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CONDENSED MATTER

Tricritical Point for the Three-Dimensional Disordered Potts Model (q = 3) on a Simple Cubic Lattice

A. B. Babaev[a, b, *] **and A. K. Murtazaev**[a, c]

[a] *Amirkhanov Institute of Physics, Dagestan Scientific Center, Russian Academy of Sciences, Makhachkala, 367003 Russia*
[b] *Dagestan State Pedagogical University, Makhachkala, 367003 Russia*
[c] *Dagestan State University, Makhachkala, 367025 Russia*
** e-mail: b_albert78@mail.ru*

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Slightly diluted magnetic systems described by the disordered three-dimensional Potts model with the number of spin states $q = 3$ are studied in the case of a simple cubic lattice. The position of the tricritical point in the phase diagram is determined using the histogram Monte Carlo technique.

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1. INTRODUCTION

Currently, the studies of phase transitions and critical phenomena in the systems with the disorder determined by quenched magnetic impurities and by various other structural defects attract a considerable attention. This occurs because modern microelectronics (and spintronics) has achieved such a miniaturization level that it is impossible to neglect the influence of such defects on the performance of microelectronic devices and circuits. Moreover, the effect of quenched disorder on different characteristics of magnetic systems is of fundamental interest [1].

The work by Harris [2] dealing with the effect of quenched disorder, which is created by nonmagnetic impurities, on the critical characteristics of magnetic materials has stimulated considerable interest in studies of the critical behavior in structurally disordered systems. According to the corresponding criterion of disorder occurring in the form of quenched nonmagnetic impurities, these defects are efficient only if the specific heat of the homogeneous system diverges at the critical point; i.e., the critical exponent of the specific heat is positive, $\alpha > 0$. Appreciable progress has already been achieved in the understanding of specific features of the effect of quenched disorder, occurring in the form of nonmagnetic impurities [1], random bonds [3], and random magnetic fields [1, 4], on the critical behavior of magnetic systems.

On the other hand, several studies [5–7] have demonstrated that the quenched disorder can give rise to the change in the order of the phase transition in the systems, which exhibit a first order phase transition in the absence of dilution. In experiment, such behavior was observed for the phase transitions in liquid crystals within a porous host material [8].

In the case of low-dimensional systems ($d \le 2$) described by the Potts model with the number of spin states $q > 4$, the presence of even infinitesimal disorder is sufficient to transform the first order phase transition to the second order one [6, 9]. For the homogeneous systems with $d \ge 3$ dimensions, which exhibit the first order phase transition, the situation can be quite different. The quenched disorder introduced in this case can give rise to the tricritical point p^*, below and above which the second and first order phase transitions occur, respectively. The main aim of the present work is to determine the position of the tricritical point for the systems described by the three-dimensional Potts model with the number of spin states $q = 3$.

The determination of the exact position of the tricritical point is quite important for the development of different new magnetic materials, as well as for studies of the effect of quenched disorder on various thermodynamic characteristics. In the available publications, the results for the tricritical point [10–12] in the systems described by the Potts model with $q = 3$ are not quite definite. The tricritical point in [10] and in [11, 12] is observed at $p^* = 0.90(1)$ and 0.76(8), respectively.

In contrast to [10–12], we implement the quenched disorder in a conventional way using nonmagnetic impurities (by specifying the relative content of magnetic sites). Note that the disorder brought about in the form of nonmagnetic impurities and the disorder of the random bond type should be characterized by the same universality class [1, 3]. Earlier, we determined the tricritical points with the accuracy of 0.01 for the Potts model with $q = 4$ in the cases of the disorder implemented in the form of nonmagnetic impurities [13] and for the disorder of the random bond type [14]. In the case of $q = 3$, the position of the tricritical point has not yet been found with a good accuracy.

The interest in the disordered Potts model with the number of spin states $q = 3$ arises because it describes the physical properties of many multicomponent alloys and liquid crystals in the aerogel host material. Structural phase transitions in some materials such as $SrTiO_3$ are also described by the Potts model with $q = 3$.

2. MODEL AND ITS ANALYSIS

For the simple cubic lattice, the Hamiltonian of the three-dimensional disordered Potts model with the number of spin states $q = 3$ can be written as [15]

$$H = -\frac{1}{2}J\sum_{i,j}\rho_i\rho_j\delta(S_i, S_j), \quad S_i = 1, 2, 3, \tag{1}$$

where J is the parameter characterizing the ferromagnetic exchange interaction of the nearest-neighbor spins and $\rho_i = 1$ and 0 (if site i is occupied by a magnetic atom and a nonmagnetic impurity, respectively).

