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Temperature dependence of nuclear spin-relaxation rates for Fe, Co and Ni

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Abstract. Numerical calculations of the temperature dependence of the longitudinal (T_1^{-1}) and transverse (T_2^{-1}) nuclear spin-relaxation rates for Fe, Co and Ni are performed for both ferromagnetic and paramagnetic states, using the first-principles density of states and various approximations of the spin-fluctuation theory. If the spin fluctuations are taken into account, the quantities $(T_1 T)^{-1}$ and $(T_2 T)^{-1}$ depend significantly on temperature. Near T_C in the ferromagnetic region they increase sharply, the increases being monotonic and similar for the two rates, just as observed experimentally.

1. Introduction

It is well known that in ferromagnetic metals the contact hyperfine interaction gives the main contribution to the nuclear spin relaxation (see, e.g., [1–6]). In this case the relaxation rate is just the Fourier transform of the electron spin correlation function at the nuclear magnetic resonance (NMR) frequency, which by the fluctuation-dissipation theorem can be expressed in terms of the magnetic susceptibility [7]. The relation between the nuclear spin-relaxation rate and magnetic susceptibility permits one to calculate the relaxation rates for ferromagnetic metals at finite temperatures using the spin-fluctuation theory (SFT) developed by the author and a co-author in [8, 9] and successfully applied to Fe, Co and Ni in [10].

Unlike the case for simple and non-magnetic transition metals, where the relaxation rates are proportional to temperature (see, e.g., [11]), for ferromagnetic metals a significant temperature dependence is found for the quantities $(T_1 T)^{-1}$ and $(T_2 T)^{-1}$ [12, 13]. While a theoretical explanation of the temperature dependence of the relaxation rates for simple and non-magnetic transition metals is available [14–16], for ferromagnetic ones it is absent even at a qualitative level. So, according to Moriya's estimates [17] (see also [18–20]), for Fe, Co and Ni the largest contribution to T_1^{-1} comes just from the orbital (not contact) interaction. In our opinion, this result is a consequence of the fact that the spin fluctuations increasing sharply with increasing temperature were not taken into account in [17]. We believe that only by correctly taking account of the spin fluctuations can one explain the temperature behaviour of the relaxation rates for ferromagnetic metals properly. We emphasize that by ferromagnetic metals we always mean the *strongly* ferromagnetic metals Fe, Co and Ni. For the *weakly* ferromagnetic metals, a quite satisfactory treatment of the temperature dependence of the relaxation rates based on the SFT is already available (see [21] and references therein).

Note that an attempt to take into account the effect of the electron–electron interaction on the nuclear spin relaxation in metals was undertaken in [7], but within a very simplified

model: the wavelength- and frequency-dependent magnetic susceptibilities were calculated within a model of a free-electron gas with interaction of δ -function type. As follows from the arguments in [7], the relaxation rate T_1^{-1} is enhanced by the electron–electron interaction. However, detailed comparison between the theory and the experimental data is absent from [7]. Moreover, at that time, experimental data were available only for multidomain Fe, Co and Ni [22, 23], since they were obtained in zero applied field. (The high-field rates which are two-to-three times less than the low-field ones [24] are intrinsic relaxation rates for ferromagnetic metals.)

Finally, calculations of the relaxation rates T_1^{-1} for most elements as impurities in ferromagnetic iron using the KKR–Green’s function method [25] revealed that almost all of the calculated rates are smaller than the experimental ones. A systematic tendency for theory to underestimate the experimental rates, including in the case of *FeFe*, suggested to the authors of [26–28] that an important relaxation mechanism is missing in the one-electron theory [25]. The contribution of spin fluctuations is a reasonable candidate for providing the missing rate, and our paper demonstrates this.

2. Theoretical model

2.1. Relaxation rates

The usual quantum mechanical consideration of the contact hyperfine interaction (see, e.g., [6]) gives the following expressions for the longitudinal (T_1^{-1}) and transverse (T_2^{-1}) nuclear spin-relaxation rates:

$$\frac{1}{T_1} = B \int_{-\infty}^{\infty} \langle \{ \Delta \hat{S}_n^+(t), \Delta \hat{S}_n^-(0) \} \rangle e^{i\omega_0 t} dt \quad (1)$$

$$\frac{1}{T_2} = \frac{1}{2T_1} + B \int_{-\infty}^{\infty} \langle \{ \Delta \hat{S}_n^z(t), \Delta \hat{S}_n^z(0) \} \rangle e^{i\omega_0 t} dt \quad (2)$$

where $\langle \{ \Delta \hat{S}_n^\alpha(t), \Delta \hat{S}_n^\beta(0) \} \rangle$ is a single-site electron spin correlator and ω_0 is the NMR frequency. The expressions (1) and (2) are derived under the assumption that the hyperfine magnetic field at a nucleus is proportional to the total spin at a site, and that the constant B effectively depends on the magnitude of the nuclear spin (not necessarily equal to 1/2). Using the fluctuation-dissipation theorem, we obtain [29, 30]

