\gamma|H_0 \quad . \quad (14.11)$$

The change of the eigenvalue m by ± 1 , of course, must accompany the absorption or emission of a single photon at frequency ω to satisfy energy conservation law. This is the principle of magnetic resonance.

14.2 Gyromagnetic ratio and g -factor

If a charged particle with a mass m makes a circular motion as shown in Fig. 14.2, the corresponding angular momentum is

$$\vec{J} = \vec{p} \times \vec{r} = m \frac{2\pi r^2}{T} \vec{z} \quad , \quad (14.12)$$

where T and r are a period and radius of circular motion. The magnetic moment is

$$\vec{\mu} = iA\vec{z} = \frac{e}{T} (\pi r^2) \vec{z} \quad , \quad (14.13)$$

where i is a current and A is an effective area. The gyromagnetic ratio γ is thus obtained from (14.12) and (14.13) as

$$\gamma = \frac{\vec{\mu}}{\vec{J}} = \frac{e}{2m} \quad . \quad (14.14)$$

Since the nuclear mass is heavier than the electron mass by three to four orders of magnitude, the electron gyromagnetic ratio is larger than the nuclear gyromagnetic ratio by a factor of $10^3 \sim 10^4$. Therefore, at a dc magnetic field of $H_0 = 1T$, the nuclear Zeeman frequency is in the range of $5 \sim 50$ MHz while the electron Zeeman frequency is ~ 50 GHz.

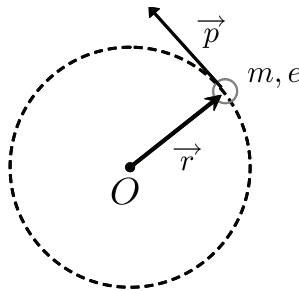


Figure 14.2: A circular motion of a charged particle.

The above classical picture addresses a so-called orbital angular momentum as shown in Fig. 14.2, but cannot address properly a spin angular momentum, which is intrinsically a quantum effect. An electron in free space has a new gyromagnetic ratio:

$$\gamma_e = -g_e \left(\frac{e}{2m} \right) \quad , \quad (14.15)$$

where $g_e = 2.002319 \dots$ is an electron g -factor [6]. An electron in solids acquires a different value for a g -factor due to the presence of spin-orbit coupling [5, 6]. The gyromagnetic ratio of a nuclear spin is defined by

$$\hat{\mu}_n = g_n \frac{e}{2M_p} \hbar \hat{I} = \gamma_n \hbar \hat{I} \quad , \quad (14.16)$$

where M_p is a proton mass. The gyromagnetic ratio $\gamma_n = g_n \frac{e}{2M_p} (> 0)$ is independent of environments and a universal value for a nucleus, because the nuclear wavefunction is so tiny and protected by surrounding valence electrons that the environment hardly affects it.

14.3 Thermal population and saturation

In a magnetic resonance experiment, a spin system continuously absorbs a photon from an alternating magnetic field and dissipates its energy to thermal reservoirs, as shown in Fig. 14.3. The steady state (thermal equilibrium) populations of the two spin states, N_- and N_+ , and those of the two reservoir states, N_a and N_b , satisfy the detailed balance:

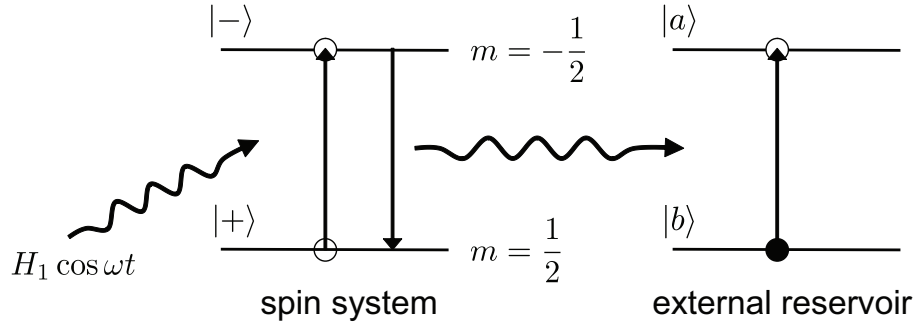


Figure 14.3: Absorption of photon and energy dissipation of a spin system.

$$N_- N_b W_{-b \rightarrow +a} = N_+ N_a W_{+a \rightarrow -b} \quad , \quad (14.17)$$

where the two transition matrix elements are identical, since

$$\begin{aligned} W_{-b \rightarrow +a} &= \frac{2\pi}{\hbar} \left| \langle +, a | \hat{\mathcal{H}}_I | -, b \rangle \right|^2 \\ &= \frac{2\pi}{\hbar} \left| \langle -, b | \hat{\mathcal{H}}_I | +, a \rangle \right|^2 \\ &= W_{+a \rightarrow -b}. \end{aligned} \quad (14.18)$$

