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Magnetization and magnetic entropy change of a three-dimensional isotropic ferromagnet near the Curie temperature in the random phase approximation

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ABSTRACT

The behavior of a three-dimensional isotropic Heisenberg ferromagnet in the presence of a magnetic field H is investigated in the random phase approximation (RPA) near the Curie temperature T_c. It is shown that the magnetization M at the Curie temperature T_c is described by the law $M(T=T_c)\sim H^{1/5}$ and the initial magnetic susceptibility χ_0 at temperatures $T\geq T_c$ is given by $\chi_0(T\geq T_c)\sim(T-T_c)^{-2}$. It means that in the RPA the critical exponents for a three-dimensional Heisenberg ferromagnet coincide with the critical exponents for the Berlin-Kac spherical model of a ferromagnet rather than with the critical exponents of the mean field approximation (MFA). Hence it follows as well that, when a magnetic field H is risen from $H=0$ to $H=H_a$, the magnetic entropy S_M will be decreased as $\Delta S_M(T=T_c)\sim -H_a^{4/5}$ at the Curie temperature T_c and as $\Delta S_M(T>T_c)\sim -(T-T_c)^{-3}H_a^2$ at temperatures $T>T_c$.

1. Introduction

The magnetocaloric effect in ferromagnets has attracted recently considerable attention both from the fundamental point of view and from the viewpoint of its practical applications [1–3]. Technical use of this effect is based on a cyclic process, which includes the isothermal magnetic entropy change ΔS_M upon magnetic field increase from H_1 to H_2 as well as adiabatic temperature change ΔT_{ad} upon magnetic field decrease from H_2 to H_1. In order to calculate the magnetic entropy change ΔS_M upon magnetic field variation from H_1 to H_2, it is necessary to know the temperature and field dependence of the magnetization $M(T,H)$ [3]:

$$\Delta S_M(T,H_2-H_1)=S_M(T,H_2)-S_M(T,H_1)=\int_{H_1}^{H_2}\left(\frac{\partial M(T,H)}{\partial T}\right)_H dH. \quad (1)$$

For obtaining $M(T,H)$ in low-dimensional magnetic systems rather sophisticated theoretical methods are used (see, for example Ref. [4]). At the same time the simplest method, namely, the mean field approximation (MFA) is used as a rule for describing $M(T,H)$ in three-dimensional ferromagnets, in which the magnetocaloric effect has a maximum in the vicinity of the Curie temperature T_c [5,6].

The shortcomings of the MFA are well known. Firstly, the MFA cannot describe correctly the low-temperature magnetization of ferromagnets in the magnetically ordered state since it does not take into consideration spin-wave excitations. Secondly, the MFA falls to account for a short-range magnetic order in the paramagnetic state of ferromagnets above the Curie temperature T_c. It is evident that neglect of the short-range magnetic order may introduce considerable errors in evaluating the magnetic entropy neat T_c.

Therefore, it is worthwhile to use a more advanced approximation—the random phase approximation (RPA) [7–9] which enables to take into account both spin waves at low temperatures and effects of the short-range magnetic order in the paramagnetic temperature region. The advantages of the RPA have been successfully displayed [10] in case of isotropic one- and two-dimensional ferro- and antiferromagnetic systems, which exhibit the short-range magnetic order in the paramagnetic state at finite temperatures $T\neq 0$, since the long-range magnetic order in these systems occurs only at $T=0$. In Ref. [10] spin–spin correlation functions, which describe the short-range magnetic order for the relevant systems in an explicit form, as well as the magnetic susceptibility has been investigated in the framework of the RPA, and the results were in very good agreement with such elaborate theoretical approximations as large-N theory and the renormalization group approach.

As regards the RPA studies of the three-dimensional ferromagnets, major efforts in these investigations have been aimed at calculating the magnetization $M(T,H)$ in the low-temperature

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region [8,9]. As a result, only the expression for the Curie temperature T_c and the high-temperature series expansion of the susceptibility $\chi(T \gg T_c)$ have been obtained at high temperatures [8,9]. The field and temperature dependence of the magnetization $M(T,H)$ as well as the similar dependence of the magnetic entropy $S_M(T,H)$ for three-dimensional ferromagnets have not been examined thoroughly in the immediate vicinity of T_c in the framework of the RPA. Hence these issues will be the main subject of our paper. One would expect that the RPA for three-dimensional ferromagnets in the paramagnetic state near $T_c \neq 0$, analogously to the RPA for one- and two-dimensional magnetic systems near $T_c = 0$ [10], will give a more exact description of the magnetization $M(T,H)$ and the magnetic entropy $S_M(T,H)$ as compared to the MFA.