$$\frac{1}{T_1} = B\hbar \coth \frac{\hbar\omega_0}{2T} \text{Im} \chi_L^{+-}(\omega_0, T)$$

$$\frac{1}{T_2} = \frac{1}{2T_1} + B\hbar \coth \frac{\hbar\omega_0}{2T} \text{Im} \chi_L^{zz}(\omega_0, T)$$

where χ_L^{+-} and χ_L^{zz} are the transverse and longitudinal local susceptibilities expressed in units of $g^2 \mu_B^2$, and T is the temperature in energy units. Since the energy $\hbar\omega_0$ is close to zero ($\hbar\omega_0 \sim 10^{-4}$ – 10^{-5} eV), with account taken of the fact that $\coth(\hbar\omega/2T) \simeq 2T/\hbar\omega$, we have

$$\frac{1}{T_1 T} = 2B\hbar \frac{\text{Im} \chi_L^{+-}(\omega_0, T)}{\hbar\omega_0} \quad (3)$$

$$\frac{1}{T_2 T} = \frac{1}{2} \frac{1}{T_1 T} + 2B\hbar \frac{\text{Im} \chi_L^{zz}(\omega_0, T)}{\hbar\omega_0}. \quad (4)$$

Thus, at a fixed temperature the relaxation rates are defined by the slopes of the imaginary parts of the local susceptibilities near zero.

As is shown in [29], for the choice of the z -axis along the magnetization direction in the cubic crystal, the imaginary parts of the enhanced local susceptibilities are calculated from the formulae

$$\text{Im } \chi_L^{+-} = \frac{\text{Im } \chi_{L0}^{+-}}{(1 - u \text{Re } \chi_{L0}^{+-})^2 + (u \text{Im } \chi_{L0}^{+-})^2} = \frac{2 \text{Im } \chi_{L0}^{xx}}{(1 - 2u \text{Re } \chi_{L0}^{xx})^2 + (2u \text{Im } \chi_{L0}^{xx})^2} \quad (5)$$

$$\text{Im } \chi_L^{zz} = \frac{1}{4} \frac{\text{Im}(\chi_{L0}^{\uparrow\uparrow} + \chi_{L0}^{\downarrow\downarrow})[1 - u^2 \text{Re}(\chi_{L0}^{\uparrow\uparrow}\chi_{L0}^{\downarrow\downarrow})] + u \text{Im}(\chi_{L0}^{\uparrow\uparrow}\chi_{L0}^{\downarrow\downarrow})[2 + u \text{Re}(\chi_{L0}^{\uparrow\uparrow} + \chi_{L0}^{\downarrow\downarrow})]}{[1 - u^2 \text{Re}(\chi_{L0}^{\uparrow\uparrow}\chi_{L0}^{\downarrow\downarrow})]^2 + [u^2 \text{Im}(\chi_{L0}^{\uparrow\uparrow}\chi_{L0}^{\downarrow\downarrow})]^2} \quad (6)$$

where χ_{L0}^{xx} and $\chi_{L0}^{\sigma\sigma}$ are zero (unenhanced) local susceptibilities, and u is the effective constant of the electron–electron interaction. At small energies, to the terms linear in $\varepsilon = \hbar\omega$, taking into account the expansion

$$\chi_{L0}^{\alpha\alpha}(\varepsilon) = \chi_{L0}^{\alpha\alpha}(0) + i\varphi_{L0}^{\alpha\alpha}\varepsilon$$

we obtain from (5) and (6)

$$\text{Im } \chi_L^{+-}(\varepsilon) = \frac{2\varphi_{L0}^{xx}}{(1 - 2u\chi_{L0}^{xx}(0))^2} \varepsilon \quad (7)$$

$$\text{Im } \chi_L^{zz}(\varepsilon) = \varepsilon \frac{1}{4} \sum_{\sigma} \left(\frac{1 + u\chi_{L0}^{\bar{\sigma}\bar{\sigma}}(0)}{1 - u^2\chi_{L0}^{\sigma\sigma}(0)\chi_{L0}^{\bar{\sigma}\bar{\sigma}}(0)} \right)^2 \varphi_{L0}^{\sigma\sigma} \quad (8)$$

($\sigma = \uparrow, \downarrow$ or ± 1 , and $\bar{\sigma}$ denotes $-\sigma$). Substituting (7), (8) into (3), (4) and going over to the shorter notation of our previous paper [10], where, in addition, all susceptibilities are expressed in units of $g^2\mu_B^2/2$, we finally obtain

$$\frac{1}{T_1 T} = c \frac{2\varphi_L^x}{(1 - u\chi_L^x(0))^2} \quad c \equiv B\hbar \quad (9)$$

$$\frac{1}{T_2 T} = \frac{1}{2} \frac{1}{T_1 T} + c \frac{1}{4} \sum_{\sigma} \left(\frac{1 + u\chi_L^{\bar{\sigma}\bar{\sigma}}(0)/2}{1 - u^2\chi_L^{\sigma\sigma}(0)\chi_L^{\bar{\sigma}\bar{\sigma}}(0)/4} \right)^2 \varphi_L^{\sigma\sigma}. \quad (10)$$

