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MAGNETISM

Mean-Field Approximation for the Potts Model of a Diluted Magnet in the External Field

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Abstract—The Potts model of a diluted magnet with an arbitrary number of states placed in the external field has been considered. Phase transitions of this model have been studied in the mean-field approximation, the dependence of the critical temperature on the external field and the density of magnetic atoms has been found, and the magnetic susceptibility has been calculated. An improved mean-field technique has been proposed, which provides more accurate account of the effects associated with nonmagnetic dilution. The influence of dilution on the first-order phase transition curve and the magnetization jump at the phase transition has been studied by this technique.

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1. INTRODUCTION

The Potts model [1] is one of the most used models in statistical physics; it is a theoretical tool applied to study a wide class of phenomena in condensed matter [2, 3] and nuclear physics [4, 5]. There are very few exact results of the Potts model. Knowingly, a first (second)-order phase transition occurs in zero external field if the number of spin states in the Potts model is greater (lower) than a certain critical value (depending on the lattice dimension) [1, 6, 7]. In contrast to the Ising model, the Potts model with a number of states no less than three also exhibits phase transitions in a nonzero external field [4, 5]. The points of these first-order phase transitions form a line in the temperature–external field plane, which ends up at the second-order phase transition point [4, 5]. The influence of nonmagnetic dilution on the critical behavior of the Potts model in zero external field was considered, in particular, in [3, 8, 9]. However, as far as we are aware of, the influence of nonmagnetic dilution on the entire first-order phase transition line has not been studied so far.

In this work, we consider the Potts model with an arbitrary number of states in the external field and nonmagnetic dilution in the mean field approximation. We implement both the classical mean-field technique and its modification, which takes into account more accurately the effect of nonmagnetic dilution.

2. POTTS MODEL

The Potts model [1] is formulated as follows. We consider a regular lattice. Each node corresponds to the quantity σ_i ("spin"), which can take s different values (e.g., 1, 2,..., s). 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 the external field H act on the state *1*. Then the total energy is

$$E = -J_p \sum_{i,j} \delta(\sigma_i, \sigma_h) = H \sum_i \delta(\sigma_i, 1).$$

We permit some lattice nodes to be occupied by nonmagnetic atoms ("impurities") instead of spins. Let b be the fraction of spins and $1 - b$, respectively, the fraction of impurities in the lattice. One can consider two types of impurities: frozen immobile impurities distributed randomly and uncorrelated over the lattice nodes and "mobile" impurities capable of moving over the nodes and occurring in the thermodynamic equilibrium with the matrix. The model with frozen impurities is of much greater interest, since the overwhelming majority of magnets with impurities belong to this particular type.

Let us consider a lattice node occupied by a magnetic atom. Let $n_1, n_2,..., n_s$ be the numbers of atoms in the first coordination sphere of this node that appear 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 $W(n_1, n_2,..., n_s)$. Let p_j be the probability of finding the magnetic atom in the state j. Obviously, for the frozen impurities,

$$\langle n_j \rangle_W = qbp_j. \quad (1)$$

We rely on the expression

$$\left\langle \frac{e^{Kn_j + h\delta(j,1)}}{\sum_i e^{Kn_i + h\delta(i,1)}} \right\rangle_W = p_j, \quad (2)$$

which is a generalization of the formula quoted in [10] with $K = j_p/kT$ and $h = H/kT$ (k is the Boltzman constant). We define the magnetization for the Potts model in the following way [3]:

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

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

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

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

$$M = \left\langle \frac{e^{Kn_1 + h} - \frac{1}{s-1}\sum_{i=2}^{s} e^{Kn_i}}{e^{Kn_1 + h} + \sum_{i=2}^{s} e^{Kn_i}} \right\rangle. \quad (3)$$

We will seek for the solution, in which all p_i for $i > 1$ are identical and equal to p. Then

$$p_1 = M + \frac{1 - M}{s} \quad \text{and} \quad p = \frac{1 - M}{s}. \quad (4)$$

