ISSN 1063-7834, Physics of the Solid State, 2014, Vol. 56, No. 7, pp. 1338–1341. © Pleiades Publishing, Ltd., 2014.
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MAGNETISM

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

S. V. Semkin and V. P. Smagin
Vladivostok State University of Economics and Service, ul. Gogolya 41, Vladivostok, 690014 Russia
e-mail: Li15@rambler.ru
Received January 16, 2014

Abstract—A method of mean field, which is a variant of a 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. The magnetization and correlations functions of both pure and diluted-bond Ising magnets have been calculated by this method.

DOI: 10.1134/S1063783414070300

1. INTRODUCTION

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

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

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

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, 5] and to calculate by these methods the correlation functions of both pure and diluted magnets.

2. MEAN-FIELD APPROXIMATION

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

$$E_n = -\sum J_{ij}\sigma_i\sigma_j - J\sum h^i_{\text{in}}\sigma_i - H_{ex}\sum\sigma_i. \qquad (2)$$

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 fields h^i_{in} are computed for each cluster atom by summing up the Ising variables corresponding to the external atoms neighboring the given atom.

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

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

Further calculation depends on the a particular approximation of the distribution function $W_n(h^i_{\text{in}})$ of the exchange fields. The simplest approximation can be obtained setting all h^i_{in} 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 a pure ($p = 1$) magnet, setting $n = 1$ and $n' = 2$ we find in this approximation

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

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

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

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 the mere magnetization but also the correlation functions of a pure and diluted Ising magnet.

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

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

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:

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

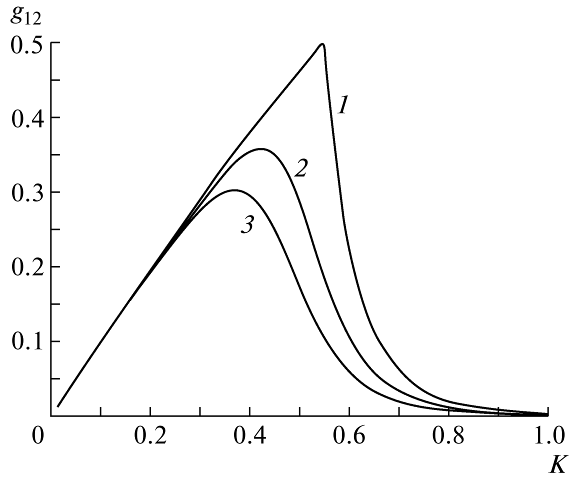

Fig. 1. Correlation function g_{12} versus the parameter $K = J/kT$ in the external field H_{ex} = (*1*) 0, (*2*) 0.1 and 0.2.

This implies that at $M = 0$ (i.e., at $H_{ex} = 0$ and $K < K_c = \frac{1}{2}\ln\frac{q}{q-2}$) $g_{12} = \tanh K$ 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

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

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

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

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

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

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

where

$$x_1 = (3q-4)K\mu + 3h, \quad x_2 = (q-2)K\mu + h,$$

$$x_3 = qK\mu + h.$$

All four functions: (9), (10) $\tanh(qK\mu + h)$ and the right-hand side of Eq. (4) coincide with each other at a certain nonzero (at $K > K_c$) value of the parameter $\mu = \mu_0$. This implies that the use of one, two and three-atom clusters in the mean-field approximation yield the same result as the Bethe approximation.

The correlation function g_{12} of the nearest atoms can be calculated now from Eq. (12) with $\mu = \mu_0$. This also leads to Eq. (7). The function g_{13} can be found from Eq. (11). The correlation functions g_{12} and g_{13} found this way for the one-dimensional Ising chain ($q = 2$) coincide with the solutions quoted in [6]. It can be readily verified that the following relation holds

$$\left(\frac{g_{12}}{1-M^2}\right)^2 = \frac{g_{13}}{1-M^2}.$$

which allows us to suggest that the function g_{ij} for an arbitrary q has the same form as for the one-dimensional chain

$$g_{ij} = (1-M^2)a^{|j-i|} = (1-M)^2\exp(-|j-i|/\xi), \quad (13)$$

where $a = \dfrac{g_{12}}{1-M^2} = \dfrac{g_{13}}{g_{12}}$ and ξ is the correlation length. We find from Eqs. (13) and (7) the dependence of ξ on K and the magnetization M

$$\xi = -\left(\ln\frac{g_{12}}{1-M^2}\right)^{-1}. \quad (14)$$

The correlation length ξ does not diverge at the critical point ($x_{ex} = 0$, $K = K_c$) but has a maximum value of $1/\ln(q-1)$.

