Problem Set 3

Handed Out: Tuesday 2015/02/10
Due: Tuesday 2015/02/24 (before class)

1. **Pulses**. Consider a sample of protons in a magnetic field which is not perfectly homogeneous. A pulse is applied to spins in the center of the magnet. The frequency of the applied radiofrequency (rf) field is adjusted so that the resonance condition is satisfied exactly for these center spins; the pulse time is adjusted to $t_p\,\omega_1 = \pi/2$ and the pulse phase is set to $\phi_p = 0$. The magnetization of the center spins after the pulse should thus be $\mathbf{M} = -\hat{\mathbf{y}}$. Plot the magnetization components ($M_x, M_y,$ and M_z) as a function of resonance offset $\Delta\omega = \omega_0 - \omega$ for $\Delta\omega = -25\,\omega_1$ to $\Delta\omega = +25\,\omega_1$. Over what range of resonance offsets is the pulse effective in creating transverse magnetization?

2. **Composite Pulses**.[1] In real experiments, the rf field created by the coil is not precisely uniform over the volume of the sample. This imperfection is called *rf inhomogeneity*. This exercise examines one strategy for rendering experiments less sensitive to rf inhomogeneity.

   (a) An NMR experiment is performed on isolated proton spins. Suppose that the peak rf field in the *center* of the sample is $B_1 = 4.697$ mT, and that a pulse of duration $t_p = 5\ \mu$s and phase $\phi_p = 0$ is applied. What is the flip angle in the center of the sample? If the magnetization vector before the pulse is $\boldsymbol{M} = \hat{\boldsymbol{z}}$, what is the magnetization vector after the pulse? Ignore off-resonance effects.

   (b) At the *edge* of the sample, the peak rf field is only $B_1 = 4.228$ mT. If the magnetization vector at the edge of the sample before the pulse is $\boldsymbol{M} = \hat{\boldsymbol{z}}$, what is the magnetization vector at the edge of the sample after the pulse? What is the angle between the magnetization vectors at the edge of the sample and at the center of the sample, after the pulse?

   (c) Now suppose that the single rf pulse is replaced by a sequence of three pulses of durations $2.5\,\mu$s, $5\,\mu$s, and $2.5\,\mu$s, with phases 0, $\pi/2$, and 0, respectively. This three-pulse sequence is an example of a *composite pulse*. If the magnetization vector before the pulse is $\boldsymbol{M} = \hat{\boldsymbol{z}}$, what is the magnetization vector at the *center* of the sample after the pulse?

   (d) Calculate the magnetization vector at the *edge* of the sample after the composite pulse. What is the angle between the magnetization vector at the the edge of the sample and the magnetization vector at the center of the sample, after the pulse?

   (e) Explain the operation of the composite pulse geometrically.

   (f) Speculate on some applications of composite pulses.

3. **Adiabatic Rapid Passage**. In class we discussed how a frequency-chirped transverse rotating magnetic field can be used to invert magnetization. Equivalently, the size of the applied longitudinal magnetic field, B_0, can be swept. In order for the magnetization to exactly follow the effective field in the rotating frame, the static field must be swept slowly enough. In this exercise we will derive an expression for the permissible speed of the longitudinal field sweep.

   (a) Suppose that the phase of the applied rf is $\phi_{\text{arp}} = 0$, so that that the effective field during the adiabatic rapid passage is given by

   $$\mathcal{H}_{\text{eff}}(t) = (\omega_0(t) - \omega)\, I_z + \omega_1 I_x, \tag{1}$$

   where $\omega_0(t) = -\gamma B_0(t)$. In order to remove the time-dependence of the $\mathcal{H}_{\text{eff}}(t)$, let us transform the density operator into a second interaction representation defined by the operator

   $$U = e^{-i\theta(t) I_{yR}}. \tag{2}$$

   Give an equation for $\theta(t)$.

   (b) Give an expression for the Coriolis term, $+i\,\dot{U}U^{\dagger}$, in the effective Hamiltonian in the quantum mechanical reference defined by U (no pun intended). Compare the size of this Coriolis term to the size of the new effective Hamiltonian near resonance when $\omega_0(t) - \omega \approx 0$.

