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MAGNETISM

Investigation of the Potts Model of a Diluted Magnet by Local Field Averaging Technique

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Abstract—Averaging of the local interatomic interaction fields has been applied to the Potts model of a diluted magnet. A self-consistent equation for the magnetization and an equation for the phase transition temperature have been derived. The temperature and magnetic atom density dependences of the spontaneous magnetization have been found for the lattices with the coordination numbers 3 and 4 and various numbers of spin states.

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1. INTRODUCTION

We consider the Potts model with nonmagnetic impurities on a regular lattice with the coordination number q. Let each lattice node be occupied by a magnetic atom with the probability b or a nonmagnetic impurity atom with the probability $1 - b$ independent of the occupation of other nodes; in other words, we consider a magnet with frozen impurities. Each node containing a magnetic atom corresponds to the quantity σ_i ("spin"), which can take s different values, say, 1, 2,..., s [1]. Two neighboring spins σ_i and σ_j interact with the energy $-J_p\delta(\sigma_i, \sigma_j)$, where

$$\delta(\sigma_i, \sigma_j) = \begin{cases} 1, & \sigma_i = \sigma_j, \\ 0, & \sigma_i \neq \sigma_j. \end{cases}$$

Let there also be the external field H acting on the state 1. Then the total energy of the system is

$$E = J_p \sum_{(i,j)} \xi_i \xi_j \delta(\sigma_i, \sigma_j) - H \sum_i \xi_i \delta(\sigma_i, 1),$$

where ξ_i are 1 for the nodes occupied by magnetic atoms and zeroes for the nodes occupied by impurity atoms.

As was found in [2, 3], the critical behavior of this model may depend on the impurity density to such an extent that the character of the phase transition may change at a certain impurity density. In our previous work [4], we considered the behavior of the Potts model of a diluted magnet on a Bethe lattice in the case of pseudorandomly distributed nonmagnetic impurities. In this work, we offer another approach to studying the critical behavior of the Potts model of a diluted magnet.

Let us consider a lattice node occupied by a magnetic atom. Let $n_1, n_2, \ldots, n_s$ be the numbers of atoms in the first coordination sphere of this node situated in the states 1, 2,..., s, respectively. All numbers n_i are random quantities varying from one node to another with a common distribution function $W(n_1, n_2, \ldots, n_s)$.

Our starting point is the relation

$$\left\langle \frac{e^{Kn_j + h\delta(j,1)}}{\sum_i e^{Kn_i + h\delta(j,1)}} \right\rangle_W = p_j, \qquad (1)$$

which is the generalization of the formula quoted in [5]. Here, p_j is the probability of finding a magnetic atom in the state j, $K = J_p/kT$, $h = H/kT$ (k is the Boltzman constant). We define the magnetization of the Potts model as [2]

$$M = \frac{sp_1 - 1}{s - 1}.$$

This definition and the normalization $p_1 + \sum_{i=2}^{s} p_i = 1$ yield

$$M = p_1 - \frac{1}{s-1}\sum_{i=2}^{s} p_i,$$

which leads, according to Eq. (1), to the expression

$$M = \left\langle \frac{e^{Kn_1 + h} - \frac{1}{s-1}\sum_{i=2}^{s} e^{Kn_i}}{e^{Kn_1 + h} + \sum_{i=2}^{s} e^{Kn_i}} \right\rangle_W. \qquad (2)$$

For the further analysis, we have to construct the function $W(n_1, n_2, ..., n_s)$, by which the averaging in the right-hand side of Eq. (2) is performed. Various approximations are possible at this point. For example, n_j can be replaced by their average values, which leads to the mean-field approximation considered in [6]. In this work, we consider another approximation similar to the one used in [7, 8] for the Ising model of a diluted magnet. More specifically, we construct the distribution function $W(n_1, n_2, ..., n_s)$ assuming that each magnetic atoms of the first coordination sphere can appear in the state j with the probability p_j independent of the states of other atoms. This leads to the distribution function of the form

$$W(n_1, n_2, \ldots, n_s) = \sum_{z=0}^{q} C_q^z b^z (1-b)^{q-z} \times \sum_{\{n_i\}} C_z^{n_1, n_2, \ldots n_s} p_1^{n_1} p_2^{n_2} \ldots p_s^{n_s}.$$

Here, $C_q^z = \dfrac{q!}{z!(q-z)!}$ are the binomial coefficients and $C_z^{n_1, n_2, \ldots n_s} = \dfrac{Z!}{n_1! n_2! \ldots n_s!}$ are the polynomial coefficients.