In [16, 17], it has been shown that this model in the absence of the structural disorder exhibits a weak first order phase transition, which could be expected based on the mean-field theory [18]. To determine the tricritical point, we studied the thermal characteristics of the system as functions of its linear size L using the histogram analysis of the data within a very narrow dilution range ($0.95 \le p \le 1.00$).

The tricritical point for disordered systems can hardly be determined using conventional theoretical and experimental techniques because it is nearly impossible to prepare the samples with the clearly specified and distributed impurity densities. Moreover, most of the conventional theoretical techniques are inapplicable to disordered systems [1]. Therefore, such systems described by microscopic Hamiltonians can be rigorously and consistently treated by the Monte Carlo methods allowing one to study the thermal parameters of the spin systems with any degree of complexity at any controlled nonmagnetic impurity densities.

In our study, we use a highly efficient Wolff cluster algorithm [19] of the Monte Carlo method. In more detail, we have described this algorithm in [20, 21].

To analyze the character of the phase transition, we employ the histogram analysis of the Monte Carlo data [22, 23]. In the histogram data analysis, the probability of finding the system with the energy U and the order parameter m is given by the expression [22]

$$\overline{P(U, m)} = \frac{1}{Z(K)}W(U, m)\exp[KU], \tag{2}$$

where $W(U, m)$ is the number of configurations with the energy U and order parameter m, $Z(K)$ is the energy distribution function for the whole system, and K is the inverse temperature.

3. RESULTS OF THE SIMULATIONS

The calculations were performed for the systems with periodic boundary conditions. We studied the $L \times L \times L = N$ systems, where L = 20–90 with the relative spin contents $p = 1.00$, 0.97, and 0.95. To drive the system to the equilibrium state, we calculated the corresponding relaxation time τ_0 for each system with the linear size L. Then, the averaging was performed over a part of the Markovian chain of length $\tau = 150\tau_0$. In addition, we performed the averaging over different initial configurations. In the case of $p = 1.0$, we used ten initial configurations for the averaging. For the system with $p = 0.97$ and 0.95, we performed the configurational averaging over 1000–3000 different configurations. The technique of averaging over the ensemble of disordered systems with different realizations of the quenched disordered is discussed in detail in [16].

To determine the critical temperatures, we used the technique based on the fourth order Binder cumulants [24]. The technique for determining the critical temperatures within the Binder cumulant approach is discussed in detail in [21, 25–27]. In Fig. 1, we show the phase diagram describing the dependence of the phase transition temperature on the spin concentration p. In this diagram, the critical temperatures at $p = 1.0$, 0.95, 0.90, 0.80, 0.70, and 0.65 are taken from [17], whereas those at $p = 0.97$ and $p = 0.60$ are determined in the present study. At $p^* = 0.95$ and below this value, the system exhibits the second order phase transition, while the first order phase transition occurs above this point. At the same figure, we also show the results predicted by the mean-field theory for the phase transition temperature $T_t(p) = p^* T_t(1)$ [11] as a function of the spin concentration p and by the effective medium theory [28]

$$K_t(p) = \log\left[\frac{(1 - p_c)e^{K_t(1)} - (1 - p)}{(p - p_c)}\right], \tag{3}$$

where p_c is the spin percolation threshold ($p_c = 0.31$) and $K_t = J/k_BT$.

From Fig. 1, it follows that, at $p \ge 0.8$, the calculated $T_c(p)$ dependence agrees well with the results both of the effective medium theory and of the mean-field theory. At $p < 0.8$, we observe an appreciable

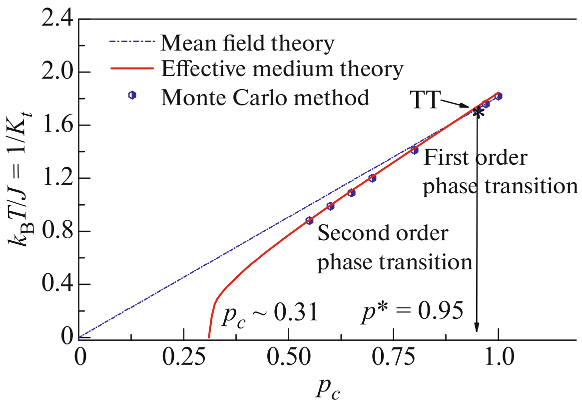

Fig. 1. (Color online) Phase diagram for the three-dimensional disordered Potts model with the number of spin states $q = 3$. The tricritical point is marked as TT.