From here, in particular, for $u \rightarrow 0$, i.e. without allowing for enhancement, it follows that

$$\frac{1}{T_1 T} = c2\varphi_L^x \quad \frac{1}{T_2 T} = \frac{1}{2} \frac{1}{T_1 T} + c\varphi_L^z \quad (11)$$

where

$$\varphi_L^z = \frac{1}{4}(\varphi_L^{\uparrow} + \varphi_L^{\downarrow}). \quad (12)$$

At first sight, the final expressions for relaxation rates (9), (10) appear to have an approximate character, since they are based on the linear approximation of the local susceptibilities. However, in numerical calculations the formulae (9), (10) are preferable to the initial formulae (3)–(6), since the calculation using the formulae (3)–(6) reduces, in fact, to numerical differentiation, and this is known to be an ill-posed problem. In addition, it is very difficult to realize the self-consistent calculation of local susceptibilities with a small ε -step.

2.2. Local susceptibilities

A method for self-consistent calculation of magnetic properties of ferromagnetic metals at finite temperatures, based on the usage of real band structure and spin fluctuations, was developed in detail in [8, 9]. Here we give only the basic ideas of the method and present the formulae

necessary for calculation of relaxation rates, or more exactly, self-consistent calculation of local susceptibilities.

The electron–electron interaction characterized by the intra-atomic electronic repulsion constant u is replaced by the interaction of electrons with the variable exchange field which is specified by the mean value $\langle V_z \rangle$ and the mean square of the thermal fluctuations of the on-site exchange field (‘fluctuations’, for short) $\zeta^\alpha \equiv \langle \Delta V_\alpha^2 \rangle$, $\alpha = x, z$, calculated using the formulae

$$\langle V_z \rangle = -u\rho_z \quad \rho_z = (n_\uparrow - n_\downarrow)/2 \quad n_\sigma = \frac{N}{\pi} \int \text{Im } g_\sigma(\varepsilon) f(\varepsilon) d\varepsilon \quad (13)$$

$$\zeta^\alpha = \frac{uT}{2\lambda_L^\alpha} \int_0^1 \frac{1}{a_\alpha^2 + b_\alpha^2 k^2} \frac{2}{\pi} \arctan \frac{c_\alpha}{a_\alpha^2 + b_\alpha^2 k^2} 3k^2 dk. \quad (14)$$

Here ρ_z is a mean on-site spin moment, n_σ is the number of electrons with spin projection σ , N is the number of energy bands,

$$g_\sigma(\varepsilon) = \int \frac{v(\varepsilon')}{\varepsilon - \sigma \langle V_z \rangle - \Delta \Sigma_\sigma(\varepsilon) - \varepsilon'} d\varepsilon' \quad (15)$$

is the mean single-site Green function, $f(\varepsilon) = [\exp((\varepsilon - \mu)/T) + 1]^{-1}$ is the Fermi function, $a_\alpha^2 = \lambda_0^\alpha / \lambda_L^\alpha$, $b_\alpha^2 = (1 - a_\alpha^2)/0.6$, $c_\alpha = u\varphi_L^\alpha \pi^2 T / (6\lambda_L^\alpha)$, $\lambda_0^\alpha = 1 - u\chi_0^\alpha(0)$, $\lambda_L^\alpha = 1 - u\chi_L^\alpha(0)$, where $v(\varepsilon)$ is the non-magnetic density of states (DOS) per unit cell, band and spin,

$$\Delta \Sigma_\sigma(\varepsilon) = \frac{g_\sigma^s(\varepsilon)\zeta^z}{1 + 2\sigma \langle V_z \rangle g_\sigma^s(\varepsilon)} + 2g_\sigma^s(\varepsilon)\zeta^x \quad (16)$$

is the fluctuation contribution to the self-energy part ($g_\sigma^s(\varepsilon)$ is determined by expression (15) at $\Delta \Sigma_\sigma(\varepsilon) = 0$), $\chi_0^\alpha(0)$ is the static uniform susceptibility determined in the paramagnetic region (in the ferromagnetic region, $\lambda_0^\alpha = 0$) by numerical differentiation of the spin moment ρ_z with respect to the magnetic field h , the mean field $\langle V_z \rangle$ is kept fixed:

$$\chi_0^z(0) = -\frac{\partial \rho_z}{\partial h} \simeq -\frac{\rho_z(\langle V_z \rangle + h/2) - \rho_z(\langle V_z \rangle - h/2)}{h} \quad (17)$$

and $\chi_L^\alpha(0)$, φ_L^α are the quantities from the expansion of the dynamic local susceptibility $\chi_L^\alpha(\varepsilon) = \chi_L^\alpha(0) + i\varphi_L^\alpha \varepsilon$, calculated from the formulae

$$\begin{aligned} \chi_L^x(0) &= -\frac{N}{\pi} \int \text{Im}(g_\uparrow g_\downarrow) f d\varepsilon & \varphi_L^x &= \frac{N}{\pi} \int \text{Im } g_\uparrow \text{Im } g_\downarrow \left(-\frac{\partial f}{\partial \varepsilon} \right) d\varepsilon \\ \chi_L^\sigma(0) &= -\frac{2N}{\pi} \int \text{Im } g_\sigma^2 f d\varepsilon & \varphi_L^\sigma &= \frac{2N}{\pi} \int (\text{Im } g_\sigma)^2 \left(-\frac{\partial f}{\partial \varepsilon} \right) d\varepsilon \\ \chi_L^z(0) &= \frac{1}{4}(\chi_L^\uparrow(0) + \chi_L^\downarrow(0)) & \varphi_L^z &= \frac{1}{4}(\varphi_L^\uparrow + \varphi_L^\downarrow). \end{aligned} \quad (18)$$