We will seek for the solution, in which all p_i for $i > 1$ are identical and equal to p. Then, having expressed p and p_1 in terms of the magnetization M, we find from Eq. (2) the self-consistent equation for M

$$M = \sum_{z=0}^{q} C_q^z b^z (1-b)^{q-z} \times \sum_{n_1=0}^{z} C_z^{n_1} \left(M + \frac{1-M}{s}\right)^{n_1} \left(\frac{1-M}{s}\right)^{z-n_1} \Lambda_{z,s}^{n_1}(K,h), \quad (3)$$

$$\Lambda_{z,s}^{n_1}(K,h) = \sum_{\{n_i\}} C_{z-n_1}^{n_2, \ldots n_s} \frac{e^{Kn_1+h} - \dfrac{1}{s-1}\sum_{i=2}^{s} e^{Kn_i}}{e^{Kn_1+h} + \sum_{i=2}^{s} e^{Kn_i}}.$$

At $h = 0$, Eq. (3) always have the solution $M = 0$, which is stable at $K < K_c(b)$, implying the absence of spontaneous magnetization at high temperatures. The equation for $K_c(b)$ can be found by equating the derivative of the right-hand side of Eq. (3) with respect to M to 1 at $M = 0$:

$$1 = \sum_{z=0}^{q} C_q^z b^z (1-b)^{q-z} \sum_{n_1=0}^{z} C_z^{n_1} \frac{n_1 s - z}{s^z} \Lambda_{z,s}^{n_1}(K_c(b), 0). \quad (4)$$

In the case of $s > 2$, the spontaneous magnetization M exhibits an abrupt jump (a first-order phase transition) at $K = K_c(b)$. At $s = 2$, which corresponds to the Ising model, the phase transition is the second-order transition.

2. LATTICES WITH COORDINATION NUMBERS OF 3 AND 4

At $q = 3$, we find from basic equation (3) the equation for the magnetization of a hexagonal lattice. This equation is rather bulky but can be greatly simplified in the $K \to \infty$ limit (i.e., at zero temperature). Setting the external field to zero, we find

$$M_0 = M_0 \left(-\frac{s-1}{s} M_0^2 + \frac{s-2}{s} M_0 + \frac{1}{s}\right)\left(\frac{b}{1-b}\right)^3. \quad (5)$$

The solution $M_0 = 0$ is the stable solution of this equation only at $b < B_c$, where B_c is found from the condition $s = \left(\dfrac{b_c}{1-b_c}\right)^3$, i.e.,

$$b_c = \frac{\sqrt[3]{s}}{1+\sqrt[3]{s}}. \quad (6)$$

The physical meaning of the quantity b_c is the percolation threshold for the lattice with the coordination number 3. Clearly, the percolation threshold by definition cannot depend on the number s of spin states; however, we obtain this particular result within the method under consideration. Figure 1 shows the phase transition temperatures $T_c(b) = 1/K_c(b)$ found from Eq. (4) versus the magnetic atom density b (the curves *1*, *2* and *3* are plotted for the $q = 3$ and the number of spin states of 2, 3 and 4, respectively). As is seen, the function $T_c(b)$ has an infinite derivative at $b = b_c$ and is nearly linear at b close to 1.

According to Eq. (5), the spontaneous magnetization at $b > b_c$, is determined by the expression

$$M_0 = \frac{s - 2 + \sqrt{s^2 - 4(s-1)s\left(\dfrac{1-b}{b}\right)^3}}{2(s-1)}. \quad (7)$$

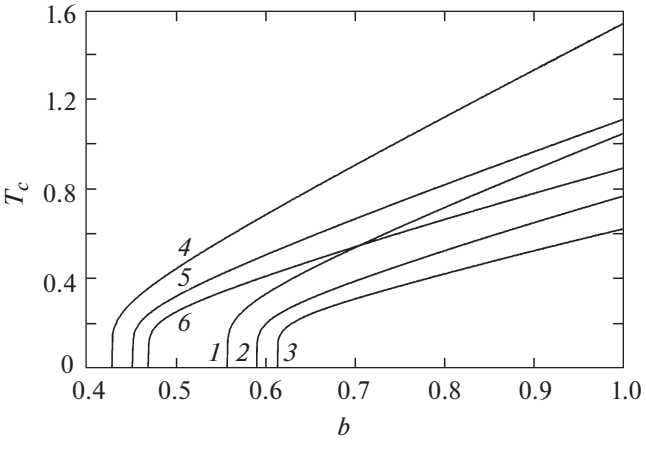

Fig. 1 Critical temperature versus the magnetic atom density for the coordination numbers $q =$ (curves *1*, *2* and *3*) 3 and (curves *4*, *5* and *6*) 4 and the number of spin states $s =$ (*1* and *4*) 2, (*2* and *5*) 3 and (*3* and *6*) 4.

