Exercises for Monday evening problem-solving session, 2013 Winter School on Biomolecular Solid State NMR. These are intended to be educational and to illustrate some of the mathematical tricks that are important in solid state NMR.

1. In analyzing NMR pulse sequences, it is often important to manipulate rotations in unusual ways. As practice, show that a 90° rotation about -y followed by a 240° rotation about x followed by a 90° rotation about -y is the same as a 180° rotation about an axis in the xy plane that makes a 30° angle with the x axis. In other words, show that $90_{270}\ 240_0\ 90_{270} = 180_{30}$, where $\theta_\phi$ means a rotation by $\theta$ degrees about an axis that makes a $\phi$ degree angle with x. [Hint: It helps to rewrite $240_0$ as a product of three rotations, first about -y, then about z, then about y.]

2. "Composite pulses" are trains of contiguous pulses that produce the same rotation as a single pulse, but are less sensitive to resonance offsets, rf inhomogeneity, or other problems. Using an Average Hamiltonian Theory-like calculation and ignoring MAS, show that $90_0\ 270_{90}\ 90_0$ is a composite $\pi$ pulse that is insensitive to chemical shifts or resonance offsets to lowest order. [Hint: Write down a Hamiltonian that includes rf and chemical shift terms, then transform to an interaction representation with respect to the rf term.]

3. Consider a train of rotor-synchronized $\pi$ pulses with XY4 phases (one $\pi$ pulse per MAS rotation period, phase pattern XYXY). By considering only the periodicities of coefficients of $I_x$, $I_y$, and $I_z$ in $\tilde{I}_z(t)$ (the interaction representation version of $I_z$), show that CSA and isotropic shift interactions average to zero, regardless of the $\pi$ pulse length. What happens to the CSA and isotropic shifts if there are two $\pi$ pulses in each rotation period, as in a REDOR sequence?

4. Consider the 2Q-HORROR technique described in this morning's lecture and in the "recoupling notes". What happens to the average dipole-dipole, CSA, and isotropic shift Hamiltonians when $\omega_1 = n\omega_R/2$, with n = 2, 3, and 4?

5. Our NMR spectrometers, probes, and samples exist in the "laboratory frame". Yet we design and analyze NMR measurements as if they were in the "rotating frame". Why is this O.K.? Show that NMR signals, as detected by a real NMR spectrometer and an NMR probe with a single rf coil along x, are equal (to an excellent approximation) to signals along both x and y in the rotating frame. [Hints: (a) Write down a nuclear spin Hamiltonian in the lab frame, including the lab-frame rf term; (b) Write down a density operator expression for the lab-frame signal; (c) Transform to a rotating frame at the rf carrier frequency; (d) Evaluate the effective rotating-frame Hamiltonian; (e) Recall that a real NMR spectrometer has two signal channels, detecting signals from the probe that are either "in-phase" or "out-of-phase" with the rf carrier.]