ISSN 1063-7761, Journal of Experimental and Theoretical Physics, 2015, Vol. 121, No. 4, pp. 636–639. © Pleiades Publishing, Inc., 2015.
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ORDER, DISORDER, AND PHASE TRANSITION IN CONDENSED SYSTEM

The Potts Model on a Bethe Lattice with Nonmagnetic Impurities

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Received April 17, 2015

Abstract—We have obtained a solution for the Potts model on a Bethe lattice with mobile nonmagnetic impurities. A method is proposed for constructing a "pseudochaotic" impurity distribution by a vanishing correlation in the arrangement of impurity atoms for the nearest sites. For a pseudochaotic impurity distribution, we obtained the phase-transition temperature, magnetization, and spontaneous magnetization jumps at the phase-transition temperature.

DOI: 10.1134/S1063776115100131

1. INTRODUCTION

The Potts model [1] is formulated as follows. Let us consider a certain regular lattice. We put in correspondence to each site a quantity σ_i ("spin") that can assume n different values (say, 1, 2, ..., n). Two neighboring spins σ_i and σ_j interact with 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 us suppose that an external field, H, is acting on state 1. The total energy is then given by

$$E = -J_p\Sigma_{(i,j)}\delta(\sigma_i,\sigma_j) - H\Sigma_i\delta(\sigma_i,1).$$

We assume that nonmagnetic atoms ("impurities") are located at some lattice sites. Let b be the fraction of spins; accordingly, $1 - b$ is the fraction of impurities in the lattice.

We can consider two types of impurities: "frozen-in" stationary impurities that are distributed at random among lattice sites without correlation and "mobile" impurities that can move over sites and are in thermodynamic equilibrium with the matrix. The model with frozen-in impurities is most interesting because most magnets with impurities belong precisely to this type. Unfortunately, the exact solution of the problem with frozen-in impurities cannot be obtained even for simple lattices. It will be shown below, however, that the exact solution to the problem with mobile impurities can be obtained on the Bethe lattice. This solution, which is probably interesting as such, makes it possible to analyze the behavior of a system with frozen-in impurities. For mobile impurities, the correlation (covariation) in the arrangement of impurities at neighboring lattice sites can be calculated. Imposing the condition of vanishing on this correlation, we obtain a impurity distribution that we called the "pseudochaotic" distribution. Although such a distribution of impurities over lattice sites is not completely random, the percolation threshold (e.g., for a pseudochaotic distribution on the Bethe lattice) coincides with the threshold for frozen-in impurities. We believe that the behavior of a system with pseudochaotic mobile impurities is a good approximation for a magnet with frozen-in impurities.

Thus, we consider the Potts model with mobile impurities. Let us suppose that variables σ_i can assume, apart from values of 1, 2, ..., n, a zero value when a nonmagnetic impurity is located at a site. We assume that the forces of interaction act only between neighboring atoms. The contribution to the system energy from two adjacent sites can then be written in the form

$$E_{ij} = -J_p\delta(\sigma_i,\sigma_j) - (U_{11} - J_p)\delta(0,\sigma_j)\delta(\sigma_i,0)$$
$$-U_{12}\{\delta(\sigma_i,0)(1-\delta(0,\sigma_j)) + \delta(0,\sigma_j)(1-\delta(\sigma_i,0))\}$$
$$-U_{22}(1-\delta(0,\sigma_j))(1-\delta(\sigma_i,0)).$$

Here, U_{11} is the energy of interaction of two adjacent impurity atoms, U_{12} is the energy of interaction of an impurity atom and a magnetic atom, and U_{22} is the energy of interaction between two magnetic atoms.

The large partition function of the system has the form

$$Z = \Sigma\exp\{K\Sigma_{(i,j)}\varphi(\sigma_i,\sigma_j) + h\Sigma_i\delta(\sigma_i,1) + x\Sigma_i\delta(\sigma_i,0)\}, \quad (1)$$

where $K = Jp/kT$, $h = H/kT$, and $x = \mu/kT$ (μ is the chemical potential),

$$\varphi(\sigma_i,\sigma_j) = \delta(\sigma_i,\sigma_j) + (\gamma-1)\delta(0,\sigma_j)\sigma(\sigma_i,0),$$

