Effect of lattice vibrations on magnetic properties of metals at finite temperatures

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Abstract. We investigate the effect of electron-phonon interaction in the dynamic spin-fluctuation theory of metallic magnetism. Electron-phonon interaction is represented by fluctuations of the crystal lattice potential. We illustrate the theoretical results in the example of Fe and Ni. We show that the effect of phonons on temperature dependence of magnetic characteristics is appreciable in Fe, but not as large as in the static single-site spin-fluctuation theory and spin dynamics using classical Hamiltonians. On the contrary, in Ni the effect of phonons is small in agreement with the results of the spin dynamics.

1. Introduction

Temperature dependence of magnetic properties in transition metals is mostly determined by the 3d electron spin fluctuations. All spin fluctuation theories (SFT) ignore the electron-phonon interaction and use the Debye-Waller factor (DWF) to compare the results with neutron scattering experiments [1]. In [2] the electron-phonon interaction was studied using the random-phase approximation (RPA), which is not enough at finite temperatures. Effect of lattice vibrations in the static single-site SFT was estimated in [3]. In Fe the estimates imply a reduction in the Curie temperature by up to 20% [4]. Self-consistent calculations of the lattice and magnetic subsystems were carried out in spin dynamics using effective Hamiltonians with classical spins [5–8], but results of these papers depend on realization of the disordered local moments approach [9] and do not agree with each other even in Fe.

We present a microscopic description of the electron-phonon interaction in the dynamic spin-fluctuation theory (DSFT) of metallic magnetism [10]. We obtain an expression that relates the self-energy part with thermal spin and lattice fluctuations. Temperature dependence of the lattice fluctuation is determined by the mean squared atomic displacement. The latter is calculated in the harmonic approximation using the realistic phonon density of states obtained from the neutron scattering measurements. The theory is illustrated in the example of bcc Fe and fcc Ni.
2. Electron-phonon interaction in DSFT

2.1. Self-energy part

In the DSFT, we consider the Hamiltonian of the system of interacting electrons \( \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \).

The first term describes the kinetic and potential energies of the electrons:

\[
\mathcal{H}_0 = \sum_{i=1}^{N_e} \left( -\frac{\hbar^2}{2m_e} \nabla_i^2 + \sum_{j=1}^{N} U(r_i - R_j) \right),
\]

where \( U(r_i - R_j) \) is the potential energy of the \( i \)th electron in the field of the \( j \)th ion (\( m_e \) is the electron mass, \( N_e \) is the number of electrons and \( N \) is the number of ions). The term \( \mathcal{H}_1 \) describes the electron-electron interaction.

We now assume that each lattice site can be displaced by vector \( u_j \) from the equilibrium position \( R_j \). Replacing \( R_j \) with \( R_j + u_j \) and using linear approximation in displacements \( u_j \), we obtain

\[
\sum_{ij} U(r_i - R_j - u_j) = \sum_{ij} U(r_i - R_j) - \sum_{ij} u_j \nabla U(r_i - R_j).
\]

The first term enters \( \mathcal{H}_0 \) and determines the electron energy spectrum. The second term,

\[
W = -\sum_{i=1}^{N_e} \sum_{j=1}^{N} u_j \nabla U(r_i - R_j),
\]

describes the electron-phonon interaction. The Hamiltonian of the system takes the form \(^1\)

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + W.
\]

As a result of the Stratonovich-Hubbard transformation \([1]\), we come to the system of noninteracting electrons in the exchange field \( V \) with the Hamiltonian

\[
\mathcal{H}(V) = \mathcal{H}_0 + V + W.
\]

The Green function corresponding to this system is

\[
G(V) = (z + \mu - \mathcal{H}(V))^{-1},
\]

where \( z = \varepsilon - i0^+ \) and \( \mu \) is the chemical potential. The initial system of interacting electrons is described by the mean Green function \( \bar{G} \equiv \langle G(V) \rangle \), where the average is carried out over the \( V \) and \( W \) configurations. The mean Green function can be expressed in the form

\[
\bar{G} = (z + \mu - \mathcal{H}_0 - \Sigma)^{-1},
\]

where \( \Sigma \) is the self-energy part (SEP). The equation for the fluctuation contribution to the SEP \( \Delta \Sigma = \Sigma - \bar{V} \) is obtained similarly to the case of the rigid lattice \([1]\) if we replace \( V \) by \( V + W \) and use the second-order perturbation theory. We represent \( \Delta \Sigma \) as the sum of two terms:

\[
\Delta \Sigma = \langle \Delta V (1 - \bar{G}(\Delta V - \Delta \Sigma))^{-1} \rangle + \langle W (1 - \bar{G}(W - \Delta \Sigma))^{-1} \rangle,
\]

where \( \Delta V = V - \bar{V} \) is the exchange field fluctuation (for details, see \([10]\)). The first term \( \Delta \Sigma^{sp} \) describes contribution from the spin fluctuations and is treated as in the DSFT \([1]\). The

