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MAGNETISM

Ising Model of a Dilute Ferromagnet in the Self-Consistent Field Approximation

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Abstract—The method of averaging over the exchange interaction fields has been considered as applied to clusters of one and two magnetic atoms in the Ising model of a dilute ferromagnet, and a variant of fixed-scale group renormalization on the basis of this method has been constructed. It has been shown that the approximation obtained makes it possible to distinguish models with the site and bond dilutions.

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1. INTRODUCTION

Phase transitions in irregular spin systems are frequently studied using the Ising model for a dilute magnet. This model is characterized by the Hamiltonian

$$E(p) = -\Sigma_{(l,l')}\xi_l\xi_{l'}J\sigma_l\sigma_{l'} - H\Sigma_l\xi_l\sigma_l, \quad (1)$$

where σ_l are ordinary Ising variables, defining the orientation of the atomic magnetic moment and assuming the values +1 and –1; J is the exchange integral; and H is proportional to the external magnetic field. The random variable ξ_l may be 0 and 1, and its mean $\langle\xi_l\rangle = p_s$ determines the probability of occupying the lth site by Ising spin; the summation in the first sum is performed over all ordered pairs of neighboring sites, and, in the second sum, over all lattice sites. We assume that magnetic and nonmagnetic atoms are arranged over lattice sites randomly without correlation and are not displaced under the action of thermal vibrations (frozen-in impurities). In addition, we will consider the model of frozen bonds, which assumes that a certain fraction, $1 - p_b$, of all exchange integrals are artificially switched off.

The critical phenomena in the Ising and Heisenberg models for dilute magnets as well as in models of ferromagnets with random bonds have been studied during several recent decades [1–6]. The researchers' attention was attracted mainly to the problem of universality and to the behavior of dilute magnets near the critical point [3, 5, 6]. In the present work, we propose a simple method for calculating the magnetization and Curie temperature of a dilute magnet, applicable in a wide range of concentrations of nonmagnetic impurities. Although details of the phase transition such as calculation of critical indices, correlation function, etc. remain beyond the scope of this work, the method proposed, theoretically, can be used for calculating the critical correlation length by constructing a fixed-scale renormalizing transformation by analogy with [7].

It is known [8] that, for a pure ($p_s = 1$) Ising magnet in a zero external filed, the following relation is satisfied:

$$\langle\sigma\rangle = \langle\tanh(\beta Jh_1)\rangle, \quad (2)$$

where $h_1 = \Sigma\sigma_j$ (the summation is performed with respect to spins neighboring to a given site) is the exchange field, $\beta = \frac{1}{kT}$, T is the temperature of the system, and k is the Boltzmann constant. The averaging on the right-hand side, in fact, is the averaging over the distribution function $W_1(h_1)$ for the exchange field.

Relation (2) can be extended as follows. We consider a cluster of n atoms. The Hamiltonian of this cluster is

$$E_n = -J\Sigma\sigma_i\sigma_j - J\Sigma h^i_{\text{in}}\sigma_i. \quad (3)$$

The summation in the first term is performed over pairs of nearest atoms of the cluster that are the nearest neighbors. The second term in (3) is described by the interaction of atoms in a cluster with their nearest neighbors not entering into the cluster. The exchange interaction fields h^i_{in} are calculated for each atom by summing the Ising variables corresponding to external atoms neighboring to the given one.

Average the quantity $\frac{\Sigma\sigma_i}{n}$ over the ensemble with Hamiltonian (3), considering h^i_{in} as constants and, then, average the resulting expression over the mutual distribution function $W_n(h_1, ..., h_n)$ for the exchange interaction fields. Equating the result of this averaging to $\langle\sigma\rangle$, we obtain

$$\langle\sigma\rangle = \left\langle \frac{\Sigma\left(\frac{\Sigma\sigma_i}{n}\right)\exp(-\beta E_n)}{\Sigma\exp(-\beta E_n)} \right\rangle. \quad (4)$$

Formula (2) may be considered as a special case of (4) when the cluster consists of one atom.

