Physics of the Solid State, 2023, Vol. 65, No. 4

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The effect of nonmagnetic disorder on phase transitions of the first-order

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Received June 16, 2022
Revised January 31, 2023
Accepted February 1, 2023

Using the Monte Carlo method, weakly dilute magnetic systems described by two-dimensional 5-state Potts model, which in the pure state undergoes a phase transition first-order. Numerical studies have revealed that an insignificant quenched disorder, realized in the form of nonmagnetic impurities, can change the order of phase transition in magnetic systems described by the two-dimensional 5-state Potts model on a square lattice, for which a phase transition of the first-order is observed in a homogeneous state. It is shown that such a phase change the transition is due to the fact that nonmagnetic disorder prevents the coexistence of local phases characteristic of a phase transition of the first-order at $T = T_l$.

Keywords: phase transitions, nonmagnetic disorder, Potts model, Monte Carlo, symmetry.

DOI: 10.21883/PSS.2023.04.56004.407

1. Introduction

Recently, there has been a significant amount of interest in studies of phase transitions (PT) and critical phenomena (CP) in magnetic systems that contain disorders in the form of quenched nonmagnetic impurities. On one hand, it is related to the fact that modern microelectronics and spintronics have reached such a level of miniaturization that the impact of different defects in structures on the behavior of microelectronic devices and elements cannot be neglected. At the same time, the effect of a quenched disorder on various characteristics of magnetic systems is also of fundamental scientific interest [1].

The study of Harris [2] devoted to the effect of quenched disorder on the critical properties of magnetics has caused much interest in the study of a critical behavior of structurally disordered systems. According to this criterion, defects realized as quenched nonmagnetic impurities are essential if the specific heat diverges at the critical point in the homogeneous variant, i.e. the specific heat exponent is positive $\alpha > 0$. Appreciable progress has already been achieved in the understanding of specific features of the effect of quenched disorder, occurring both in the form of nonmagnetic impurities, random bonds and in the form of random magnetic fields [1–4], on the critical behavior of magnetic systems.

However, unlike the effect of quenched disorder on continuous PTs, much less is known about its influence on first-order transitions. In particular, there are reasons to suggest that disorder has a completely different effect up to the change of a PT order in spin systems exhibiting a first-order PT in the homogeneous state [5–7]. The first-order PT is characterized by the existence of different local phases [6,7]. Such a change in the PT is experimentally observed in liquid crystals with aerogel [8]. In addition, the exact values of the nonmagnetic impurity concentrations c, $c = 1-p$, where p is the concentration of spins, at which the physical properties of the considered systems can change greatly, are important for the development of various new magnetic materials. As an example, we can consider high-temperature superconductors formed when nonmagnetic Sr atoms are substituted for a small amount of La atoms in the $LaCuO_4$ antiferromagnetic dielectric [9]. Also, the combination of phase coexistence and a certain chemical disorder is important for colossal magnetoresistance oxides [10]. Therefore, the question is clear: how does disorder affect a first-order phase transition, and whether the coexistence of different phases is possible at a disorder in the system under consideration? An attempt to answer this question on the basis of numerical experiment through the analysis of magnetic configurations described by homogeneous and doped Potts models is the main goal of this work.

When studying the effect of disorder in the form of nonmagnetic impurities on first-order phase transitions the experimental and theoretical methods of investigation meet significant and formidable challenges. The point is that the experimental findings depend strongly on the method and the specific sample as well as on the way the sample is prepared (see references in [3]). In addition, the experimental studies based on a unified methodical approach on a series of single-type samples at a strictly controlled content of the impurities are not practically performed. And theoretical approaches are nearly all based on the application of some or other computational schemes within the field-theory renormalization-group method. The applicability of these schemes for quenched disorder models is much more complicated than for pure systems. This results in an extensive investigation of phase transitions and critical phenomena in dilute systems by various Monte Carlo (MC) methods [3,11]. An important advantage of these methods is the availability to control all parameters in the course of the experiment.

2. Model and numerical investigation technique

This study considers a two-dimensional 5-state ($q = 5$) Potts model on a square lattice in pure (with a spin concentration of $p = 1.00$) and weakly diluted mode ($p = 0.95,\ 0.90$). In this model a first-order PT is observed in the homogeneous state [12,13]. When building up ferromagnetic Potts models with a number of spin states equal to q, the following features must be taken into account [12]:

– spins S_i are present in the sites of the lattice in question, which can be oriented in q symmetric directions of the hypertetrahedron with a dimension of $q - 1$, so that the angles between any two spin directions are equal to each other;

– the bond energy between two sites is zero, if they are in different states (no matter in which exactly) or, if at least one site contains a nonmagnetic atom, and is equal to J, if the interacting sites are in the same state (again, no matter in which exactly).

