Problem Set #6
Rad 226a

1. **Miscellaneous spectra**
What is the resulting observed spectrum for a I-S spin system if the density operator at the start of acquisition is:

a. $\hat{\sigma}_0 = \hat{I}_x$

b. $\hat{\sigma}_0 = 2\hat{I}_x \hat{S}_z$

c. $\hat{\sigma}_0 = \hat{I}_x + 2\hat{I}_x \hat{S}_z$

d. $\hat{\sigma}_0 = \hat{I}_x + 2\hat{I}_y \hat{S}_z$

Note as always for this class, this problem and the ones the follow use the following sign conventions:

- Chemical shift
- $\omega_0 = \gamma B_0$
- $\Omega$
- Left handed rotation

- J coupling
- $2\hat{I}_z \hat{S}_z$
- $\frac{1}{2} J$
- Right handed rotation

- Rf
- $\omega_1$
- Left handed rotation
2. SNR revisited

Show that the SNR for a 90-acquire measurement of a collection of $N$ spin $\frac{1}{2}$ particles with gyromagnetic ratio $\gamma$ can be expressed as

$$SNR \propto N \frac{\gamma \hbar}{2} P \sqrt{1 - \frac{Q_L}{Q_U}}$$

where $P$=polarization, $Q_U$ = unloaded quality factor ($Q$) of the Rf coil, and $Q_L$ = loaded $Q$ of the Rf coil.

Note, in general there is also a term to account for the noise factors of the preamp. This term is typically less than 0.5 dB, and for our purposes can be neglected.
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3. **Distortionless Enhanced by Polarization Transfer (DEPT)**
   For this problem, we are going to examine the inverse DEPT pulse sequence, which is useful if we have $^{13}$C signals that we wish to detect via coupling to more sensitive $^1$H nuclei.

a) Given a system of $^{13}$C-$^1$H J-coupled spin pairs, show the full branch diagram and compute the relative sensitivity of direct $^{13}$C detection versus the sequence shown below known as inverse DEPT.

\[
\begin{aligned}
\text{inverse DEPT} \\
^{13}\text{C} & \rightarrow \left(\frac{\pi}{2}\right)_x \rightarrow \frac{1}{2J} \rightarrow (\pi)_x \rightarrow \frac{1}{2J} \\
^{1H} & \rightarrow (\theta)_x \rightarrow \left(\frac{\pi}{2}\right)_y \rightarrow \frac{1}{2J} \rightarrow \frac{1}{2J} \rightarrow \text{acquire}
\end{aligned}
\]

where $\theta = \frac{\pi}{2}$

b. In general, the value of $\theta$ in an inverse DEPT sequence needs to be optimized for different spin systems. Show that the inverse DEPT coherence transfer efficiency as a function of $\theta$ for a CH spin system is as shown in the plot below. (extra credit): Repeat (b) for CH$_2$, and CH$_3$ systems.

![Coherence Transfer Efficiency Plot]

c. What is the relative SNR of inverse DEPT (CH system, $\theta=\pi/2$) compared to direct $^{13}$C detection?
4. **C$_2$ Lactate Imaging**

A lactate molecule labeled at the 2$^{nd}$ carbon position, [2-$^{13}$C]Lac, is coupled to the attached $^1$H nucleus with a coupling constant $J=140$Hz.

The effect of J-coupling on the carbon (or proton) spectrum is to split the peak into a doublet.

a) What is the effect of the J-coupling on a single shot imaging sequence like the Echo Planar Imaging (EPI) sequence? Assume readout time is $\sim$10ms.

b) Propose a method to eliminate the artifact seen in part a).

c) Suppose you only excite a narrow Rf band ($\sim$100Hz), centered at the center of lactate doublet, what do you expect to see? What would happen if this narrow band excitation is now centered at one of the peaks? Simulate the two cases using full density matrix with J-coupling included in the Hamiltonian and show the results.