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Numerical calculation of local magnetic characteristics of Fe, Co and Ni at finite temperatures

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Abstract

The transverse and longitudinal local susceptibilities, the dynamic spin correlation function and the local magnetic moment of Fe, Co and Ni are calculated, using the first-principles density of states and the dynamic non-local approximation of the spin-fluctuation theory. A remarkable agreement between theory and experiments on magnetovolume effect and neutron scattering has been found.

1. Introduction

Magnetic properties of ferromagnetic transition metals at *zero* temperature are fairly successfully described [1–5] within the framework of the local spin-density approximation (LSDA) to the density functional theory [6–9]. However, attempts to describe the *temperature* dependence of the magnetic properties within the framework of this approximation do not lead to satisfactory results. In order to explain the magnetic properties of ferromagnetic metals at finite temperatures one usually uses the spin-fluctuation approach (see, e.g. [10, 11]). Unfortunately, the spin-fluctuation theory (SFT) is very complicated and one has to introduce a number of significant simplifications in actual calculations (the Hubbard's Hamiltonian, the static local approximation, a model density of states (DOS), a step Fermi function etc). On the other hand, part of the electron–electron correlation has already been taken into account in the self-consistent LSDA potential, and the question is how important the remaining part is for the ferromagnetic metals.

In order to find out the relative contributions of the spin fluctuations and the singularities of the electron structure in forming the on-site local magnetic moment, in paper [12] we performed dynamic spin correlator calculations. The calculations showed that in the one-electron approximation the value of the local moment is reproduced well enough, but the time of its damping is comparable with the time of electron hopping from one site to another, $\tau_e \sim \hbar/W \sim 0.1\text{--}1$ fs (W is the bandwidth and 1 fs = 10^{-15} s). Then, to take into account the electron correlations, which substantially slow down the damping of the local moment, we developed a model, based on the single-site approximation of multiple

scattering theory, and applied it, first, to study the paramagnetic state [13], and then also the ferromagnetic one [14, 15]. However, the numerical calculations carried out at that time had a preliminary character and were fairly simplified. In particular, the basic initial parameter of the model, the mean spin-polarized DOS, was calculated only within the *implicit* account of spin fluctuations. Recently we developed a *rigorous* method for calculation of magnetic characteristics at finite temperatures [16], based on the dynamic non-local approximation (DNA) of the SFT. In this method the mean spin-polarized DOS is obtained *self-consistently* from a system of nonlinear equations only slightly more complicated than the standard mean-field-theory system of equations. The initial parameters of the calculation are the DOS and the magnetic moment at $T = 0$ for a specific metal. In our papers [17, 18] the developed method was successfully applied for calculations of some magnetic properties of Fe, Co and Ni. In the present paper, it is applied for calculations of the *local* magnetic characteristics such as the transverse and longitudinal susceptibilities, the dynamic spin correlation function and the local magnetic moment. In fact, for the first time a self-consistent calculation of the local magnetic characteristics of Fe, Co and Ni is performed with account taken of the real band structure and spin fluctuations. Note that almost all of the recent calculations of the local magnetic characteristics of Fe, Co and Ni (see, e.g. [10, 11, 19–22]) have been performed in the static approximation, i.e. the spin fluctuations have been treated classically. A more detailed comparison of our approach with the ones of [10, 11, 19–22] is given in [17].

2. Calculation formulae

2.1. Local magnetic characteristics

A detailed derivation of the formulae for the local magnetic characteristics of ferromagnetic metals at finite temperatures is given in our paper [14]. Here we present only the initial formulae and the final expressions necessary for numerical calculations. Note that all expressions are obtained for the choice of the z -axis along the magnetization direction in the cubic crystal.

The Fourier transform of the local susceptibility is given by

$$\chi_L^{\alpha\beta}(\omega) \equiv \chi_{nm}^{\alpha\beta}(\omega) = \frac{i}{\hbar} \int_0^\infty \langle [\hat{S}_n^\alpha(t), \hat{S}_n^\beta(0)] \rangle e^{i\omega t} dt \quad (1)$$

where $\hat{S}_n^\alpha(t)$ is the spin moment operator on the n th site of the lattice, taken in the Heisenberg representation, index α ($= x, y, z$) specifies components of the spin operator, angle brackets denote quantum statistical averaging and square brackets denote commutation. From (1) for the imaginary parts of zero (unenhanced) local susceptibilities we obtain

$$\text{Im } \chi_{L0}^{+-}(\omega) = N\pi \int f(\varepsilon) [v_\uparrow(\varepsilon)v_\downarrow(\varepsilon + \hbar\omega) - v_\downarrow(\varepsilon)v_\uparrow(\varepsilon - \hbar\omega)] d\varepsilon \quad (2)$$

$$\text{Im } \chi_{L0}^{\sigma\sigma}(\omega) = N\pi \int f(\varepsilon)v_\sigma(\varepsilon)[v_\sigma(\varepsilon + \hbar\omega) - v_\sigma(\varepsilon - \hbar\omega)] d\varepsilon. \quad (3)$$

Here $f(\varepsilon) = [\exp((\varepsilon - \mu)/T) + 1]^{-1}$ is the Fermi function, where T is the temperature in energy units and μ is the chemical potential, $\sigma = \uparrow, \downarrow$ or ± 1 is the spin projection index, N is the number of energy bands, and

$$v_\sigma(\varepsilon) = \frac{1}{\pi} \text{Im } g_\sigma(\varepsilon) \quad (4)$$

is the mean spin-polarized DOS of the one band, where $g_\sigma(\varepsilon)$ is the mean single-site Green function (see section 2.2).

