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SPIN-SPIN INTERACTIONS AND NUCLEAR MAGNETIC RELAXATION IN MAGNETICS

In present short note we consider the influence of spin-spin interactions (the Suhl-Nakamura interaction and the dipole-dipole interaction) on the relaxation of the magnetic nuclei with spin $I = 1/2$ in magnetically ordered solids.

The interaction Hamiltonian of the two magnetic nuclei with spin $I = 1/2$ in magnetic solids can be written as [9]

$$H_0 = H_{HF} + H_{S-N} + H_{d-d}, \tag{1}$$

where the first term is the hyperfine magnetic interaction (*HF*) Hamiltonian, $H_{S\text{-}N}$ is the Suhl-Nakamura interaction (*SN*) Hamiltonian and $H_{d\text{-}d}$ is dipole-dipole interaction (*DD*) Hamiltonian.

For simplicity we shall assume that the *HF* Hamiltonian is isotropic and has the form ($\hbar = 1$)

$$H_{HF} = -\omega_0 I_Z. \tag{2}$$

Here $I_Z = I_{1Z} + I_{2Z}$ and ω_0 is the NMR frequency of nuclei.

Usually $||H_{HF}|| >> ||H_{S-N}||$, $||H_{d-d}||$ and the full interaction Hamiltonian can be written as [3, 9]

$$H_0 = -\omega_0 I_Z + V_{12}(I_{1+}I_{2-} + I_{1-}I_{2+}) - D_{12}[4I_{1Z}I_{2Z} - (I_{1+}I_{2-} + I_{1-}I_{2+})]. \quad (3)$$

In Eq. (3) V_{12} is the constant of the *SN*-interaction between nuclear magnetic moments. The dipolar coupling constant D_{12} is given by

$$D_{12} = \frac{\gamma^2 \hbar}{8 r_{12}^3}(3\cos^2 \vartheta_{12} - 1). \quad (4)$$

It should be noted that in the interaction Hamiltonian (3) the *Z*-axis is the quantization axis for the nuclear spins and in magnetically ordered materials this axis coincides with the direction of the electron magnetization $\vec{M}_e$ [9].

Now we assume that there are the thermal fluctuations in the electron magnetization vector $\vec{M}_e$ [1, 2, 6, 9]. We want to show that the thermal fluctuations in the direction of the quantization axis for the nuclear spins lead to the temporal fluctuations of *SN* and *DD* interaction Hamiltonians.

Consider two coordinate system *X*, *Y*, *Z* and *X'*, *Y'*, *Z'*. In the „rigid" coordinate system *X*, *Y*, *Z* the *Z*-axis coincides with the equilibrium direction of an electron magnetization $\vec{M}_e(0)$. The „fluctuated" coordinate system *X'*, *Y'*, *Z'* is obtained by the rotation of the coordinate system *X*, *Y*, *Z* around the axis at angle φ with the axis *X*. In this „fluctuated" coordinate system the *Z'*-axis coincides with the direction of an electron magnetization $\vec{M}_e(t)$ at the time *t*. The transformation from the coordinate system *X*, *Y*, *Z* to the coordinate system *X'*, *Y'*, *Z'* is defined by the rotation operator [4, 8]

$$R(\theta, \varphi) = \exp(-i\varphi I_Z)\exp(-i\theta I_Y)\exp(i\varphi I_Z). \quad (5)$$

Here θ is the angle between *Z*-axis and *Z'*-axis.

The interaction Hamiltonian in the „fluctuated" coordinate system has the form

$$H' = R(\theta, \varphi) H_0 R^{-1}(\theta, \varphi). \quad (6)$$

Using Eq. (5) and assuming that fluctuations in the angle θ is small ($\cos\theta \approx 1$, $\sin\theta \approx \theta$) we obtain

$$H'(t) = H_0 + H_1(t). \tag{7}$$

The static part of interaction Hamiltonian (7) coincides with Hamiltonian (3). The time-dependent part in Hamiltonian (7) contains three terms

$$H_1(t) = H_{HF}(t) + H_{S-N}(t) + H_{d-d}(t). \tag{8}$$

Here the term

$$H_{HF}(t) = \frac{\omega_0}{\sqrt{2}} \cdot \theta(t) \cdot (e^{-i\varphi(t)} \cdot T_{1,+1} - e^{i\varphi(t)} \cdot T_{1,-1}) \tag{9}$$

