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Problem Set #2
BioE 326B/Rad 226B

1. Secular approximation
2. Dipolar coupling
3. Classical relaxation

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A Secular Approximation

In a uniform magnetic field B_0 (assumed to be in the +z direction), the Hamiltonian for a J-coupled 2-spin system of spin ½ nuclei can be written in the rotating frame as:

$$\hat{H}_0 = \hat{A} + \hat{B}$$

where

$$\hat{A} = -\Omega_I \hat{I}_z - \Omega_S \hat{S}_z \quad \text{and} \quad \hat{B} = 2\pi J\left(\hat{I}_x\hat{S}_x + \hat{I}_y\hat{S}_y + \hat{I}_z\hat{S}_z\right)$$

for $\Omega_I = \gamma(1-\sigma_I)B_0 - \omega_0$ and $\Omega_S = \gamma(1-\sigma_S)B_0 - \omega_0$.

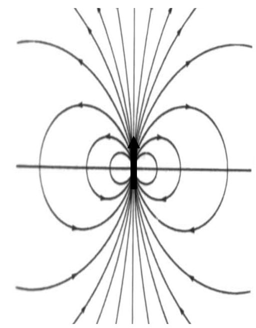
a. Find a secular approximation for the Hamiltonian, i.e.

$$\hat{H}_0 \approx \hat{A} + \hat{B}^s.$$

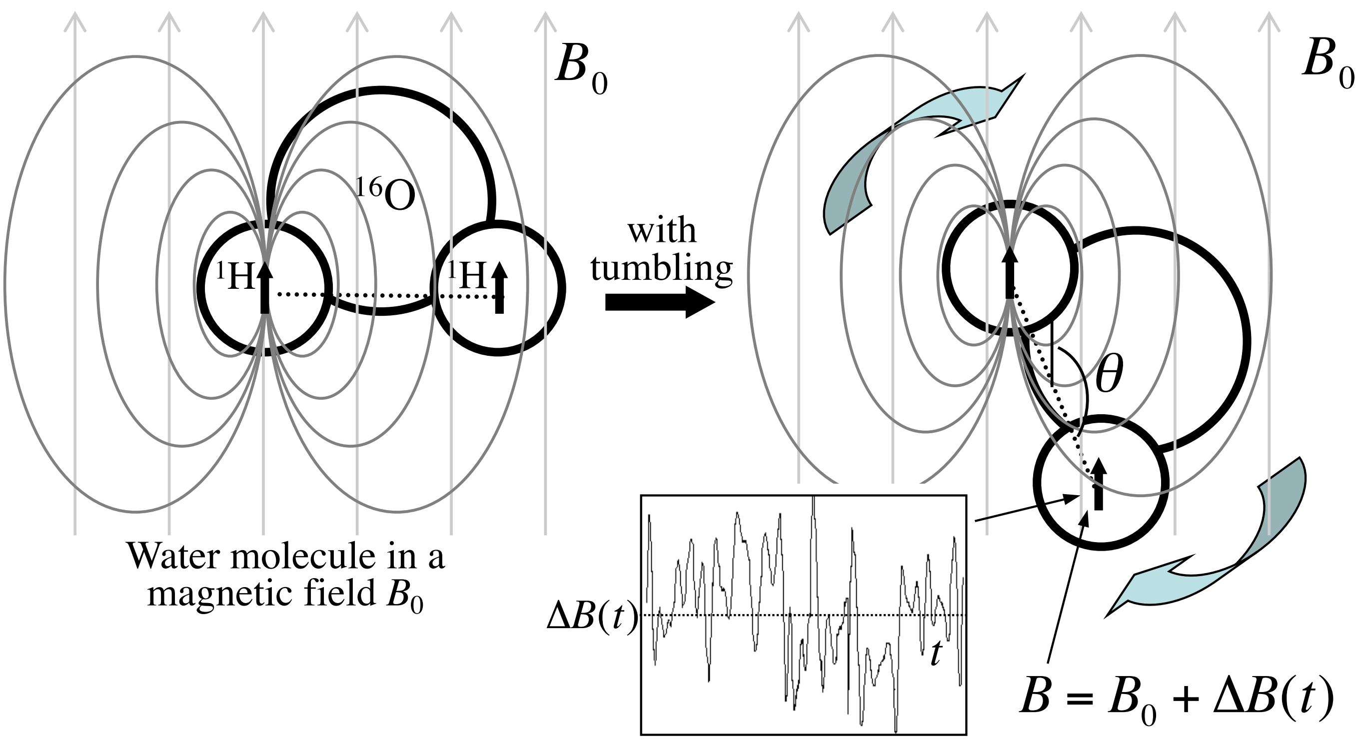
a. Under what conditions is the secular approximation valid? How does this compare to the strong versus weak coupling approximation?