Therefore, the spin population ratio is identical to the reservoir population ratio (Boltzman factor) as it should be at thermal equilibrium:

$$\frac{N_-}{N_+} = \frac{N_a}{N_b} = e^{-E/k_B T} \quad . \quad (14.19)$$

If we begin with a non-thermal population, the transient behavior is described by the following rate equation:

$$\frac{d}{dt} N_+ = N_- W_{\downarrow} - N_+ W_{\uparrow} \quad , \quad (14.20)$$

$$\frac{d}{dt}N_- = N_+W_\uparrow - N_-W_\downarrow \quad , \quad (14.21)$$

where $W_\downarrow = N_bW_{-b \rightarrow +a} > W_\uparrow = N_aW_{+a \rightarrow -b}$. The population difference $n = N_+ - N_-$ is governed by the rate equation:

$$\frac{d}{dt}n = -\frac{n - n_0}{T_1} \quad . \quad (14.22)$$

Here $n_0 = N \frac{W_\downarrow - W_\uparrow}{W_\downarrow + W_\uparrow}$ is a thermal equilibrium population difference and $T_1 = (W_\downarrow + W_\uparrow)^{-1}$ is a spin relaxation time. Equation (14.22) indicates that any departure of n from n_0 can be removed with a time constant T_1 due to the coupling of the spin system to external reservoirs.

The rate equation for photon absorption and emission processes is given by

$$\frac{d}{dt}N_+ = W_{-\rightarrow+}N_- - W_{+\rightarrow-}N_+ \quad , \quad (14.23)$$

$$\frac{d}{dt}N_- = W_{+\rightarrow-}N_+ - W_{-\rightarrow+}N_- \quad . \quad (14.24)$$

The two transition matrix elements are also identical with each other, $W_{-\rightarrow+} = W_{+\rightarrow-} = W$, so that the population difference n is governed by

$$\frac{d}{dt}n = -2Wn \quad . \quad (14.25)$$

Equation (14.25) means that the population difference n disappears (population saturation) if only absorption and emission of photons from the alternating magnetic field is taken into account and the dissipation to external reservoirs is neglected.

If we combine the two effects, we have a complete rate equation:

$$\frac{d}{dt}n = -2Wn - \frac{n - n_0}{T_1} \quad . \quad (14.26)$$

The steady state solution of the above equation is

$$n = \frac{n_0}{1 + 2WT_1} \quad . \quad (14.27)$$

The energy absorption rate per second is now calculated as

$$\frac{d}{dt}E = \hbar\omega nW = \frac{\hbar\omega n_0 W}{1 + 2WT_1} = \begin{cases} \hbar\omega n_0 W \left(W \ll \frac{1}{2T_1} \right) \\ \frac{\hbar\omega n_0}{2T_1} \left(W \gg \frac{1}{2T_1} \right) \end{cases} \quad . \quad (14.28)$$

The energy absorption rate $\frac{dE}{dt}$ initially increases with the incident field energy W but saturates at the value determined by T_1 time constant. A short T_1 is essential to detect a weak absorption signal.

14.4 Manipulation of a single spin

14.4.1 Heisenberg equation of motion

The motion of an isolated spin in a static magnetic field is governed by the Zeeman Hamiltonian,

$$\hat{\mathcal{H}} = -\hbar\gamma H_0 \hat{I}_z \quad . \quad (14.29)$$

Using the commutation relations,

$$[\hat{I}_x, \hat{I}_y] = i\hat{I}_z \quad , \quad (14.30)$$

$$[\hat{I}_y, \hat{I}_z] = i\hat{I}_x \quad , \quad (14.31)$$

$$[\hat{I}_z, \hat{I}_x] = i\hat{I}_y \quad , \quad (14.32)$$

we obtain the Heisenberg equations of motion:

$$\frac{d}{dt}\hat{I}_x = \frac{1}{i\hbar} [\hat{I}_x, \hat{\mathcal{H}}] = \gamma H_0 \hat{I}_y \quad , \quad (14.33)$$

$$\frac{d}{dt}\hat{I}_y = \gamma H_0 \hat{I}_x \quad , \quad (14.34)$$

$$\frac{d}{dt}\hat{I}_z = 0 \quad . \quad (14.35)$$

Combining (14.33), (14.34) and (14.35), we have the famous operator torque equation:

$$\frac{d}{dt}\hat{I} = \vec{i} \frac{d\hat{I}_x}{dt} + \vec{j} \frac{d\hat{I}_y}{dt} + \vec{k} \frac{d\hat{I}_z}{dt} = \gamma H_0 \hat{I} \times \vec{k} \quad , \quad (14.36)$$

or equivalently

$$\frac{d}{dt}\hat{\mu} = \gamma H_0 \hat{\mu} \times \vec{k} \quad , \quad (14.37)$$

where $\vec{i}, \vec{j}, \vec{k}$ are the unit vectors along x, y, z directions and $\hat{\mu} = \gamma\hbar\hat{I}$ is the magnetic moment operator. Equation (14.36) or (14.37) suggest that the spin precesses along a static magnetic field with right-handed circulation for $\gamma < 0$ or left-handed circulation for $\gamma > 0$ as shown in Fig. 14.4.

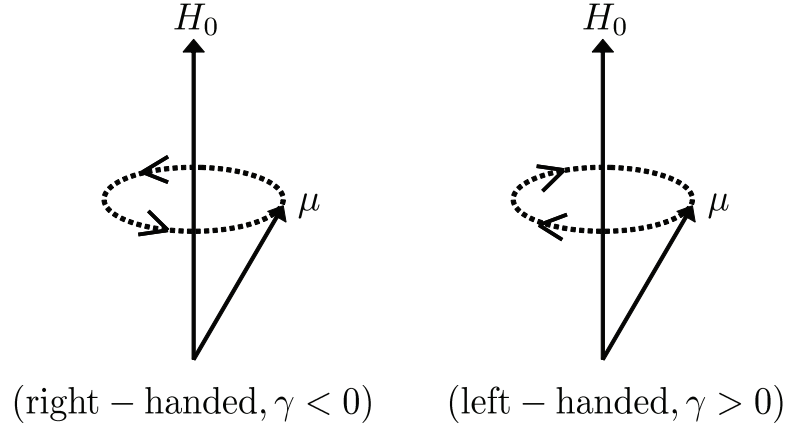


Figure 14.4: Spin precession about a static magnetic field with a Larmor frequency $\omega_L = |\gamma|H_0$.