Formula (4) can be used as a basis for approximate methods for finding the spontaneous magnetization and the phase transition point of the Ising model, if we replace the distribution function $W_n(h_1, ..., h_n)$ by various approximate expressions in which the mean magnetization $m = \langle\sigma\rangle$ enters as an unknown parameter. For example, setting in (2) $W_1(h_1) = \delta(h_1 - qm)$, where q is the coordination number of the lattice, we will obtain the known approximation of the field, described in [9]. The same method can also be used for studying dilute magnets. In [9], a dilute magnet is considered in the approximation based on (2). In the present work, we will study dilute magnets in the approximation based on (4), using clusters of one and two atoms. The use of clusters of different sizes also makes it possible to construct a fixed-scale renormalizing transformation [7]. This possibility is also studied in the present work.

2. BOND AND SITE DILUTIONS

Let us consider clusters of one and two sites in the Ising model with the site dilution. The result of averaging in (4) with respect to approximate exchange field distribution functions will be denoted by $\langle\sigma_n\rangle$. Then,

$$\langle\sigma_1\rangle = \langle\tanh(Kh)\rangle_{W_1^q(h)} \quad (5)$$

and

$$\langle\sigma_2\rangle = p_b\left\langle \frac{\sinh[K(h_1+h_2)]}{\cosh[K(h_1+h_2)] + e^{-2K}\cosh[K(h_1-h_2)]} \right\rangle_{W_2^q(h_1,h_2)} + (1-p_b)\left\langle \frac{\sinh[K(h_1+h_2)]}{\cosh[K(h_1+h_2)] + \cosh[K(h_1-h_2)]} \right\rangle_{W_2^q(h_1,h_2)}$$

or

$$\langle\sigma_2\rangle = p_b\left\langle \frac{\sin[K(h_1+h_2)]}{\cosh[K(h_1+h_2)] + e^{-2K}\cosh[K(h_1-h_2)]} \right\rangle_{W_2^q(h_1,h_2)} + (1-p_b)\frac{1}{2}\langle\tanh(Kh_1) + \tanh(Kh_2)\rangle_{W_2^q(h_1,h_2)}, \quad (6)$$

where $K = J\beta$. The presence of two terms on the right of (6) is caused by the fact that, in the set of clusters from neighboring atoms on the lattice, the fraction of clusters with a broken exchange bond is $1 - p_b$.

In the model with the site dilution for a one-atom cluster, we obtain

$$p_s\langle\sigma_1\rangle = p_s\langle\tanh(Kh)\rangle_{W_1^q(h)}, \quad (7)$$

and, for a two-site cluster,

$$p_s\langle\sigma_2\rangle = p_s^2 \times\left\langle \frac{\sinh[K(h_1+h_2)]}{\cosh[K(h_1+h_2)] + e^{-2K}\cosh[K(h_1-h_2)]} \right\rangle_{W_2^q(h_1,h_2)} + p_s(1-p_s)\frac{1}{2}\langle\tanh(Kh_1) + \tanh(Kh_2)\rangle_{W_2^q(h_1,h_2)}. \quad (8)$$

In these expressions, $\langle\sigma_1\rangle$ and $\langle\sigma_2\rangle$ are the mean magnetization of an atom; the magnetization per site is obtained by the multiplication by p_s.

3. MEAN-FIELD METHOD

In the mean-field approximation, the exchange fields h_1 and h_2 in expressions (5)–(8) are replaced by their mean values, which corresponds to using delta-function in these expression as the exchange field distribution functions:

$$W_1^q(h) = \delta(h - mqp), \quad (9)$$

$$W_2^q(h_1, h_2) = W_1^{q-1}(h_1)W_1^{q-1}(h_2) = \delta(h_1 - m(q-1)p)\delta(h_2 - m(q-1)p). \quad (10)$$

In this approximation, the problems of the site and bond dilution lead to the same expressions, therefore p_b and p_s are denotes simply by p. Using expressions (5) (or (7)), we obtain an extension of the mean-field approximation to the case of dilute magnets:

$$m = \tanh(Kqpm). \quad (11)$$

This equation has a nonzero solution for $K > K_c = 1/qp$, which, as is known [1], does not agree with the real behavior of spontaneous magnetization of dilute magnets, which must vanish at concentrations below