\(^1\) We investigate the effect of phonons on electrons. We neglect the effect of the electronic subsystem on the lattice vibrations, just as in \([3]\).
second term $\Delta \Sigma_{ph}$ describes contribution from the phonons. Retaining only linear and quadratic in $W$ terms and using $\langle W \rangle = 0$, we obtain $\Delta \Sigma_{ph} = \langle WGW \rangle$. Since the Wannier functions $w_j(\mathbf{r}) = w(\mathbf{r} - \mathbf{R}_j)$ are localized at lattice sites, $W$ is site-diagonal:

$$W_j = -u_j \cdot \mathbf{J}, \quad \mathbf{J} \equiv \int w^*(\mathbf{r})\nabla_r U(\mathbf{r})w(\mathbf{r})\, d\mathbf{r},$$  (1)

just as the exchange potential $V$. Therefore, proceeding similarly to [1], in the momentum representation we obtain

$$\Delta \Sigma_{ph}^k(z) = \sum_q \langle W_q \tilde{G}_{k-q}(z)W_{-q} \rangle.$$

Next we apply the single-site approximation. We replace the Green function $\tilde{G}_{k-q}(z)$ by the single-site Green function $g(z) = N^{-1} \sum_k \tilde{G}_{k}(z)$, and SEP $\Sigma_{ph}(z)$ by the coherent potential $\Sigma(z) = N^{-1} \sum_k \Sigma_k(z)$. Then the expression for phonon contribution (2) takes the form [3,10]

$$\Delta \Sigma_{ph}^k(z) = g(z) \langle W^2 \rangle,$$

where

$$\langle W^2 \rangle = \sum_q \langle |W_q|^2 \rangle = \frac{1}{N} \sum_j \langle W_j^2 \rangle.$$

In the absence of correlations of atomic displacements in different directions, using relation (1), we come to

$$\langle W^2 \rangle = \frac{1}{3} J^2 \langle u^2 \rangle,$$

where $J^2$ is squared gradient of the cellular potential.

2.2. Mean-squared atomic displacement

Temperature dependence of the lattice fluctuation (4) is determined by the mean-squared atomic displacement $\langle u^2 \rangle$, which can be calculated in the harmonic or anharmonic approximation.

In the harmonic approximation, the mean-squared displacement is given by (see, e.g., [11])

$$\langle u^2 \rangle = \frac{3\hbar}{2M} \int \frac{1}{\omega} \coth \left( \frac{\hbar \omega}{2k_B T} \right) g(\omega)\, d\omega,$$

where $g(\omega)$ is the phonon density of states (DOS), $M$ is the atomic mass and $T$ is temperature (in units of K).

The simplest way of calculating $\langle u^2 \rangle$ is to use the Debye phonon DOS $g_D(\omega) = 3\omega^2/\omega_D^3$, $0 \leq \omega \leq \omega_D$, where $\omega_D$ is the Debye frequency. In this case, expression (5) takes the form

$$\langle u^2 \rangle = \frac{9\hbar}{2M \omega_D^3} \int_0^{\omega_D} \omega \coth \left( \frac{\hbar \omega}{2k_B T} \right)\, d\omega.$$

Passing to the dimensionless variable $x = \hbar \omega/k_B T$ in the integral, we obtain

$$\langle u^2 \rangle = \frac{9\hbar^2}{2Mk_B \Theta_D x_D} \int_0^{x_D} x \coth(x/2)\, dx,$$

where $x_D = \Theta_D/T$ ($\Theta_D$ is the Debye temperature determined by the relation $\hbar \omega_D = k_B \Theta_D$). Using the identity $\coth(x/2) = 1 + 2/(e^x - 1)$, we come to the formula in the Debye model

$$\langle u^2 \rangle = \frac{9\hbar^2}{Mk_B \Theta_D} \left( \frac{1}{4} + \frac{\Phi(x_D)}{x_D} \right), \quad \Phi(x_D) \equiv \int_0^{x_D} \frac{x}{e^x - 1}\, dx.$$  (6)
At $T \ll \Theta_D$ we have $\Phi(x_D)/x_D^2 \to 0$, and the mean-squared displacements at $T = 0$ is given by the formula (the effect of zero-point vibrations)

$$\langle u^2 \rangle_0 = \frac{9h^2}{4Mk_B\Theta_D}.$$  

At $T \gg \Theta_D$ we have $x_D \to 0$ and $\Phi(x_D)/x_D^2 \sim x_D^{-1} = T/\Theta_D$. As a result, we obtain linear temperature dependence of the mean-squared displacements at $T \gg \Theta_D$:

$$\langle u^2 \rangle = \frac{9h^2T}{Mk_B\Theta_D^2}. \tag{7}$$

Instead of the Debye phonon DOS one can use a realistic phonon DOS calculated from the phonon spectrum measurements in the neutron scattering experiment. In this case, it is necessary to directly calculate integral (5) using the table-valued function $g(\omega)$.