The zero susceptibility is fully reconstructed from its imaginary part by application of the Hilbert transformation

$$\chi(z) = -\frac{1}{\pi} \int \frac{\text{Im } \chi(\omega')}{z - \omega'} d\omega' \quad (5)$$

where z is a complex number from the upper half-plane.

Enhanced susceptibilities are calculated from the formulae

$$\chi_L^{+-}(\omega) = \frac{\chi_{L0}^{+-}(\omega)}{1 - u\chi_{L0}^{+-}(\omega)} \quad (6)$$

$$\chi_L^{zz}(\omega) = \frac{1}{4} \frac{\chi_{L0}^{\uparrow\uparrow}(\omega) + \chi_{L0}^{\downarrow\downarrow}(\omega) + 2u\chi_{L0}^{\uparrow\uparrow}(\omega)\chi_{L0}^{\downarrow\downarrow}(\omega)}{1 - u^2\chi_{L0}^{\uparrow\uparrow}(\omega)\chi_{L0}^{\downarrow\downarrow}(\omega)} \quad (7)$$

where u is the effective constant of the electron–electron interaction (see section 2.2).

Note that in the standard random-phase approximation (RPA) the formulae of (6) and (7) type are obtained [23] for susceptibilities $\chi(\mathbf{q}, \omega)$, where \mathbf{q} is the wavevector, i.e. the usual RPA susceptibility contains enhancement for one fixed \mathbf{q} -mode only. This approach is suitable for an ideal crystal. But at finite temperatures ideality is broken and the strong interaction of modes with different \mathbf{q} takes place. At finite temperatures our enhanced local susceptibility $\chi_L(\omega)$ is preferable to $\chi_L^{RPA}(\omega) = \frac{1}{N_a} \sum_{\mathbf{q}} \chi(\mathbf{q}, \omega)$, N_a being the number of \mathbf{q} -vectors in the Brillouin zone, since the main contribution to thermodynamic quantities in this case is due to short-wave spin excitations.

The dynamic spin correlation function is determined as

$$F_{nn}^{\alpha\beta}(t) = \frac{1}{2} \langle \{\hat{S}_n^\alpha(t), \hat{S}_n^\beta(0)\} \rangle \quad (8)$$

where the braces denote anticommutator. Taking into account the fluctuation–dissipation theorem (see, e.g. [24]) for the single-site frequency correlation function, we obtain

$$F(\omega) \equiv \sum_{\alpha} F_{nn}^{\alpha\alpha}(\omega) = \sum_{\alpha} \int F_{nn}^{\alpha\alpha}(t) e^{i\omega t} dt = \left(\frac{n_{\uparrow} - n_{\downarrow}}{2} \right)^2 \delta(\omega) + A(\omega) \quad (9)$$

where

$$n_{\sigma} = \frac{N}{\pi} \int \text{Im } g_{\sigma}(\varepsilon) f(\varepsilon) d\varepsilon \quad (10)$$

is the number of electrons with spin projection σ , and

$$\begin{aligned} A(\omega) &= \sum_{\alpha} \int \frac{1}{2} \langle \{\Delta \hat{S}_n^{\alpha}(t), \Delta \hat{S}_n^{\alpha}(0)\} \rangle e^{i\omega t} dt \\ &= \hbar \coth \frac{\hbar\omega}{2T} \text{Im} \left[\frac{1}{2} (\chi_L^{+-}(\omega) + \chi_L^{*-+}(-\omega)) + \chi_L^{zz}(\omega) \right] \end{aligned} \quad (11)$$

($\Delta \hat{S}_n^{\alpha} = \hat{S}_n^{\alpha} - \langle \hat{S}_n^{\alpha} \rangle$ is the fluctuation of the spin moment operator.) By inverse Fourier transformation of function (9) we find the time correlation function

$$F(t) = \frac{1}{2\pi} \int F(\omega) e^{-i\omega t} d\omega = \left(\frac{n_{\uparrow} - n_{\downarrow}}{2} \right)^2 + \frac{1}{\pi} \int_0^{\infty} A(\omega) \cos \omega t d\omega. \quad (12)$$

One of the basic characteristics measured by polarized neutron scattering is the local spin moment. We determine the effective local spin moment in a frequency interval $[-\omega, \omega]$ by the formula

$$S_L(\omega) = \left(\frac{1}{\pi} \int_0^{\omega} F(\omega') d\omega' \right)^{1/2} = \left[\left(\frac{n_{\uparrow} - n_{\downarrow}}{2} \right)^2 + \frac{1}{\pi} \int_0^{\omega} A(\omega') d\omega' \right]^{1/2}. \quad (13)$$

It is clear that in the infinite frequency interval this quantity coincides with a root mean square of the local spin moment

$$S_L \equiv S_L(\infty) = (F(t=0))^{1/2} = \langle \hat{S}^2(t=0) \rangle^{1/2}. \quad (14)$$

2.2. Mean single-site Green function and effective constant of the electron–electron interaction

A method for self-consistent calculation of magnetic properties of ferromagnetic metals at finite temperatures, based on the usage of real band structure and the DNA of the SFT, was developed in detail in [16]. Here we present only the formulae necessary for calculation of the mean single-site Green function and effective constant of the electron–electron interaction.

