Chapter 11

Manipulating Spin

11.1 Larmor Precession

Turning on a magnetic field $\vec{B}$, the qubit state rotates. There are two steps to understanding this process, essentially the same steps we make to understand any quantum process:

1. Find $\hat{H}$
2. Solve Schrödinger equation

For the second step, we first solve the "time-independent" Schrödinger equation; that is, we find energy eigenstates

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle \quad .$$

The "time-dependent" Schrödinger equation

$$i\hbar \tfrac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

has solution

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}}{\hbar}t} |\psi(t=0)\rangle \quad .$$

Expanding $|\psi(t=0)\rangle = \sum_n c_n |\psi_n\rangle$, we get

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |\psi_n\rangle \quad .$$

(This assumes that $\hat{H}$ is time-independent. If the Hamiltonian is itself a function of t, $\hat{H} = \hat{H}(t)$, then we must directly solve the time-dependent Schrödinger equation.)

Find $\hat{\mathcal{H}}$

Assume there is only potential energy, not kinetic energy. Classically, $E = -\vec{\mu} \cdot \vec{B}$. Quantumly, the magnetic moment is in fact a vector *operator*, $\hat{\vec{\mu}} = \frac{gq}{2m}\hat{\vec{S}} = -\frac{e}{m}\hat{\vec{S}}$. Hence we set the quantum Hamiltonian to be

$$\hat{H} = \tfrac{e}{m}\hat{\vec{S}} \cdot \vec{B} \quad .$$

We may choose our coordinate system so $\vec{B} = B\hat{z}$; then

$$\hat{H} = \tfrac{eB}{m}\hat{S}_z \ .$$

Solve Schrödinger Equation

Following the recipe we gave above, we start by finding the eigendecomposition of $\hat{H}$. The eigenstates of $\hat{H}$ are just those of $\hat{S}_z$: $|0\rangle$ (up) and $|1\rangle$ (down). The corresponding eigenenergies are $E_0 = \frac{eB}{2m}\hbar$, $E_1 = -\frac{eB}{2m}\hbar$.

Next we solve the time-dependent Schrödinger equation. Write

$$|\psi(t=0)\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \ .$$

Then

$$\begin{aligned} |\psi(t)\rangle &= \alpha e^{-i\frac{eB}{2m}t}\,|0\rangle + \beta e^{i\frac{eB}{2m}t}\,|1\rangle \\ &\propto \alpha\,|0\rangle + \beta e^{i\frac{eB}{m}t}\,|1\rangle \ , \end{aligned}$$

where the proportionality is up to a global phase. On the Bloch sphere,

$$|\psi(t=0)\rangle = \cos\tfrac{\theta}{2}\,|0\rangle + \sin\tfrac{\theta}{2}e^{i\varphi}\,|1\rangle$$

evolves to

$$|\psi(t)\rangle = \cos\tfrac{\theta}{2}\,|0\rangle + \sin\tfrac{\theta}{2}e^{i(\varphi+\frac{eB}{m}t)}\,|1\rangle \ .$$

Thus the state rotates counterclockwise around the z axis, at frequency $\omega_0 \equiv \frac{eB}{m}$ (ω_0 is known as the cyclotron frequency, since it is the same frequency with which a classical e^- cycles in a magnetic field, due to the Lorentz force).

Therefore $\hat{R}_z(\Delta\varphi) = e^{-i\frac{\hat{S}_z}{\hbar}\Delta\varphi}$ is a unitary operation which rotates by $\Delta\varphi$ about the z axis. (Proof: $\hat{R}_z(\Delta\varphi)$ is exactly $e^{-i\frac{\hat{H}}{\hbar}t}$ for $t = \Delta\varphi/\omega_0$.) Being unitary means $\hat{R}_z(\Delta\varphi)^\dagger = \hat{R}_z(\Delta\varphi)^{-1} = \hat{R}_z(-\Delta\varphi)$.