$$\gamma = \frac{U}{J_p}, \quad U = U_{11} - 2U_{12} + U_{22}.$$

2. SOLUTIONS FOR THE BETHE LATTICE

We construct a Bethe lattice in the following manner. We consider two adjacent sites with spin variables σ_1 and σ_2. Joining each site with $q - 1$ outer neighbors (sites of the first shell), each site of the first shell with $q - 1$ sites of the second shell, and continuing this process N times. We obtain the so-called Cayley tree: the Bethe lattice is the inner (far from boundary sites) part of the Cayley tree for $N \to \infty$. To evaluate the partition function (1) on the Bethe lattice, we will use an approach that is analogous to that employed in [1] for the Ising model. The large partition function (1) is the sum over all of the possible spin configurations $\{\sigma\}$:

$$Z = \Sigma_{\{\sigma\}} P(\sigma);$$

$$P(\sigma) = \Sigma \exp\{K\Sigma_{(i,j)}\varphi(\sigma_i, \sigma_j) \\ + h\Sigma_i \delta(\sigma_i, 1) + x\Sigma_i \delta(\sigma_i, 0)\}.$$

Separating the terms that contain σ_1 and σ_2 in this expression, we can write it in the form

$$P(\sigma) = e^{\psi(\sigma_1,\sigma_2)} \Pi_{j=1}^{q-1} Q_N(\sigma_1|s_1^{(j)}) \Pi_{l=1}^{q-1} Q_N(\sigma_2|s_2^{(j)}),$$

where

$$\psi(\sigma_1, \sigma_2) = K\varphi(\sigma_1, \sigma_2) \\ + h(\delta(\sigma_1, 1) + \delta(\sigma_2, 1)) + x(\delta(\sigma_1, 0) + \delta(\sigma_2, 0)),$$

and $s_1^{(j)}$ and $s_2^{(l)}$ denote the aggregates of spins at the jth and lth branches of sites 1 and 2, respectively.

Denoting $G_N(\sigma) = \Sigma_{\{s\}} Q_N(\sigma|s)$, we can write the partition function in the form

$$Z_N = \Sigma_{\sigma_1,\sigma_2} e^{\psi(\sigma_1,\sigma_2)} G_N^{q-1}(\sigma_1) G_N^{q-1}(\sigma_2). \tag{2}$$

Using this relationship, we can find the probability, p_i, that spin σ_1 assumes the value i (in view of the symmetry, the probabilities of the relevant values of variable σ_2 are exactly the same):

$$p_i = \frac{1}{Z_N} \Sigma_{\sigma_1,\sigma_2} \frac{1}{2}(\delta(\sigma_1, 1) + \delta(\sigma_2, i)) \\ \times e^{\psi(\sigma_1,\sigma_2)} G_N^{q-1}(\sigma_1) G_N^{q-1}(\sigma_2) - p_0^2. \tag{3}$$

In accordance with the above arguments, the concentration of magnetic atoms in the lattice is $b = 1 - p_0$. We calculate the covariance in the arrangement of impurities at sites 1 and 2 as

$$g_{12} = \frac{1}{Z} \Sigma_{\sigma_1,\sigma_2} \delta(\sigma_1, 0)\delta(\sigma_2, 0) \\ \times e^{\psi(\sigma_1,\sigma_2)} G_N^{q-1}(\sigma_1) G_N^{q-1}(\sigma_2) - p_0^2. \tag{4}$$

For the function $G_N(\sigma)$, we can construct recurrent relationships by representing $Q_N(\sigma|s)$ in the form

$$Q_N(\sigma|s) \\ = \exp\{K\varphi(\sigma, s_1) + h\delta(s_1, 1) + x\delta(s_1, 0)\}\Pi_{j=1}^{q-1} Q_{N-1}(s_1|t^{(j)}),$$

where s_1 is one of the spins of the first shell and $t^{(j)}$ is the aggregate of spins of one of its branches. Summing this expression over the aggregate of spins s, we obtain

$$G_N(\sigma) = \Sigma_{s_1} \exp\{K\varphi(\sigma, s_1) \\ + h\delta(s_1, 1) + x\delta(s_1, 0)\} G_{N-1}^{q-1}(s_1). \tag{5}$$

Since we will further pass to the thermodynamic limit ($N \to \infty$), we introduce the relationships $y_{i,N} = G_N(i)/G_N(1)$ instead of the function $G_N(\sigma)$. We can derive the recurrent relationships that express $y_{i,k}$ in terms of $y_{i,k-1}$ from expression (5) (obviously, $y_{i,0} = 1$) and the expression for p_i and g_{12} in terms of $y_{i,N}$ from expressions (3) and (4).

