1 Readings

Liboff, Introductory Quantum Mechanics, Ch. 11

Stolze and Suter, Quantum Computing, Ch. 10

Nielsen and Chuang, Quantum Computation and Quantum Information, Ch. 7.7.2, 7.7.3

2 Spin Resonance and single qubit gates

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 we saw in the last lecture that this allows us to rotate qubit state from one point on the Bloch sphere to another via Larmor precession:

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

This rotation has to occur at a rate determined by the magnitude of B_0 which is fast. To get better control we would like to have a slower rotation. *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 $\omega_o = \frac{eB_o}{m}$:

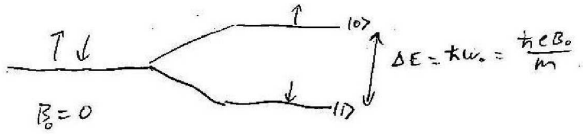

Figure 1:

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:

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

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 as before, together with 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 $\left|\psi\right\rangle$.

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

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?

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

So, we can conclude that we NEED to have a field perpendicular to the large bias field $\vec{B} = B_o\hat{z}$ in order to induce "spin flips" or to mix up $\left|0\right\rangle$ and $\left|1\right\rangle$ states in $\left|\psi\right\rangle$. 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.

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

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 these coupled first order differential equations we make a substitution followed by an approximation. The substitution is

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

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

and amounts to transforming to a frame rotating around the z axis with frequency ω_o.

The approximation involves a recognition that ω_o is much larger than ω_1 and so these fast rotations average to zero on the timescales $1/\omega_1$ (which are the relevant experimental timescales) and can be neglected relative to unity. This is referred to as the 'rotating wave approximation':

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

Using this transformation to a rotating frame and the rotating wave approximation, after a little algebra we obtain the following differential equations for a(t) and b(t)):

$$\begin{aligned} \frac{\partial^2 a(t)}{\partial t^2} + \frac{\omega_1^2}{4}a(t) &= 0 \\ b(t) &= \frac{2i}{\omega_1}\frac{\partial a(t)}{\partial t}. \end{aligned}$$

The equation for $a(t)$ is a familiar second order differential equation, with solutions

$$a(t) = c_1 e^{i\omega_1 t/2} + c_2 e^{-i\omega_1 t/2}$$

and hence

$$b(t) = -c_1 e^{i\omega_1 t/2} + c_2 e^{-i\omega_1 t/2}.$$

The coefficients c_1 and c_2 are determined by the initial coniditions. We may then obtain the general solution for any initial conditions $\alpha(0), \beta(0)$. Now we can construct the 2x2 matrix corresponding to the unitary evolution operator $U(t)$ by solving first for the initial conditions i) $\alpha(0) = 1, \beta(0) = 0$, and then ii) for the

initial conditions $\alpha(0)=1,\beta(0)=1$. The solution to i) gives the first column of $U(t)$ and the solution to ii) gives the second column of $U(t)$:

$$\begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} \begin{bmatrix} \alpha(0) \\ \beta(0) \end{bmatrix}.$$

i) initial condition $\alpha(0)=1,\beta(0)=0$ (this is $\left|+1/2\right\rangle = \left|0\right\rangle \equiv$ north pole on the Bloch sphere).

This corresponds to $c_1 = c_2 = 1/2$ and yields the following solution:

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

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

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

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

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

which apart from the global phase factor is of the same form as the previous equation, with azimuth $\phi = \omega_o t - \pi/2$. Therefore we can conclude that the qubit state is rotating (precessing) around $\hat{z}$ at a rate ω_o.

What about θ? $\theta = \omega_1 t$, so the qubit state is simultaneously traveling down the sphere at a rate $\omega_1 = \frac{eB_1}{m}$ at the same time that it is much more rapidly precessing about $\hat{z}$ at the fast ω_o, the *Larmor frequency*. We can control ω_1 very precisely by changing the amplitude of the weak field B_1. Even though ω_0 is very large, ω_1 can be very small, allowing a greater degree of control. *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.

ii) initial condition $\alpha(0)=0,\beta(0)=1$ (this is $\left|-1/2\right\rangle = \left|1\right\rangle \equiv$ south pole on the Bloch sphere).

This corresponds to $c_1 = -1/2, c_2 = +1/2$ and yields the following solution:

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

Putting the solutions for the two initial conditions together, we obtain

$$\begin{aligned} U(t) &= = \begin{bmatrix} e^{-i\frac{\omega_o}{2}t} cos\frac{\omega_1}{2}t & -ie^{-i\frac{\omega_o}{2}t} sin\frac{\omega_1}{2}t \\ -ie^{+i\frac{\omega_o}{2}t} sin\frac{\omega_1}{2}t & e^{+i\frac{\omega_o}{2}t} cos\frac{\omega_1}{2}t \end{bmatrix} \\ &= e^{-i\omega_o t/2} \begin{bmatrix} cos\frac{\omega_1}{2}t & -isin\frac{\omega_1}{2}t \\ -ie^{+i\frac{\omega_o}{2}t} sin\frac{\omega_1}{2}t & e^{+i\frac{\omega_o}{2}t} cos\frac{\omega_1}{2}t \end{bmatrix}. \end{aligned}$$