The mean single-site Green functions are calculated from the formula

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

where $\nu(\varepsilon)$ is the non-magnetic DOS (per unit cell, band and spin),

$$\langle V_z \rangle = -u(n_{\uparrow} - n_{\downarrow})/2 \quad (16)$$

is the mean value of the variable exchange field, and

$$\Delta \Sigma_{\sigma}(\varepsilon) = \frac{g_{\sigma}^s(\varepsilon) \langle \Delta V_z^2 \rangle}{1 + 2\sigma \langle V_z \rangle g_{\sigma}^s(\varepsilon)} + 2g_{\sigma}^s(\varepsilon) \langle \Delta V_x^2 \rangle \quad (17)$$

is the fluctuation contribution to the self-energy part ($g_{\sigma}^s(\varepsilon)$ is determined by expression (15) at $\Delta \Sigma_{\sigma}(\varepsilon) = 0$). The mean square of the thermal fluctuations of the on-site exchange field ('fluctuations', for short) in their turn are expressed in terms of $g_{\sigma}(\varepsilon)$. So, equations (15)–(17), complemented by the equations for $\langle \Delta V_{\alpha}^2 \rangle$, $\alpha = x, z$, and by the condition of the conservation of the total number of electrons:

$$n_{\uparrow} + n_{\downarrow} = n_e \quad (18)$$

make up a system of nonlinear equations.

At zero temperature the fluctuations $\langle \Delta V_{\alpha}^2 \rangle$ vanish, and the system of equations (15)–(18) turn into the mean-field-theory system of equations (10), (16) and (18). This gives one an opportunity to find the effective constant u from a known magnetic moment $m_0 = g\mu_B(n_{\uparrow} - n_{\downarrow})/2$; after that, at any fixed temperature, equations (15)–(18) make up a closed system, whose solution gives the function $g_{\sigma}(\varepsilon)$. Details of the calculations are given in [17, 18, 25].

3. Results and discussion

As the initial DOS, we take the DOS of non-magnetic metal calculated in the local-density approximation by the KKR method with a self-consistent potential [5]. The smoothed DOSs of the d band $\nu(\varepsilon)$ used for calculation are represented in figures 1, 6 and 8 of [17] for Fe, Co and Ni, respectively. (With the help of smoothing we take into account the damping of one-electron states resulting from electron–electron correlations.) The experimental values of the magnetic moment m_0 used are given in table 2 of [17].

The results of our calculation of the effective constant u for Fe, Co and Ni are given in table 1. In the same table, for comparison, we present the values of the effective Stoner parameter I , obtained in the LSDA calculations [1, 3, 4]. The deviations of our values of u from the corresponding ones of I are considerable. However, one should not attach much importance to this fact. Firstly, as it was shown in [4] by Cr as an example, the approximate values of I given in table 1 are probably within about 10% of the correct values for the assumed form for the exchange–correlation functional. (The exact value of I for Cr is 10% *greater* than the approximate one.) Secondly, and above all, our values for the constant u depend on the degree of smoothing of the DOS. So, in our paper [26] the DOS for Fe was smoothed with

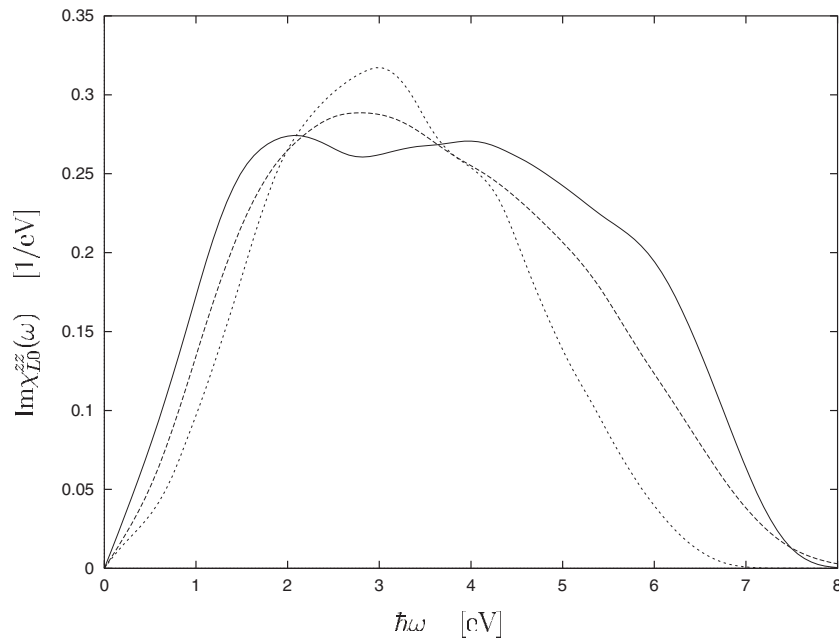


Figure 1. The imaginary part of the zero longitudinal local susceptibility of iron at $T/T_C = 0.0$ (.....), 0.93 (---), and 1.0 (—).