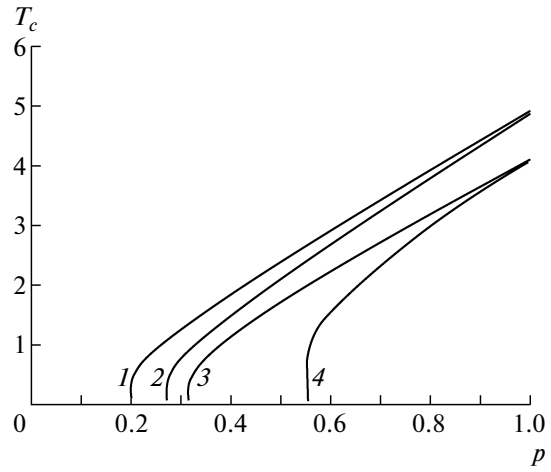

Fig. 1. Curie temperature as a function of the concentration for $q = 6$: (*1*) Bethe approximation; (*2*) field averaging, cubic lattice; (*3*) triangular lattice, site dilution; and (*4*) triangular lattice, bond dilution.

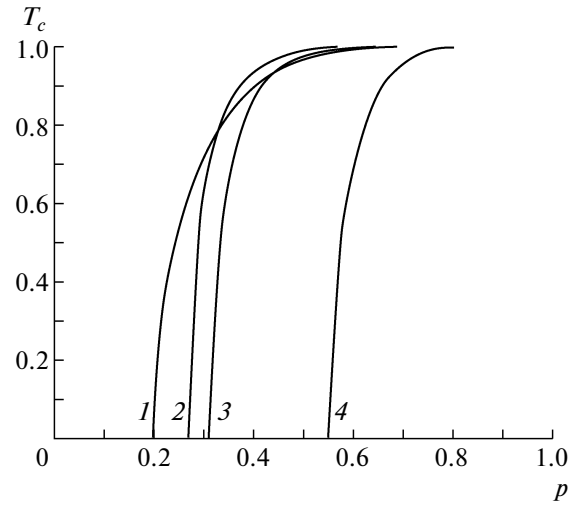

Fig. 2. Spontaneous magnetization at zero temperature as a function of the concentration for $q = 6$: (*1*) Bethe approximation; (*2*) field averaging, cubic lattice; (*3*) triangular lattice, site dilution; and (*4*) triangular lattice, bond dilution.

the percolation threshold p_c. The use of a cluster of two atoms (relations (6) or (8)) does not lead to substantially different results. The equation for magnetization in this case,

$$m = (1-p)\tanh[K(q-1)pm] + p\frac{\sinh[2k(q-1)pm]}{\cosh[2K(q-1)pm] + e^{-2K}}, \quad (12)$$

has a nonzero solution for any p. Replacing on the right-hand sides of (11) and (12) the magnetization m by the parameter μ and equating these parts, we obtain

$$\tanh[Kqp\mu] = (1-p)\tanh[K(q-1)p\mu] + p\frac{\sinh 2K(q-1)p\mu}{\cosh[2K(q-1)p\mu] + e^{-2K}}. \quad (13)$$

We may equate the mean magnetization m of one magnetic atom to μ, the solution of (13), or assume that $m = \tanh(Kqp\mu)$: in this case, for a pure magnet ($p = 1$), we come to the well known Bethe approximation [10]. For dilute magnets, a nonzero solution of (13) exists under the condition $K > K_c$, where

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

where p_c is the percolation threshold in the mean-field approximation. The graph of the function $T_c(p) = K_c^{-1}(p)$ for $q = 6$ is shown in Fig. 1 (curve *1*). As is known [1], the dependence of the magnetization at zero temperature ($K \longrightarrow \infty$) on the concentration $m(p)$ is the probability that a certain magnetic atom belongs to an infinite cluster $P(p)$. According to (13), this function is found from the solution of the equation

$$\begin{cases} \tanh(qpx) = (1-p)\tanh[(q-1)px] \\ \quad + p\tanh[2(q-1)px], \\ P(p) = \tanh(qpx). \end{cases} \quad (14)$$

The graph of this function for $q = 6$ is shown in Fig. 2 (curve *1*).

