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MAGNETISM

Correlation Functions of Pure and Diluted Ising Magnets in the Mean-Field Approximation

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Abstract—A mean-field method, which is a variant of the fixed-scale renormalization group transformation and is applied to both pure and diluted magnets, has been considered. It has been shown that, for pure magnets, the method is equivalent to the Bethe approximation. This method has been used to calculate the magnetization and correlation functions of both pure and bond-diluted Ising magnets.

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1. INTRODUCTION

Investigation of phase transitions in diluted and disordered magnets has been the subject of theoretical and experimental works for many years [1–3]. In our previous works [4, 5], we suggested a classification of self-consistent methods for calculating the magnetization and critical points of pure and diluted magnets. However, in these works, we disregarded the problem of calculating correlation functions and their behavior near the critical point. However, as will be shown below, some methods described in [4, 5] can be applied to calculate spin correlations.

We consider the bond-diluted Ising model. The Hamiltonian of this model has the form

$$E = -\sum J_{ij}\sigma_i\sigma_j - H_{ex}\sum\sigma_i. \tag{1}$$

Here, σ_i are Ising variables, which take the values +1 or −1; J_{ij} are the exchange interaction constants; and H_{ex} is proportional to the external magnetic field. The quantities J_{ij} are nonzero only for the nearest neighbors in the crystal lattice and for these neighbors J_{ij} amounts to J and zero with the probability p and $1-p$, respectively. The probability p is the fraction of "magnetic" bonds in the lattice; the magnet is pure at $p = 1$. The aim of this work is to apply to this model some of the self-consistent methods described in [4] to this model and, using these methods, to calculate the correlation functions of both pure and diluted magnets.

2. MEAN-FIELD APPROXIMATION

According to [4], one of the ways of approximately solving the problem with Hamiltonian (1) is the following. Let us consider a cluster consisting of n atoms. The Hamiltonian of this cluster is

$$E_n = -\sum J_{ij}\sigma_i\sigma_j - J\sum h_{in}^i\sigma_i - H_{ex}\sum\sigma_i. \tag{2}$$

Summation in the first term of this expression is performed over the pairs of atoms within the cluster, which are the nearest neighbors. The second term in Eq. (2) describes interaction of the cluster atoms with their nearest neighbors outside the cluster, and the third term is for the interaction with the external field. The exchange interaction fields h_{in}^i are computed for each cluster atom by summing up the Ising variables corresponding to the external atoms neighboring with the given atom.

We average the quantity $\frac{\Sigma\sigma_i}{n}$ over the ensemble with Hamiltonian (2) regarding h_{in}^i as constants and then average the resulting expression over the simultaneous distribution function $W_n(h_{in}^i)$ of the exchange interaction fields. Having constructed a similar expression for another cluster containing $n' \neq n$ atoms and equating these two expressions, we find

$$\langle\sigma\rangle = \left\langle\frac{\sum\left(\frac{\Sigma\sigma_i}{n}\right)\exp(-\beta E_n)}{\sum\exp(-\beta E_n)}\right\rangle = \left\langle\frac{\sum\left(\frac{\Sigma\sigma_i}{n'}\right)\exp(-\beta E_{n'})}{\sum\exp(-\beta E_{n'})}\right\rangle. \tag{3}$$

Further calculation depends on the particular approximation of the distribution function $W_n(h_{in}^i)$ of the exchange interaction fields. The simplest approximation can be obtained setting all h_{in}^i constants equal to $q_i\mu$, where q_i is the number of "external" neighbors of the nth atom and μ is the parameter characterizing the magnetization, which is found from the solution of self-consistent equation (3). For the pure ($p = 1$) magnet, setting $n = 1$ and $n' = 2$, we find in this approximation

$$M = \tanh(qK\mu + h) = \frac{\sinh(2(q-1)K\mu + 2h)}{\cosh(2(q-1)K\mu + 2h) + e^{-2K}}. \quad (4)$$

Here, $M = \langle\sigma\rangle$ is the average magnetization per lattice site, $K = J/kT$ (k is the Boltzmann constant), $h = H_{ex}/kT$, and q is the coordination number of the lattice. It is easily shown that approximation (4) is nothing else than the Bethe approximation [6]. Indeed, denoting $x = \exp(-2K\mu)$, we can rewrite Eq. (4) as

$$M = \frac{e^{h} - e^{-h}x^{q}}{e^{h} + e^{-h}x^{q}} = \frac{e^{2h}(x^{-(q-1)} - e^{-2h}x^{q-1})}{e^{2h}x^{-(q-1)} + e^{-2h}x^{q-1} + 2e^{-2K}}$$

or

$$M = \frac{e^{h} - e^{-h}x^{q}}{e^{h} + e^{-h}x^{q}}, \quad x = \frac{e^{-K+h} + e^{K-h}x^{q-1}}{e^{K+h} + e^{-K-h}x^{q-1}}, \quad (5)$$

which coincides with the solution for the Ising model on the Bethe lattice, as quoted in [6]. That is, as far as the calculation of the magnetization M is concerned, approximation (4) can be regarded as a variant of the derivation of the Bethe approximation. The Bethe approximation can be also obtained as a solution of the Ising problem on the Bethe lattice (tree) [6] or as a relation between the magnetizations of the central atom and the atom of the first coordination sphere [7]. Yet our method (4), as will be shown below, allows calculating not only the magnetization but also the correlation functions for the pure and diluted Ising magnets.