Now for $\omega_o t = 2\pi$, $e^{i\omega_o t} = 1, e^{i\omega_o t/2} = -1$, and we obtain

$$U_{\omega_o t=2\pi} = (-1)\begin{bmatrix} cos\frac{\omega_1}{2}t & -isin\frac{\omega_1}{2}t \\ -isin\frac{\omega_1}{2}t & cos\frac{\omega_1}{2}t \end{bmatrix}.$$

Now recall from Homework 1, that a rotation around the x-axis corresponds to the operator

$$e^{-i\frac{\gamma}{2}X} = (-1)\begin{bmatrix} cos\frac{\gamma}{2} & -isin\frac{\gamma}{2} \\ -isin\frac{\gamma}{2} & cos\frac{\gamma}{2} \end{bmatrix}.$$

So we have arrived at the gate $U_{\omega_o t=2\pi} = (-1)e^{-i\frac{\gamma}{2}X}$, where the angle $\gamma = \omega_1 t$, i.e., we have a gate corresponding to a rotation about the x-axis of the amount $\omega_1 t$.

We have already specified the product $\omega_o t$, but we still have one more parameter to play with, namely ω_1. Hence we can choose the value of this such that $\omega_1 t = \pi$, to arrive at the X gate:

$$U_{\omega_0 t=2\pi} = (-1)(-i)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Note the global phase of +i. These phases must be kept track of when gates are performed sequentially on different qubits, i.e., when they are no longer 'global' on the entire qubit array.

Thus an alternating magnetic field along the x-axis allows us to realize an X gate for a physical spin realization of a qubit. Similarly, an alternating magnetic field along the y-axis allows us to realize a Y gate. Together, these allow any arbitrary unitary transformation to be made on a single qubit, i.e., any arbitrary transformation on the Bloch sphere. Note that a rotation about the z-axis can now be made either by combining x- and y-rotations, e.g., with

$$e^{-i\frac{\phi}{2}Z} = e^{-i\frac{\pi}{4}Y} e^{i\frac{\phi}{2}X} e^{i\frac{\pi}{4}Y}$$

or by a free Larmor precession for a finite time.

In principle, the fields should be switched off when the gate is achieved, if one wishes to preserve the final state and not further time evolve it under the two fields. The weak alternating field is usually easy to switch off, hence the term 'RF pulse'. The large static field is not so easy to turn off and one has to then keep track of the accumulated phase on the qubit resulting from further Larmor precession.

3 Two qubit gates for coupled spins

Electron and nuclear spins can interact directly via a dipolar coupling, or indirectly through chemical bonds (electron density) connecting them in some structure. In liquids both of these can often be approximated by the Ising-type interaction

$$H_{int} = JS_{z1}S_{z2}.$$

where J measures the strength of the coupling. The Hamiltonian for two coupled spins is then $H = H_1 + H_2 + H_{int}$. Consider two spins A and B with possibly different Larmor frequencies ω_A, ω_B (due, e.g., to different g factors, or for nuclear spins to different local magnetic field strengths within a molecule). In the S_z basis the Hamiltonian matrix is given by

$$\begin{aligned} H &= -\omega_A S_{zA} - \omega_B S_{zB} + J S_{zA} S_{zB} \\ &= \frac{\hbar}{2}\begin{bmatrix} -\omega_A - \omega_B + \frac{J\hbar}{2} & 0 & 0 & 0 \\ 0 & -\omega_A + \omega_B - \frac{J\hbar}{2} & 0 & 0 \\ 0 & 0 & \omega_A - \omega_B - \frac{J\hbar}{2} & 0 \\ 0 & 0 & 0 & \omega_A + \omega_B + \frac{J\hbar}{2} \end{bmatrix} \end{aligned}$$

where the two-qubit basis states are ordered as usual as

$$\begin{bmatrix} 00 \\ 01 \\ 10 \\ 11 \end{bmatrix}.$$

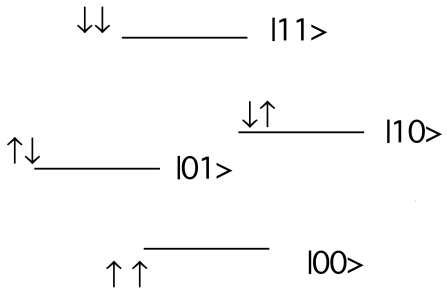

Figure 2: Energy levels of 2 spins coupled by Ising-like interaction

Now suppose, e.g., that $\omega_A > \omega_B$ and $J > 0$. Then the energy levels are of the form in Figure 2. There are 4 possible single spin resonance transitions: their energies Δ are