14.4.2 Rotating reference frame

Suppose a fictitious frame $(\vec{i}, \vec{j}, \vec{k})$ rotates along z-axis (or \vec{k}) with an angular frequency $\vec{\Omega}$, their dynamics are described by

$$\frac{d}{dt} \vec{i} = \vec{\Omega} \times \vec{i} \quad , \quad (14.38)$$

$$\frac{d}{dt} \vec{j} = \vec{\Omega} \times \vec{j} \quad , \quad (14.39)$$

$$\frac{d}{dt} \vec{k} = \vec{\Omega} \times \vec{k} \quad , \quad (14.40)$$

Then a dynamical variable $\vec{F} = \vec{i} F_x + \vec{j} F_y + \vec{k} F_z$ follows the equation,

$$\begin{aligned} \frac{d}{dt} \vec{F} &= \vec{i} \frac{dF_x}{dt} + \vec{j} \frac{dF_y}{dt} + \vec{k} \frac{dF_z}{dt} + F_x \frac{d\vec{i}}{dt} + F_y \frac{d\vec{j}}{dt} + F_z \frac{d\vec{k}}{dt} \\ &= \frac{\partial \vec{F}}{\partial t} + \vec{\Omega} \times \vec{F} \quad . \end{aligned} \quad (14.41)$$

Here $\frac{d\vec{F}}{dt}$ and $\frac{\partial \vec{F}}{\partial t}$ are considered as the time rates of change of \vec{F} with respect to a (fixed) laboratory frame and (rotating) fictitious frame $(\vec{i}, \vec{j}, \vec{k})$, respectively.

If we substitute $\vec{F} = \hat{\mu}$ in (14.41) and use (14.37), we have

$$\frac{d}{dt} \hat{\mu} = \frac{\partial \hat{\mu}}{\partial t} + \vec{\Omega} \times \hat{\mu} = \gamma H_0 \hat{\mu} \times \vec{k} \quad . \quad (14.42)$$

The above result leads to the Heisenberg equation of motion for $\hat{\mu}$ in a rotating frame:

$$\begin{aligned} \frac{\partial \hat{\mu}}{\partial t} &= \hat{\mu} \times (\gamma H_0 \vec{k} + \vec{\Omega}) \\ &= \gamma H_{\text{eff}} \hat{\mu} \times \vec{k} \quad , \end{aligned} \quad (14.43)$$

where $H_{\text{eff}} \vec{k} = H_0 \vec{k} + \vec{\Omega}/\gamma$ is an effective field. If a fictitious frame rotates with an angular frequency $\vec{\Omega} = -\gamma H_0 \vec{k}$, the effective field H_{eff} disappears and the spin remains fixed, $\frac{\partial \hat{\mu}}{\partial t} = 0$, in this rotating frame.

Alternatively, the spin $\hat{\mu}$ rotates along a static field (\vec{k}) with an angular frequency $\vec{\Omega} = -\gamma H_0 \vec{k}$ in the (fixed) laboratory frame. This oscillation frequency is called a Larmor frequency and given by

$$\omega_L = |\gamma| H_0 \quad . \quad (14.44)$$

14.4.3 Effect of alternating magnetic fields

Suppose an alternating magnetic field is applied along x -axis (\vec{i}) ,

$$H_x(t) = \vec{i} H_{x0} \cos \omega t \quad . \quad (14.45)$$

This ac field can be decomposed into two circularly rotating fields:

$$H_R(t) = H_1 \left(\vec{i} \cos \omega t + \vec{j} \sin \omega t \right) \quad , \quad (14.46)$$

$$H_L(t) = H_1 \left(\vec{i} \cos \omega t - \vec{j} \sin \omega t \right) \quad , \quad (14.47)$$

where $H_1 = H_{x0}/2$. If $H_R(t)$ rotates synchronously as the precession of the spin, then $H_L(t)$ rotates in an opposite direction so that we can neglect the effect of $H_L(t)$ on the spin.

The torque equation in the laboratory frame is now

$$\frac{d}{dt} \hat{\mu} = \hat{\mu} \times \gamma \left[H_0 \vec{k} + H_1 \left(\vec{i} \cos \omega_z t + \vec{j} \sin \omega_z t \right) \right] \quad . \quad (14.48)$$

The above equation can be translated into the one in the rotating frame with an angular frequency ω_z :

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\mu} &= \hat{\mu} \times \left[(\gamma H_0 + \omega_z) \vec{k} + \gamma H_1 \vec{i} \right] \\ &= \hat{\mu} \times \gamma \left[\left(H_0 + \frac{\omega_z}{\gamma} \right) \vec{k} + H_1 \vec{i} \right] \end{aligned} \quad (14.49)$$