Table 1. Our results for the effective constant of the electron–electron interaction u of Fe, Co and Ni, compared to the corresponding results for the exchange–correlation (effective Stoner) parameter I obtained in LSDA (all values in units of eV).

	Fe	Co	Ni
Present calculation	1.08	1.25	1.16
Gunnarsson [1]	0.92	0.99	1.01
Andersen <i>et al</i> [3]	0.91	—	0.99
Janak [4]	0.92	0.98	1.01

Table 2. The local magnetic moment M_L for Fe, Co and Ni at zero, near critical and Curie temperatures. (T_C is the Curie temperature calculated in the DNA and given in the last column of table 1 in [17].)

T/T_C	Fe		Co		Ni	
	T/T_C	$M_L(T)/M_L(0)$	T/T_C	$M_L(T)/M_L(0)$	T/T_C	$M_L(T)/M_L(0)$
0.00	1.00	1.00	0.00	1.00	0.00	1.00
0.93	0.98	0.98	0.78	1.06	0.88	1.06
1.00	0.99	0.99	1.00	1.14	1.00	1.12

the Lorentz function of half-width $\Gamma = 0.0675$ eV (in the present paper $\Gamma = 0.0742$ eV), and $u = 0.96$ eV was obtained, which agrees closely with the value $I = 0.92$ eV obtained in [1,4].

Within the framework of an article, a detailed analysis of all complex susceptibilities of the three metals at various temperatures does not seem possible. Let us illustrate the behaviour of the local susceptibilities by an example of the imaginary part of the zero and enhanced longitudinal susceptibilities of iron represented in figures 1 and 2. As can be seen from figure 1, the temperature dependence of the imaginary part of zero susceptibility

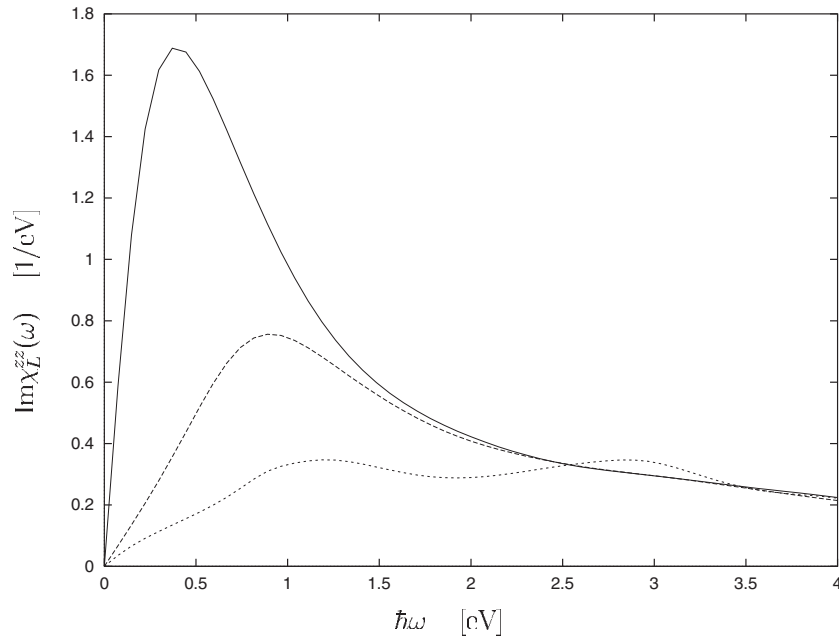


Figure 2. The imaginary part of the *enhanced* longitudinal local susceptibility of iron. (The notation is as for figure 1.)

$\text{Im } \chi_{L0}^{zz}(\omega) = \frac{1}{4} \sum_{\sigma} \text{Im } \chi_{L0}^{\sigma\sigma}(\omega)$ is weak. (Since $\text{Im } \chi_{L0}^{\sigma\sigma}(\omega)$ is an odd function, the calculations of $\text{Im } \chi_{L0}^{zz}(\omega)$ and $\text{Im } \chi_L^{zz}(\omega)$ are performed only at $\omega \geq 0$.) According to the formula

$$\text{Im } \chi_{L0}^{\sigma\sigma}(\omega) \simeq \frac{\pi}{N} v_{\sigma}^2(\mu) \hbar \omega \quad (19)$$

