Evening problem-solving session, January 8, 2018

I will do AHT/recoupling calculations for the DRAMA pulse sequence (see page 14 of "tycko_recoupling_notes4"), the 2Q-HORROR sequence (see page 18), and rotational resonance (see page 23). I may also do an AHT/recoupling calculation for Hartmann-Hahn cross polarization under MAS. I will also answer questions regarding this morning's lecture.

And here are several practice problems, some of which I may discuss at the problem-solving session:

1. For a spin-1/2, let $|a\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$ and $|b\rangle = (|+\rangle + i|-\rangle)/\sqrt{2}$. What is $\langle a|b\rangle$? What are $S_x|a\rangle$, $S_y|a\rangle$, $S_x|b\rangle$, and $S_y|b\rangle$?

2. Suppose you have a system of two spin-1/2 nuclei in a mixed state, with equal probabilities of being in each of the two states $|\psi_1\rangle = (|++\rangle + |--\rangle + |-+\rangle)/\sqrt{3}$ and $|\psi_2\rangle = (|++\rangle - |--\rangle - |-+\rangle)/\sqrt{3}$. What is the corresponding density operator ρ? What do $|\psi_1\rangle$ and $|\psi_2\rangle$ look like as 4-dimensional vectors in the direct-product basis? What is ρ as a 4X4 matrix in the direct-product basis?

3. Let $\rho(0) = 1 - \beta\omega_0 S_z$ as discussed in this morning's lecture. Show that the "1" part of this initial density operator does not contribute to NMR signals, regardless of the pulse sequence and the spin Hamiltonian.

4. Using commutation relations among angular momentum components, show that $[S^2,S_z] = 0$. {Hint: use the identity $[A^2,B] = A[A,B] + [A,B]A$} Does this mean that S^2 must also commute with S_x and S_y?

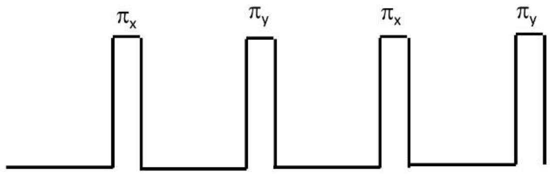
5. Show that $R_y(-\pi/2)R_x(-\pi/2)R_y(\pi)R_z(\pi/2) = R_x(\pi/2)$.

6. Show that, for any spin system, $Tr\{S_x,S_y\} = Tr\{S_x,S_z\} = 0$. [Hint: write S_x and S_y in terms of S_+ and S_-]

7. Based on the expression for the truncated dipole-dipole coupling in this morning's slides, show that the dipole-dipole coupling under MAS can be written as

$$H_D(t) = [A\cos(\omega_R t + \gamma) + B\sin(\omega_R t + \gamma) + C\cos(2\omega_R t + 2\gamma) + D\sin(2\omega_R t + 2\gamma)](3S_{z1}S_{z2} - \mathbf{S}_1 \cdot \mathbf{S}_2)$$

8. Consider the following XY4 sequence in a non-spinning sample



a. Show that the four π pulses together produce no net rotation.
b. Show that the four pulses together produce approximately no rotation even if their flip angles are $\pi+\varepsilon$, where ε is a small number. (Hence, the XY4 sequence is insensitive to rf inhomogeneity.)
c. Show that the XY4 sequence averages out chemical shifts and resonance offsets (to lowest order in average Hamiltonian theory), even if the π pulses have non-negligible lengths. (Hence, the XY4 sequence is insensitive to chemical shifts.)