4. AVERAGING OVER THE EXCHANGE INTERACTION FIELDS

Another approximate method for finding the distribution functions and a method for finding the spontaneous magnetization on its basis was proposed in [9]. The quantities σ_j entering into the expression for $h_1 = \Sigma\sigma_j$ are considered as random variables taking the values $+1$ and -1 with the probabilities $(1 + m)/2$ and $(1 - m)/2$, respectively. The number of terms in the sum for h_1 is a random variable distributed by the binomial law from 0 to q with the parameter p. In this case, the distribution function $W_1^q(h)$ has the form

$$W_1^q(h) = \sum_{i=0}^{q} C_q^i p^i (1-p)^{q-i} \times \sum_{j=0}^{i} C_i^j \left(\frac{1+m}{2}\right)^j \left(\frac{1-m}{2}\right)^{i-j} \delta(h-(2j-i)). \quad (15)$$

Substituting this expression into (5), we obtain an equation for spontaneous magnetization as a function of concentration and temperature. This method for

Exact site (upper value) and bond (lower value) percolation thresholds [1] (first column) and the percolation thresholds in the Bethe approximation (second column) (for columns 1, 2, and 1–2, see explanation in text)

Lattice type (coordination number)	Exact value	Bethe approximation	1	2	1–2
Hexagonal (3)	0.700 0.653	0.500	0.557	0.571	0.629
Square (4)	0.590 0.500	0.333	0.428	0.429	0.434
Tetrahedron (4)	0.430 0.390	0.333	0.428	0.429	0.434
Cubic (6)	0.310 0.250	0.200	0.293	0.290	0.272
Triangular (6)	0.500 0.347	0.200	0.293	0.310 0.295	0.556 0.315

obtaining equations of spontaneous magnetization will be called below as the exchange-field-averaging method. As was shown in [9], in contrast to (11) and (12), the equation obtained from (5) by means of (15) has a nonzero solution only for $p > p_c$. Moreover, in most cases, approximate values of p_c obtained from this equation are more accurate than those found from (14) (table, column 1).

Since Bethe approximation (13) is more accurate than the mean-field approximation for clusters of one (11) and two (12) atoms and the exchange-field averaging gives more accurate results even for a one-atom cluster, we may hope that the combination of these methods will be a sufficiently good approximation.

Let us consider the distribution function $W_2^q(h_1, h_2)$ for clusters of two neighboring atoms. Two cases are possible. In one case, it may happen that, among external atoms neighboring to the first atom of the cluster, there are no nearest neighbors of its second atom. This takes place in the hexagonal ($q = 3$), tetrahedral ($q = 4$), and cubic ($q = 6$) lattices. Below, this situation will be called "the absence of overlapping of coordination spheres". In the other case, it may happen that atoms neighboring to one site of the cluster simultaneously are neighboring to its second site; for example, this takes place in the case of the planar triangular ($q = 6$) lattice. In the first case, the fields h_1 and h_2 are statistically independent (in the framework of the exchange-field averaging method): $W_2^q(h_1, h_2) = W_1^{q-1}(h_1) W_1^{q-1}(h_2)$. In the second case, $h_{1,2} = h'_{1,2} + h_{1,2}^{\text{com}}$, where $h_{1,2}^{\text{com}}$ are the exchange fields produced by atoms neighboring simultaneously to both the atoms of the cluster. The fields h'_1, h'_2, and $h_{1,2}^{\text{com}}$ in the framework of the averaging method are assumed statistically independent and having binomial distributions similar to (15).

For dilute magnets in the first case, the joint distribution function for the fields is constructed by (15) and the model of a site dilute magnet is identical to the dilute bonds model. In the second case, the field distribution functions on the site and bond dilution are different.

Consider the approximation obtained from (6) and (8) by substituting in these expressions of the distribution function $W_2^q(h_1, h_2) = W_1^{q-1}(h_1) W_1^{q-1}(h_2)$, i.e., in the absence of overlapping of coordination spheres. The expression obtained in this case can be used for calculating the spontaneous magnetization as a function of concentration and temperature. It turns out that the spontaneous magnetization is nonzero only if $p > p_c$. The values of p_c found in this way are presented in the table (column 2).