resulting from (3) at low $\hbar\omega$ and with neglect of the temperature broadening of the Fermi function, the linear dependence of $\text{Im } \chi_{L0}^{zz}(\omega)$ is retained in a sufficiently large energy interval, and in full accordance with the behaviour of the DOS on the chemical-potential level (see figure 4 of [17]) the susceptibility $\text{Im } \chi_{L0}^{zz}(\omega)$ increases with increasing temperature. From comparison of figure 2 with 1, it is seen that the enhancement of the susceptibility due to electron-electron correlations occurs predominantly in the region $\hbar\omega < 2$ eV. As for the temperature variations, they are qualitatively similar to those of the zero susceptibility, but quantitatively they are considerable. Besides, with the increase of temperature the enhancement increases. This is due to the fact that with the increase of temperature the *real* part of the zero susceptibility in the energy region $\hbar\omega < 2$ eV increases considerably, and this, due to the resonance denominator of the formula

$$\text{Im } \chi_L^{zz}(\omega) = \frac{\pi}{N} \hbar \omega \frac{1}{4} \sum_{\sigma} \left(\frac{1 + u \text{Re } \chi_{L0}^{\bar{\sigma}\bar{\sigma}}(0)}{1 - u^2 \text{Re } \chi_{L0}^{\sigma\sigma}(0) \text{Re } \chi_{L0}^{\bar{\sigma}\bar{\sigma}}(0)} \right)^2 v_{\sigma}^2(\mu) \quad (20)$$

resulting from (7) at small $\hbar\omega$, leads to the sharp increase of the enhancement.

The results of the calculation of the effective local spin moment $S_L(\omega)$ are represented in figures 3–5. As can be seen from the figures, the local spin moment in a wide energy interval varies only slightly with the increase of temperature. This is due to the fact that a decrease in the first term in (13) is compensated for by an increase in the second one. However, in a small energy interval such a compensation does not occur. Here the local moment depends strongly on the temperature, and the smaller the interval, the sharper the dependence.

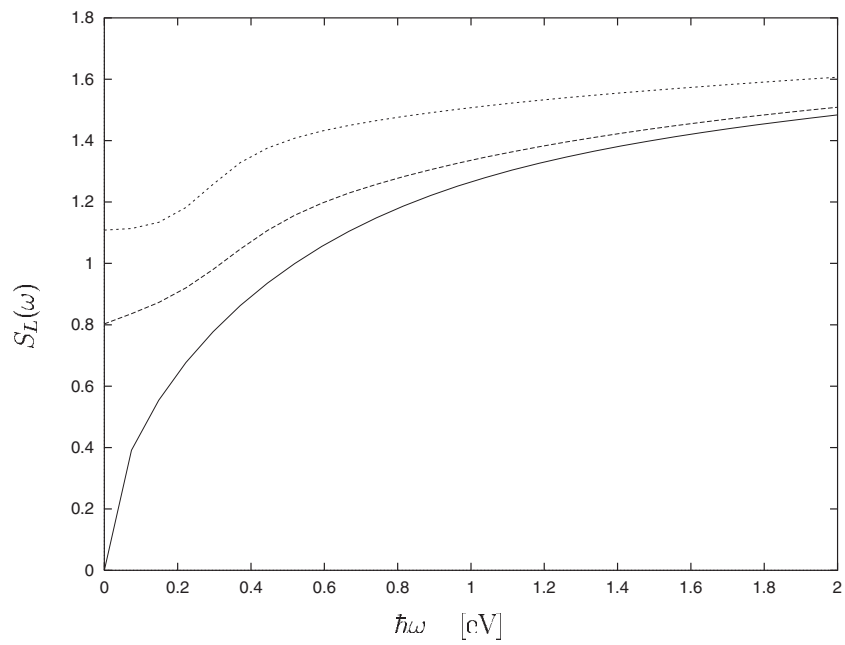


Figure 3. The effective local spin moment $S_L(\omega)$ in a frequency interval $[-\omega, \omega]$ for iron. (The notation is as for figure 1.)

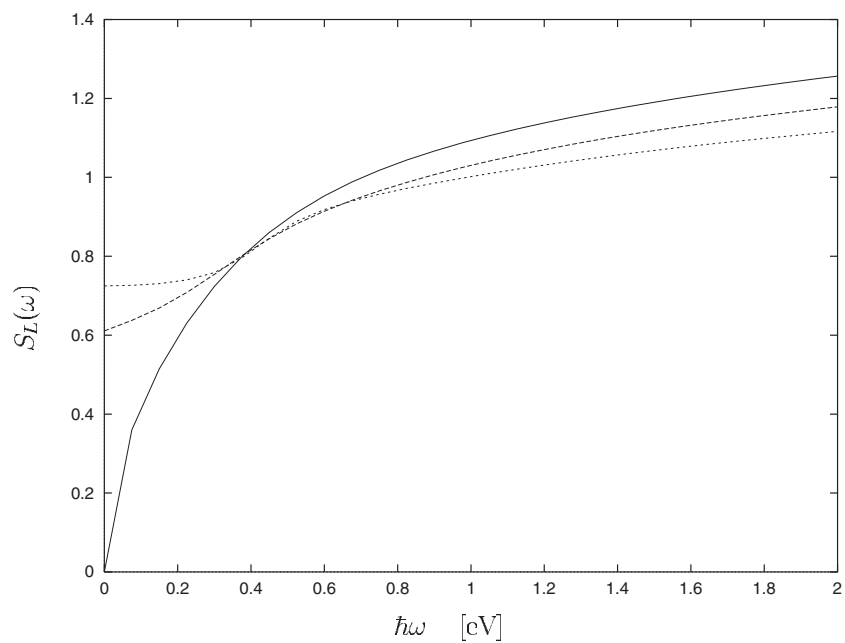


Figure 4. The effective local spin moment $S_L(\omega)$ in a frequency interval $[-\omega, \omega]$ for cobalt at $T/T_C = 0.0$ (\cdots), 0.78 ($---$), and 1.0 ($---$).