In this rotating frame, $H_R(t)$ is a static field along x -axis while the field along z -axis is offset by $\frac{\omega_z}{\gamma}$, so that the effective static is now

$$H_{\text{eff}} = \left(H_0 + \frac{\omega_z}{\gamma} \right) \vec{k} + H_1 \vec{i} \quad . \quad (14.50)$$

At resonance condition, $\omega_z = -\gamma H_0$, the effective static field H_{eff} along z -axis disappears and only $H_1 \vec{i}$ survives. In such a case, the spin simply rotates about x -axis in the rotating frame (Fig. 14.5(a)). If there is a slight detuning, $\omega_z \neq -\gamma H_0$, the effective static field $H_{\text{eff}} = \left(H_0 + \frac{\omega_z}{\gamma} \right) \vec{k} + H_1 \vec{i}$ is in the $x-z$ plane and the spin precesses in a cone of fixed angle about the direction of H_{eff} with an angular frequency γH_{eff} (Fig. 14.5(b)).

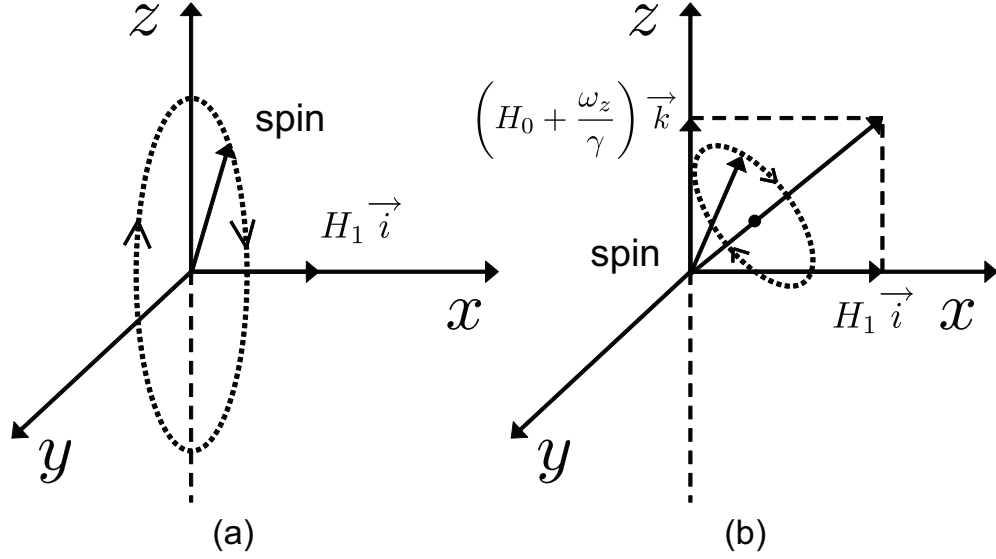


Figure 14.5: Spin precession at resonance condition, $\omega_z = -\gamma H_0$ (a), and at off-resonance condition $\omega_z \neq -\gamma H_0$ (b), where $\gamma > 0$ is assumed.

14.4.4 Bloch equations

A macroscopic magnetization consisting of many spins can be described by the phenomenological model called “Bloch equations”. The magnetization along z -axis is expressed as an ensemble averaged quantity:

$$M_z = \hbar\gamma\langle\hat{I}_z\rangle N = \hbar\gamma\frac{n}{2} \quad , \quad (14.51)$$

where N is the total number of spins in a sample and $n = N_+ - N_-$ is the population difference. The equation of motion for M_z is driven by the spin precession term due to an external field and spin relaxation term due to dissipative coupling to heat reservoirs:

$$\frac{d}{dt}M_z = \gamma\left(\vec{M} \times \vec{H}\right)_z - \frac{M_z - M_0}{T_1} \quad , \quad (14.52)$$

where $\vec{M} = \vec{i}M_x + \vec{j}M_y + \vec{k}M_z$, M_0 is the thermal equilibrium magnetization and T_1 is the spin relaxation time. Similarly, the equation of motions for M_x and M_y are given by

$$\frac{d}{dt}M_x = \gamma\left(\vec{M} \times \vec{H}\right)_x - \frac{M_x}{T_2} \quad , \quad (14.53)$$

$$\frac{d}{dt}M_y = \gamma\left(\vec{M} \times \vec{H}\right)_y - \frac{M_y}{T_2} \quad , \quad (14.54)$$

where T_2 is the spin decoherence time.

When there is a static field H_0 along z -axis and an alternating field H_1 with a slight detuning $h_0 = H_0 + \frac{\omega_z}{\gamma} \neq 0$, (14.52)-(14.54) are reduced to

$$\frac{d}{dt}M_z = -\gamma H_1 M_y - \frac{M_z - M_0}{T_1} \quad , \quad (14.55)$$

$$\frac{d}{dt}M_x = \gamma h_0 M_y - \frac{M_x}{T_2} \quad , \quad (14.56)$$

$$\frac{d}{dt}M_y = \gamma H_1 M_z - \gamma h_0 M_x - \frac{M_y}{T_2} \quad , \quad (14.57)$$

in the rotating frame.