The anharmonic approximation [12] allows to take into account the corrections due to thermal expansion and fourth-order term in the crystal lattice potential $^2$. In [14] the following formula was obtained for the mean-squared displacement

$$\langle u^2 \rangle_{\text{anh}} = \langle u^2 \rangle_h \left[1 + T \left(2\chi\gamma_G - 20k_B\gamma_0o_0^{-2}\right)\right], \tag{8}$$

where $\langle u^2 \rangle_h$ is the mean-squared displacement in the harmonic approximation, $\chi$ is the thermal expansion coefficient (in units of $K^{-1}$), $\gamma_G$ is the (dimensionless) Grüneisen coefficient, $\gamma_0$ is the anharmonic parameter (in units of eV·Å$^{-4}$) and $\alpha_0$ is the coefficient of proportionality at $T$ in formula (7) for $\langle u^2 \rangle_h$ (in units of eV·Å$^{-2}$). The parameters $\chi$ and $\gamma_G$ are table-valued, and parameter $\gamma_0$ is taken in such a way as to make the curve $\langle u^2 \rangle_{\text{anh}}$ pass through the experimental point at the highest temperature.

2.3. Computational formulae

For calculating magnetic characteristics we use the local Gaussian approximation of the DSFT [1]. The equations with respect to the chemical potential $\mu$, mean field $\bar{V}$, transverse $\zeta^{\text{dp}} = \langle \Delta V^2 \rangle'$ and longitudinal $\zeta^{\text{dp}} = \langle \Delta V^2 \rangle'$ local spin fluctuations remain unchanged. Taking (3) into account, we write the equation for the coherent potential in the form $^3$

$$\Delta \Sigma_\sigma(z) = \frac{g_\sigma(z)\zeta^{\text{dp}}}{1 + 2\sigma V^2 g_\sigma(z)} + 2g_\sigma(z)\zeta^{\text{sp}} + g_\sigma(z)\zeta^{\text{ph}}, \tag{9}$$

where $\bar{\sigma} = -\sigma$. Here, $\zeta^{\text{ph}} \equiv \langle W^2 \rangle$ is lattice fluctuation, and the local Green function is calculated by the formula

$$g_\sigma(z) = \int \frac{\nu(\varepsilon')}{z - \sigma V^2 - \Delta \Sigma_\sigma(z) - \varepsilon'} d\varepsilon', \tag{10}$$

where $\nu(\varepsilon')$ is the nonmagnetic electron DOS of the d band at $T = 0$. The quantity $\langle W^2 \rangle$ is calculated by formula (4). An average of the squared gradient of the cellular potential $J^2$ is estimated as $\langle J^2 \rangle = \eta/n(\varepsilon_F)$, where $\eta$ is the Hopfield parameter and $n(\varepsilon_F)$ is the value of the electron DOS at the Fermi level (for details, see [1]).

$^2$ Thermal expansion also modifies the lattice potential and hence modifies the electron and phonon spectra. This is left for further study.

$^3$ For the spin contribution $\Delta \Sigma^{sp}$ we use a more accurate expression in the second-order with respect to $\Delta V$ and infinite order with respect to $\bar{V}$ that takes into account the asymmetry of the exchange potential distribution along the magnetization direction (for details, see [1]).
Calculation in the DSFT with phonons reduces to finding the quantities $\mu$, $\bar{V}^z$, $\zeta^x$ and $\zeta^z$ at each temperature. We solve a system of equations only with respect to the four variables $\mu$, $\bar{V}^z$, $\zeta^x$ and $\zeta^z$ choosing a sufficiently small step in temperature and taking the values from the previous step as the initial guess. In the DSFT [1], the functions $\Delta \Sigma_\sigma(z)$ and $g_\sigma(z)$ for current values of $\mu$, $\bar{V}^z$, $\zeta^x$ and $\zeta^z$ were updated by formulae (10) and (9) only once, starting from $\Delta \Sigma_\sigma(z) = 0$. In iron and some of its alloys, this leads to hysteresis in temperature dependence of magnetic characteristics at high temperatures [14]. In this paper, the functions $\Delta \Sigma_\sigma(z)$ and $g_\sigma(z)$ are recalculated by formulae (10) and (9) until the self-consistency is achieved (for details, see [15]). This removes the temperature hysteresis and gives a proper temperature dependence without applying high-order terms in the free energy [16].

