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Spin-density correlations in the dynamic spin-fluctuation theory: Comparison with polarized neutron scattering experiments

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ABSTRACT

To study the spin-density correlations in the ferromagnetic metals above the Curie temperature, we relate the spin correlator and neutron scattering cross-section. In the dynamic spin-fluctuation theory, we obtain explicit expressions for the effective and local magnetic moments and spatial spin-density correlator. Our theoretical results are demonstrated by the example of bcc Fe. The effective and local moments are found in good agreement with results of polarized neutron scattering experiment over a wide temperature range. The calculated short-range order is small (up to 4 Å) and slowly decreases with temperature.

1. Introduction

Spin-fluctuation theories of metallic magnetism support the existence of the short-range order (SRO) above the Curie temperature in the ferromagnetic metals but there is no agreement about the extent of the SRO (see, e.g., [1]). The fluctuating-local-band theory [2,3] is based upon the existence of very strong SRO well above T_C but it is unlikely to apply to any real material [4]. The static spin-fluctuation theories [5,6] describe the paramagnetic phase as having no appreciable SRO outside the critical region. The situation is similar in the dynamic theories [7–9], all based on the single-site approximation. The dynamic spin-fluctuation theory (DSFT) [10–13] takes into account both single-site and nonlocal interactions without mapping of the itinerant-electron system onto an effective Hamiltonian with classical spins [8,14–17].

In the previous paper [18], we applied the DSFT to study the SRO. Here we present new theoretical results on the spin-density correlations in the DSFT and compare our calculations with polarized neutron scattering experiments [19,20], which play a major role in testing the theory.

The polarized neutron scattering experiments have been mainly interpreted using the spin-wave theory [19,21]. Analyzing the peak of the scattering function, the SRO of about 15–20 Å was obtained in the ferromagnetic metals. This interpretation was criticized because the peak position and width of the curve are about equal [22]. However, in [14,15] the authors still claim that spin wave excitations persist in paramagnetic bcc Fe above T_C.

Theoretical treatment of the neutron magnetic scattering for *itinerant-electron* magnets in literature is rather limited (see, e.g., [23,24]). Here, we fill in this gap by deriving an expression for the *magnetic* neutron scattering cross-section in the itinerant-electron theory.

Our theoretical results are demonstrated by the example of bcc Fe. We calculate the spin-density correlator as a function of distance and temperature and calculate its Fourier transform (effective moment) as a function of wavevector and temperature in a systematic way.[1] A number of magnetic characteristics, such as effective moment and local moment, are compared with experiment over a large temperature range.

The paper is organized as follows. In Section 2, we derive explicit expressions for the effective and local magnetic moments and spatial spin-density correlator in the DSFT. We show that, at high temperatures, the spin-density correlator reduces to the well-known Ornstein–Zernike form and the spin-correlator in the momentum representation is given by the Lorentzian function. In Section 3, we relate the *magnetic* neutron scattering cross-section to the energy-integrated scattering function. In Section 4, we present numerical results for bcc Fe and compare them with experiment. In Section 5, we summarize the present work.

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[1] For selected temperatures, calculations of the spin-density correlator and its Fourier transform in static and dynamic approximations of spin-fluctuation theory were carried out in [25] and [10,26], respectively.

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2. Spatial spin-density correlator

2.1. Spin-density correlations in metals

We consider the spatial correlator $\langle s^\alpha(\mathbf{r}) s^\alpha(0)\rangle$ of the spin-density operator $s^\alpha(\mathbf{r}) = \sum_i s_i^\alpha \delta(\mathbf{r} - \mathbf{r}_i)$, $\alpha = x, y, z$. Here, $s_i^\alpha = \frac{1}{2}\sigma_\alpha$ is the α component of the spin operator of the i-th electron (σ_α is the Pauli matrix), the angle brackets denote the canonical average $\langle\ldots\rangle = Z^{-1}\,\mathrm{Tr}(\ldots \mathrm{e}^{-H/T})$, where $Z = \mathrm{Tr}\,\mathrm{e}^{-H/T}$ is the partition function, H is the Hamiltonian of the system of interacting electrons, and T is temperature (in energy units).