describes the fluctuations in the hyperfine interaction Hamiltonian. In Eq. (9)

$$T_{1,\pm 1} = \mp \frac{1}{\sqrt{2}} I_{\pm} = \mp \frac{1}{\sqrt{2}} (I_{1\pm} + I_{2\pm}) \tag{10}$$

are components of irreducible tensor operator of the first rank [4, 5, 8].
The term

$$H_{S-N}(t) = 2V_{12} \cdot \theta(t) \cdot (e^{-i\varphi(t)} \cdot T_{2,+1} - e^{i\varphi(t)} \cdot T_{2,-1}) \tag{11}$$

is the fluctuating part of the Suhl-Nakamura interaction Hamiltonian. In Eq. (11) the $T_{2,\pm 1}$ are components of irreducible tensor operator of the second rank [4, 5, 8]:

$$T_{2,\pm 1} = \mp \frac{1}{2} (I_{1Z} I_{2\pm} + I_{1\pm} I_{2Z}). \tag{12}$$

In Eq. (8) the term

$$H_{d-d}(t) = 6D_{12} \cdot \theta(t) \cdot (e^{-i\varphi(t)} \cdot T_{2,+1} - e^{i\varphi(t)} \cdot T_{2,-1}) \tag{13}$$

describes the fluctuations in the dipolar interaction Hamiltonian.

From Eq. (11) and Eq. (13) we see that these fluctuating Hamiltonians have the same forms. So we will use the new Hamiltonian

$$H_{\text{int}}(t) = A_{12} \cdot \theta(t) \cdot (e^{-i\varphi(t)} \cdot T_{2,+1} - e^{i\varphi(t)} \cdot T_{2,-1}), \tag{14}$$

where

$$A_{12} = 2 \cdot (V_{12} + 3D_{12}). \tag{15}$$

In order to derive the expressions for the spin-lattice relaxation rates we use the well-known expression for the reduced spin density matrix [5, 9]

$$\frac{d\tilde{\rho}}{dt} = -\int_0^\infty d\tau \cdot \overline{[\tilde{H}_1(t),[\tilde{H}_1(t-\tau),\tilde{\rho}]]}. \tag{16}$$

Here

$$\tilde{\rho}(t) = e^{i\omega_0 t I_Z} \rho(t) e^{-i\omega_0 t I_Z} \tag{17}$$

and

$$\tilde{H}_1(t) = e^{i\omega_0 t I_Z} H_1(t) e^{-i\omega_0 t I_Z}. \tag{18}$$

In Eq. (16) the upper bar denotes the average on the random fluctuations of the Hamiltonian $H_1(t)$.

Using Eq. (18) we obtain from Eq. (9) and Eq. (14)

$$\tilde{H}_1(t) = F(t) \cdot T_+ \cdot e^{i\omega_0 t} + F^*(t) \cdot T_- \cdot e^{-i\omega_0 t}, \tag{19}$$

where

$$F(t) = \frac{\omega_0}{\sqrt{2}} \cdot \theta(t) \cdot e^{-i\varphi(t)}, \tag{20}$$

and

$$T_\pm = \pm(T_{1,\pm 1} + \alpha \cdot T_{2,\pm 1}). \tag{21}$$

In Eqs. (21)

$$\alpha = \frac{\sqrt{2} \cdot A_{12}}{\omega_0}. \tag{22}$$

Using the definition

$$J(\omega_0) = \int_0^{\infty} \overline{F(t)F^*(t-\tau)} \cdot e^{i\omega_0\tau} d\tau \tag{23}$$

and retaining in Eq. (16) only time independent terms (secular terms [5, 9]) we obtain

$$\frac{d\rho}{dt} = -J(\omega_0) \cdot [T_+,[T_-,\rho]] - J^*(\omega_0) \cdot [T_-,[T_+,\rho]]. \tag{24}$$

Multiplying both sides of Eq. (24) by $I_Z = I_{1Z} + I_{2Z}$ and taking the trace, we obtain the equations of motions for the expectation values of I_Z:

$$\left\langle \frac{dI_Z}{dt} \right\rangle = -J(\omega_0) \cdot \langle [T_+,[T_-,I_Z]] \rangle - J^*(\omega_0) \cdot \langle [T_-,[T_+,I_Z]] \rangle, \tag{25}$$

Here $\langle C \rangle = Tr(C\rho)$.