Aligning $\vec{B}$ with the z axis rotates the spin about the z axis. Each state is restricted to the line of latitude it starts on, as illustrated above. For a more general rotation about a different axis, simply point the $\vec{B}$ field in a different direction. For example, the unitary operator

$$\hat{R}_n(\Delta\gamma) = e^{-i\frac{\hat{\vec{S}}\cdot\hat{n}}{\hbar}\Delta\gamma}$$

rotates by $\Delta\gamma$ about the axis $\hat{n}$. To achieve this unitary transformation, set $\vec{B} = B\hat{n}$ for exactly time $t = \Delta\gamma/\omega_0$.

Any unitary transformation on a single qubit, up to a global phase, is a rotation on the Bloch sphere about some axis; mathematically, this is the well-known isomorphism $SU(2)/\pm 1 \cong SO(3)$ between 2×2 unitary matrices up to phase and 3×3 real rotation matrices. Hence Larmor precession, or spin rotation, allows us to achieve any single qubit unitary gate. While theoretically simple, Larmor precession can unfortunately be inconvenient in real life, mostly because of the high frequencies involved and the susceptibility to noise. A more practical method for achieving rotations on the Bloch sphere is spin resonance, which we will describe next.

11.2 Spin Resonance

How do we control qubit states in the lab? If $|psi(t)\rangle = \alpha(t)\,|0\rangle + \beta(t)\,|1\rangle$, how do we deterministically change α and β?

We know that the Hamiltonian evolves things in time, so if we turn on a field then the Hamiltonian will evolve the state via $e^{-i\hat{H}t/\hbar}$.

For a static magnetic field this allows us to rotate qubit state from one point on the Bloch sphere to another via rotations:

$$\hat{R}_i(\Delta\theta) = e^{-i\hat{S}_i\Delta\theta/\hbar}, \Delta\theta = \frac{eB_o}{m}\Delta t, \vec{B} = B_o\hat{x}_i$$

Question: How can we maintain energy level splitting between $|0\rangle$ and $|1\rangle$ and *control* the rate at which a qubit rotates between states? (i.e. change it at a rate different from $\omega_o = \frac{eB_o}{m}$.)

Answer: Spin Resonance gives us a new level of control (most clearly seen in NMR).

How it works: Turn on a big DC field B_o and a little AC field $\vec{B}$ sin(ω_o t) that is tuned to the resonance $\omega_o = \frac{eB_o}{m}$:

The small AC field induces controlled mixing between $|0\rangle$ and $|1\rangle$... "SPIN FLIPS".

We must solve the Schrodinger equation to understand what is going on:

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle$$

It is convenient to use column vector notation:

$$|psi(t)\rangle = \alpha(t)\,|0\rangle + \beta(t)\,|1\rangle = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}$$

What's the Hamiltonian? $\hat{H} = -\vec{\mu}\cdot\vec{B} = \frac{e}{m}\vec{S}\cdot\vec{B}$

We now let the magnetic field be composed of the large bias field and a small oscillating transverse field:

$$\vec{B} = B_o\hat{z} + B_1 cos\omega_o t\hat{x}$$

With this we obtain the Hamiltonian:

$$\hat{H} = \frac{e}{m}B_o\hat{S}_z + \frac{e}{m}B_1 cos\omega_o t\hat{S}_x$$

Now use 2×2 matrix formulation, where the Pauli matrices ($\hat{S}_z = \frac{\hbar}{2}\sigma_z$, etc.) are of course eminently useful:

$$\hat{H} = \frac{e}{m} B_o \cdot \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{e}{m} B_1 cos\omega_o t \cdot \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The two terms sum to give the following 2×2 Hamiltonian matrix (expressed in the $\hat{S}_z$ basis):

$$\hat{H} = \frac{e\hbar}{2m} \begin{pmatrix} B_o & B_1 cos\omega_o t \\ B_1 cos\omega_o t & -B_o \end{pmatrix}$$

Now we can plug this Hamiltonian into the Schr. equation and solve for $|psi\rangle$.

A bit of intuition on QM: If you construct a Hamiltonian matrix out of some basis, then the matrix element H_{ij} tells us how much application of the Hamiltonian tends to send a particle from state $|j\rangle$ to state $|i\rangle$. (The units are of course energy $\Rightarrow$ rate of transitions $\propto$ frequency $\propto \frac{E}{\hbar} \propto \frac{H_{ij}}{\hbar}$.)