According to the group representation [8], the correlation function of three neighboring spins is

$$g_{123} = \langle\sigma_1\sigma_2\sigma_3\rangle - M(g_{12}+g_{13}+g_{23}) - M^3. \quad (15)$$

We first consider a one-dimensional spin chain. The average value $\langle\sigma_1\sigma_2\sigma_3\rangle$ of the product of spins situated at three neighboring sites can be calculated as [6]

$$\langle\sigma_1\sigma_2\sigma_3\rangle = \frac{\mathrm{Tr}\mathbf{SVSVSVV}^{N-3}}{\mathrm{Tr}\mathbf{V}^n},$$

where

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \mathbf{V} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$$

is the transfer matrix. Performing calculations as described in [6], we find the three-body correlation function

$$g_{123} = -2Mg_{13}. \quad (16)$$

Considering now the cluster with $n = 3$ for an arbitrary q we find similarly to Eqs. (9)–(12)

$$\langle\sigma_1\sigma_2\sigma_3\rangle = \frac{\sinh x_1 - 2e^{-2K}\sinh x_2 - e^{-4K}\sinh x_3}{\cosh x_1 + 2e^{-2K}\cosh x_2 + e^{-4K}\cosh x_3}. \quad (17)$$

Calculating g_{123} with the use of this expression we see that Eq. (16) holds for an arbitrary q.

4. DILUTED BONDS

Let us consider now the diluted bond Ising model with $p \neq 1$. By the same reasoning as in the case of a pure magnet we find the self-consistent equation for the magnetization M [5]

$$\tanh(Kqp\mu + h) = (1-p)\tanh(K(q-1)p\mu + h)$$
$$+ p\frac{\sinh(2K(q-1)p\mu + 2h)}{\cosh(2K(q-1)pm + 2h) + e^{-2K}}, \quad (18)$$
$$M = \tanh(Kqp\mu + h).$$

This equation transforms to Eq. (4) at $p = 1$ and has a nonzero solution at $h = 0$ under the condition $K > K_c$, where

$$K_c(p) = \frac{1}{2}\ln\frac{p+p_c}{p-p_c}, \quad (19)$$

And $p_c = 1/(q-1)$ is the percolation threshold of the Bether lattice [9]. It is noteworthy that although Eqs. (18) yield the exact solution for the Ising model on the Bethe lattice with $p = 1$ and the exact percolation threshold p_c for this lattice, they still cannot be regarded as the exact solution of the Ising problem for a diluted magnet on the Bethe lattice [5].

The density dependence of the magnetization at zero temperature ($K \longrightarrow \infty$) and zero external field ($h = 0$) is knowingly [9] the probability $P(p)$ that a certain magnetic atom belongs to an infinite cluster. This function is found by solving the equation

$$\begin{cases} \tanh(qpx) \\ = (1-p)\tanh((q-1)px) + p\tan(2(q-1)px) \\ P(p) = \tanh(qpx). \end{cases}$$

Calculating the average value of the spin product in the two-atom cluster we find

$$\langle\sigma_1\sigma_2\rangle = (1-p)\tanh^2((q-1)p\mu K + h)$$
$$+ p\frac{\cosh(2(q-1)pK\mu + 2h) - e^{-2K}}{\cosh(2(q-1)pK\mu + 2h) + e^{-2K}}. \quad (20)$$