3. CLASSICAL MEAN-FIELD METHOD

The simplest way of using formula (3) is the mean-field technique. It consists of replacing n_i in the right-hand side of Eq. (3) by their average values (1) expressed in terms of the magnetization M via formulas (4). This replacement results in the self-consistent equation for M:

$$M = \frac{e^{yM + h} - 1}{e^{yM + h} - 1 + s}, \quad (5)$$

where $y = qKb$. This equation determines the temperature dependence of the magnetization M on temperature, density and the external magnetic field. As is seen from Eq. (5), the dependence of the magnetization on temperature, density and the coordination number of the lattice is reduced to the dependence on y, which is typical for the mean-field approximation. This method was implemented to a pure ($b = 1$) Potts magnet both in the absence of the external field [2] and (for $s = 3$) in the nonzero external field [5]. However, as is seen from Eq. (5), its direct generalization to the case of a diluted magnet does not lead to any nontrivial results: the concentration b enters Eq. (5) only in the product. In this work, we propose the modification of the mean-field method, which will hopefully provide a more accurate description of the influence of nonmagnetic dilution on the critical behavior of the Potts model. Yet before introducing this modification we consider what can be obtained in the classical mean-field approximation (5) applied to a diluted magnet.

At $h = 0$, Eq. (5) always have the solution $M = 0$. However, this solution is stable only if the derivative of the right-hand side of Eq. (5) with respect to M is less than one at $M = 0$. It can be verified by calculating this derivative that the zero solution is stable at $y \leqslant s$, which leads to the following dependence of the phase transition temperature $T_0 = 1/K_0$ on the density b, the number s of spin states and the coordination number q:

$$T_0 = \frac{qb}{s}, \quad (6)$$

i.e., the phase transition temperature at $h = 0$ in the present approximation is simply proportional to the density b of magnetic atoms.

At $y < s$ ($T < T_0$), the spontaneous magnetization is determined by a nonzero solution of Eq. (5) at $h = 0$. This nonzero solution vanishes at $s = 2$ and $y \to s + 0$, which implies the absence of a discontinuity at the critical point $y = s$; i.e., this is the second-order phase transition. Let us recall that the Potts model with $s = 2$ is equivalent to the Ising model, which exhibits the second-order magnetic phase transition. If, on the contrary, $s > 2$, the nonzero solution of Eq. (5) at $y \to s + 0$ tends to the finite value M^* detemined by the equation

$$M^* = \frac{e^{sM^*} - 1}{e^{sM^*} - 1 + s}, \quad (7)$$

i.e., the phase transition is the first-order transition. A similar dependence $M_1^*(s) = \frac{s-2}{s-1}$ was derived in [2] by a method somewhat different from the mean-field method.

The susceptibility

$$\chi = \left.\frac{\partial M}{\partial H}\right|_{H=0} = \frac{K}{J_p}\left.\frac{\partial M}{\partial h}\right|_{h=0}$$

at $y < s$ can be found from Eq. (5) and amounts to $\chi = \frac{K}{J_p}\frac{1}{s-y}$. If $y > s$, the expression for the susceptibility becomes

$$\chi = \frac{K}{J_p}\left(\frac{s}{(1 + (s-1)M)(1 - M)} - y\right)^{-1}. \quad (8)$$

At $s = 2$ and $y \to 2 + 0$, this expression approximately reads as $\chi \approx \frac{1}{2}\frac{K}{J_p}\frac{1}{y-2}$. If, on the contrary, $s > 2$, susceptibility (8) remains finite at $y \to s + 0$ and has the maximum value at $y = s$ determined by substituting $M = M^*$ into Eq. (8).