The equations (13)–(18), complemented by the condition of the conservation of the total number of electrons:

$$n_\uparrow + n_\downarrow = n_e \quad (19)$$

which determines the value of the chemical potential μ entering into the Fermi function, make up a closed system with respect to four variables ζ^x , ζ^z , $\langle V_z \rangle$ and μ . The algorithm and the details of the calculation for this system are given in the appendix. Note that in the various approximations of the SFT, only the formula for spin fluctuations ζ^α is modified. In the dynamic non-local approximation (DNA) it has the form (14), and in the static local approximation (SLA) is simplified to

$$\zeta_{SL}^\alpha = \frac{uT}{2\lambda_L^\alpha}. \quad (20)$$

3. Results and discussion

The initial parameters of the calculation are the electron DOS calculated in the local density approximation by the KKR method with a self-consistent potential [31] and the experimental value of the magnetic moment m_0 at zero temperature. After elimination of the sp background, convolution with the Lorentz function of half-width $\Gamma = 0.01W$ (W is the bandwidth) and normalization to one d band of unit width, we obtain the DOSs represented in figures 1, 6 and 8 in [10] for Fe, Co and Ni, respectively. The values of m_0 used are given in table 2 in [10]. Since in the present paper the temperature dependence (not numerical values) of the relaxation rates is investigated, the constant c in the formulae (9)–(11) is taken for simplicity to be equal to unity.

The results of the calculation of the relaxation rates in the SLA and DNA using the zero and enhanced susceptibilities are represented in figures 1–6. As can be seen from the figures, the relaxation rates exhibit qualitatively similar behaviours for all three metals. The quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ calculated without allowing for the enhancement depend only slightly on temperature, which is consistent with the known Korringa formula [14] for the nuclear spin-relaxation rate for simple metals. If the enhancement is taken into account, the quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ considerably increase and manifest significant temperature dependence in the ferromagnetic region, the increases near T_C being monotonic and similar for the two rates, just as was observed experimentally [13]. For Fe and Ni near T_C , the longitudinal and transverse relaxation rates completely coincide: $T_1^{-1} = T_2^{-1}$.

As can be seen from figures 1, 3 and 5, in the SLA the quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ depend on temperature too strongly. This is connected with the fact that in the SLA, spin fluctuations increase linearly with temperature (see (20)), and, as a consequence, over a wide temperature interval the magnetization decreases too fast.

Let us analyse the results obtained in the DNA (figures 2, 4 and 6) in greater detail. We begin with the ferromagnetic region. In agreement with experiment [13], at low temperatures the temperature dependence of the quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ is weak; at room and higher temperatures it is considerably enhanced, sharply increasing in the critical region. On the whole, the temperature dependences of the quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ are similar for the three metals. However, for Fe the curve $(T_1T)^{-1}$ is far above the curve $(T_2T)^{-1}$; for Co these curves come together, and for Ni they change places. This is connected with the fact that in Fe the transverse fluctuations dominate, while in Ni the longitudinal fluctuations dominate, and in Co the intermediate situation is realized: the transverse and longitudinal fluctuations are close in value [10].

The strong temperature dependence of the relaxation rates is principally due to resonance behaviour of the imaginary parts of the enhanced susceptibilities (7) and (8) at low energies. This behaviour was analysed in detail in [30] with iron as an example.

It should be noted that near T_C the relaxation rates calculated in the present paper, particularly for Co, do not increase as sharply as those in [13]. This is possibly due to the single-site approximation (SSA), which insufficiently takes into account the *space* spin-density correlations. (Compare the results obtained in the DNA with those obtained in the SLA where the intersite correlations are not taken into account at all.)

In the paramagnetic region, the computed quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ are equal to each other, not changing with the increase of temperature for Fe and Ni, and slowly decreasing for Ni. The experimental data for Co and Ni [12, 13] confirm this temperature behaviour. (The data for paramagnetic iron are absent from the literature.) However, the fact that over a wide range of temperatures the computed quantities $(T_1T)^{-1}$ and $(T_2T)^{-1}$ remain on a level with critical ones attracts our attention. This is connected with the fact that in the paramagnetic

