Exercise 3:

This exercise aims to recapitulate some pulse design and QM aspects of NMR.

^{129}Xe is a nucleus with a gyromagnetic ratio of 11.86 MHz/T and a very large chemical shift range. Using xenon in gas phase as a reference signal at 0 ppm, atoms that penetrate red blood cells in solution appear at ca. 225 ppm.

Question 3.1: What is the bandwidth in Hz that you need to acquire the signal of a blood sample with xenon gas on top of it at a spectrometer field strength of 9.4T?

Question 3.2: What is the dwell time required for this bandwidth?

Question 3.3: If you want to make sure that the resonances with the largest offset experience an effective field that is not tilted by more than 5° out of the transverse plane, what is the B_1 field amplitude that you need to apply for an excitation pulse? Give the results in Hz and µT.

Consider ^{13}C atoms at a field strength corresponding to 600 MHz for proton spectra (the gyromagnetic ratio of ^{13}C is 10.7 MHz/T, that for ^{1}H is 42.6 MHz/T)

Question 3.4: What is the thermal spin polarization at 300 K?

Question 3.5: To what temperature do you have to cool down the sample to achieve 50% spin polarization?

The Dirac notation allows compact formulation of many QM problems of spin physics.

Question 3.6: Write the following expressions in Dirac notation:

a) $\hat{I}_z\psi_\beta = -\frac{1}{2}\psi_\beta$ b) $\int \psi_\beta^*\psi_\alpha \, d\tau$ c) $\int \psi^* \, \hat{Q}\psi \quad d\tau$

Question 3.7: Use the Dirac notation to express the following statements

a) ψ_α is normalized
b) ψ_α and ψ_β are orthogonal
c) ψ_α is an eigenfunction of $\hat{I}_z$ with eigenvalue ½.
d) ψ can be expressed as a linear combination of ψ_α and ψ_β.

Consider the spin-½ state $|\theta\rangle$ which is defined as $|\theta\rangle = \cos\frac{\theta}{2}|\alpha\rangle + i\sin\frac{\theta}{2}|\beta\rangle$.

Question 3.8: Show that $|\theta\rangle$ is an eigenstate of $\hat{I}_z \cos\theta + \hat{I}_y \sin\theta$ and give the eigenvalue.

Question 3.9: Give a pictorial representation of the state $|\theta\rangle$.

Question 3.10: What pulse transforms the state $|\theta\rangle$ into an eigenstate of $\hat{I}_y$? Derive the result geometrically.

Note:
the following page might be helpful http://en.wikipedia.org/wiki/List_of_trigonometric_identities