

Problem Set #3

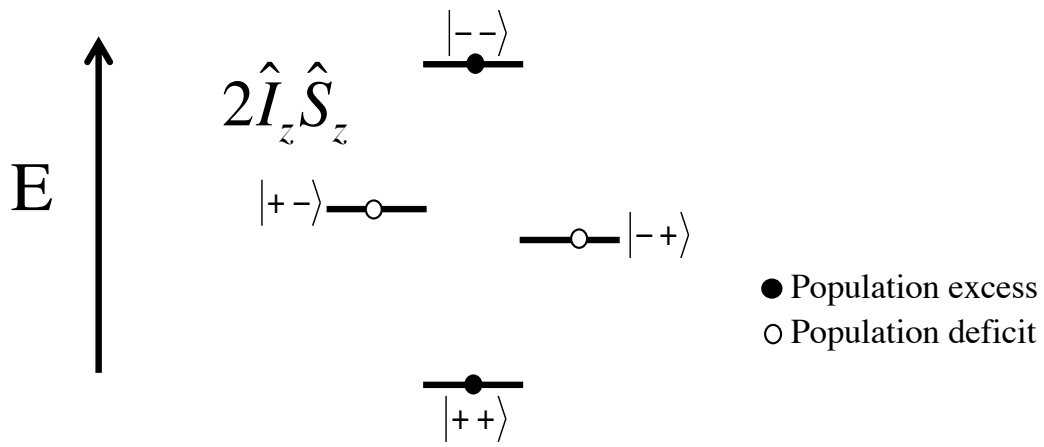
BioE 326B/Rad 226B

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:



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 $|m_n\rangle$, $n = 1 \dots N$ 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:

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

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.

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

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

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

T_1 and T_2 of bone (from de Graaf, problem 3.3)

- a. Given a longitudinal relaxation time constant T_1 of 4.0 s for free water ($\tau_c = 10^{-11}$ s) at 7.05 T, calculate the T_1 for bone ($\tau_c = 10^{-6}$ s) under the condition of pure dipolar relaxation. Assume equal dipolar distances r for all compounds.
- b. Calculate the minimum T_1 relaxation time constant at 7.05 T as a result of pure dipolar relaxation.
- c. Calculate the transverse relaxation time constants T_2 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:

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

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