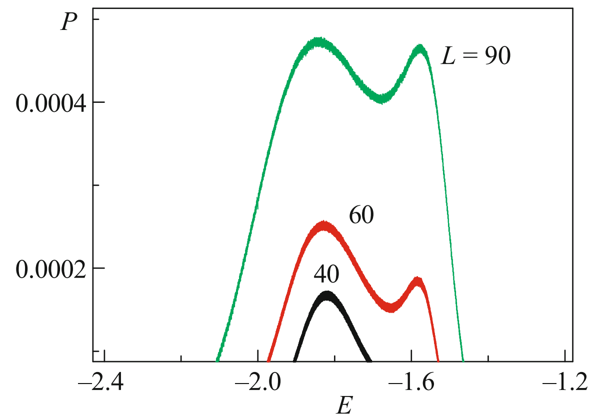

Fig. 2. (Color online) Histograms for the energy distribution characterizing the three-dimensional Potts model with $q = 3$ at the relative spin content $p = 0.97$ and at different linear sizes L of the system.

deviation of the predictions of the mean-field theory from those based on the effective medium theory and from the Monte Carlo data.

The histogram analysis of the Monte Carlo data [22, 23] allows us to reliably determine the range of the spin concentration p at which the transformation of the first order phase transition to the second order one occurs. This method also makes it possible to estimate the minimum sizes of the system at which it is still possible to determine correctly the order of the phase transition. The histogram analysis for the three-dimensional Potts model with the number of spin states $q = 3$ at the relative spin content $p = 0.97$ indicates the first order phase transition as for the pure undiluted system at $p = 1.0$. This conclusion is illustrated in Fig. 2, where we show the histogram of the energy distribution near the phase transition point for the systems with different linear sizes L. In Fig. 2, we can see that the bimodality in the energy distribution is observed in the systems with $L = 60$ and 90, whereas it is absent at $L = 40$. Therefore, the histogram data analysis is appropriate for the systems with the sizes not smaller than $L = 60$. The bimodality in the energy distribution is the sufficient condition for the first order phase transition. At the same time, for all systems under discussion with the spin content $p = 0.95$ and the lineal sizes $L = 40$, 60, and 90, we observe the energy distribution with only one peak (Fig. 3), which is characteristic of the second order phase transition. Such behavior was also observed at all other spin contents meeting the condition $p \leq 0.95$. For the Potts model with $q = 4$, the bimodality in the energy distribution is observed at $p^* \sim 0.70(1)$ [13] in the case of disorder coming from nonmagnetic impurities and at $p^* \sim 0.74(2)$ for the disorder of the random bond type [14].

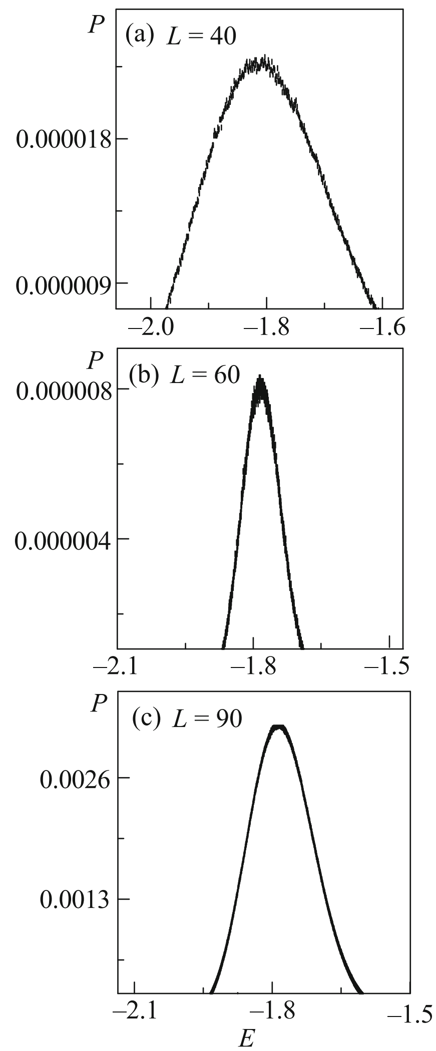

Fig. 3. Histograms for the energy distribution for the three-dimensional Potts model with $q = 3$ at the relative spin content $p = 0.95$ and at different linear sizes L of the system.

4. CONCLUSIONS

The histogram analysis of the Monte Carlo data for the spin systems described by the three-dimensional slightly disordered Potts model with $q = 3$ has demonstrated that the transformation of the first order phase transition to the second order one within the Potts model under study occurs at $p^* = 0.95(1)$. A minor increase in the relative spin content with respect to this value results in the first order phase transition. This leads us to the conclusion that p^* is the tricritical point for this model.

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