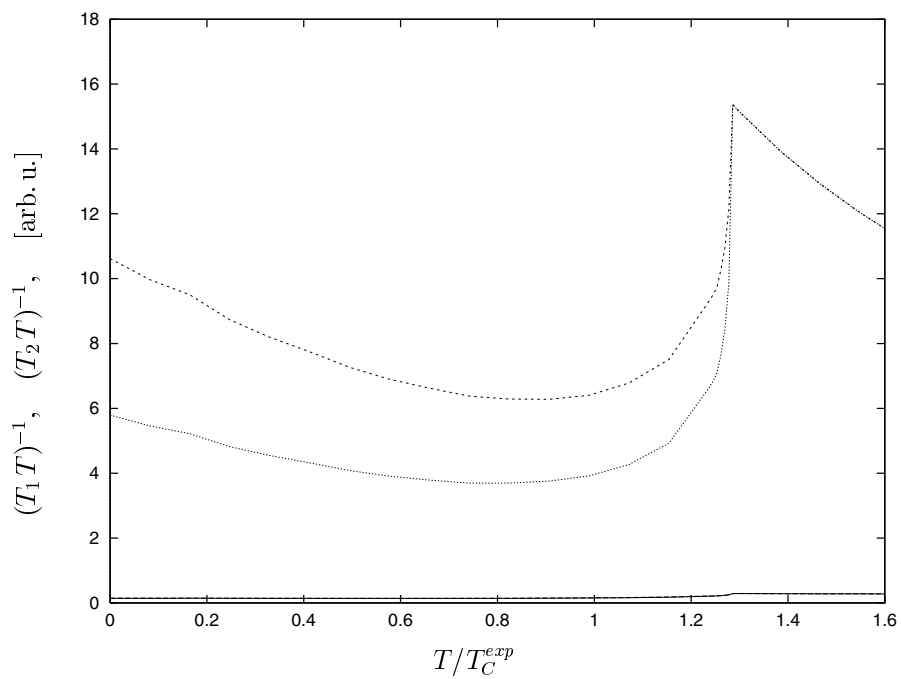


Figure 1. The temperature dependence of the longitudinal $(T_1T)^{-1}$ and transverse $(T_2T)^{-1}$ nuclear spin-relaxation rates (divided by T) for Fe, calculated in the SLA using the zero (— and - - -) and enhanced (· · · · · and ·····) susceptibilities. (The solid curve coincides with the fine dotted one.)

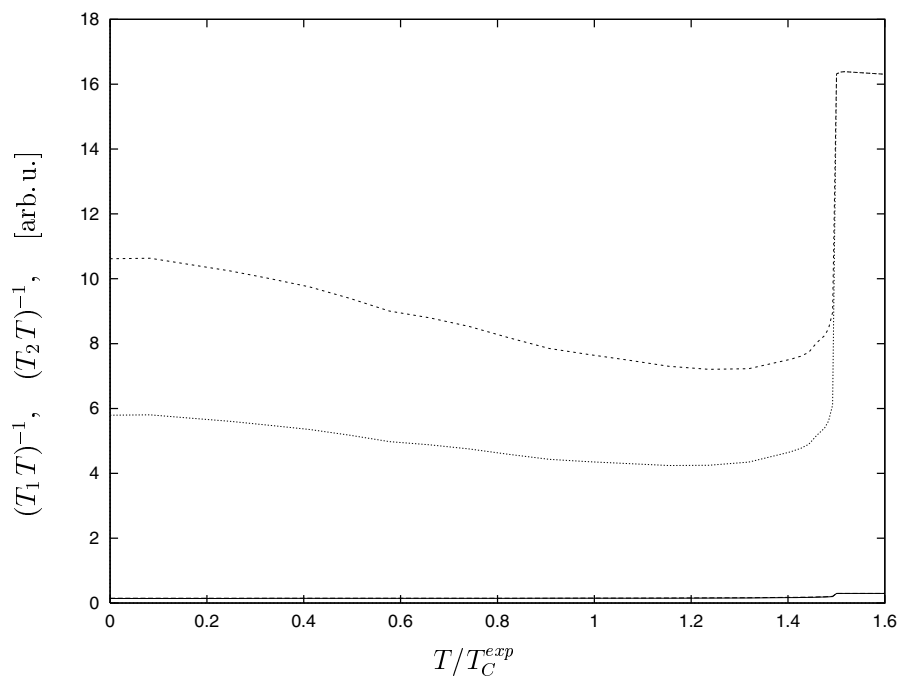


Figure 2. As figure 1, but calculated in the DNA.