3. Numerical results

First, we illustrate the theoretical results in the example of bcc Fe. The initial data for the DSFT calculation are the value of the magnetic moment $m(0) = 2.217 \mu_B$ [17] and the first-principle electron DOS at $T = 0$. The DOS of nonmagnetic Fe is calculated by the Korringa-Kohn-Rostoker method with a self-consistent potential taken from [18]. The DOS of the d band is next smoothed using the Lorentzian function with the halfwidth $\delta = 0.005$ to take the damping of one-electron states into account (see, e.g., [19]). The effective interaction constant $u$ determined from the DSFT equations at $T = 0$ is equal to 1.07 eV.

The additional initial data for taking phonons into account are the phonon DOS and the average of the mean-squared gradient of the cellular potential $\langle J^2 \rangle$. The phonon DOS for Fe was calculated based on the neutron scattering results in [20] (we use the tabular data from [21]). The Hopfield parameter for Fe is $\eta = 5.62$ eV/Å² [22]. The value of the electron DOS at the Fermi level for Fe is $n(\varepsilon_F) = 1.92$ eV$^{-1}$ [23]. Hence $\langle J^2 \rangle = 2.93$ eV²/Å².

In figure 1a, we present the calculation results for temperature dependence of magnetic characteristics, where the lattice fluctuation $\zeta^{ph}$ is calculated using formula (5) in the harmonic approximation with a realistic phonon DOS. Also, for comparison, we present the DSFT results without lattice vibrations. As can be seen from figure 1a, lattice vibrations have a dual effect. In addition to explicit contribution to the SEP, lattice vibrations lead to an enhancement of the spin fluctuations in the ferromagnetic state and their weakening in the paramagnetic state.

**Figure 1.** Magnetization $m/m_0$ (-----), spin fluctuations $\zeta^x$ (-----) and $\zeta^z$ (-----) in units of $\bar{V}^z(0)$, local magnetic moment $m_L/m_0$ (-----) and inverse paramagnetic susceptibility $\chi^{-1}$ (-----) in units of $T_C^{\exp}/\mu_B^2$ for (a) Fe and (b) Ni calculated in the Gaussian approximation of the DSFT. Red lines show results of the DSFT with phonons, where the lattice fluctuation $\zeta^{ph}$ (-----) in units of $\bar{V}^z(0)$ is calculated in the harmonic approximation (5) with a realistic phonon DOS.
Taking lattice vibrations into account in the DSFT for Fe has a substantial effect on magnetic characteristics at high temperatures (Table 1). For instance, the calculated Curie temperature $T_C$ decreases by about 8%. However, this variation is almost twice as low as estimated in the static single-site SFT [3] and more than three times lower compared to the one obtained in [7]. The local magnetic moment $m_L$ in the paramagnetic state decreases only by 2% in contrast to about 10% in calculations using the effective Heisenberg Hamiltonian [6]. The paramagnetic Curie temperature $\Theta_C$ decreases by 6% and the effective moment $m_{\text{eff}}$ in the Curie-Weiss law decreases by 12%. For all above-mentioned characteristics the electron-phonon interaction taken into account in the DSFT leads to a better agreement with experiment. The effect of phonons in the DSFT is weakly dependent on temperature in contrast to the correction from the Debye-Waller factor, which increases with temperature above $T_C$.

Table 1. Ferromagnetic $T_C$ and paramagnetic $\Theta_C$ Curie temperatures, effective $m_{\text{eff}}$ and local $m_L(T_C)$ magnetic moments for Fe calculated in the DSFT with phonons taken into account in different approximations.

| DSFT            | $T_C/T_C^{\text{exp}}$ | $\Theta_C/T_C^{\text{exp}}$ | $m_{\text{eff}}/m_{\text{eff}}^{\text{exp}}$ | $m_L(T_C)/m_L(0)$ |
|-----------------|------------------------|------------------------------|-----------------------------------------------|-------------------|
| GA             | 1.64                   | 1.74                         | 1.23                                          | 1.09              |
| GA+Harm.       | 1.51                   | 1.64                         | 1.08                                          | 1.07              |
| GA+Debye       | 1.50                   | 1.64                         | 1.05                                          | 1.07              |
| GA+Anharm.     | 1.47                   | 1.61                         | 0.98                                          | 1.06              |

For comparison, we carried out calculations with the mean-squared displacement $\langle u^2 \rangle$ in expression (4) calculated by formula (6) in the Debye model and by formula (8) in the anharmonic approximation (figure 2a). In the Debye model, the temperature dependence of magnetic characteristics stays practically unchanged (for details, see [10]).