So, if we only had $\vec{B} = B_o\hat{z}$ and $\vec{B}_1 = 0$, then what would the rate of spin flip transitions be?

$$rate_{i \leftarrow j} \propto \langle i| \hat{H} |j\rangle = |1\rangle \hat{H} |0\rangle = H_{21} = 0!$$

So, we can conclude that we NEED to have a field perpendicular to the large bias field $\vec{B} = B_o\hat{z}$ to induce "spin flips" or to mix up $|0\rangle$ and $|1\rangle$ states in $|\psi\rangle$. This is perhaps more obvious in case of spin, but not as obvious for other systems. It is important to develop our quantum mechanical intuition which can easily get lost in the math!

Now let's solve the Schr. equation for Spin Resonance.

$$\hat{H} |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \frac{e\hbar}{2m} \begin{pmatrix} B_o & B_1 cos\omega_o t \\ B_1 cos\omega_o t & -B_o \end{pmatrix} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}$$

We get two coupled differential equations. First, we define $\omega_o = \frac{eB_o}{m}$ and $\omega_1 = \frac{eB_1}{2m}$, where the latter quantity is defined with a seemingly annoying factor of 1/2. It'll make sense later, though.

$$i\frac{\partial \alpha(t)}{\partial t} = \frac{\omega_o}{2}\alpha(t) + \omega_1 cos(\omega_o t)\beta(t)$$

$$i\frac{\partial \beta(t)}{\partial t} = \omega_1 cos(\omega_o t)\alpha(t) - \frac{\omega_o}{2}\beta(t)$$

To solve we make a substitution. This may seem weird, but it involves the recognition that the system has a natural rotating frame in which the system should be viewed.

$$a(t) = \alpha(t)e^{i\omega t/2}$$

$$b(t) = \alpha(t)e^{-i\omega t/2}$$

Now we're going to use a dubious approximation, but it involves a recognition that ω_o is much larger than ω_1 and these fast rotations average to zero on the timescales $1/\omega_1$ (which are the relevant experimental timescales). Anyway, here's the dubious approximation:

$$cos(\omega_o t)e^{i\omega_o t} \approx \frac{1}{2}$$

Using these definitions and dubious approximations and we obtain the following differential equation for a(t) (and correspondingly b(t)):

$$\frac{\partial^2 a(t)}{\partial t^2} + \frac{\omega_1^2}{4}a(t) = 0$$

This is a familiar second order differential equation. Our initial conditions have yet to be specified, but let's say $\alpha(0) = \beta(0) = 0$. This gives the following solution:

$$\begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\omega_o}{2}t}cos\frac{\omega_1}{2}t \\ -e^{+i\frac{\omega_o}{2}t}sin\frac{\omega_1}{2}t \end{pmatrix}$$

What does this mean geometrically? Let's go to the Bloch sphere! Our generalized Bloch vector looks like:

$$|\psi\rangle = cos\frac{\theta}{2}|0\rangle + e^{i\phi}sin\frac{\theta}{2}|1\rangle$$

Our time-dependent state which is a solution to the Schr. equation looks like:

$$|\psi(t)\rangle = cos\frac{\omega_1 t}{2}|0\rangle + e^{i(\omega_o+\pi)}sin\frac{\omega_1 t}{2}|1\rangle$$

Geometrically we can say that $\phi = \omega_o t + \pi$, so we conclude that the qubit is spinning around $\hat{z}$ at a rate ω_o.

What about θ? $\theta = \omega_1 t$, so we're crawling up the sphere at a rate $\omega_1 = \frac{eB_1}{m}$ at the same time we're spinning rapidly about $\hat{z}$ at the fast ω_o, the *Larmor frequency.* We can control ω_1 precisely by changing the amplitude of B_1.

Even though ω_0 is very large, ω_1 can be very small. If we're really good, we can flip spins by applying a "π-pulse": $\omega_1 \Delta t = \pi$.

Note: As spins flip out of ground state they suck energy out of the "RF field" ($B_1 cos\omega_o$). This is easily detected and forms the basis of NMR.