The spatial Fourier transformation is defined by

$$s_{\mathbf{q}}^\alpha = \int s^\alpha(\mathbf{r}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{r}} \mathrm{d}\mathbf{r}, \quad s^\alpha(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{q}} s_{\mathbf{q}}^\alpha \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}},$$

where $V = N\Omega_{\mathrm{WS}}$ is the volume of the crystal (N is the number of unit cells and Ω_{WS} is the volume of the Wigner–Seitz cell). Translational invariance of the system leads to

$$\langle s^\alpha(\mathbf{r}) s^\alpha(\mathbf{r}')\rangle = \frac{1}{V^2}\sum_{\mathbf{q}} \langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle \mathrm{e}^{\mathrm{i}\mathbf{q}(\mathbf{r}-\mathbf{r}')}.$$

Transforming the sum into an integral over the Brillouin zone and replacing the latter by the equal-volume sphere with radius q_{B}, we have

$$\langle s^\alpha(\mathbf{r}) s^\alpha(0)\rangle = \frac{1}{2\pi^2 N\Omega_{\mathrm{WS}}}\int_0^{q_{\mathrm{B}}} \langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle \frac{q\sin(qr)}{r}\,\mathrm{d}q. \tag{1}$$

The local spin moment s_{L} is defined by the formula

$$s_{\mathrm{L}}^2 = \iint_{\mathrm{WS}} \langle \mathbf{s}(\mathbf{r})\mathbf{s}(\mathbf{r}')\rangle\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}', \tag{2}$$

where both integrals are taken over the same Wigner–Seitz cell. Replacing the integral by the value of the integrand at the site multiplied by the cell volume, we write formula (2) as

$$s_{\mathrm{L}}^2 = \Omega_{\mathrm{WS}}^2 \langle \mathbf{s}(\mathbf{R}_j)\mathbf{s}(\mathbf{R}_j)\rangle = \Omega_{\mathrm{WS}}^2 \langle \mathbf{s}(0)\mathbf{s}(0)\rangle. \tag{3}$$

Passing to the limit in (1) as $r \to 0$ and using $\sin(rq) \approx rq$, we have

$$\langle s^\alpha(0) s^\alpha(0)\rangle = \frac{1}{2\pi^2 N\Omega_{\mathrm{WS}}}\int_0^{q_{\mathrm{B}}} \langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle q^2\,\mathrm{d}q. \tag{4}$$

Substituting the latter into formula for the local moment (3) and taking into account $\Omega_{\mathrm{WS}} = (2\pi)^3/\Omega_{\mathrm{BZ}}$, we obtain

$$s_{\mathrm{L}}^2 = \frac{4\pi}{N\Omega_{\mathrm{BZ}}}\int_0^{q_{\mathrm{B}}} \langle \mathbf{s}_{\mathbf{q}}\mathbf{s}_{-\mathbf{q}}\rangle q^2\,\mathrm{d}q. \tag{5}$$

Thus, in order to calculate the spatial correlator and local moment, it is necessary to find the spin-density operator in the momentum representation $\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle$. In agreement with the fluctuation-dissipation theorem, the spin-density correlator $\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle$ is related to the imaginary part of the enhanced susceptibility $\chi_{\mathbf{q}}^\alpha(\varepsilon)$, in the units of $\frac{1}{2}g^2\mu_{\mathrm{B}}^2$ (g is the electron g-factor, and μ_{B} is the Bohr magneton), by

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{1}{2\pi}\int B(\varepsilon)\,\mathrm{Im}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)\,\mathrm{d}\varepsilon, \tag{6}$$

where $B(\varepsilon) = (\mathrm{e}^{\varepsilon/T} - 1)^{-1}$ is the Bose function (in the DSFT, we assume $\hbar = 1$).

Next, we derive an exact expression for $\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle$ in the DSFT and obtain its high-temperature approximation.

2.2. Spin-density correlator in the DSFT

In the DSFT, the enhanced susceptibility $\chi_{\mathbf{q}}^\alpha(\varepsilon)$ is expressed in terms of the unenhanced one $\chi_{\mathbf{q}}^{0\alpha}(\varepsilon)$ by the formula

$$\chi_{\mathbf{q}}^\alpha(\varepsilon) = \frac{\chi_{\mathbf{q}}^{0\alpha}(\varepsilon)}{1 - \tilde{u}\chi_{\mathbf{q}}^{0\alpha}(\varepsilon)}, \tag{7}$$

where $\tilde{u} = u/N$ is the Fourier transform of the effective interaction constant u. Due to strong localization of the Bose function at zero energy, we replace it and the susceptibility $\chi_{\mathbf{q}}^{0\alpha}(\varepsilon)$ by the Taylor series in ε. As a result, formula (6) takes the form:

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{T}{2\tilde{u}\lambda_{\mathbf{q}}^\alpha}\frac{2}{\pi}\arctan\frac{\tilde{u}\varphi_{\mathbf{q}}^\alpha \pi^2 T}{6\lambda_{\mathbf{q}}^\alpha},$$

where $\lambda_{\mathbf{q}}^\alpha = 1 - \tilde{u}\chi_{\mathbf{q}}^{0\alpha}(0)$ and $\varphi_{\mathbf{q}}^\alpha = \mathrm{d}\chi_{\mathbf{q}}^{0\alpha}(0)/\mathrm{d}\varepsilon$.