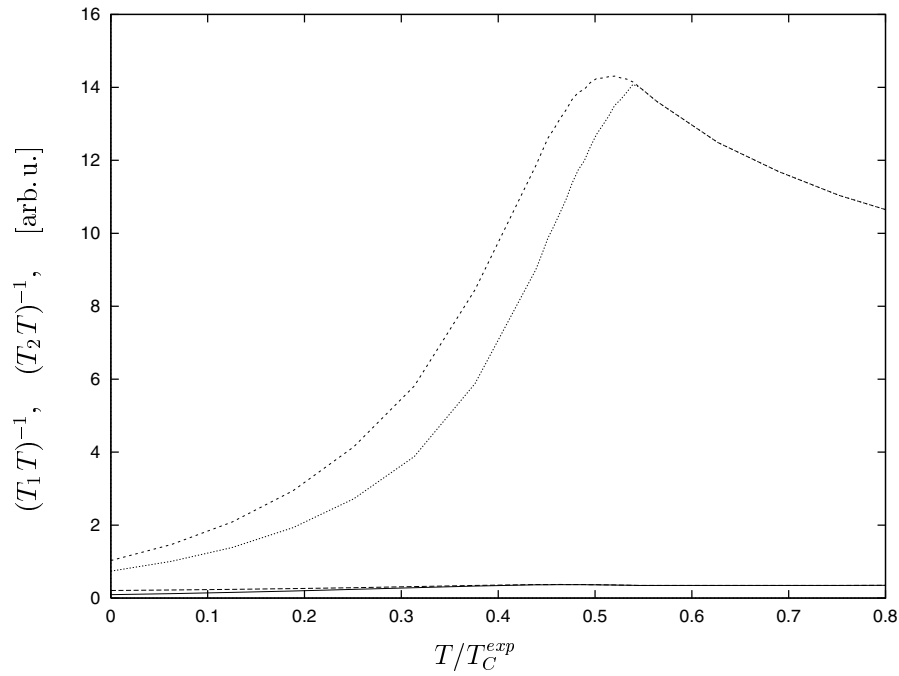


Figure 3. The temperature dependence of the longitudinal (T_1^{-1}) and transverse (T_2^{-1}) nuclear spin-relaxation rates (divided by T) for Co, calculated in the SLA using the zero (— and - - -) and enhanced (· · · · · and · · · · ·) susceptibilities.

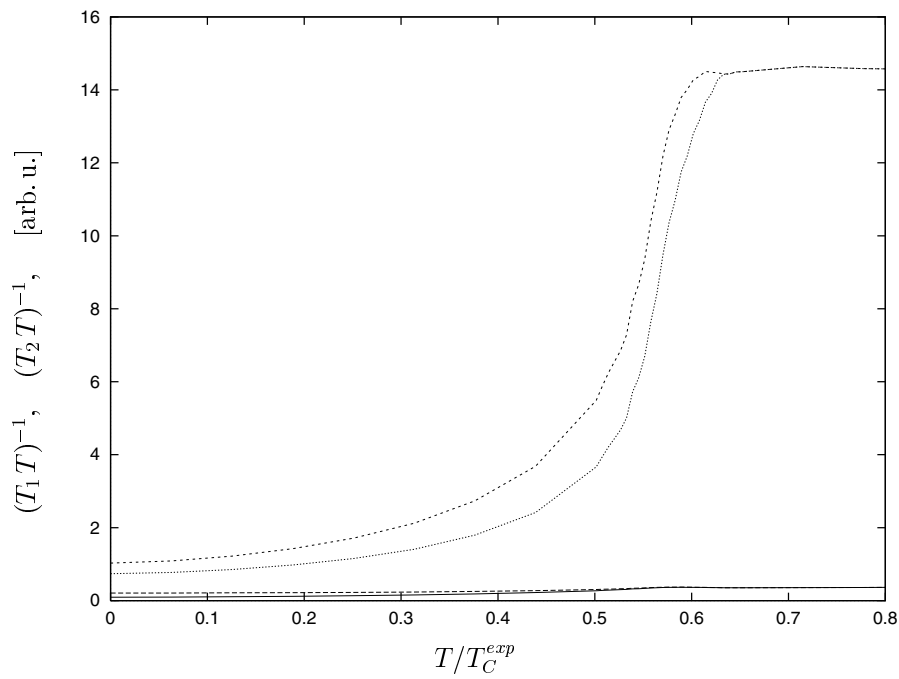


Figure 4. As figure 3, but calculated in the DNA.