Using the following commutation relations

$$[T_\pm, I_Z] = \mp T_\pm,$$

we have from Eq. (25)

$$\begin{aligned} \left\langle \frac{dI_Z}{dt} \right\rangle &= -2\,\mathrm{Re}[J(\omega_0)] \cdot \langle [T_+,T_-] \rangle = \\ &= -2J(\omega_0) \cdot \{\langle [T_{1,-1},T_{1,+1}] \rangle + \alpha \cdot (\langle [T_{1,-1},T_{2,+1}] \rangle + \\ &\quad + \langle [T_{2,-1},T_{1,+1}] \rangle) + \alpha^2 \cdot \langle [T_{2,-1},T_{2,1}] \rangle\}. \end{aligned} \tag{26}$$

Using the relation [7]

$$\langle [T_{1,-1},T_{1,+1}] \rangle = \langle I_z \rangle,$$

$$\langle [T_{1,-1}, T_{2,+1}] \rangle = \langle [T_{2,-1}, T_{1,+1}] \rangle = 0,$$

$$\langle [T_{2,-1}, T_{2,1}] \rangle = \frac{2}{3} I(I+1) \cdot \langle I_Z \rangle,$$

we obtain

$$\left\langle \frac{dI_Z}{dt} \right\rangle = -2\,\mathrm{Re}[J(\omega_0)] \cdot [1 + \frac{2}{3} I(I+1)\alpha^2] \cdot \langle I_Z \rangle. \tag{27}$$

From Eq. (27) it follows that the spin-lattice relaxation rate is defined by equation

$$T_1^{-1} = (T_1^{-1})_{HF} + (T_1^{-1})_{\text{int}}, \tag{28}$$

where

$$(T_1^{-1})_{HF} = 2\,\mathrm{Re}[J(\omega_0)] \tag{29}$$

is the spin-lattice relaxation rate defined by the fluctuations in the hyperfine interaction Hamiltonian;

$$(T_1^{-1})_{\text{int}} = \mathrm{Re}[J(\omega_0)] \cdot \frac{4}{3} I(I+1) \cdot \alpha^2 \tag{30}$$

is the spin-lattice relaxation rate defined by the fluctuations in the Suhl-Nakamura and dipolar interaction Hamiltonians.

From Eq. (29) and Eq. (30) we have

$$\frac{(T_1^{-1})_{\text{int}}}{(T_1^{-1})_{HF}} = \frac{1}{\omega_0^2}[\frac{4}{3} I(I+1)A_{12}^2] = \frac{4M_2}{\omega_0^2}, \tag{31}$$

where

$$M_2 = \frac{4}{3} I(I+1) \cdot (V_{12} + 3D_{12})^2. \tag{32}$$

Usually the NMR resonance frequency for nuclei ^{57}Fe is $\omega_0 \approx 10^8$ *rad* · *sec*$^{-1}$ Assuming that $\sqrt{M_2} \approx (10^3 \div 10^6)\, rad \cdot \sec^{-1}$ [9], we have from Eq. (31)

$$\frac{(T_1^{-1})_{\text{int}}}{(T_1^{-1})_{HF}} = \frac{4M_2}{\omega_0^2} \approx 4 \cdot 10^{-4} \div 4 \cdot 10^{-10}. \qquad (33)$$

It follows from obtained results (Eq. (33)) that spin-spin interactions (the Suhl-Nakamura interaction and the dipole-dipole interaction) give negligibly small contribution to the relaxation of the magnetic nuclei with spin $I = 1/2$ in magnetically ordered solids.

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ODDZIAŁYWANIE SPINOWO-SPINOWE I RELAKSACJA MAGNETYCZNA JĄDROWA W MAGNETYKACH

Streszczenie

Zakładając, że w magnetycznie uporządkowanych ciałach relaksacja jest uwarunkowana oddziaływaniami Suhl-Nakamura oraz oddziaływaniami dipolowymi, wyprowadzono analityczne wyrażenie na prędkość relaksacji spin-sieć (T_1^{-1}) jąder ze spinem $I = 1/2$.