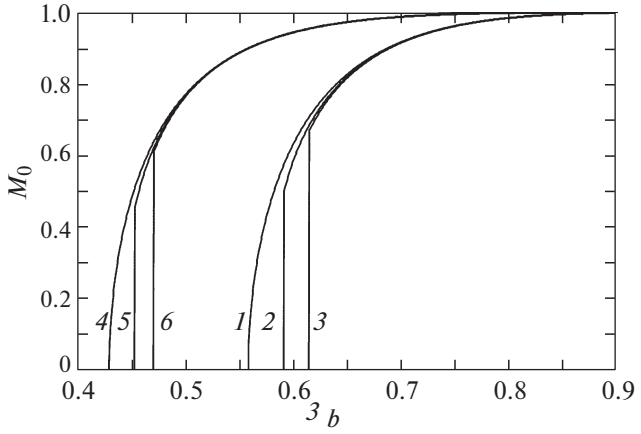

Fig. 2. Spontaneous magnetization versus the magnetic atom density at zero temperature for the coordination numbers q = (curves *1*, *2* and *3*) 3 and (curves *4*, *5* and *6*) 4 and the number of spin states s = (*1* and *4*) 2, (*2* and *5*) 3 and (*3* and *6*) 4.

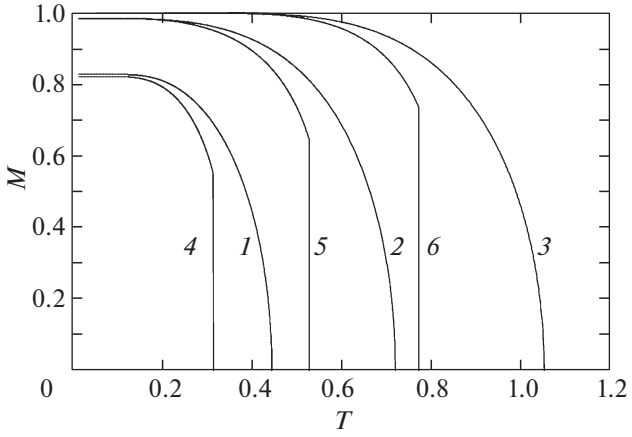

Fig. 3. Temperature dependence of the spontaneous magnetization of a diluted magnet with the lattice coordination number $q = 3$, magnetic atom densities of (*1* and *4*) 0.65, (*2* and *5*) 0.8 and (*3* and *6*) 1.0 and s = (the Ising model, curves *1*, *2* and *3*) 2 and (curves *4*, *5* and *6*) 3.

At $b = b_c$, M_0 increases abruptly from zero to $\Delta M_0 = \frac{s-2}{s-1}$. Figure 2 shows the functions $M_0(b)$ for $s = 2$, 3 and 4 (curves *1*, *2* and *3*, respectively). As is seen, the curves nearly coincide at high densities b but differ significantly near the percolation thresholds.

Figure 3 shows the temperature dependence of spontaneous magnetization at various densities b and the numbers s of spin states. As is seen in Fig. 3, the phase transition at $s = 2$ (the Ising model) and $s = 3$ is the second and first-order transition, respectively. Although we did not obtain a change in the character of the phase transition with a decrease in the density of magnetic atoms, as was found in [2] and [3], yet the magnitude of the magnetization jump at the critical point decreases with b.

At $q = 4$, we find from Eq. (3) at $K \to \infty$ the equation for the spontaneous magnetization at zero temperature

$$(1-b)^4 = 4b^3(1-b)\left(-\frac{s-1}{s}M_0^2 + \frac{s-2}{s}M_0 + \frac{1}{s}\right) + b^4\left(\frac{2(s-2)(s-1)}{s^2}M_0^3 - \frac{5s^2-15s+12}{s}M_0^2 + \frac{3(s-2)^2}{s^2}M_0 + \frac{3s-4}{s^2}\right), \quad (8)$$

This equation has a solution for $b > b_c$, which is in turn found from the equation

$$(1-b_c)^4 = 4b_c^3(1-b_c)\frac{1}{s} + \frac{3s-4}{s^2}b_c^4. \quad (9)$$

As in the case of $q = 3$, the percolation threshold b_c appears to be dependent on s. For $s = 2$, Eq. (8) is reduced to the explicit relation

$$M_0(b) = \sqrt{1 - \frac{2(1-b)^4}{4b^3(1-b) + b^4}}. \quad (10)$$

The plot of this function and the solutions of Eq. (8) for $s = 3$ and 4 are shown in Fig. 2 (curves *4*, *5* and *6*, respectively); as is seen, the magnitude of the jump at $b = b_c$ increases with s. The density dependences of the phase transition temperature and the temperature dependences of the spontaneous magnetization at $q = 4$ are similar to the respective dependences at $q = 3$ (Figs. 1 and 3).

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