As is known [4, 5], in contrast to the Ising model with its single phase transition point at $h = 0$, the Potts model with $s > 2$ exhibits a line of first-order phase transitions in the (K, h) plane, which starts at the point $(K_0, 0)$ and ends up at the point (K_e, h_e), where the second-order phase transition occurs. The points of the phase transition line are found from the conditions

$$\begin{cases} F(M,h) = M, \\ \dfrac{dF(M,h)}{dM} = 1, \end{cases}$$

where $F(M, h) = 1 - s/(e^{yM + h} - 1 + s)$. Hence,

$$e^h = \left(\frac{s}{1-M} - s + 1\right)e^{-yM}, \qquad (9)$$

and the magnetization is determined by the equation

$$y(s-1)x^2 - ysx + s = 0 \quad (x = 1 - M). \qquad (10)$$

This equation has a solution only for $y \in \left[\frac{4(s-1)}{s}, s\right]$. The upper boundary of this interval corresponds to phase transition temperature (6) at $h = 0$ and the lower one corresponds to the temperature $T_e = \frac{qbs}{4(s-1)}$. As follows from Eqs. (9) and (10), $h_e = \ln(s-1) - 2(s-2)/s$. The terminating point of the first-order phase transition line in the special case of $s = 3$ and $q = 6$ (a cubic lattice) of the Potts model without dilution ($b = 1$) was found in [5]. Substituting these values into our result we find exactly the same as in [5]. Using Eqs. (9) and (10), the equation of the first-order phase transition line can be written in the form

$$h(y) = \ln\left(\frac{s}{x_c(y)} - s + 1\right) - y(1 - x_c(y)),$$

$$x_c(y) = \frac{ys + \sqrt{y^2s^2 - 4ys(s-1)}}{2y(s-1)}, \quad y = qKb,$$

i.e., the influence of the density b of magnetic atoms (and the coordination number q of the lattice) in the classical mean-field approximation is reduced to rescaling the temperature axis. In particular, h_e is independent of b and the magnetization at the point (K_e, h_e) is independent of b and q and amounts to

$$M_e = 1 - \frac{s}{2(s-1)}.$$

4. MODIFIED MEAN-FIELD METHOD

The function $W(n_1, n_2,..., n_s)$, by which averaging in Eq. (3) is performed, can be expressed as

$$W(n_1, n_2, \ldots, n_s) = \sum_{z=0}^{q} P(z) W_z(n_1, n_2, \ldots, n_s), \qquad (11)$$

where $P(z)$ is the probability of finding z magnetic atoms in the first coordination sphere of the node occupied by the magnetic atom. For frozen impurities, obviously,

$$P(z) = C_q^z b^z (1-b)^{q-z}, \qquad (12)$$

where $C_q^z = \frac{q!}{z!(q-z)!}$ are the binomial coefficients.

Let us construct $W_z(n_1, n_2,..., n_s)$ approximately as follows. We denote the set of magnetic atoms, which are the neighbors of magnetic atoms having exactly z magnetic neighbors as Ω_z. Let $p_j(z)$ be the probability of finding an atom from Ω_z in the state j. We assume that $p_j(z) = p_j$. Then the average values of n_j calculated with the distribution function $W_z(n_1, n_2,..., n_s)$ are zp_j. Let us specify the function $W_z(n_1, n_2,..., n_s)$ as

$$W_z(n_1, n_2, \ldots, n_s) = \prod_{j=1}^{s} \delta(n_j - zp_j), \qquad (13)$$

i.e., for each specific z value we equate n_j to their average values. This is exactly our modification of the classical mean-field method. For a pure ($b = 1$) Potts magnet, this corresponds to an ordinary mean-field approximation. Using Eq. (4), we come to the self-consistent equation for finding M

$$M = \sum_{z=0}^{q} C_q^z b^z (1-b)^{q-z} \frac{e^{KzM+h} - 1}{e^{KzM+h} - 1 + s}. \qquad (14)$$

The phase transition temperature at $h = 0$ is found similar to the previous case:

$$1 = \frac{K_0}{s}\sum_{z=0}^{q} z C_q^z b^z (1-b)^{q-z} = \frac{K_0 qb}{s},$$

i.e., the phase transition temperature is given by formula (6), like in the previous case. Similar to Eq. (5), Eq. (14) has a stable nonzero solution at $T < T_0$, which determines the spontaneous magnetization. If $s = 2$ (the Ising model), this solution vanishes at $T \to T_0 - 0$, whereas $M \to M^* > 0$ at $s > 2$; i.e., the phase transition is the second-order transition at $s = 2$ and the first-order transition at $s > 2$.