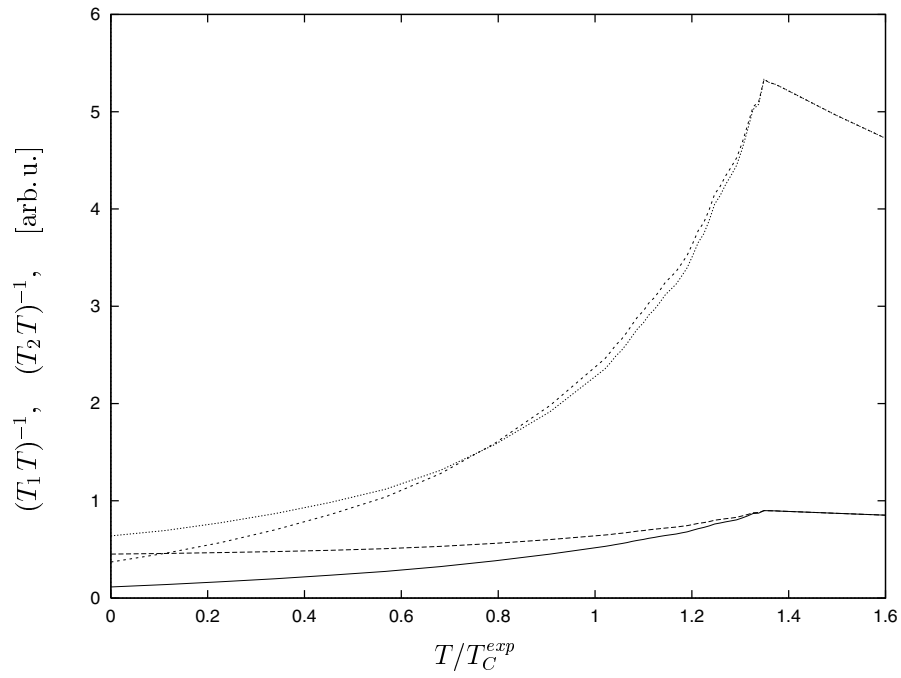


Figure 5. The temperature dependence of the longitudinal (T_1^{-1}) and transverse (T_2^{-1}) nuclear spin-relaxation rates (divided by T) for Ni, calculated in the SLA using the zero (— and - - -) and enhanced (· · · · · and · · · · ·) susceptibilities.

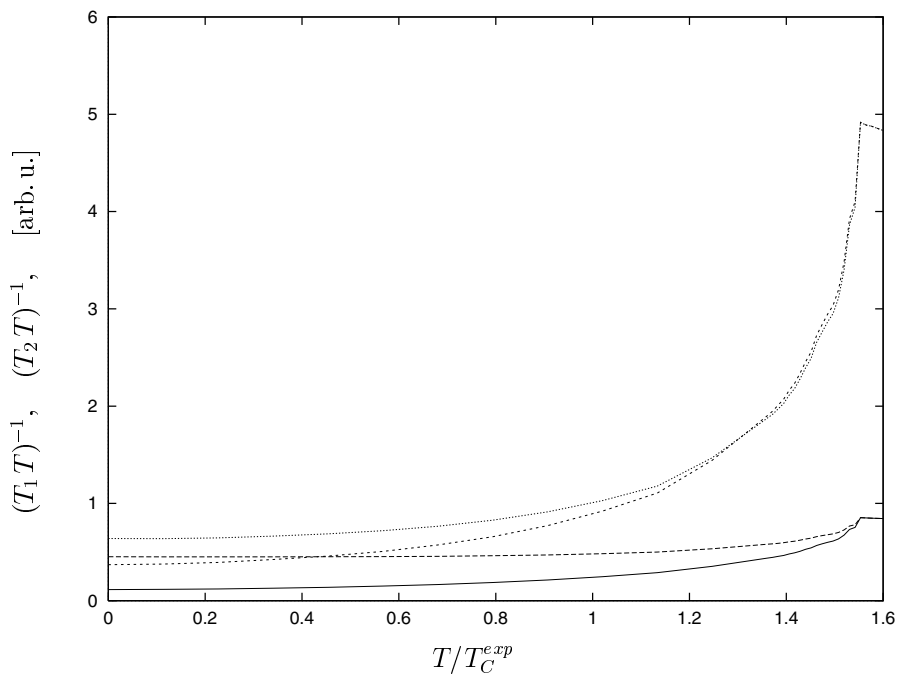


Figure 6. As figure 5, but calculated in the DNA.

region the imaginary part of the local susceptibility $\text{Im } \chi_L(\omega, T)$ with temperature increasing decreases too slowly. Such behaviour of $\text{Im } \chi_L(\omega, T)$ is observed in all local models of the SFT (see, e.g., [21] and references therein). It is possible that in Fe, Co and Ni the short-range magnetic order is retained far above T_C (see, e.g., [32,33] and references therein). In this case, the temperature behaviour of the local susceptibility more closely resembles the behaviour of the static uniform susceptibility which rapidly decreases with increasing temperature.

4. Conclusions

Taking account of spin fluctuations permits one to explain the general temperature behaviour of the nuclear spin-relaxation rates for Fe, Co and Ni. From the four approximations of the SFT considered, the DNA turned out to be the best approximation for all three metals. In the DNA a qualitative agreement with experimental data [12, 13] is found. In calculating the relaxation rates for ferromagnetic metals, one could hardly expect better agreement. Firstly, the SSA used in our method is not justified for all temperatures: at low temperatures, spin-wave consideration is preferable [23], and near T_C , taking account of the so-called critical spin fluctuations is preferable [34]. Even in the region of intermediate temperatures where the SSA is most appropriate, one should not forget the Hubbard model used in this approximation and that the dependence of the magnetic characteristics upon u is fairly strong [35]. Secondly, in addition to relaxation due to the electron spin fluctuations, important nuclear relaxation mechanisms due to the crystal imperfections, e.g. the relaxation due to the magnetic impurities [36], exist. Thirdly, and above all, the very experimental data on the relaxation rates differ for ferromagnetic metals. (See, e.g., the data for Ni in figure 5 in [12] and figure 8 in [13].)

As for the principal result of our numerical calculations, it is as follows: the temperature behaviour of the nuclear spin-relaxation rates for ferromagnetic metals is determined by the electron–electron correlations; over a wide range of temperatures these correlations can be adequately described within the SSA of the SFT.

