D. Spielman
spielman@stanford.edu

Problem Set #6
BioE 326B/Rad 226B

1. Chemical shift anisotropy
2. Scalar relaxation of the 2^{nd} kind
3. $T_{1\rho}$ Relaxation by scalar coupling of the 2nd kind (extra credit)

D. Spielman
spielman@stanford.edu

Chemical Shift Anisotropy

The Hamiltonian a single-spin system in a magnetic field subject to both the isotropic part of the chemical shift shielding tensor, σ, and an anisotropic component, Δσ, is given by:

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t) \quad \text{where} \quad \hat{H}_0 = -\gamma B_0 (1-\sigma)\hat{I}_z$$

and $\hat{H}_1(t) = \gamma B_0 \Delta\sigma \left(\tfrac{1}{3}\sqrt{\tfrac{2}{3}} F_0(t)\hat{I}_z - \tfrac{1}{6} F_1(t)\hat{I}_+ - \tfrac{1}{6} F_{-1}(t)\hat{I}_- \right)$

wit
h $F_0(t) = \sqrt{\tfrac{3}{2}}\left(3\cos^2\theta - 1\right)$ and $F_{\pm 1}(t) = 3\sin\theta\cos\theta e^{\mp i\phi}$

Find:

$$\frac{1}{T_1} = ?$$

$$\frac{1}{T_2} = ?$$

D. Spielman
spielman@stanford.edu

Scalar relaxation of the 2nd kind

Consider a system of J-coupled spins.

$$\hat{H} = -\omega_I \hat{I}_z - \omega_S \hat{S}_z + 2\pi J\left(\hat{I}_z\hat{S}_z + \hat{I}_x\hat{S}_x + \hat{I}_y\hat{S}_y\right)$$

In this case, the T_1 relaxation time of the S spin is very short ($T_{1S} << 1/J$). One way of analyzing this system is to assume the S spin is in continuous equilibrium with the lattice because of its short relaxation time. By assuming the S spin is part of the lattice, the perturbing Hamiltonian can be rewritten as:

$$\hat{H}_1 = S_z(t)\hat{I}_z + S_x(t)\hat{I}_x + S_y(t)\hat{I}_y$$

where $S_z(t)$, $S_x(t)$, and $S_y(t)$ are well modeled as stochastic functions with the following correlation functions:

$$\left\langle S_z(t)S_z(t+\tau)\right\rangle = \frac{(2\pi J)^2 S(S+1))}{3} e^{-\tau/T_{1,S}}$$

$$\left\langle \left(S_x(t)+iS_y(t)\right)\left(S_x(t+\tau)-iS_y(t+\tau)\right)\right\rangle = \left\langle S_+(t)S_-(t+\tau)\right\rangle = \frac{2(2\pi J)^2 S(S+1))}{3} e^{i\omega_s\tau}e^{-\tau/T_{2,S}}$$

Show:

$$\frac{1}{T_1} = \frac{2(2\pi J)^2 S(S+1))}{3}\frac{T_{2,S}}{1+(\omega_I-\omega_s)^2 T_{2,S}^2}$$

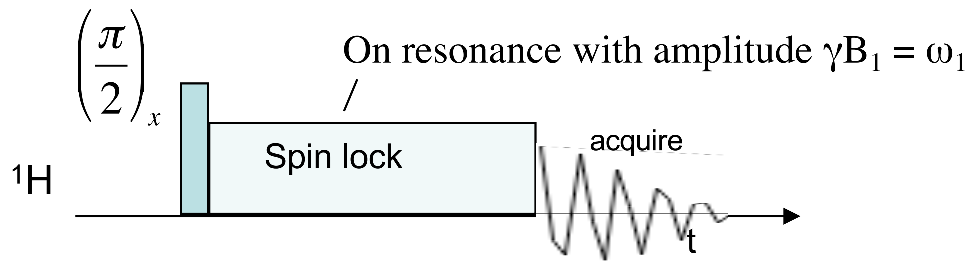
$$\frac{1}{T_2} = \frac{(2\pi J)^2 S(S+1))}{3}\left(T_{1,S} + \frac{T_{2,S}}{1+(\omega_I-\omega_s)^2 T_{2,S}^2}\right)$$

Note: the S(S+1)/3 factor comes from $\mathrm{Tr}\left(\hat{S}_p^2\right) = \frac{S(S+1)}{3}$, p = product operator where S = spin of the unpaired electron system or nucleus.

D. Spielman
spielman@stanford.edu

$T_{1\rho}$ Relaxation by scalar coupling of the 2nd kind (extra credit)

We now wish to perform a spin lock experiment and measure relaxation in the rotating frame ($T_{1\rho}$).



a) What is the Hamiltonian in the laboratory frame with the spin-lock pulse on?

b) What is the Hamiltonian in a frame of reference rotating around the z axis at a frequency ω_0?

c) What is the Hamiltonian in the doubly rotating frame (i.e. also rotating around the x axis at a frequency ω_1)?

d) Find an expression for the relaxation superoperator in the doubly rotating frame. Hint: the following transformation may help simplify your result: $z' = x$, $y' = z$, and $x' = y$.

e) Assuming an exponential correlation time for the perturbation fields of τ_c, find an expression for $1/T_{1\rho}$ ("longitudinal" relaxation rate in the doubly rotating frame).

f) What is $1/T_{1\rho}$ in the limit of $\omega_1 = 0$?