In the anharmonic approximation, the parameters for Fe in formula (8) were taken from [13]. The anharmonic contribution to the mean-squared displacement becomes substantial at high temperatures (figure 2a). For instance, at $T/T_C^{\text{exp}} = 1.5$ it is about 30%. However, the anharmonicity does not lead to serious changes in the temperature dependence of magnetic
characteristics. The value of $T_C$ in Fe decreases by 3%, paramagnetic Curie temperature $\Theta_C$ by 2%, and local magnetic moment $m_L$ in the paramagnetic state only by 1% compared to the harmonic approximation (see Table 1). Most of all, taking the anharmonicity in the DSFT into account affects the effective moment $m_{\text{eff}}$ and leads to its reduction by 9% compared to the harmonic approximation.

For Ni the value of the magnetic moment is $0.616 \mu_B$ [17] and electron DOS of nonmagnetic Ni is taken from [18]. The DOS of the d band is next smoothed using the Lorentzian function with the halfwidth $\delta = 0.005$. The effective interaction constant $u$ determined from the DSFT equations at $T = 0$ is equal to 1.02 eV. The additional initial data for taking phonons into account are the phonon DOS and mean-squared gradient of the cellular potential. The phonon DOS was calculated based on the neutron scattering results in [26] (we use the tabular data from [21]). The Hopfield parameter for Ni is $\eta = 1.76 \text{ eV/\AA}^2$ [22] and value of the electron DOS at the Fermi level is $n(\varepsilon_F) = 2.0 \text{ eV}^{-1}$ [23]. Thus, $\langle J^2 \rangle = 0.88 \text{ eV}^2/\text{\AA}^2$.

As we see from Table 2, the ratio of the lattice fluctuation $\zeta_{\text{ph}}$ to the spin fluctuation $\zeta_{\text{sp}} = 2\zeta_{\text{sp}}^x + \zeta_{\text{sp}}^z$ is larger in Ni than in Fe: 7% in Ni vs. 4% in Fe at $T_C^{\text{cal}}$ and 18% in Ni vs. 7% in Fe at $2T_C^{\text{cal}}$. But the effect of lattice vibrations on magnetic properties in Ni is smaller: of about 1–2% for all magnetic characteristics (figure 1b). These results are in agreement with the Curie temperature calculations obtained from the spin dynamics [7,8]. Our calculations show that use of the Debye model or anharmonic approximation brings some differences in the mean-squared displacement (figure 2b) but does not change the results for magnetic characteristics.

**Table 2.** Lattice fluctuation $\zeta_{\text{ph}}$ and spin fluctuation $\zeta_{\text{sp}}$ (in units of $\bar{V}_z^2(0)$) calculated for Fe and Ni in the DSFT with phonons.

|          | Fe | Ni |
|----------|----|----|
| $T_C^{\text{cal}}$ | 0.045 | 1.137 | 0.137 | 1.980 |
| $2T_C^{\text{cal}}$ | 0.090 | 1.239 | 0.274 | 1.521 |

4. Conclusion

We present dynamic spin fluctuation theory with thermal lattice fluctuations and apply it to Fe and Ni.

The effect of lattice vibrations on magnetic properties in Fe is substantial but not as large as predicted by the static single-site SFT and spin dynamics simulations. In the DSFT with phonons, the Curie temperature $T_C$ decreases by 8%, paramagnetic Curie temperatures by 6%, effective magnetic moment in the Curie-Weiss law by 12%, and local magnetic moment $m_L$ above the Curie temperature by only 2%, relative to the DSFT without phonons. For comparison we calculate the mean squared atomic displacement using (a) Debye model and (b) anharmonic approximation. If we replace the realistic phonon DOS by the Debye DOS, temperature dependence of the magnetic characteristics stays practically unchanged. In the anharmonic approximation, the mean squared atomic displacement increase substantially above $T_C$, but most of magnetic characteristics do not change much compared to the results in the harmonic approximation.

In contrast to Fe, the effect of lattice vibrations on magnetic properties in Ni is small: of about 1–2% for all magnetic characteristics, which is in agreement with the spin dynamics simulations. Calculation of the mean squared atomic displacement using Debye model or anharmonic approximation does not change the results.
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