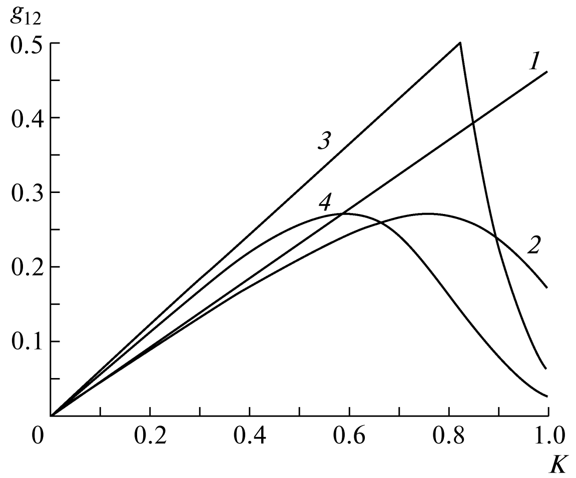

Fig. 2. Correlation function g_{12} versus the density p of magnetic bonds at (*1*) $K = 0.5$, $H_{ex} = 0$, (*2*) $K = 0.5$, $H_{ex} = 0.05$, (*3*) $K = 0.7$, $H_{ex} = 0$, and (*4*) $K = 0.7$, $H_{ex} = 0.7$.

Introducing the notation $\gamma = (q - 1)p\mu K + h$ in Eqs. (18) and (20) we write the expressions for the magnetization M and the correlation function $g_{12} = \langle\sigma_1\sigma_2\rangle - M^2$ in the form

$$g_{12} = (1-p)\tanh^2\gamma + p\frac{\cosh(2\gamma) - e^{-2K}}{\cosh(2\gamma) + e^{-K}} - M^2,$$
$$M = (1-p)\tanh\gamma + p\frac{\cosh(2\gamma)}{\cosh(2\gamma) + e^{-2K}}. \quad (21)$$

As follow from these equations, g_{12} can be expressed as a function of K, M and p independent of q, similarly to Eq. (7). In the absence of the external magnetic field in the temperature range $K < K_c$

$$g_{12}(p) = pg_{12}(1) = p\tanh K.$$

At $K > K_c$, the dependence of g_{12} on p is more complicated (Fig. 2).

5. CONCLUSIONS

Thus, we have studied both pure and diluted-bond Ising magnet in the mean-field approximation. As a result of this investigation, we have drawn the following basic conclusions:

(1) For a pure Ising magnet, the mean-field approximation can be regarded as a variant of the derivation of the Bethe approximation. This variant is advantageous in that the correlation functions and correlation length (relations (7) and (14)) can be easily found.

(2) In the present approximation, the correlation length remains finite at the phase transition and has a maximum at this point.

(3) In the absence of the external magnetic field, the maximum correlation of the adjacent spins (and the correlation length) is reached at $K = K_c$. At $H_{ex} \neq 0$, the maximum is shifted to the left (toward lower K values) and its magnitude decreases.

(4) In the present approximation, the correlation function g_{12} of a pure or diluted magnet can be expressed as function (7) of K and M independent of q or as function (21) of K, M and p, respectively.

(5) The dependence of the correlation function g_{12} on the density p of magnetic bonds is linear in zero external field in the temperature range $K < K_c(p)$ and is shown in Fig. 2 is a more general case.

REFERENCES

1. Yu. A. Izyumov and M. V. Medvedev, *Theory of Magnetically Ordered Crystals with Impurities* (Nauka, Moscow, 1970) [in Russian].
2. R. Fol'k, Yu. Golovach, and T. Yavorskii, Phys.—Usp. **46** (2), 169 (2003).
3. B. N. Shalaev, Phys. Solid State **52** (1), 87 (2010).
4. S. V. Semkin and V. P. Smagin, Phys. Solid State **55** (5), 970 (2013).
5. S.V. Semkin and V. P. Smagin, Russ. Phys. J. **56** (2), 118 (2013).
6. R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982; Mir, Moscow, 1985).
7. I. A. Kvasnikov, *Thermodynamics and Statistical Physics*, Vol. 2: *Theory of Equilibrium Systems* (Editorial URSS, Moscow, 2002) [in Russian].
8. R. Balesçu, *Equilibrium and Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1975; Mir, Moscow, 1978), Vol. 1.
9. J. M. Ziman, *Models of Disorder: The Theoretical Physics of Homogeneously Disordered Systems* (Cambridge University Press, Cambridge, 1979; Mir, Moscow, 1982).

Translated by A. Safonov

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