For the triangular axis, the field distribution function of a site-diluted magnet is calculated as follows:

$$W_2^6(h_1, h_2) = W_1^3(h'_1) W_1^3(h'_2) W_1^2(h^{\text{com}})\delta \times (h_1 - (h'_1 + h^{\text{com}}))\delta(h_2 - (h'_2 + h^{\text{com}})). \quad (16)$$

In this case, $h_1^{\text{com}} = h_2^{\text{com}} = h^{\text{com}}$. For bond-dilute magnets with a triangular lattice, the situation is somewhat more complicated: h_1^{com} may be not equal to h_2^{com}. The joint field distribution function can be defined by the direct calculation of the probabilities $W(h_1^{\text{com}}, h_2^{\text{com}})$ as

$$W(-2, 0) = 2(1-p)^2 p^2 \left(\frac{1-m}{2}\right)^2,$$

$$W(-1, -1) = (1-p)^2 p^2 ((1-m)^2 + (1-m^2)/2),$$

$$W(-1, 0) = (1-p)^3 p(1-m) + (1-p)p^3(1-m^2/2),$$

$$W(-1, 1) = (1-p)^2 p^2 (1-m^2)/2,$$

$$W(-2,-1) = 2(1-p)p^3\left(\frac{1-m}{2}\right)^2,$$

$$W(0,0) = (1-p)^2p^2(1-m^2) + p^4(1-m^2)/2 + (1-p)^4,$$

$$W(-2,-2) = p^4\left(\frac{1-m}{2}\right)^2.$$

The remaining probabilities are either zero or found from the symmetry condition $W(h_1^{\text{com}}, h_2^{\text{com}}) = W(h_2^{\text{com}}, h_1^{\text{com}})$ and the fact that, on the replacement of m by $-m$, the probability $W(h_1^{\text{com}}, h_2^{\text{com}})$ passes into $W(-h_1^{\text{com}}, -h_2^{\text{com}})$. In column 2 of the table, two values of the critical concentration for the triangular lattice are presented: the upper one, for the site dilution and, the lower one, for the bond dilution.

Now let us construct the combination of the Bethe approximation and the exchange-field averaging method. To that end, equate the right-hand sides of (7) and (8) averaged with respect to the exchange fields defined above. In column 1–2 of the table, percolations thresholds of different lattices, calculated by this method, are presented. For the triangular lattice, two values are presented: the upper one, on the site dilution, and, the lower one, on the bond dilution.

In the same approximation, we calculated concentration dependences of the Curie temperature (Fig. 1). Curve *2* in this figure corresponds to $q = 6$ and the absence of the overlapping of coordination spheres. Curve *3* was calculated for the triangular lattice on the site dilution, and curve *4*, on the bond dilution. In addition, we calculated the magnetization at zero temperature, i.e., the fraction of atoms belonging to an infinite cluster as a function of concentration p (Fig. 2). The curve numbers in this figure correspond to the same cases as in Fig. 1.

5. CONCLUSIONS

Thus, from the results obtained, we can draw the following conclusions.

(1) All approximations based on the averaging with respect to the interaction field give more accurate results for the concentration dependence of the Curie temperature and magnetization temperature than the mean-field method in the form of the Bethe approximation.

(2) Although the use of two-cluster atoms in the exchange-field averaging method does not lead to a substantial improvement of the accuracy of approximation (see the table) as compared to a one-atom cluster, in some cases, it nevertheless makes it possible to distinguish between the problems of site and bond percolation.

(3) The method based on the comparison of cluster of one and two sites (which, in fact, is a group renormalization transformation of a fixed scale) makes it possible to obtain more accurate results also with the use of the mean-field approximation (the Bethe method) and the exchange-field averaging. In the latter case, for the triangular lattice, we obtain the most accurate values of both the site and bond percolation thresholds.

REFERENCES

1. J. M. Ziman, *Models of Disorder: The Theoretical Physics of Homogeneously Disordered Systems* (Cambridge University Press, Cambridge, 1979; Mir, Moscow, 1982).
2. Yu. A. Izyumov and M. V. Medvedev, *Theory of Magnetically Ordered Crystals with Impurities* (Nauka, Moscow, 1970) [in Russian].
3. R. Folk, Yu. Holovatch, and T. Yavorskii, Phys.—Usp. **46** (2), 169 (2003).
4. Vik. S. Dotsenko, Phys.—Usp. **38** (5), 457 (1995).
5. B. N. Shalaev, Phys. Solid State **52** (1), 87 (2010).
6. B. N. Shalaev, Sov. Phys. JETP **46** (6), 1204 (1977).
7. L. A. Serkov, Theor. Math. Phys. **92** (1), 759 (1992).
8. H. B. Callen, Phys. Lett. **4**, 161 (1963).
9. V. I. Belokon' and S. V. Semkin, Sov. Phys. JETP **75** (4), 680 (1992).
10. R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982; Mir, Moscow, 1985).

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