If H_1 is small so that saturation along x -axis is negligible (weak probing case), we have the approximate solution for M_z :

$$M_z \simeq M_0 \quad . \quad (14.58)$$

We now introduce

$$M_+ = M_x + iM_y = \hbar\gamma\langle\hat{I}_+\rangle N \quad , \quad (14.59)$$

which satisfies the equation of motion

$$\frac{d}{dt}M_+ = -\left(i\gamma h_0 + \frac{1}{T_2}\right)M_+ + i\gamma H_1 M_0 \quad . \quad (14.60)$$

The steady state solution of (14.60) is given by

$$M_+ = \frac{\gamma M_0}{\gamma h_0 - i\frac{1}{T_2}} H_1 \quad . \quad (14.61)$$

The in-phase and quadrature-phase responses to the small external probe field H_1 are now expressed as

$$M_x = \chi_0 \omega_0 T_2 \frac{(\omega_0 - \omega) T_2}{1 + (\omega_0 - \omega)^2 T_2^2} H_1 \quad , \quad (14.62)$$

$$M_y = \chi_0 \omega_0 T_2 \frac{1}{1 + (\omega_0 - \omega)^2 T_2^2} H_1 \quad , \quad (14.63)$$

where $\chi_0 = M_0/H_0$ is the magnetic susceptibility at dc and $\omega_0 = \gamma H_0$ is the spin Larmor frequency. Equations (14.62) and (14.63) represent the linear dispersion and absorption spectrum for a small external probe field.

14.5 Optical manipulation of semiconductor spin qubits

S.M. Clark et al., PRL 99, 040501 (2007)

D. Press et al., Nature 456, 218 (2008)

14.6 Double resonance

14.6.1 Hyperfine interaction

Let us consider a magnetic coupling between two spins, say a nuclear spin and an electron spin, as shown in Fig. 14.6

Suppose a nucleus with a magnetic moment μ_n at $\vec{r} = 0$ has a finite radius ρ_0 , there exist two kinds of magnetic fields: uniform internal field H_i inside the nucleus and external dipole field H_e outside the nucleus, as shown in Fig. 14.7. The continuity of magnetic flux

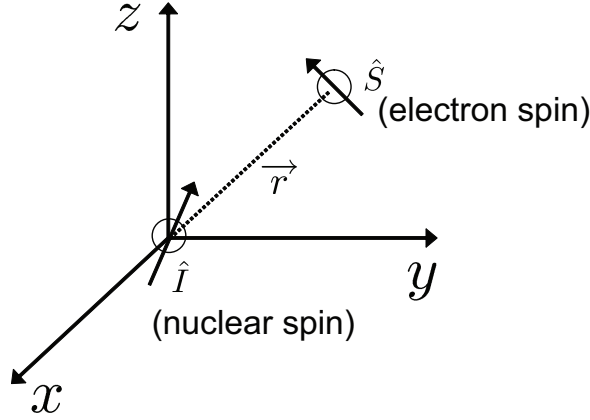


Figure 14.6: A magnetic coupling between a nuclear spin \hat{I} and electron spin \hat{S} .

requires the integrated magnetic fields inside and outside the nucleus exactly cancel with each other out:

$$\phi_i(\rho_0) + \phi_e(\rho_0) = 0. \quad (14.64)$$

The internal flux is given by

$$\phi_i(\rho) = \pi\rho_0^2 H_i, \quad (14.65)$$

while the external flux is

$$\begin{aligned} \phi_e(\rho) &= 2\pi \int_{\rho_0}^{\infty} \left(-\frac{\mu_n}{r^3}\right) r dr \\ &= -\mu_n \frac{2\pi}{\rho_0}. \end{aligned} \quad (14.66)$$

From (14.64), (14.65) and (14.66), we have the internal field

$$H_i = \frac{2\mu_n}{\rho_0^2}. \quad (14.67)$$

If an electron wavefunction overlaps with a nuclear wavefunction, the effective nuclear magnetic field which an electron spin feels is given by

$$H_z = H_i \left(\frac{4}{3}\pi\rho_0^3\right) |u_e(0)|^2, \quad (14.68)$$

where $|u_e(0)|^2$ is the electron density at $\vec{r} = 0$ and thus $\left(\frac{4}{3}\pi\rho_0^3\right) |u_e(0)|^2$ is the probability of finding an electron inside the nucleus. The magnetic interaction between the nucleus and the electron outside the nucleus is identically equal to zero, when the electron wavefunction spreads isotropically to a much larger space than the nuclear wavefunction, which is the case for a s -wave symmetry electron wavefunction. Then, the space integration cancels out exactly due to the continuity of magnetic flux. Form (14.67) and (14.68), the effective interaction Hamiltonian.

$$\begin{aligned} \hat{\mathcal{H}} &= -\mu_e H_z = -\frac{8\pi}{3} \hat{\mu}_e \cdot \hat{\mu}_n |u_e(0)|^2 \\ &= \frac{8\pi}{3} \gamma_e \gamma_n \hbar^2 \hat{I} \cdot \hat{S} |u_e(0)|^2, \end{aligned} \quad (14.69)$$

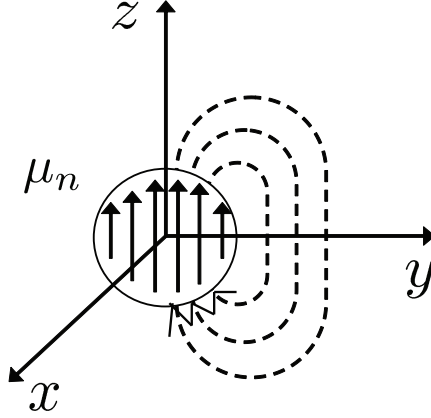


Figure 14.7: The internal and external magnetic fields created by a single nuclear spin with a magnetic moment μ_n .

where $\hat{\mu}_e = -\hbar\gamma_e\hat{S}$ and $\hat{\mu}_n = \hbar\gamma_n\hat{I}$ are used. The Hamiltonian (14.69) is called a contact Hyperfine interaction, which exists only for the case that the electron and nucleus wavefunctions overlap.