- $\uparrow\uparrow \longleftrightarrow \uparrow\downarrow$, ie., $00 \longleftrightarrow 01$

$$\begin{aligned}\Delta &= \left[\left(-\omega_A+\omega_B-\frac{J\hbar}{2}\right)-\left(-\omega_A-\omega_B+\frac{J\hbar}{2}\right)\right]\frac{\hbar}{2} \\ &= \left[2\omega_B - J\hbar\right]\frac{\hbar}{2} \\ &= \left(\omega_B-\frac{J\hbar}{2}\right)\hbar\end{aligned}$$

- $\uparrow\uparrow \longleftrightarrow \downarrow\uparrow$, ie., $00 \longleftrightarrow 10$

$$\begin{aligned}\Delta &= \left[\left(+\omega_A-\omega_B-\frac{J\hbar}{2}\right)-\left(-\omega_A-\omega_B+\frac{J\hbar}{2}\right)\right]\frac{\hbar}{2} \\ &= \left[2\omega_A - J\hbar\right]\frac{\hbar}{2} \\ &= \left(\omega_A-\frac{J\hbar}{2}\right)\hbar\end{aligned}$$

- $\uparrow\downarrow \longleftrightarrow \downarrow\downarrow$, ie., $01 \longleftrightarrow 11$

$$\begin{aligned}\Delta &= \left[\left(+\omega_A+\omega_B+\frac{J\hbar}{2}\right)-\left(-\omega_A+\omega_B-\frac{J\hbar}{2}\right)\right]\frac{\hbar}{2} \\ &= \left[2\omega_A + J\hbar\right]\frac{\hbar}{2} \\ &= \left(\omega_A+\frac{J\hbar}{2}\right)\hbar\end{aligned}$$

- $\downarrow\uparrow \longleftrightarrow \downarrow\downarrow$, ie., $10 \longleftrightarrow 11$

$$\begin{aligned}\Delta &= \left[\left(+\omega_A+\omega_B+\frac{J\hbar}{2}\right)-\left(+\omega_A-\omega_B-\frac{J\hbar}{2}\right)\right]\frac{\hbar}{2} \\ &= \left[2\omega_B + J\hbar\right]\frac{\hbar}{2} \\ &= \left(\omega_B+\frac{J\hbar}{2}\right)\hbar\end{aligned}$$

The resulting spin resonance spectrum will look like Figure 3. Then selectively exciting the spin B at frequency $\omega_B + J\hbar/2$ will give the transition $10 \longleftrightarrow 11$ but will not affect spin A. This therefore gives us a CNOT gate:

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

In practice, frequency selective pulses require relatively long time to realize which has disadvantages (allowing more bad interactions with the environment that can destroy the quantum coherence). Experimentalists implementing quantum gates with nuclear spins usually prefer to work with shorter pulses that then possess a broader 'bandwidth', i.e., include many resonance frequencies and address mutliple transitions. See Stolze and Suter, Ch. 10.2.5 for an example of how the CNOT gate can be achieved in this situation.

4 Refocusing spin interactions

The spin-spin interaction is always on. So how can we implement a single qubit gate in the presence of coupling to the second qubit? In Homework 4 you showed that for spins interacting with an Ising coupling, the effect of this coupling can be removed by conjugating with an X gate. Specifically, with

$$H_{int} = g\sigma_z^{(1)} \otimes \sigma_2^{(2)}.$$

you showed $X^{(2)}U(t)X^{(2)} = U^{-1}(t)$, where $U(t) = e^{-iH_I t}$ and hence $X^{(2)}U(t)X^{(2)}U(t) = 1$. Thus if we have the full two-qubit interaction,

$$H = aZ_1 + bZ_2 + H_{int}$$

and apply the above conjugation by an X gate on qubit 2, you will be left with the free spin precession of qubit 1:

$$e^{-iHt/\hbar}X^{(2)}e^{-iHt/\hbar}X^{(2)} = e^{-ibZ_1 t/\hbar}.$$

Using another set of refocusing pulses on spin 2 can further remove this free spin precession of qubit 1. See Stolze and Suter, Ch. 10.1.7, and/or Nielsen and Chuang, Ch. 7.7.3.

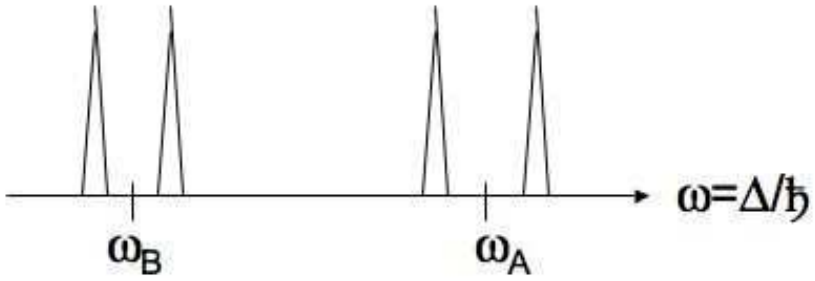

Figure 3: Spin resonance spectrum of two spins coupled by Ising interaction. Each single spin resonance line ω_i is split into two lines, $\omega_i - J\hbar/2$ and $\omega_i + J\hbar/2$.