RANDOM AND ROTARY RESONANCE

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Introduction

We consider the spin dynamics of a nuclear quadrupole with spin 3/2 under the effect of an rf pulse and magic angle spinning. The MQ excitation is maximal between resonance conditions $\omega_1 = n\omega_2 / 2, n = 1, 2, \ldots$ (Fig. 1), where $\omega_1$ is the frequency of the rf pulse, and $\omega_2$ is the spinning frequency. This has been successfully explained earlier using Floquet theory [1]. We present an alternative analysis here.

Theory

Our analysis is based on considering the spinning as a random perturbation to the rf Hamiltonian. The Hamiltonian can be written in the form

$$H(t) = q(t)(3S_z^2 - S_z^2) / 6 + \omega_3 S_z$$

where $q(t)$ is the quadrupole coupling frequency, and is modulated by the spinning. The period of $q(t)$ is the spinning frequency $\omega_2$.

As in [1], the dynamics can be written in terms of spin $1/2$ subsystems by going to a rotating frame of reference. The Hamiltonians of the spin $1/2$ subsystems can be written as

$$-\omega_1 I_z + \sqrt{3}U_q I_x U_q^*$$

where $U_q = \exp(\pm i\int q(t)dt)$. Since $q(t)$ is large, it is convenient to think of $\int q(t)dt$ as a random, equally distributed phase angle for a perturbation in the $xy$ plane to the Hamiltonian $-\omega_1 I_z$. The propagator for (2) is of the form

$$\exp(-i\omega_2 I_z t)U$$

where the Hamiltonian for $U$ is again of the form $\sqrt{3}\omega_3 U I_x U^*$. Here, $U_r = \exp(\pm i\phi(t)I_z)$, where $\phi(t)$ is a random, equally distributed phase angle.

We show that $U(2\pi / \omega_2)$ is of the form $\exp(i\phi_0 X \cdot I)$ where $\phi_0$ is a random small phase and the vector $X$ represents a random direction. Thus after 1 rotor period, (3) represents a small perturbation of $U(-2\pi i\omega_1 / \omega_2)$. An analysis of the expression

$$\exp(-\pi i\omega_1 / \omega_2)\exp(i\phi_0 X \cdot I)$$

gives an explanation of resonance conditions without the use of Floquet theory.

References