The interaction of the modes is taken into account by interpolating the static susceptibility $\chi_{\mathbf{q}}^{0\alpha}$ between the uniform susceptibility $\chi_0^{0\alpha}$ and local susceptibility $\chi_{\mathrm{L}}^{0\alpha} = N^{-2}\sum_{\mathbf{q}}\chi_{\mathbf{q}}^{0\alpha}$, i.e. the function $\lambda_{\mathbf{q}}^\alpha = 1 - \tilde{u}\chi_{\mathbf{q}}^{0\alpha}(0)$ is calculated by the formula [11]

$$\lambda_{\mathbf{q}}^\alpha = \lambda_0^\alpha + (\lambda_{\mathrm{L}}^\alpha - \lambda_0^\alpha)q^2/\overline{q^2}, \tag{8}$$

where $\overline{q^2} = 0.6q_{\mathrm{B}}^2$ is the average of q^2 over the Brillouin zone approximated by the equal-volume sphere. The function $\varphi_{\mathbf{q}}^\alpha$ is replaced, for simplicity, by its mean value $N\varphi_{\mathrm{L}}^\alpha$, where $\varphi_{\mathrm{L}}^\alpha = N^{-2}\sum_{\mathbf{q}}\varphi_{\mathbf{q}}^\alpha(0)$. The final expression for spin-density correlator (6) takes the form (for details, see [27])

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{NT}{2u\lambda_{\mathrm{L}}^\alpha}\frac{1}{a_\alpha^2 + b_\alpha^2(q/q_{\mathrm{B}})^2}\frac{2}{\pi}\arctan\frac{c_\alpha}{a_\alpha^2 + b_\alpha^2(q/q_{\mathrm{B}})^2}, \tag{9}$$

where

$$a_\alpha^2 = \lambda_0^\alpha/\lambda_{\mathrm{L}}^\alpha, \quad b_\alpha^2 = (1 - a_\alpha^2)/0.6, \quad c_\alpha = u\varphi_{\mathrm{L}}^\alpha \pi^2 T/(6\lambda_{\mathrm{L}}^\alpha).$$

2.3. High-temperature approximation

We consider the high-temperature approximation ($T \gg T_{\mathrm{C}}$). Using the explicit expression for the Bose function, we write spin-density correlator (6) as

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{1}{2\pi}\int \frac{1}{\mathrm{e}^{\varepsilon/T} - 1}\,\mathrm{Im}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)\,\mathrm{d}\varepsilon.$$

Taking into account $\mathrm{e}^{\varepsilon/T} \approx 1 + \varepsilon/\mathrm{T}$, we have

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{T}{2\pi}\int \frac{\mathrm{Im}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)}{\varepsilon}\,\mathrm{d}\varepsilon.$$

Using the Kramers–Kronig relation (see, e.g., [24])

$$\mathrm{Re}\,\chi_{\mathbf{q}}^\alpha(0) = \frac{1}{\pi}\int \frac{\mathrm{Im}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)}{\varepsilon}\,\mathrm{d}\varepsilon$$

and taking into account that $\mathrm{Im}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)$ is an odd function and $\mathrm{Re}\,\chi_{\mathbf{q}}^\alpha(\varepsilon)$ is an even one, we obtain the high-temperature (classical) version of the fluctuation–dissipation theorem:

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{T}{2}\chi_{\mathbf{q}}^\alpha(0). \tag{10}$$

Expressing the enhanced susceptibility in terms of the unenhanced one according to (7), we have

$$\langle s_{\mathbf{q}}^\alpha s_{-\mathbf{q}}^\alpha\rangle = \frac{T}{2}\frac{\chi_{\mathbf{q}}^{0\alpha}(0)}{1 - \tilde{u}\chi_{\mathbf{q}}^{0\alpha}(0)} = \frac{T}{2\tilde{u}}\frac{1}{1 - \tilde{u}\chi_{\mathbf{q}}^{0\alpha}(0)} - \frac{T}{2\tilde{u}}.$$

Neglecting the second term, which is responsible for the intrinsic fluctuations of the field (for details, see [13]), and using (8), we obtain the Lorentzian function