   (c) Show that the Coriolis term has a negligible effect on the evolution of the density matrix when the following condition is met:

   $$\frac{dB_0}{dt} \ll \gamma B_1^2 \tag{3}$$

4. **The Driven Undamped Harmonic Oscillator**. The Hamiltonian for the harmonic oscillator is

$$\begin{aligned}\mathcal{H} &= \omega_0(a^{\dagger}a + \frac{1}{2}) - F(t)X \\ &= \omega_0(a^{\dagger}a + \frac{1}{2}) - \frac{F(t)X_0}{\hbar\sqrt{2}}(a^{\dagger} + a)\end{aligned} \tag{4}$$

where $F(t)$ is an applied force and $X_0 = (\hbar\omega_0/k)^{1/2}$.

[1] Adapted from Problem 10.2 in Malcolm H. Levitt's *Spins Dynamics*. IMPORTANT: Assume linearly polarized rf. See the Appendix.

(a) In class we have been working in the Schrödinger representation: operators are time independent and the density operator (or the wavefunction) evolves in time. Alternatively, one may work in a representation — the Heisenberg representation – in which operators of interest evolve in time and the density operator (or wavefunction) is static.

By working the Heisenberg representation, show that the evolution of the Harmonic oscillator under the action of an applied dc force $F(t) = F_0$ is described by

$$\langle X \rangle(t) = \langle X \rangle(0) \cos \omega_0 t + \frac{\omega_0}{k} \langle P \rangle(0) \sin \omega_0 t + \frac{F_0}{k} \quad (5)$$

The applied force displaces the initial position of the oscillator by an amount F_0/k.

(b) Now let the applied force oscillate at the resonance frequency of the oscillator:

$$F(t) = F_0 \cos(\omega_0 t + \phi) \quad (6)$$

Invent an interaction representation that removes the time dependence of $\mathcal{H}(t)$. What unitary operator U is used to transform the density operator into the new frame of reference?

(c) What is the effective Hamiltonian in the new frame of reference?

(d) Again working in the Heisenberg representation, show that, for an oscillator initially at rest,

$$\langle X \rangle(t) = \frac{F_0\, t}{2m\omega_0} \, \sin(\omega_0 t + \phi) \quad (7)$$

In other words, the resonantly driven oscillator's response in ninety degrees out of phase with the driving force and the amplitude of the response grows linearly in time.

— revision 2015/01/14:
change due date from 02/19 to 02/24

Appendix A: A Linearly vs. Circularly Polarized Radiofrequency Transverse Magnetic Field

In class we used a **circularly polarized** radiofrequency magnetic field to excite the spin:

$$\boldsymbol{B}_{\text{rf}} = B_1 (\cos(\omega t + \phi)\, \hat{x} + \sin(\omega t + \phi)\, \hat{y}). \tag{A1}$$

This form for the applied field resulted in a laboratory-frame Hamiltonian for the applied rf magnetic field of

$$\begin{aligned}\mathcal{H}_{\text{rf}} &= -\boldsymbol{\mu} \cdot \boldsymbol{B}_{\text{rf}} \\ &= \omega_1 (I_x \cos(\omega t + \phi) + I_y \sin(\omega t + \phi)) \\ &= \omega_1 \left\{ \frac{I_+}{2} e^{-i\omega t} e^{-i\phi} + \frac{I_-}{2} e^{+i\omega t} e^{+i\phi} \right\}\end{aligned} \tag{A2}$$

where $\omega_1 \equiv -\gamma B_1$. The associated rotating-frame Hamiltonian is

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= U(\omega_0 I_z + \mathcal{H}_{\text{rf}}) U^\dagger + i \dot{U} U^\dagger \\ &= (\omega_0 - \omega) I_z + \omega_1 \{ I_x \cos\phi + I_y \sin\phi \}\end{aligned} \tag{A3}$$

with

$$U = e^{\, i \omega t I_z}. \tag{A4}$$

In the laboratory, it is more common to employ a **linearly polarized** radiofrequency magnetic field to excite the spins. Such a field is easily manufactured using a solenoid coil, for example. In the case of a linearly polarized rf magnetic field

$$\boldsymbol{B}_{\text{rf}} = B_1 \, \cos(\omega t + \phi)\, \hat{x}. \tag{A5}$$