If an electron is distant from a nucleus or an electron and a nucleus are co-located but the electron wavefunction is a p -wave, d -wave or other symmetries with non-zero angular momentum, the space integration for an external dipole field H_e is non-zero. We have a new interaction Hamiltonian [6]:

$$\begin{aligned}\hat{\mathcal{H}} &= \frac{\hat{\mu}_e \cdot \hat{\mu}_n}{r^3} - \frac{3(\hat{\mu}_e \cdot \vec{r})(\hat{\mu}_n \cdot \vec{r})}{r^5} \\ &= \frac{\gamma_e\gamma_n\hbar^2}{r^3} \left[\frac{3(\hat{S} \cdot \vec{r})(\hat{I} \cdot \vec{r})}{r^2} - \hat{S} \cdot \hat{I} \right],\end{aligned}\quad (14.70)$$

The Hamiltonian (14.70) has the terms such as $-\frac{\gamma_e\gamma_n\hbar^2}{r^3}\hat{S}_x\hat{I}_x$ and $\frac{\gamma_e\gamma_n\hbar^2}{r^5}\hat{S}_x\hat{I}_yxy$. If $\hat{I}_x = \frac{1}{2}(\hat{I}_+ + \hat{I}_-)$ and $\hat{I}_y = \frac{1}{2i}(\hat{I}_+ - \hat{I}_-)$ and similar expressions for \hat{S}_x and \hat{S}_y are used in (14.70) and we introduce a polar coordinate (r, θ, φ) as shown in Fig. 14.8, we have the new expression:

$$\hat{\mathcal{H}} = -\frac{\gamma_e\gamma_n\hbar^2}{r^3}(A + B + C + D + E + F), \quad (14.71)$$

where

$$A = \hat{S}_z\hat{I}_z(1 - 3\cos^2\theta), \quad (14.72)$$

$$B = -\frac{1}{4}(\hat{S}_+\hat{I}_- + \hat{S}_-\hat{I}_+)(1 - 3\cos^2\theta), \quad (14.73)$$

$$C = -\frac{3}{2}(\hat{S}_+\hat{I}_z + \hat{S}_z\hat{I}_+)\sin\theta\cos\theta e^{-i\phi}, \quad (14.74)$$

$$D = -\frac{3}{2}(\hat{S}_-\hat{I}_z + \hat{S}_z\hat{I}_-)\sin\theta\cos\theta e^{-i\phi}, \quad (14.75)$$

$$E = -\frac{3}{4}\hat{S}_+\hat{I}_+\sin^2\theta e^{-2i\phi}, \quad (14.76)$$

$$F = -\frac{3}{4}\hat{S}_-\hat{I}_-\sin^2\theta e^{2i\phi} \quad . \quad (14.77)$$

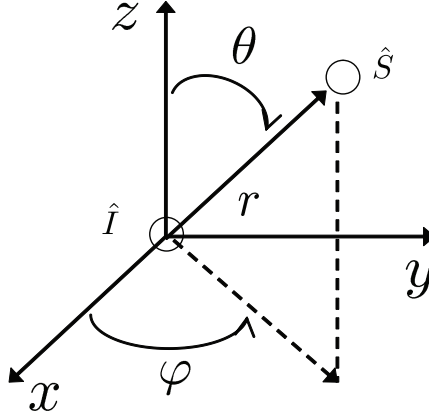


Figure 14.8: A polar coordinate for an electron spin and a nuclear spin.

If there is a strong static field H_0 along z -axis, the Zeeman Hamiltonian

$$\hat{\mathcal{H}}_z = -\gamma_n\hbar H_0\hat{I}_z + \gamma_e\hbar H_0\hat{S}_z \quad , \quad (14.78)$$

dominates over the hyperfine interaction Hamiltonian. In this case we can solve the Zeeman problem first and then treat the hyperfine coupling as a perturbation. The eigenenergy of the unperturbed state is

$$E_z = -\gamma_n\hbar H_0 m_I + \gamma_e\hbar H_0 m_s \quad , \quad (14.79)$$

where m_I and m_s are the eigenvalues of \hat{I}_z and \hat{S}_z . The energy level diagram is shown in Fig. 14.9 for $m_I = \pm 1/2$ and $m_s = \pm 1/2$. The matrix elements A to F connect these Zeeman eigenstates, as shown in Fig. 14.10