However, there is still some difference between the behaviors of the solutions of Eqs. (5) and (14). The solution of Eq. (5) depends only on the parameter $y = qKb$, whereas the dependence of the solution of Eq. (14) on q, K and b is a more complicated. In particular, the quantity M^* depends now not only on s, as

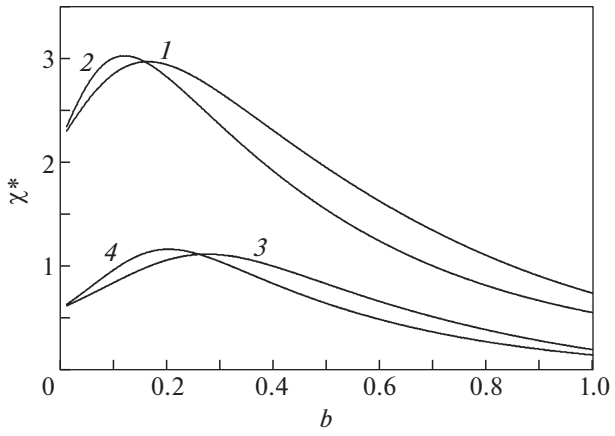

Fig. 1. Magnetic susceptibility multiplied by J_p at $T = T_c - 0$ versus the density b of magnetic atoms according to the modified mean-field approximation for (*1*) $q = 3$, $s = 3$; (*2*) $q = 4$, $s = 3$; (*3*) $q = 3$, $s = 4$; (*4*) $q = 4$, $s = 4$.

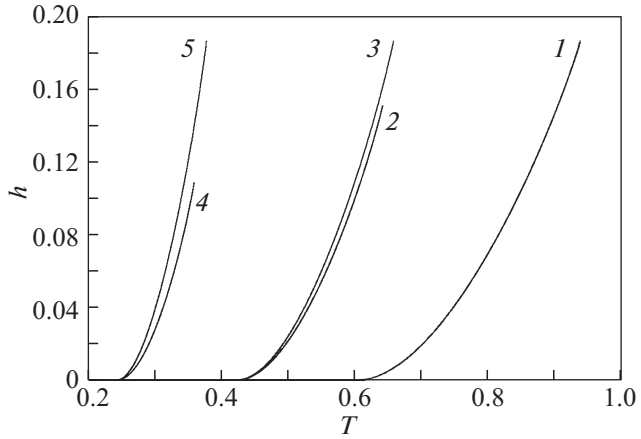

Fig. 2. First-order phase transition lines in the temperature T – external field h plane calculated for the Potts model with $s = 5$ and $q = 3$ calculated in the (curves *1*, *3*, *5*) classical and (curves *1*, *2*, *4*) modified mean-field approximation for the magnetic atom densities $b =$ (*1*) 1, (*2* and *3*) 0.7 and (*4* and *5*) 0.4. Both methods yield identical results for $b = 1$ (curve *1*).

in the previous case, but also on q and b and is given by the equation

$$M^* = \sum_{z=0}^{q} C_q^z b^z (1-b)^{q-z} \frac{\exp\left(\frac{zsM^*}{qb}\right) - 1}{\exp\left(\frac{zsM^*}{qb}\right) - 1 + s}, \quad (15)$$

which coincides with Eq. (7) only at $b = 1$.

Taking the derivative of Eq. (14) with respect to H, we find the magnetic susceptibility. At $T > T_c$ (in this case, the spontaneous magnetization vanishes), we find

$$\chi = \frac{K}{J_p} \sum_{z=0}^{q} \frac{Kz\chi + 1}{s} C_q^z b^z (1-b)^{q-z},$$

which is reduced to $\chi = \frac{K}{J_p} \frac{1}{s - y}$, as in the previous case. At $T < T_c$, we find the following equation for the susceptibility:

$$\chi = \frac{K}{J_p} \frac{\langle \varphi(z) \rangle}{1 - K\chi \langle z\varphi(z) \rangle}, \quad (16)$$

where

$$\varphi(z) = \frac{e^{KzM}}{e^{KzM} - 1 + s} - \frac{(e^{KzM} - 1)e^{KzM}}{(e^{KzM} - 1 + s)^2},$$

and the brackets denote averaging over the binomial distribution (12).