We will seek the solution in which all values of p_i for $i > 1$ are identical; we denote $y_{i,k}$ for $i > 1$ just by y_k and, in addition introduce the notation $t_k = e^x y_{0,k}^{q-1}$. Then relationships (3) and (4) yield

$$p_1 = \frac{1}{\tilde{Z}_N}(e^{K+2h} + t_N e^h + (n-1)e^h y_N^{q-1}), \tag{6}$$

$$1 - b = \frac{1}{\tilde{Z}_N}(t_N^2 e^{K\gamma} + t_N e^h + (n-1)t_N y_N^{q-1}), \tag{7}$$

$$g_{12} = \frac{t_N^2 e^{K\gamma}}{\tilde{Z}_N} - (1-b)^2, \tag{8}$$

$$\tilde{Z}_N = t_N^2 e^{K\gamma} + e^{K+2h} + 2t_N e^h \\ + (n-1)y_N^{q-1}(2t_N + 2e^h + e^K y_N^{q-1} + (n-2)y_N^{q-1}). \tag{9}$$

From relationship (5), we obtain the recurrent relationships

$$y_{0,N} = \frac{e^{\gamma K} t_{N-1} + e^h + (n-1)y_{N-1}^{q-1}}{t_{N-1} + e^{K+h} + (n-1)y_{N-1}^{q-1}}, \tag{10}$$

$$y_N = \frac{t_{N-1} + e^h + (e^K + (n-2))y_{N-1}^{q-1}}{t_{N-1} + e^{K+h} + (n-1)y_{N-1}^{q-1}}. \tag{11}$$

Let us consider relationships (6)–(11) in the thermodynamic limit ($N \to \infty$). In this limit, $y_{0,N} \to y_0$, $y_N \to \mathbf{y}$, $t_N \to t$, and $Z_N \to Z$. In accordance with the above arguments, we choose the value of γ so that g_{12} vanishes. We denote this value of γ by γ_0. Then, relationships (7) and (8) give

$$1 - b = \frac{te^{K\gamma_0}}{te^{K\gamma_0} + e^h + (n-1)y^{q-1}}.$$

from which

$$e^{K\gamma_0} = \frac{1-b}{bt}(e^h + (n-1)y^{q-1}). \tag{12}$$

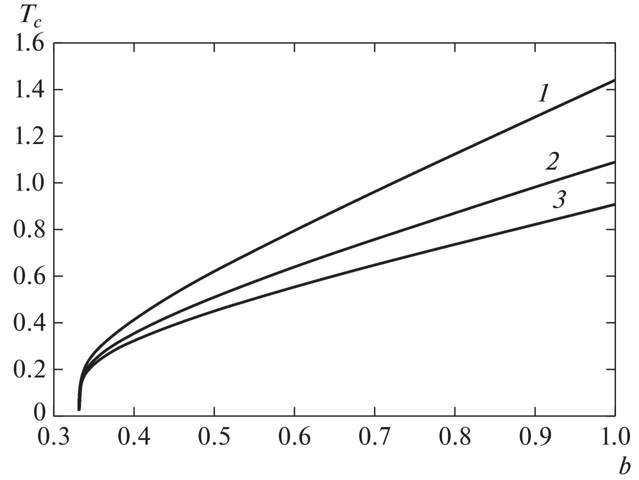

Fig. 1. The dependence of the Curie temperature on the concentration of magnetic atoms for $q = 4$. Curves *1–3* correspond to $n = 2$ (Ising model), $n = 3$, and $n = 4$, respectively.

Substituting this relationship into (8), we obtain

$$t = \frac{1-b}{b}\frac{e^{K+2h} + (n-1)y^{q-1}(2e^h + y^{q-1}(e^K + n - 2))}{e^h + (n-1)y^{q-1}}, \quad (13)$$

while relationship (6) gives

$$p_1 = \frac{1}{\tilde{Z}_0}(e^{K+2h} + te^h + (n-1)e^h y^{q-1}); \quad (14)$$

or

$$\tilde{Z}_0 = t\frac{1+b}{b}(e^h + (n-1)y^{q-1}) \\ +[e^{K+2h} + (n-1)y^{q-1}(2e^h + y^{q-1}(e^K + n - 2))] \quad (15)$$

In addition, from recurrent relationship (11), we obtain for $N \to \infty$

$$p_1 = b^2 \frac{e^{K+2h} + te^h + (n-1)e^h y^{q-1}}{e^{K+2h} + (n-1)y^{q-1}(2e^h + y^{q-1}(e^K + n - 2))}. \quad (16)$$

Expressions (13)–(16) give the solution to the problem of determining the quantities that characterize the state of the Potts magnet depending on the temperature, external field, and atomic concentration of an impurity in the case of a pseudochaotic impurity distribution. In addition, these formulas make it possible to determine the phase-transition temperature $K_c(b) = J_p/kT_c(b)$ as a function of the concentration of magnetic atoms.