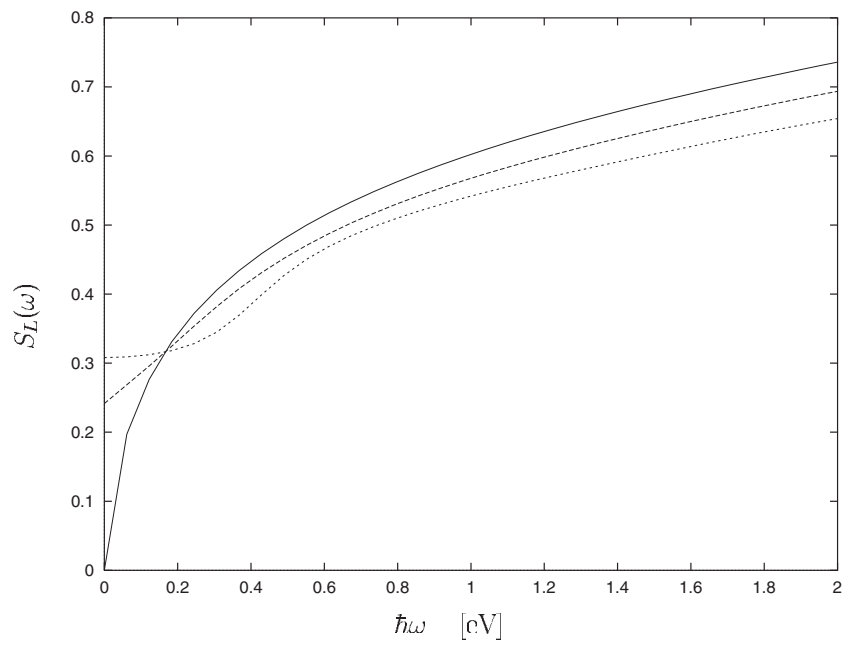


Figure 5. The effective local spin moment $S_L(\omega)$ in a frequency interval $[-\omega, \omega]$ for nickel at $T/T_C = 0.0$ (\cdots), 0.88 ($---$), and 1.0 ($—$).

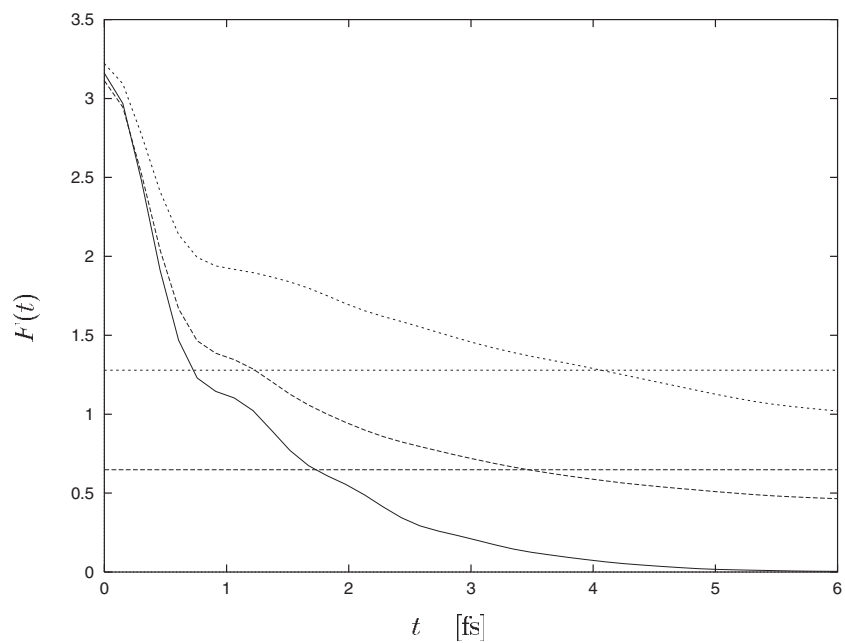


Figure 6. Time-dependent spin correlation function $F(t)$ for iron. The horizontal line indicates the asymptotic value $[(n_\uparrow - n_\downarrow)/2]^2$. (The notation is as for figure 1.)

Table 3. Calculated and experimental values of the square of the local spin moment for Fe, Co and Ni at the Curie temperature.