At $T < T_0$, the susceptibility χ increases monotonically with temperature reaching the limiting value at $T = T_0 - 0$. This limiting value χ^* is shown in Fig. 1 as a function of the density of magnetic atoms. As is seen, χ^* is nonmonotonic and tends to a finite limit at $b \to 0$. As is seen from Eqs. (7) and (8), the limiting susceptibility χ_c^* in the classical mean-field approximation is inversely proportional to b

$$\chi_c^*(b) = \frac{\chi^*(1)}{b}$$

And diverges at $b \to 0$.

Let us now consider finding the first-order phase transition lines in the modified mean-field approximation. To find the points of this line it is necessary to find the common solution of Eq. (14) and the condition that the derivative of the right-hand side of Eq. (14) with respect to M is unity. The calculation results are shown in Fig. 2. The classical mean-field approximation does not exhibit the dependence of h_e on b (Fig. 2, curves *1*, *3*, *5*), whereas in the modified mean-field approximation h_e decreases with b (curves *1*, *2*, *4*).

The magnitude of the magnetization jump at the first-order phase transition lines is illustrated in Fig. 3. The upper and lower branches of the curves in Fig. 3 correspond to the magnetization when the phase transition lines are approached from above (from lower temperatures or higher external fields) and below, respectively. The magnitude of the magnetization jump at a particular $h \in [0, h_e]$ is the difference between these two values. In the classical mean-field approximation, the jump is independent of the density b and the magnetization at the phase transition line is shown by the curve *1* in Fig. 3 at an arbitrary density. In the modified mean-field approximation, the jump appears to decrease with b (curves *2* and *3*).

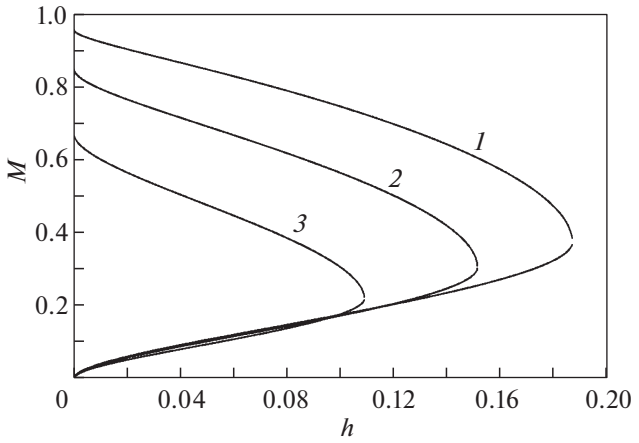

Fig. 3. Magnetization jump M at the first-order phase transition line of the Potts model with $s = 5$, $q = 3$ versus the external magnetic field h in the mean-field approximation at the magnetic atom density $b = (1)$ 1, (2) 0.7 and (3) 0.4.

5. CONCLUSIONS

We have analyzed the critical behavior of a diluted Potts magnet with an arbitrary number of states in a nonzero magnetic field with the use of the classical mean-field approximation. The results of this analysis can be regarded as the generalization of the results obtained in the earlier works [2, 5].

We have elaborated a modification of the mean-field method for a diluted Potts magnet, which coincides with the classical technique at $b = 1$. By this technique, we have analyzed the influence of nonmagnetic dilution on the first-order phase transition curve and found the following basic results:

1. The magnetic susceptibility in zero external field at $T = T_0 - 0$ is a nonmonotonic function of the density b and has a maximum at a certain b value depending on s and q (Fig. 1).

2. The coordinates (T_e, h_e) of the terminating point of the phase transition lines are functions of the density b and both functions decrease with b (Fig. 2).

3. The jump of the magnetization at the phase transition line depends on b and its magnitude decreases at all $h \in [0, h_e(b)]$ (Fig. 3).

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