Dipole coupling

Molecules in a glass of water undergo *random isotropic tumbling* due to Brownian motion. Magnetically, hydrogen nuclei behave as simple dipoles. Hence, if water is placed in a uniform magnetic field, the B field at one hydrogen nucleus due to the dipole field of the other hydrogen nucleus is given by ΔB(t) (see figure below).



B field of a magnetic dipole



where $\Delta B(t) = b\left(3\cos^2\theta(t) - 1\right)$

(b: constant)

What is the average value of ΔB(t) as defined by:

$$\overline{\Delta B(t)} = \frac{1}{\tau}\int_0^{\tau} \Delta B(t)dt = ?$$

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Classical Description of NMR Relaxation

For this problem, let's use a simplified model in which each spin, in addition to the main magnetic field B_0, sees a small field ΔB ($\Delta B << B_0$) whose amplitude and orientation change suddenly and randomly at random time intervals of average duration τ_c (τ_c is known as the correlation time).

a) T_1: consider the longitudinal magnetization M_z and the component of ΔB perpendicular to B_0, $\Delta B_\perp$.

During the first time interval of duration τ_c, the magnetization will precess around the effective field $B_0 + \Delta B_{\perp,1}$ resulting in forming an angle $\Delta\phi_1$ with respect to B_0. This process continues such that, after the *n*th time interval, the magnetization precesses around the field $B_0 + \Delta B_{\perp,n}$ making an angle $\Delta\phi_n$ with respect to its prior direction.

Assuming that $\Delta\phi_1, \Delta\phi_2, \ldots, \Delta\phi_n$ are independent and identically distributed,

show:

$$\frac{dM_z(t)}{dt} \approx -\frac{\overline{\Delta\phi^2}}{2\tau_c} M_z(t), \quad \text{hence} \quad \frac{1}{T_1} = \frac{\overline{\Delta\phi^2}}{2\tau_c}.$$

Hint: $$\frac{1}{n}\left(\sum_{i=1}^{n} \Delta\phi_i\right)^2 \approx \overline{\Delta\phi^2}$$

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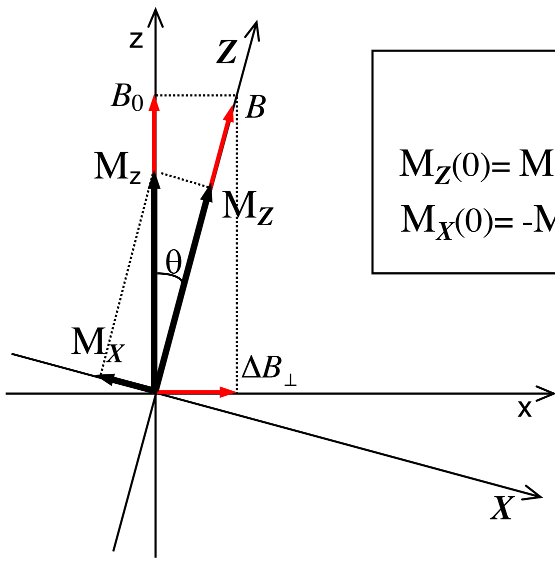
Classical Description of NMR Relaxation

b) Use the diagram below and the fact that $\theta \approx \Delta B_{\perp} / B_0 << 1$

to show: $$\frac{1}{T_1} = \frac{\overline{\Delta B_{\perp}^2}\left(1 - \cos\gamma B_0 \tau_c\right)}{B_0^2 \tau_c}.$$



Hint

$M_Z(0) = M_z(0)\cos\theta$	find	$M_Z(\tau_c) = ?$
$M_X(0) = -M_z(0)\sin\theta$		$M_X(\tau_c) = ?$

c) What is T_1 for the limiting cases of $\omega_0\tau_c << 1$ and $\omega_0\tau_c >> 1$? What value of $\omega_0\tau_c$ corresponds to the minimum value of T_1?

d) What's missing from this classical derivation of T_1?

e) T_2: Now consider the transverse magnetization and the component of ΔB parallel to B_0, $\Delta B_{\|}$. The Larmor frequency during the *i*th time interval is now given by:

$$\omega_i = -\gamma(B_0 + \Delta B_{\|,i}) = \omega_0 + \Delta\omega_i.$$

Defining the transverse relaxation time T_2 as the time at which the root-mean-square dephasing is equal to one radian, show:

$$\frac{1}{T_2} = \overline{\Delta\omega^2}\tau_c$$