2. Calculations of the magnetization near T_c

For obtaining the magnetization $M(T,H)$ in a system of N localized magnetic moments with isotropic exchange interactions it is necessary to know the thermodynamic average value of the Z spin projection $\sigma \equiv \langle S_n^z \rangle$ on the magnetic field H direction:

$$M(T,H) = N\mu_0 \langle S_n^z \rangle \equiv N\mu_0 \sigma \tag{2}$$

(here $\mu_0 = g\mu_B$, g—the Lande factor, μ_B—the Bohr magneton).

The Hamiltonian of the isotropic Heisenberg ferromagnet with the exchange interaction $J > 0$ of the z nearest neighbors is

$$\mathcal{H} = -\mu_0 H \sum_{n=1}^{N} S_n^z - \frac{1}{2} J \sum_{n=1}^{N} \sum_{\Delta=1}^{z} \mathbf{S_n S_{n+\Delta}}. \tag{3}$$

A self-consistent equation for σ, corresponding to the Hamiltonian (3), can be obtained in the framework of the RPA, using the method of the double-time-temperature spin Green functions and the so-called Tyablikov decoupling [7–9]. For arbitrary quantum spin S this equation has the form [7–11]:

$$\sigma = \frac{(S-\Phi)(1+\Phi)^{2S+1} + (S+1+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1} - \Phi^{2S+1}}, \tag{4}$$

where

$$\Phi = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\exp(E_{\mathbf{k}}/k_BT) - 1}, \quad E_{\mathbf{k}} = \mu_0 H + Jz\sigma(1-\gamma_{\mathbf{k}}),$$
$$\gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\Delta} \exp(i\mathbf{k}\Delta). \tag{5}$$

For the linear ferromagnetic chain and the square ferromagnetic lattice the behavior of $\sigma(T,H) \sim M(T,H)$ and, respectively, $\chi(T)$ for $T > 0$ has been investigated in Ref. [10] with the help of Eq. (4). In order to solve this task for the three-dimensional ferromagnetic lattices it is useful in Eq. (4) to introduce a quantity

$$\Gamma = \frac{1}{N}\sum_{\mathbf{k}} \coth\left(\frac{E_{\mathbf{k}}}{2k_BT}\right), \tag{6}$$

connected with Φ by the relation

$$\Phi = \tfrac{1}{2}(\Gamma - 1). \tag{7}$$

Substituting Eq. (7) in Eq. (4) gives

$$\sigma = \frac{1}{2}\frac{(2S+1-\Gamma)(\Gamma+1)^{2S+1} + (2S+1+\Gamma)(\Gamma-1)^{2S+1}}{(\Gamma+1)^{2S+1} - (\Gamma-1)^{2S+1}}. \tag{8}$$

At high temperatures, near the Curie temperature T_c, when $\mu_0 H/k_BT \ll 1$ and $Jz\sigma/k_BT \ll 1$, it follows from Eq. (5) that $E_{\mathbf{k}}/2k_BT \ll 1$ and, correspondingly, $\Gamma \gg 1$. Then Eq. (8) can be expanded in powers of $1/\Gamma \ll 1$:

$$\sigma \approx \frac{2S(S+1)}{3\Gamma} - \frac{2S(S+1)(2S-1)(2S+3)}{45\Gamma^3} + \cdots. \tag{9}$$

In its turn, expanding $\coth(E_{\mathbf{k}}/2k_BT)$ in Eq. (6) in powers of $E_{\mathbf{k}}/2k_BT \ll 1$, one can obtain

$$\Gamma \approx \frac{1}{N}\sum_{\mathbf{k}}\left[\left(\frac{2k_BT}{E_{\mathbf{k}}}\right) + \left(\frac{E_{\mathbf{k}}}{6k_BT}\right) + \cdots\right]$$
$$\approx \frac{2k_BT}{Jz\sigma}\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{1+\mu_0 H/Jz\sigma - \gamma_{\mathbf{k}}} + \frac{Jz\sigma + \mu_0 H}{6k_BT}$$
$$= \frac{2k_BT}{Jz\sigma} L_{nn}\left(1 + \frac{\mu_0 H}{Jz\sigma}\right) + \frac{Jz\sigma + \mu_0 H}{6k_BT}. \tag{10}$$

One can see that the leading term in the sum (10) contains a diagonal matrix element of the lattice Green function $L_{nn}(1+\mu_0 H/Jz\sigma)$, which, in the general case, is determined by the following expression for a complex variable ϵ [12]:

$$L_{nn}(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\epsilon - \gamma_{\mathbf{k}}} = \frac{\Omega_0}{(2\pi)^3}\int d\mathbf{k}\frac{1}{\epsilon - \gamma_{\mathbf{k}}} \tag{11}$$

(here Ω_0—the unit cell volume for a three-dimensional lattice).