3. CORRELATION FUNCTIONS

The correlation function of the neighboring spins in approximation (4) can be found as follows. Averaging the product of spin variables of the cluster atoms over the ensemble with Hamiltonian (2) and equating $h_{in}^{1} = h_{in}^{2} = (q-1)\mu$, we find

$$\langle\sigma_1\sigma_2\rangle = \frac{\cosh(2(q-1)K\mu + 2h) - e^{-2K}}{\cosh(2(q-1)K\mu + 2h) + e^{-K}}. \quad (6)$$

The correlation function $g_{12} = \langle\sigma_1\sigma_2\rangle - M^2$ is computed according to Eq. (6), in which the parameter μ is the solution of Eq. (4). This correlation function can be also expressed in terms of K and the magnetization M:

$$g_{12} = \tanh K + \frac{1 - \sqrt{1 - (1 - \exp(-4K))M^2}}{\sinh 2K} - M^2. \quad (7)$$

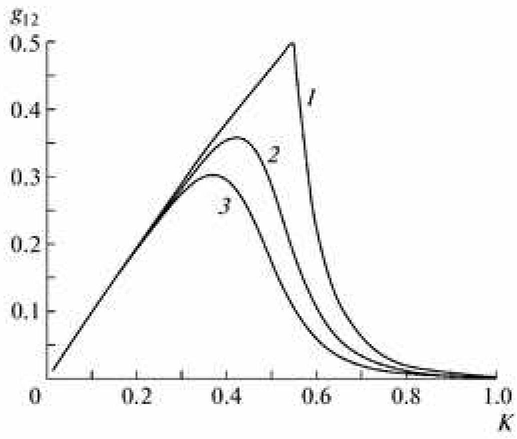

Fig. 1. Correlation function g_{12} versus the parameter $K = J/kT$ in external fields H_{ex} = (*1*) 0, (*2*) 0.1 and (*3*) 0.2.

This implies that at $M = 0$ (i.e., at $H_{ex} = 0$ and $K < K_c = \frac{1}{2}\ln\frac{q}{q-2}$), we have $g_{12} = \tanh K$ for any $q \geq 2$. At $K = K_c$ and $H_{ex} = 0$, g_{12} reaches a maximum value of $1/(q - 1)$. At $H_{ex} \neq 0$, the maximum of $g_{12}(K)$ is shifted to the left and its magnitude decreases (Fig. 1).

We consider now a three-atom cluster with the Hamiltonian

$$E_3 = -J\sigma_1\sigma_2 - J\sigma_2\sigma_3 - J(q-1)\mu(\sigma_1 + \sigma_3) - J(q-2)\mu\sigma_2 - H_{ex}(\sigma_1 + \sigma_2 + \sigma_3). \quad (8)$$

The central spin σ_2 of the cluster is coupled by exchange interactions with the side spins σ_1 and σ_3 and is situated in the field $J(q-2)\mu + H_{ex}$, whereas each of the side spins appears in the field $J(q-1)\mu + H_{ex}$. We calculate the averages $\langle\sigma_2\rangle$, $\left\langle\frac{\sigma_1 + \sigma_2}{2}\right\rangle$, $\langle\sigma_1\sigma_2\rangle$, and $\langle\sigma_1\sigma_3\rangle$ over the ensemble with Hamiltonian (8) and find

$$\langle\sigma_2\rangle = \frac{\sinh x_1 + 2e^{-2K}\sinh x_2 - e^{-4K}\sinh x_3}{\cosh x_1 + 2e^{-2K}\cosh x_2 + e^{-4K}\cosh x_3}, \quad (9)$$

$$\left\langle\frac{\sigma_1 + \sigma_3}{2}\right\rangle = \frac{\sinh x_1 + e^{-4K}\sinh x_3}{\cosh x_1 + 2e^{-2K}\cosh x_2 + e^{-4K}\cosh x_3}, \quad (10)$$

$$\langle\sigma_1\sigma_3\rangle = \frac{\cosh x_1 - e^{-4K}\cosh x_3}{\cosh x_1 + 2e^{-2K}\cosh x_2 + e^{-4K}\cosh x_3}, \quad (11)$$

$$\langle\sigma_1\sigma_2\rangle = \frac{\cosh x_1 - 2e^{-2K}\cosh x_2 + e^{-4K}\cosh x_3}{\cosh x_1 + 2e^{-2K}\cosh x_2 + e^{-4K}\cos x_3}, \quad (12)$$

where