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Appendix. Algorithm and computational details

The equations (13)–(19) represent a system of four non-linear equations for the fluctuations ζ^x and ζ^z , the mean exchange field $\langle V_z \rangle$, the chemical potential μ and the effective constant u :

$$\zeta^x = \frac{uT}{2\lambda_L^x} I^x \quad (\text{A.1})$$

$$\zeta^z = \frac{uT}{2\lambda_L^z} I^z \quad (\text{A.2})$$

$$\langle V_z \rangle = -u(n_\uparrow - n_\downarrow)/2 \quad (\text{A.3})$$

$$n_e = n_\uparrow + n_\downarrow \quad (\text{A.4})$$

where

$$I^\alpha = \int_0^1 \frac{1}{a_\alpha^2 + b_\alpha^2 k^2} \frac{2}{\pi} \arctan \frac{c_\alpha}{a_\alpha^2 + b_\alpha^2 k^2} 3k^2 dk \quad 0 < a_\alpha^2 < 1. \quad (\text{A.5})$$

At $T = 0$, the fluctuations ζ^α vanish, and the system of equations (A.1)–(A.4) turn into the mean-field-theory system of equations (A.3), (A.4). This gives one an opportunity to find the effective constant u from a known magnetic moment $m_0 = g\mu_B\rho_z(0) = g\mu_B(n_\uparrow - n_\downarrow)/2$; after that the equations (A.1)–(A.4) make up a closed system with respect to the variables $\zeta^x, \zeta^z, \langle V_z \rangle$ and μ , which at fixed temperature is simply solved, e.g., by repeatedly using the bisection method.

For analytic calculation of the integral (A.5), let us replace the variable of integration k by $x = bk$ and approximate the function $2 \arctan(c/(a^2 + x^2))/\pi$ by its two asymptotes matched (together with their derivatives) at the point $c/(a^2 + x^2) = 1$:

$$I = \frac{3}{b^3} \int_0^b dx \frac{x^2}{a^2 + x^2} \begin{cases} \frac{1}{2} \frac{c}{a^2 + x^2} & \frac{c}{a^2 + x^2} \leq 1 \\ 1 - \frac{1}{2} \frac{a^2 + x^2}{c} & \frac{c}{a^2 + x^2} > 1. \end{cases}$$

Then, introducing the notation

$$\begin{aligned} F_1(x) &= \frac{c}{2} \int \frac{x^2}{(a^2 + x^2)^2} dx = \frac{c}{2} \left(-\frac{x}{2(a^2 + x^2)} + \frac{1}{2} \arctan \frac{x}{a} \right) \\ F_2(x) &= \int \frac{x^2}{a^2 + x^2} dx - \frac{1}{2c} \int x^2 dx = x - a \arctan \frac{x}{a} - \frac{x^3}{6c} \end{aligned} \quad (\text{A.6})$$

we finally obtain

$$I = \frac{3}{b^3} \begin{cases} F_1(b) & x_0^2 \leq 0 \\ F_2(x_0) + F_1(b) - F_1(x_0) & 0 < x_0 < b \\ F_2(b) & x_0 \geq b \end{cases} \quad (\text{A.7})$$

where $x_0^2 = c - a^2$.

The calculation of the Green function (15) straight from the formula

$$g(z) = \int \frac{v(\varepsilon')}{z - \varepsilon'} d\varepsilon' \quad (\text{A.8})$$

(where z is an arbitrary complex number) is very difficult. Following [30], we obtain a formula suitable for numerical calculations. For this purpose, using a linear interpolation, we transform the tabular function $v(\varepsilon')$ into a piecewise-linear function:

$$v(\varepsilon') = \begin{cases} a_i(\varepsilon' - \varepsilon_i) + b_i & \varepsilon_i \leq \varepsilon' \leq \varepsilon_{i+1} \\ 0 & \varepsilon' < \varepsilon_1 \text{ and } \varepsilon' > \varepsilon_{n+1} \end{cases} \quad (\text{A.9})$$

where $a_i = (b_{i+1} - b_i)/(\varepsilon_{i+1} - \varepsilon_i)$, $b_i = v(\varepsilon_i)$, $i = 1, \dots, n + 1$, and n is the number of intervals. The substitution of (A.9) into (A.8) gives

$$g(z) = \sum_{i=1}^n \int_{\varepsilon_i}^{\varepsilon_{i+1}} \frac{a_i(\varepsilon' - \varepsilon_i) + b_i}{z - \varepsilon'} d\varepsilon'.$$

After simple calculations with $b_1 = b_{n+1} = 0$ we obtain

$$g(z) = \sum_{i=1}^{n+1} A_i(z - \varepsilon_i) \ln(z - \varepsilon_i) \quad (\text{A.10})$$

where $A_1 = a_1$, $A_i = a_i - a_{i-1}$, $i = 2, \dots, n$, $A_{n+1} = -a_n$.

Repeated calculations of the Fermi integrals (18) with tabular functions also represent a very complicated problem. A general numerical method for calculation of the integrals,

involving the Fermi function, was developed in [37]. A simple method for calculation of the integrals, involving the derivative of the Fermi function, was given in [10]. These methods are just what we used in the present paper.

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