Modern methods in experimental physics:
site-directed spin labeling EPR

WS 2014-15 FU Berlin 22.10.2014

Problem Set 1

Questions

a. We consider an external magnetic field along the z axis $(0, 0, B_0)$ and a fixed coordinate frame. Protons have positive gyromagnetic ratio, therefore negative frequencies (clockwise rotation around the positive z axis). Electrons have the opposite sign of γ, thus positive frequencies. List the spin and the values of γ of some biologically relevant nuclei (consider also different isotopes of the same nucleus). How is the magnetization vector $(M_x(t), M_y(t), M_z(t))$ of ^{15}N rotating in the presence of B_0? Clockwise or anticlockwise? What about the magnetization vector of ^1H and ^{12}C?

b. A linearly polarized pulse is considered as the sum of two circularly polarized fields. Can you explain why the component rotating in the opposite way as the magnetization has a negligible effect on the magnetization? Consider its effect in a frame rotating with the "correct" rotation direction.

c. In an external magnetic field $B_0 = 0.34\ T$ the Larmor frequency of the proton is -14 MHz and of a free electron is 9.4 GHz. The lengths of the corresponding $\pi/2$ pulses are: 2.5 μs for the proton and 10 ns for the electron. Calculate the applied B1 (in T) in both cases.

Problem 1: On- and off-resonance pulses in nuclear magnetic resonance

On-resonance pulses

For a radio frequency (rf) pulse on-resonant with the Larmor frequency ($\omega_{rf} = \omega_0$), the trajectory of the magnetization during the pulse can be easily calculated because the effective field $\vec{B}_{eff}$ is simply $\vec{B}_1$.

a. For a nucleus with a negative gyromagnetic ratio, calculate the *flip angle* of the magnetization for an on-resonance pulse with an amplitude $|\omega_1|/2\pi = 100$ kHz, oriented along the +y-axis, and a length $\tau = 2.5\ \mu$s.

b. Calculate the resulting magnetization vector $\vec{M}(\tau)$ in the xyz rotating frame after the 2.5 μs pulse starting from an equilibrium magnetization $\vec{M}(0) = (0, 0, 1)$. All relaxation terms must be considered negligible during the pulse length.
Hint:

(i) Calculate the nutation of $\vec{M}(0)$ at the end of the pulse (t=τ) : $\vec{M}(\tau) = \mathbf{R}_y(\beta_1)\vec{M}(0)$ where

$$\mathbf{R}_y(\beta_1) = \begin{pmatrix} \cos\beta_1 & 0 & \sin\beta_1 \\ 0 & 1 & 0 \\ -\sin\beta_1 & 0 & \cos\beta_1 \end{pmatrix} \quad (1)$$

Off-resonance pulses

For a radio frequency (rf) pulse off-resonant with the Larmor frequency ($\omega_{rf} \neq \omega_0$), the trajectory of the magnetization during the pulse is more complicated than when the pulse is on-resonant ($\omega_{rf} = \omega_0$).

a. Calculate for the same nucleus characterized by negative gyromagnetic ratio, the effective amplitude ω_{eff} for a pulse with an amplitude $|\omega_1|/2\pi = 100$ kHz, oriented along the +y-axis and a resonance offset $\Omega/2\pi = (\omega_0 - \omega_{rf})/2\pi = 100$ kHz.
What is the orientation of the effective field $\vec{B}_{eff}$? (Hint: estimate the angle θ between $\vec{B}_{eff}$ and the z-axis).
What is the *flip angle* ($\beta_{eff} = \omega_{eff}\tau$) of the magnetization around the effective pulse field, $\vec{B}_{eff}$, if the pulse is $\tau = 2.5$ μs long?

b. For the off-resonance case, calculate the resulting magnetization vector $\vec{M}(\tau)$ in the xyz rotating frame after the 2.5 μs pulse starting from an equilibrium magnetization $\vec{M}(0) = (0, 0, 1)$. All relaxation terms must be considered negligible during the pulse length.

Hint:
The nutation of the magnetization can be calculated most conveniently in a coordinate system tilted to the normal rotating frame, with the z-axis defined by the effective field vector (see figure 1).

A vector $\vec{M}$ in the rotating frame (xyz) can be expressed in the tilted frame (x′y′z′) by the transformation $\vec{M}' = \mathbf{R}_x(\theta)\vec{M}$ where

$$\mathbf{R}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \quad (2)$$

c. By which angle is the resulting magnetization vector $\vec{M}(\tau)$ tilted from $\vec{M}(0)$?

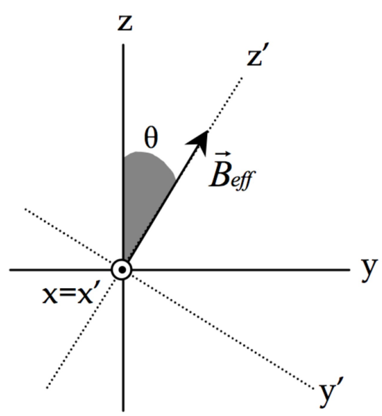

Figure 1: Orientation of the effective magnetic field in the two coordinate frames.