Problem Set #3
BioE 326B/Rad 226B

1. Solomon equations
2. Time-dependent perturbation theory
3. $T_1$ and $T_2$ of bone
4. Temperature mapping
Solomon equations

Using the Solomon equations, derive the relaxation rate of longitudinal two-spin order $2\hat{I}_z\hat{S}_z$.

Hint, the energy diagram for this coherence is:

\[ 2\hat{I}_z\hat{S}_z \]

- Population excess
- Population deficit
Time-dependent Perturbation Theory

Given a Hamiltonian of the form $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$ where $\hat{H}_1(t)$ is a perturbation small compared to $\hat{H}_0$ and $|m_n\rangle$, $n = 1\ldots N$ are the eigenkets of the unperturbed Hamiltonian $\hat{H}_0$ with eigenvalues $E_n/\hbar$, the goal is to show that if the system starts at time $t=0$ in the state $|m_j\rangle$, then the probability of finding the system in state $|m_k\rangle$ at time $t$ is given by:

$$P_{kj} = \left| \int_0^t \langle m_k(0)|\hat{H}_1(t')|m_j(0)\rangle e^{-i(E_j-E_k)t'/\hbar} \, dt' \right|^2$$

a) Consider an arbitrary wavefunction $|\psi\rangle = \sum_{n=1}^N c_n(t)|m_n\rangle$.

Using Schrodinger’s equation: $i \frac{\partial |\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$,

show $\dot{c}_k(t) = -i \sum_{n=1}^N c_n(t)\langle m_k|\hat{H}_1(t)|m_n\rangle$.

b) Given the state of the system at $t = 0$ is specified by $c_{j=1}$, $c_{n\neq j} = 0$, the perturbation assumption is that the $\hat{H}_1(t)$ will only have a small effect on the dynamics, i.e.

$c_n(t) \ll c_j(t)$ for $n \neq j$ and $c_j(t) \approx 1$.

Using these assumptions and the results from (a), show

$$P_{kj} = \left| \int_0^t \langle m_k(0)|\hat{H}_1(t')|m_j(0)\rangle e^{-i(E_j-E_k)t'/\hbar} \, dt' \right|^2$$
**T<sub>1</sub> and T<sub>2</sub> of bone** (from de Graaf, problem 3.3)

a. Given a longitudinal relaxation time constant T<sub>1</sub> of 4.0 s for free water (τ<sub>c</sub> = 10<sup>-11</sup> s) at 7.05 T, calculate the T<sub>1</sub> for bone (τ<sub>c</sub> = 10<sup>-6</sup> s) under the condition of pure dipolar relaxation. Assume equal dipolar distances r for all compounds.

b. Calculate the minimum T<sub>1</sub> relaxation time constant at 7.05 T as a result of pure dipolar relaxation.

c. Calculate the transverse relaxation time constants T<sub>2</sub> for water and bone at 7.05 T.
Temperature mapping (from de Graaf, problem 2.1)

In a proton spectrum acquired from rat brain at 7.05 T, the water resonance appears on-resonance while the NAA methyl resonance appears –801 Hz off-resonance. On a phantom the relation between the temperature T (in Kelvin) and the chemical shift difference (in ppm) between water and NAA, \( \delta_{\text{water-NAA}} \), was established as:

\[
T = -95.24 \delta_{\text{water-NAA}} + 564.15
\]

a. Calculate the brain temperature (in Kelvin) using the phantom calibration data.

b. Following a period of ischemia a proton spectrum is acquired in which the water appears +11 Hz off-resonance. The NAA methyl resonance now appears at –796 Hz off-resonance. Calculate the brain temperature (in Kelvin).