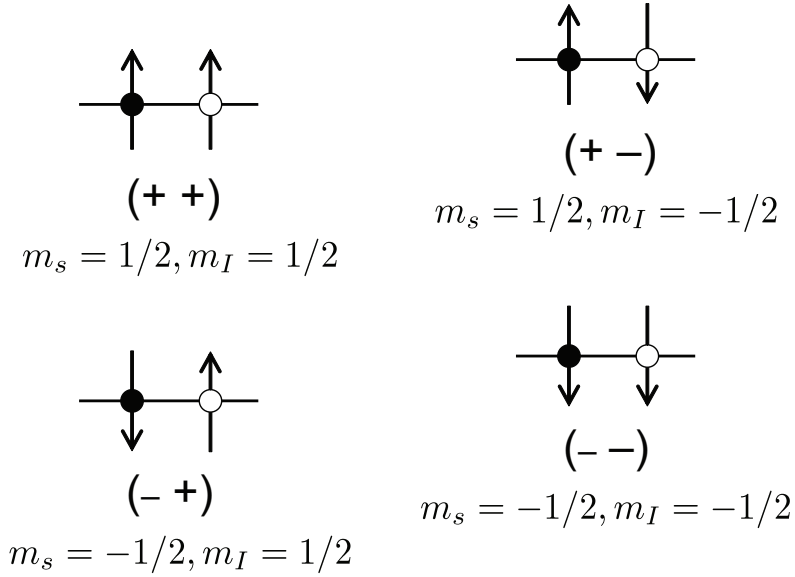


Figure 14.9: The Zeeman energy level diagram for a pair of nuclear and electron spins ($m_I = \pm 1/2, m_s = \pm 1/2$)

14.6.2 Spin Hamiltonian and hyperfine spectrum

When a nucleus is located at $\vec{r} = 0$ and an electron wavefunction $\chi(r)$ is located at an arbitrary position, both contact and dipolar hyperfine coupling terms are non-negligible, the over-all electron-nuclear interaction Hamiltonian is given by

$$\begin{aligned}
 \hat{\mathcal{H}}_{IS} &= \int |\psi(r)|^2 \left\{ \frac{8\pi}{3} \gamma_e \gamma_n \hbar^2 \hat{I} \cdot \hat{S} \delta(r) + \frac{\gamma_e \gamma_n}{r^3} \hbar^2 \right. \\
 &\quad \times \left[3 \frac{(\hat{I} \cdot \vec{r})(\hat{S} \cdot \vec{r})}{r^2} - \hat{I} \cdot \hat{S} \right] \left. \right\} \\
 &= A_x \hat{S}_x \hat{I}_x + A_y \hat{S}_y \hat{I}_y + A_z \hat{S}_z \hat{I}_z \quad .
 \end{aligned} \tag{14.80}$$

In most cases of interest, the electron Zeeman energy $\gamma_e \hbar H_0$ is much larger than the hyperfine interaction energy A_x, A_y, A_z . Therefore, the z -component of the electron spin operator commutes with the spin Hamiltonian:

$$[\hat{\mathcal{H}}, \hat{S}_z] \simeq 0 \quad . \tag{14.81}$$

This fact leads to a reduced spin Hamiltonian

$$\hat{\mathcal{H}} = \gamma_n \hbar H_0 \hat{I}_z + \gamma_e \hbar H_0 \hat{S}_z + A_z \hat{S}_z \hat{I}_z \quad . \tag{14.82}$$

The eigenstates and corresponding eigen-energies of the above Hamiltonian are

$$|m_s\rangle |m_I\rangle \quad (m_s = \pm 1/2, m_I = \pm 1/2) \quad , \tag{14.83}$$

$$E = -\gamma_n \hbar H_0 m_I + \gamma_e \hbar H_0 m_s + A_z m_s m_I \quad . \tag{14.84}$$

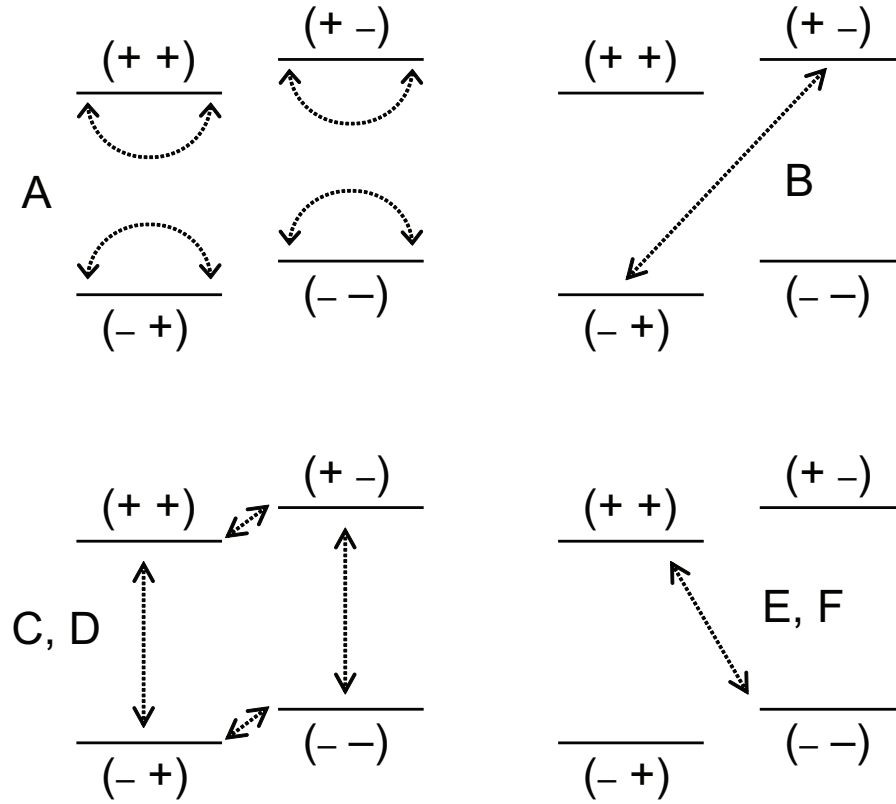


Figure 14.10: The Zeeman energy eigenstates connected by the matrix elements $A-F$.