Analysis of expressions (13)–(16) shows that for $K < K_c(b)$ and $h = 0$, the only stable solution to Eq. (16) is $y = 1$ and $p_1 = b/n$ (this follows from relationship (15)). For $K = K_c(b)$, probability p_1 increases jumpwise (a first-order phase transition) for $n > 2$. Using expressions (13) and (16), we can find the phase-transition temperature. For $K = K_c$, the derivative of the right-hand side of expression (16) with respect to y must be equal to unity for $y = 1$ (if this derivative is greater than unity, the solution $y = 1$ becomes unstable). Taking the derivative of expression (16) (using formula (13) for determining $t(y)$), we obtain

$$K_c(b) = \ln\frac{n - 1 + (q-1)b}{(q-1)b - 1}. \quad (17)$$

For $b = 1$ (i.e., for the Potts model without impurities), expression (17) coincides with the critical temperature of the Potts model on the Bethe lattice in [2]. For $n = 2$ (in this case, the Potts model is equivalent to the Ising model), relationship (17) leads to the same result as that in [3]. Figure 1 shows the curves that depict the critical temperature $T_c(b) = 1/K_c(b)$ for $q = 4$ and $n = 2, 3, 4$ (curves *1–3*, respectively). It can be seen that quantities $T_c(b)$ have an infinite derivative at $b = b_c$ and are almost linear functions of Δ near $b = 1$, which corresponds to the familiar properties of the dependence of the critical temperature on the concentration of magnetic atoms [4]. In addition, expression (17) shows that for an arbitrary n, the critical temperature vanishes for a concentration that coincides with the percolation threshold of the Bethe lattice ($b_c = 1/(q - 1)$); in this sense, the pseudochaotic impurity distribution behaves as a truly chaotic distribution [5, 6]. The difference between these distributions can be illustrated by calculating the probability that a magnetic atom that is chosen at random belongs to an infinite cluster of magnetic atoms. If we define the magnetization in the Potts model with n states analogously to [7],

$$M = \frac{np_1 - b}{b(n-1)},$$

it can easily be proven that the probability that a magnetic atom belongs to an infinite cluster is just the magnetization M at $T = 0$ and $h = 0$. Passing in relationships (13), (15), and (16) to the limit $K \to \infty$, we obtain

$$M_0(y) = \frac{1}{b(y)(n-1)} \\ \times\left(\left(\frac{1-b(y)}{1+(n-1)y^{q-1}} + \frac{b(y)}{1+(n-1)y^{2(q-1)}}\right)n - b(y)\right),$$

$$b(y) = \left(1 + \frac{1+(n-1)y^{q-1}}{1+(n-1)y^{2(q-1)}}\Sigma_{i=1}^{q-2} y^i\right)^{-1},$$

$$0 < y < 1.$$

These expressions define the $M_0(B)$ dependence in parametric form. Figure 2 shows the $M_0(b)$ curves for $n = 2$ (curve *2*) and $n = 4$ (curve *3*). The same figure shows the function $P(b)$ (curve *1*) that defines the probability that a magnetic atom belongs to an infinite cluster for a chaotic distribution of impurity atoms over the Bethe lattice sites. (This probability can be determined by the formulas [4] $P(b) = 1 - s^q$ and