	Fe	Co	Ni
Hasegawa [31, 32]	3.6	—	0.2
Present calculation	3.16	2.20	0.81
Experiment [33]	2.45	2.45	0.65

For Fe at $T = T_C = 1.49T_C^{exp}$, the computed values 1.0 and 1.3 μ_B of the local magnetic moment $M_L = g\mu_B S_L$ in the energy intervals $\hbar\omega = 0.12$ and 0.2 eV agree fairly well with the experimental values 1.3 and 1.55 μ_B , obtained at $T = 1.25T_C^{exp}$ in [27, 28]. Note that the value of the local magnetic moment in the energy window 0.1 eV in our one-electron calculations [13] was only 0.36 μ_B , which is much less than the experimental value. A good agreement with the experimental data on the polarized neutron scattering is also obtained for nickel (the experimental data for Co are absent from the literature): the values of $M_L(\hbar\omega = 0.12 \text{ eV}) = 0.55 \mu_B$ and $M_L(\hbar\omega = 0.2 \text{ eV}) = 0.7 \mu_B$, computed at $T = T_C = 1.54T_C^{exp}$, are in good agreement with the values 0.6 and 0.9 μ_B , respectively, measured at $T = 2T_C^{exp}$ [10].

The results of the calculation of the local magnetic moment in the *infinite* energy interval, $M_L(T)/M_L(0)$, of Fe, Co and Ni by formula (13) are given in table 2. As can be seen from table 2, the local moment in the infinite energy interval depends only slightly on the temperature, being almost constant for Fe, and slightly increasing for Co and Ni. The fact that $\langle M_L^2 \rangle^{1/2}$ only slightly changes with temperature is supported by experiments on magnetovolume effect (see, e.g. [11, 29, 30] and references therein). Note that for Fe the weak change of the local magnetic moment with increasing temperature was obtained in other theoretical calculations as well. However, for Ni the calculated values of $M_L(T_C)/M_L(0)$ were nowhere near unity [30].

The results of the calculation of the time correlation function $F(t)$ for Fe, Co and Ni are represented in figures 6–8. As can be seen from figure 6, the square of the local spin moment $S_L^2 = F(t = 0)$ for iron at $T = 0$ equals 3.22, which almost coincides with the value 3.18 obtained in our one-electron calculation [12] using the constant-matrix-element approximation. At $T = T_C$, the square of the local spin moment of iron varies inconsiderably and reaches the value 3.16, which is close to the value $S_L^2 \simeq 3.6$ obtained by Hasegawa [31] in the two-field method at $T = 1.1T_C^{exp}$. For Co and Ni, the computed values of $S_L^2(T_C)$ are equal to 2.20 and 0.81, respectively. The latter value substantially differs from the value $S_L^2 \simeq 0.2$ obtained by Hasegawa [32] for Ni at $T = 1.1T_C^{exp}$. However, as can be seen from table 3, our values for $S_L^2(T_C)$ are in better agreement with the experimental values obtained from the relation $m_{eff} = g\mu_B\sqrt{S(S+1)}$ for the effective magnetic moment than the ones of Hasegawa [31, 32]. The estimate of the square of the local spin moment in the paramagnetic region using the formula $S_L^2 = S(S+1) = m_{eff}^2/(g\mu_B)^2$ for ferromagnetic metals is, of course, rough enough, but a better estimate is apparently not available.

As for the time correlation function $F(t)$ at $t \neq 0$, its fluctuating part $A(t)$ is large enough beyond the main maximum, determined by the bandwidth, as well. So, while, in iron at $T = 0$ in one-electron approximation, $A(t)$ vanishes during $t_0 \simeq 0.3$ fs (see footnote 3 in [15]), with account taken of spin fluctuations, it vanishes during 4 fs. With an increase of the temperature, the damping time of the local spin moment increases. This is due to the rise in the fluctuating part of the frequency correlation function $A(\omega)$ in the low-frequency region. According to (11), the temperature dependence of the function $A(\omega)$ is determined by two factors: the hyperbolic cotangent and the sum of the imaginary parts of the susceptibilities.

