Quantum dynamical echoes

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Introduction:

I develop this question from articles witch describes polarization echoes in NMR. It is demonstrate that it is possible to revers the time evolution of polarization in a dipole-coupled nuclear spin system.

Question:

Consider a static solid that containing two nuclear spins species, I and S. The I spins are abundant and the S spins rare. The system is simultaneously irradiated with two rf fields B_{1I} and B_{2I} of frequencies ω_{1I} and ω_{2S} that close to Larmor frequencies and The resonant offsets are small.

A. Write the hamiltonian of the system and explain its terms.

B. What are the condition for time reversal.

C. Give quality explanation of the phenomena and give simple classical example that help to understanding this nature.

Answer:

A. The S spins are rare so we can ignore the S-S interactions, and we can treat the system as an ensemble of subsystems, each consisting of a single S spin and a large number of I spins. after the high-field truncations the hamiltonian compose from 4 terms:

$$H = H_I + H_S + H_{IS} + H_{II} \tag{1}$$

while:

$$H_I = \sum_k \Omega_k I_{kz} + \omega_{1I} \sum_k I_{kz} \tag{2}$$

$$H_S = \Omega_s S_z + \omega_{1s} S_{kz} \tag{3}$$

is the interaction of the spins I and spin S with the rf-fields. Ω_k and Ω_s are the resonance offsets and ω_{1I} and ω_{1s} are the rf-field strengths. According to the question the Ω_k and Ω_s are negligibly small and may be ignored.

The other two terms are the hetronuclear dipolar coupling between the spin S and the I spins.

$$H_{IS} = \sum_k b_k 2 I_{kz} S_z \tag{4}$$

with the hetronuclear dipolar constant:

$$b_k = -\frac{\mu_0 \gamma_I \gamma_S \hbar^2}{4\pi r_k^3} \frac{1}{2}(3\cos^2\theta_k - 1) \tag{5}$$

and the homonuclear dipolar coupling of the I spins.

$$H_{II} = \sum_J \sum_K d_{jk}[2I_{jz}I_{kz} - \frac{1}{2}(I_j^+ I_k^- + I_j^- I_k^+)] \tag{6}$$

with the homonuclear II dipolar coupling constant:

$$d_{jk} = -\frac{\mu_0 \gamma_I^2 \hbar^2}{4\pi r_{jk}^2}\frac{1}{2}(3\cos^2\theta_{jk} - 1) \tag{7}$$

where the r_k and r_{jk} are the internuclear distances and θ_k and θ_{jk} are the angels between the internuclear vectors and the static magnetic field.

B.In the case of strong irradiation on both channels,

$|\omega_{1I}| \gg |d_{jk}|$ and $|\omega_{1s}| \gg |b_k|$

we will write the hamiltonian in a frame rotated about the y axis which defined as:

$$A^T = exp[i\frac{\pi}{2}(\sum_k I_{ky} + S_y)] \cdot A \cdot exp[-i\frac{\pi}{2}(\sum_k I_{ky} + S_y)] \tag{8}$$

so that:

$$H^T = H_I^T + H_S^T + H_{IS}^T + H_{II}^T \tag{9}$$

$$H_I^T = \omega_{1I}\sum_k I_{kz} \tag{10}$$

$$H_S^T = \omega_{1s} S_{kz} \tag{11}$$

$$H_{IS}^T = \sum_k b_k 2I_{kx}S_x \tag{12}$$

The homonuclear dipolar interaction hamiltonian in the tilted frame H_{II}^T divide into two terms $H_{II}^{T'}$ and $H_{II}^{T''}$ secular and nonsecular with respect to the large hamiltonian H_I^T.

$$H_{II}^{T'} = -\frac{1}{2}\sum_J \sum_{Kj} d_{jk}[2I_{jz}I_{kz} - \frac{1}{2}(I_j^+ I_k^- + I_j^- I_k^+)] \tag{13}$$

$$H_{II}^{T''} = \frac{3}{2}\sum_J \sum_{Kj} d_{jk}\frac{1}{2}[(I_j^+ I_k^+ + I_j^- I_k^-)] \tag{14}$$

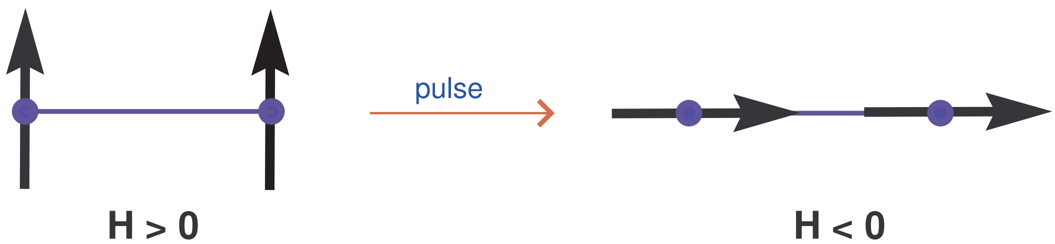
$$\tag{15}$$

For large I spin fields ($|\omega_{1I}| \gg |d_{jk}|$) the nonsecular terms $H_{II}^{T''}$ may usually be ignored. After we neglected the nonsecular terms we have the factor $-\frac{1}{2}$ that multiply the homonuclear dipolar interaction hamiltonian and experimentally switching the evolution from one situation to the other, which leads to a polarization echoes.

C. The magnetic dipolar interaction is anisotropic. Any network homologous spins can be describe, in the quantization axis of the external field, by the hamiltonian [6]. Now if a $\pi/2$ pulse is applied and then irradiation is maintained in the direction of the polarization (spin lock) with reasonable rf power, the quantization axis should be taken along the rf field. During the time, the spin dynamics is described (after we neglect the non-secular terms) by:

$$H_{II}^{'} = -[\frac{1}{2}]H_{II} \tag{16}$$

simple classical system that can demonstrate this phenomena is of two magnetic moments that repel or attract each other depending on the angle between their orientation and the internuclear vector.



two magnets constrained to a plane: in the left side the magnets are repel each other and the energy is positive. when the magnets rotate in a $\pi/2$ angle (right side) they are aligned along their internuclear vector and they attract each other (negative energy).