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

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Problem Set 5

In this problem we consider a system of one electron and one nucleus both with spins 1/2. We assume an isotropic g-tensor and an anisotropic hyperfine interaction. If the high-field approximation is valid for the electron spin, then one can neglect the non-secular terms in the Hamiltonian and it can therefore be written as

$$\hat{H}_0 = \Omega_s \hat{S}_z + \omega_I I_z + A_{zz}\hat{S}_z\hat{I}_z + A_{zx}\hat{S}_z\hat{I}_x + A_{zy}\hat{S}_z\hat{I}_y \tag{1}$$

By rotating the coordinate system around the z-axis this Hamiltonian is reduced to the form of (see lecture):

$$\hat{H}_0 = \Omega_s \hat{S}_z + \omega_I I_z + A\hat{S}_z\hat{I}_z + B\hat{S}_z\hat{I}_x \tag{2}$$

a. How would the equilibrium density matrix $\sigma_0 = -S_z$ and the operator for the $(\frac{\pi}{2})_x$ pulse look like when transformed into the eigenframe of this Hamiltonian (eq. 2)?

b. Compute σ_1 - the density matrix immediately after the application of the $(\pi/2)\hat{S}_x$ pulse - in the eigenframe of the Hamiltonian.

   Instructive point: one can follow the application of the $(\pi/2)\hat{S}_x$ on the initial density operator either in the eigenframe of the Hamiltonian or in the lab frame and then transform the resulting σ_1 in the Hamiltonian eigenframe. The latter solution is the easiest to compute.

c. Calculate the $\sigma(\tau)$ during the free evolution time period τ in the eigenframe of the Hamiltonian.

   Hint: perform the calculation in the rotating frame of the electron and neglect the resonance offsets, thus removing the electron Zeeman term from the Hamiltonian. The spin Hamiltonian in its eigenbasis can be written as:

$$\hat{H}_0 = \omega_\alpha \hat{S}^\alpha \hat{I}_z + \omega_\beta \hat{S}^\beta \hat{I}_z = \frac{\omega_+}{2}\hat{I}_z + \frac{\omega_-}{2} 2\hat{S}_z\hat{I}_z \tag{3}$$

   Here we used abbreviations $\omega_+ = \omega_\alpha + \omega_\beta$ and $\omega_- = \omega_\alpha - \omega_\beta$.

d. The detection takes place in laboratory frame. Transform the result of (c) from the eigenframe of the Hamiltonian back to the laboratory frame. Calculate all detectable terms using the detection operator -$\hat{S}_y$.

e. Plot the Fourier transform of the FID.