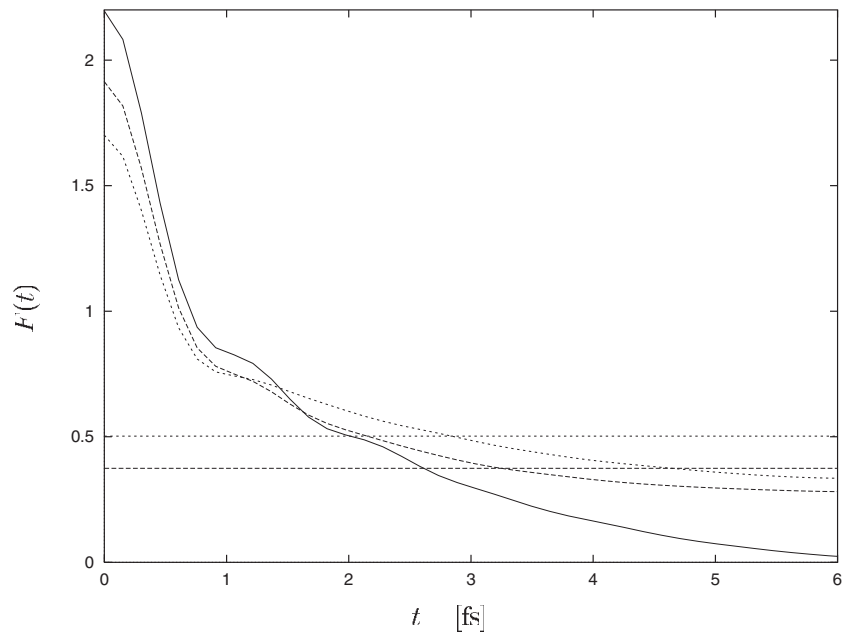


Figure 7. Time-dependent spin correlation function $F(t)$ for cobalt. The horizontal line indicates the asymptotic value $[(n_{\uparrow} - n_{\downarrow})/2]^2$ (the notation is as for figure 4).

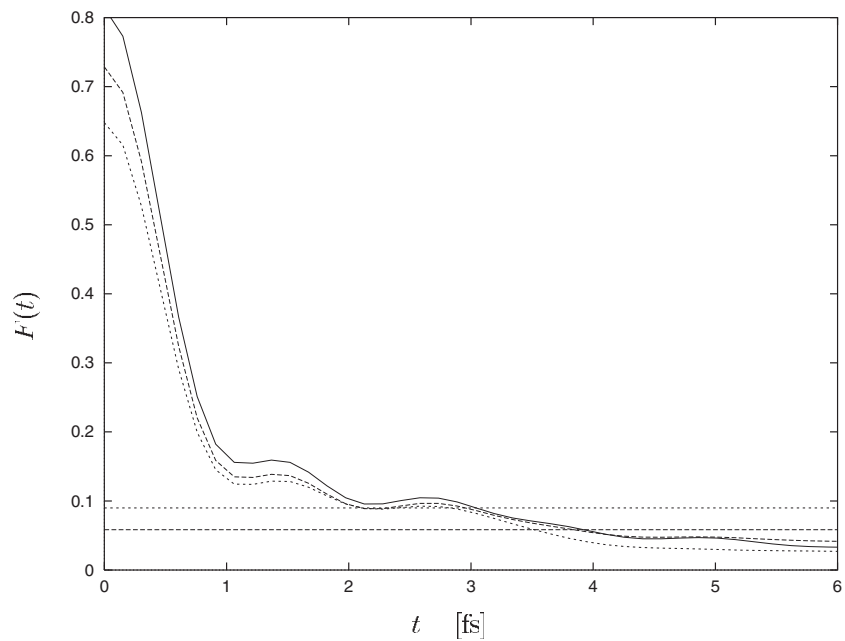


Figure 8. Time-dependent spin correlation function $F(t)$ for nickel. The horizontal line indicates the asymptotic value $[(n_{\uparrow} - n_{\downarrow})/2]^2$ (the notation is as for figure 5).

At the temperatures under consideration, the hyperbolic cotangent differs from unity only in the low-energy region: $\hbar\omega < 2T \sim 0.1$ eV. Outside this energy region, the temperature dependence of $A(\omega)$ is determined by the sum of the imaginary parts of the susceptibilities, whose behaviour is similar to $\text{Im } \chi_L^{zz}(\omega)$ represented in figure 2.

4. Conclusions

The numerical investigation of local magnetic characteristics of Fe, Co and Ni at finite temperatures using the mean single-site Green function, calculated self-consistently in the framework of the DNA of the SFT, has shown that correlation effects significantly change the local characteristics especially at low energies, and allowed us to obtain, for example, for the Fe local magnetic moment M_L at $T = T_C$ in the energy windows 0.12 and 0.2 eV, the values 1.0 and 1.3 μ_B , in accordance with values 1.3 and 1.55 μ_B , obtained in polarized neutron scattering experiments at $T = 1.25T_C$ [27, 28]. Note that the value of $M_L(\omega)$ in the energy window 0.1 in our one-electron calculations is only 0.36 μ_B , which is much less than the experimental one. Since for Fe and Ni the values of the local moment in the energy windows 0.12 and 0.2 eV are in good agreement with the experimental values, the results of our calculation can be considered as predictive for future experiments on neutron scattering for Fe, Co and Ni in sufficiently large energy windows.

The value of $M_L(T_C)/M_L(0)$ for Ni is near unity in full agreement with experimental data on the magnetovolume effect, whereas in previous treatments it is substantially smaller (see table 1 of [30]).

The calculated damping time for the spin correlation function is one order greater than the electron hopping time, but is still less than the characteristic value determined by the Curie temperature: $\tau \sim \hbar/T_C \sim 10^{-13}$ s.

Finally, note that the present calculation gives clear evidence that the DNA of the SFT is valid for adequate description of the local magnetic characteristics of ferromagnetic metals at finite temperatures. In a future paper, we intend to use this approach for the numerical calculation of the temperature dependence of the local magnetic moments in Fe–Ni invar alloys, which have attracted increasing interest recently (see, e.g. [34–37] and references therein).

Acknowledgments

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