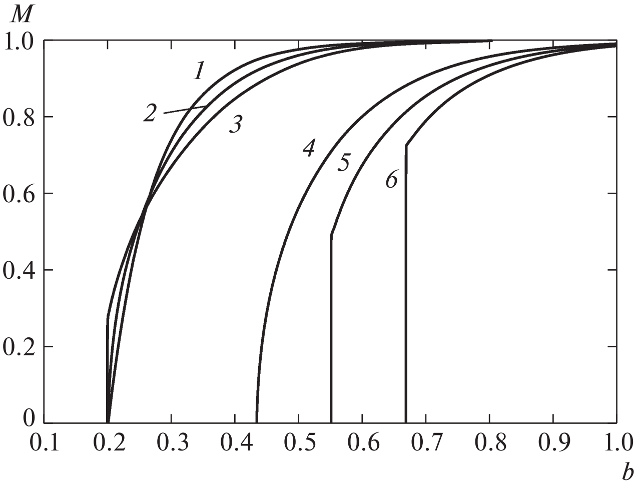

Fig. 2. The concentration dependence of spontaneous magnetization. The concentration, b, of magnetic atoms is on the abscissa axis and the magnetization is on the ordinate axis. Curve *1* describes the probability that a magnetic atom belongs to an infinite cluster in the Bethe lattice with random dilution; curves *2* and *3* describe the magnetization at zero temperature in the Potts model with a pseudochaotic distribution for $n = 2$ and 3, respectively. Curves *4*–*6* describe the magnetization at $K = 1$ for $n = 2$, 3, and 4, respectively.

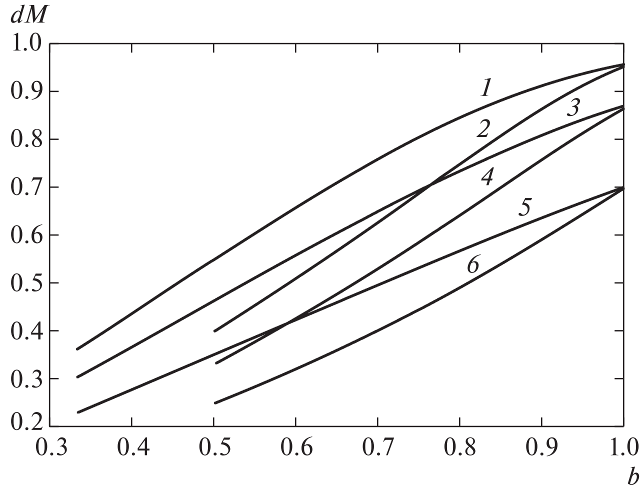

Fig. 3. The concentration dependence of the magnetization jump during the phase transition in the Potts model with a pseudochaotic impurity distribution. The concentration, b, of magnetic atoms is on the abscissa axis and the magnetization jump dM is on the ordinate axis. Curves *1*, *3*, and *5* are plotted for coordination number $q = 4$, while curves *2*, *4*, and *6* are plotted for $q = 3$. The number of states is $n = 6$ for curves *1* and *2*, $n = 4$ for curves *3* and *4*, and $n = 3$ for curves *5* and *6*.

$\Sigma_{i=0}^{q-2} s^i = 1/b$.) It can be seen that although functions $M_0(b)$ and $P(b)$ are quite similar and vanish for any n at the same value of $b_c = 1/(q-1)$, which corresponds to the percolation threshold for the Bethe lattice, there is still some difference in their details.

Figure 2 also shows the magnetization at a finite temperature ($K = 1$) as a function of the concentration of magnetic atoms for $n = 2$ (curve *4*), $n = 3$ (curve *5*) and $n = 4$ (curve *6*). It can be seen that the phase transition is of the second order for $n = 2$ (Ising model) and of the first order for $n > 2$. Expression (17) shows that the value of the concentration $b_0(K)$ for which spontaneous magnetization occurs for a finite K is defined by the expression

$$b_0(K) = b_c \frac{1 + (n-1)e^{-K}}{1 - e^{-K}}. \quad (18)$$

It can be seen that $b_0(K)$ increases with n for any n exceeding b_c as well. For $K \to \infty$, we have $b_0(K) \to b_c$ for any $n > 1$.

Figure 3 shows the dependence of the jump of the magnetization, M, upon a phase transition as a function of the concentration of magnetic atoms for different coordination numbers, q, of the lattice and the number of spin states, n. It should be noted that the phase-transition temperature (17) itself depends on the concentration, b, of magnetic atoms; for this reason, in each curve in Fig. 3, different points of the curve correspond to different temperatures. It can be seen that the jump for all values of parameters decreases monotonically with decreasing concentration b to a certain nonzero value for $b = b_c$. At a fixed b, the jump increases with n at a constant q, as well as with increasing q at a constant n. The dependence of the jump on the coordination number q of the lattice (for the same n) is manifested weakly for a pure magnet ($b = 1$), but becomes noticeable for $b < 1$.

ACKNOWLEDGMENTS

This work was supported financially by the Ministry of Education and Science of the Russian Federation under assignment no. 2014/292 for research in the sphere of scientific activity in the base of the state contract.

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Translated by N. Wadhwa

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