Generally speaking, the behavior of $L_{nn}(\epsilon)$ as a function of the complex variable ϵ is strongly dependent on the lattice dimensionality. It is known that for the linear ferromagnetic chain this matrix element is equal to $L_{nn}^{(1)}(\epsilon) = 1/\sqrt{\epsilon^2 - 1}$ in the region $\epsilon \geq 1$ and for the square ferromagnetic lattice it is equal to $L_{nn}^{(2)} = 2/\pi\epsilon K(1/\epsilon)$ at $\epsilon \geq 1$ [13], where $K(1/\epsilon)$ is the first-kind complete elliptic integral. These matrix elements $L_{nn}^{(1)}(\epsilon)$ and $L_{nn}^{(2)}(\epsilon)$ are divergent at $\epsilon \to 1^+$, so that Γ in Eq. (10) goes to infinity and σ in Eq. (9) goes to zero at $\epsilon \to 1^+$. Since the limit $\epsilon \to 1^+$ corresponds to $H \to 0$, it means that the spontaneous long-range ferromagnetic order is absent in the one- and two-dimensional lattices at finite temperatures $T \neq 0$.

However, for the three-dimensional cubic lattices the matrix elements $L_{nn}^{(3)}(\epsilon = 1^+) \equiv L_{nn}(1^+)$ take finite values, and the singular behavior of these diagonal matrix elements of the three cubic lattice Green functions in a sufficiently small neighborhood of the singularity $\epsilon = 1$ is described by the expansion in powers of $(\epsilon - 1)$ [12,14]:

$$L_{nn}(\epsilon) = \sum_{n=0}^{\infty} A_n(\epsilon-1)^n - \sum_{n=0}^{\infty} B_n(\epsilon-1)^{n+1/2}$$
$$\approx I_W - B_0(\epsilon-1)^{1/2} + A_1(\epsilon-1) - B_1(\epsilon-1)^{3/2} + \cdots. \tag{12}$$

Here $A_0 = L_{nn}(1^+) \equiv I_W$ are the well-known Watson integrals for the cubic lattices, and A_n, B_n are constants. It has been calculated [12] that I_W and B_0 are equal to $I_W^{sc} \simeq 1.517$, $B_0^{sc} = 3\sqrt{3}/\pi\sqrt{2} \simeq 1.169$ for the simple cubic lattice, $I_W^{bcc} \simeq 1.393$, $B_0^{bcc} = 2\sqrt{2}/\pi \simeq 0.910$ for a body-centered lattice, and $I_W^{fcc} \simeq 1.345$, $B_0 = 3\sqrt{3}/2\pi \simeq 0.827$ for the face-centered lattice.

Therefore, taking into account $\mu_0 H/Jz\sigma \ll 1$ near T_c (since $\mu_0 H/Jz\sigma(T) \sim \chi^{-1}(T)$ is proportional to the inverse magnetic susceptibility per spin and goes to zero at $T \to T_c^+$) and the expansion (12), we can approximate $L_{nn}(1+\mu_0 H/Jz\sigma)$ in Eq. (10) as

$$L_{nn}\left(1 + \frac{\mu_0 H}{Jz\sigma}\right) \approx I_W - B_0\left(\frac{\mu_0 H}{Jz\sigma}\right) \tag{13}$$

and the function Γ itself as

$$\Gamma \cong \frac{2k_BT}{Jz\sigma}\left[I_W - B_0\left(\frac{\mu_0 H}{Jz\sigma}\right)^{1/2}\right] + \frac{Jz\sigma}{6k_BT}. \tag{14}$$

Henceforward we keep only the maximum field contribution from $(\mu_0 H/Jz\sigma)^{1/2} \ll 1$, since, in its turn, $\mu_0 H/k_BT = (\mu_0 H/Jz\sigma)\cdot(Jz\sigma/k_BT) \ll (\mu_0 H/Jz\sigma)^{1/2}$.

Thereafter the inverse function $1/\Gamma$ can be approximated as

$$\frac{1}{\Gamma} \cong \frac{Jz\sigma}{2k_BTI_W}\left[1 + \frac{B_0}{I_W}\left(\frac{\mu_0 H}{Jz\sigma}\right)^{1/2} - \frac{1}{12I_W}\left(\frac{Jz\sigma}{k_BT}\right)^2\right]. \tag{15}$$