Now

$$\begin{aligned}\mathcal{H}_{\text{rf}} &= \omega_1 I_x \cos(\omega t + \phi) \\ &= \omega_1 \frac{1}{2}(I_+ + I_-) \, \frac{1}{2} \left\{ e^{+i\omega t} e^{+i\phi} + e^{-i\omega t} e^{-i\phi} \right\}.\end{aligned} \tag{A6}$$

Transforming the total Hamiltonian into the rotating frame,

$$I_+ \xrightarrow{U} I_+ e^{+i\omega t} \tag{A7}$$

$$I_- \xrightarrow{U} I_- e^{-i\omega t}, \tag{A8}$$

and the resulting effective Hamiltonian is

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= (\omega_0 - \omega) I_z + \frac{\omega_1}{4} \left\{ I_+ e^{-i\phi} + I_- e^{+i\phi} \right\} \\ &\quad + \frac{\omega_1}{4} \left\{ I_+ e^{+2i\omega t} e^{+i\phi} + I_- e^{-2i\omega t} e^{-i\phi} \right\}\end{aligned} \tag{A9}$$

We can see that unlike with circularly polarized rf, $\mathcal{H}_{\text{eff}}$ is not now time independent. Let us nevertheless neglect the time-dependent part of $\mathcal{H}_{\text{eff}}$. This is called the *rotating wave approximation*. We will learn to derive correction terms to the resulting (approximately correct) Hamiltonian in class. Making the rotating wave approximation,

$$\mathcal{H}_{\text{eff}}^{\text{rwa}} = (\omega_0 - \omega) I_z + \frac{\omega_1}{4} \left\{ I_+ e^{-i\phi} + I_- e^{+i\phi} \right\}. \tag{A10}$$

Using $I_\pm = I_x \pm i I_y$ and trigonometric identities, this result simplifies to

$$\mathcal{H}_{\text{eff}}^{\text{rwa}} = (\omega_0 - \omega) I_z + \frac{\omega_1}{2} \left\{ I_x \cos\phi + I_y \sin\phi \right\}. \tag{A11}$$

The (new) factor of 1/2 is significant: only half of the applied linearly polarized rf gets "used" in the rotating frame.

We can summarize the two rf Hamiltonians by defining a **nutation frequency** ω_{nut} such that

$$\boxed{\mathcal{H}_{\text{eff}} = (\omega_0 - \omega) I_z + \omega_{\text{nut}} \{ I_x \cos\phi + I_y \sin\phi \}} \tag{A12}$$

with

$$\text{cirularly polarized rf} \;\rightarrow\; \omega_{\text{nut}} = -\omega B_1, \tag{A13}$$

$$\text{linearly polarlized rf} \;\rightarrow\; \omega_{\text{nut}} = -\omega B_1 / 2. \tag{A14}$$

Levitt's "composite pulse" problem — Problem 4 above – assumes linearly polarized rf. For part (a), this will give a flip angle of

$$\begin{aligned}\theta_{\text{pulse}} &= 2\pi \times \frac{1}{2} \times 4.697 \times 10^{-3}\,\text{T} \\ &\qquad \times\; 42.56 \times 10^6 \, \frac{\text{Hz}}{\text{T}} \;\times\; 5 \times 10^{-6}\,\text{s} = \pi.\end{aligned}$$

Note that without the factor of 1/2 (to account for the rf being linearly, not circularly, polarized), you would compute $\theta_{\text{pulse}} = 2\pi$, which is a funny pulse angle to apply since it would take $M_z \rightarrow M_z$. If the pulse is applied using linearly polarized rf, then the pulse will take M_z to $-M_z$, that is, it will invert the magnetization — much more sensible.