The hyperfine energy diagrams for a high field case ($\gamma_n \hbar H_0 > A_z$) and for a low field case ($\gamma_n \hbar H_0 < A_z$) are shown in Fig. 14.11, where $A_z > 0$ is assumed.

The ESR resonance spectrum splits into double peaks,

$$\omega_{\text{ESR}} = \gamma_e H_0 + \frac{A_z}{\hbar} m_I \quad , \quad (14.85)$$

while the NMR resonance spectrum splits into the two kinds of doublets depending on the field strength:

$$\omega_{\text{NMR}} = \begin{cases} \gamma_n H_0 + \frac{A_z}{\hbar} m_s & (\text{high field}) \\ \frac{A_z}{2\hbar} \pm \gamma_n H_0 & (\text{low field}) \end{cases} . \quad (14.86)$$

Figure 14.12 shows the ESR spectrum and the two kinds of NMR spectra. If the alternating transverse field at $\omega_{\text{ESR}} = \gamma_e H_0 \pm \frac{A_z}{2\hbar}$ is sent to the coupled electron-nuclear spin system, the conditional rotation of the electron spin depending on the nuclear spin state is realized. Similarly, if the alternating transverse field at $\omega_{\text{NMR}} = \gamma_n H_0 \pm \frac{A_z}{2\hbar}$ is sent, the conditional rotation of the nuclear spin depending on the electron spin state is realized. This is a basic principle of double resonance, which can be extended to an electron-electron coupling and nuclear-nuclear coupling, too.

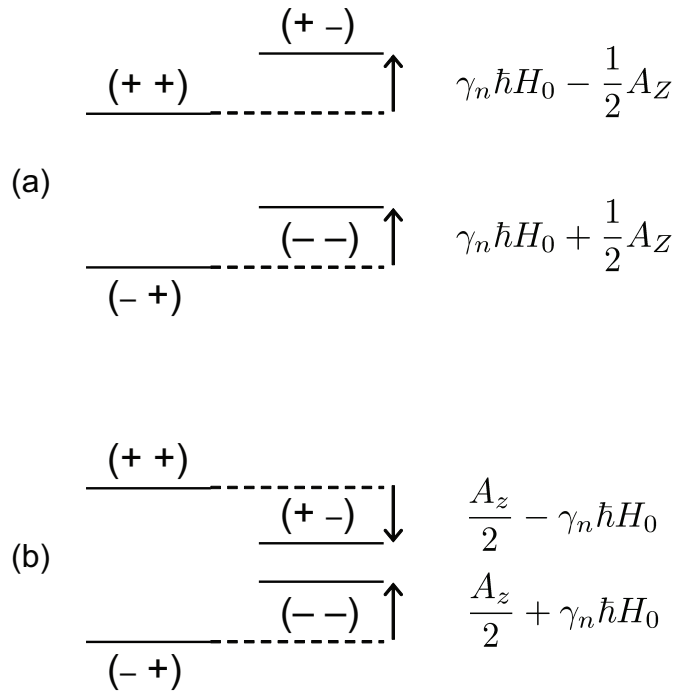


Figure 14.11: The hyperfine energy diagrams for (a) high field case ($\gamma_n \hbar H_0 > A_z$) and (b) low field case ($\gamma_n \hbar H_0 < A_z$).

14.6.3 Optical control of two semiconductor spins

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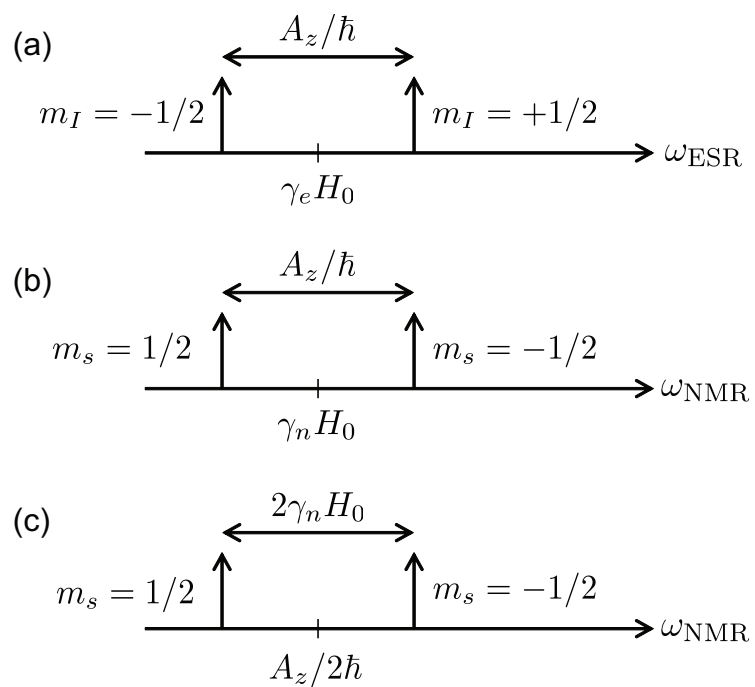


Figure 14.12: The ESR and two kinds of NMR spectra for a hyperfine coupling electron-nuclear spin system.

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