Taking into account these features, the Hamiltonian of 5-state ($q = 5$) Potts model can be represented as follows:

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

$$S_i = P_1, P_2, P_3, P_4, P_5, \tag{1}$$

where J is parameter of exchange ferromagnetic interaction of the closest spins, P_q is number of different states of the spin S_i, $\rho_i = 1$, if the site i is occupied by a magnetic atom, and $\rho_i = 0$ if the site i contains a nonmagnetic impurity, and

$$\delta(S_i, S_j) = \begin{cases} 1, & \text{if } S_i = S_j, \\ 0, & \text{if } S_i \neq S_j. \end{cases}$$

In computer simulation, we used the Wolff cluster algorithm of the Monte Carlo method [14]. This algorithm is considered in more detail in [15]. The initial configurations were set in such a way that all spins were in the same states. To bring the system to an equilibrium, a nonequilibrium section with a length of τ_0 was cut off for the system with a linear dimension of L. This nonequilibrium section was discarded. In each chain an averaging was performed over a section of Markov chain with a length of $\tau = 500\tau_0$. For the biggest system: $L = 160$, $\tau_0 = 1.8 \cdot 10^3$ MC steps/spin. In addition, configurational averaging was carried out over 1000 various impurity configurations. Then these data was used to calculate the average values of thermodynamic parameters. In the process of modeling, for two-dimensional and impurity samples various individual unique configurations of spin structures obtained by visualization of numerical data in the graphic mode were analyzed. At the end of the configurational averaging, the data was output in the graphic mode.

3. Results of numerical modelling

In [16,17] it has been found using fourth-order Binder cumulants and the method of histogram data analysis that a first-order PT is observed in the two-dimensional 5-state Potts model in the homogeneous state in accordance with the analytical forecast of [12,13], and an injection of a nonmagnetic disorder results in a change in of the first-order PT to the second-order PT. However, in these studies spin configurations observed in the computational experiments have not been analyzed and causes of the change of first-order PT to the second-order PT have not been found out. Visualizations of magnetic structures for the 5-state Potts model on a square lattice in the homogenous state ($p = 1.0$) and at a spin concentration of $p = 0.9$ are shown in Fig. 1 and 2, respectively. As can be seen from Fig. 1, the spin structures corresponding to different temperature modes — $T > T_l$, $T = T_l$ and $T < T_l$, where T_l is temperature that corresponds to first-order PT (see Fig. 1, *a*, Fig. 1, *b* and Fig. 1, *c*) allow vividly tracking the successive changes in magnetic configurations taking place with a change in the temperature mode and with introduction of a nonmagnetic disorder (see Fig. 2). As can be seen from Fig. 1, no individual ordered clusters of atoms exist in the case of homogeneous ($p = 1.0|$) magnetic structures at a temperature of $T > T_l$. Such a pattern is kept until the point of phase transition T_l. At the point of phase transition itself $T = T_l$ the coexistence of individual local phases can be noticed, each composed of atoms in strictly one of five different spin states, which is typical for the first-order PT.

The introduction of a disorder in the form of nonmagnetic impurities in the considered two-dimensional structure described by the Potts model with a number of spin states of $q = 5$ results in a noticeable change in the observed pattern for the first-order PT (see Fig. 2). In this case at a spin concentration of $p = 0.90$ and $T = T_c$ an extended cluster of atoms starts to be formed, where atoms are in only one of five possible spin states throughout the entire sample (see Fig. 2, *b*). With a decrease in temperature T (at $T < T_c$) the two-dimensional system under consideration is completely embraced by this cluster, in this case with a state $q = 5$ (see Fig. 2, *c*). A similar behavior is also observed at a spin concentration of $p = 0.95$.

In the case of three-dimensional structures described by Potts models with a number of spin states of $q > q_c$, $q_c = 2.45$ [12,13] the situation is significantly different. In this case the presence of a nonmagnetic disorder can

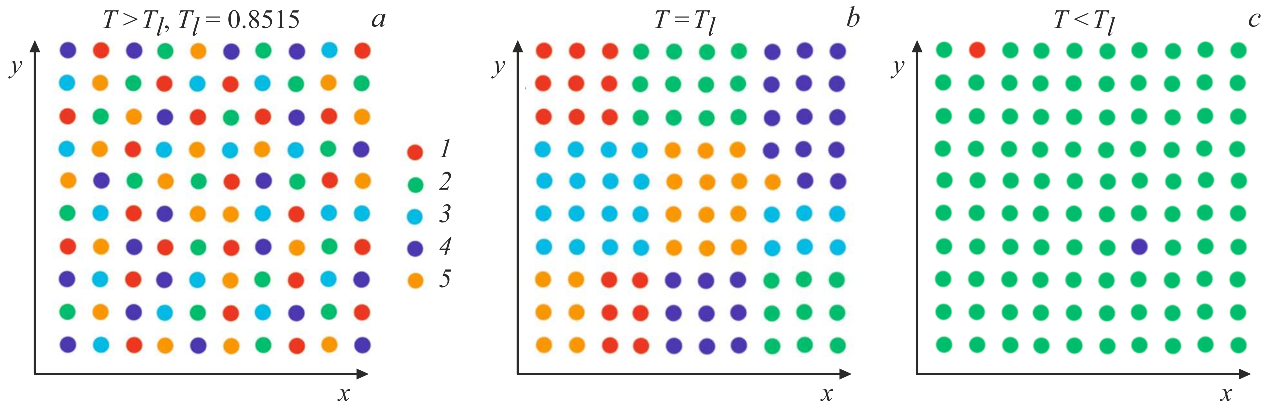

Figure 1. Magnetic structures described by a homogeneous ($p = 1.0$) 5-state Potts model on a square lattice at various temperature modes. With $T = T_l$ different spin phases exist simultaneously.

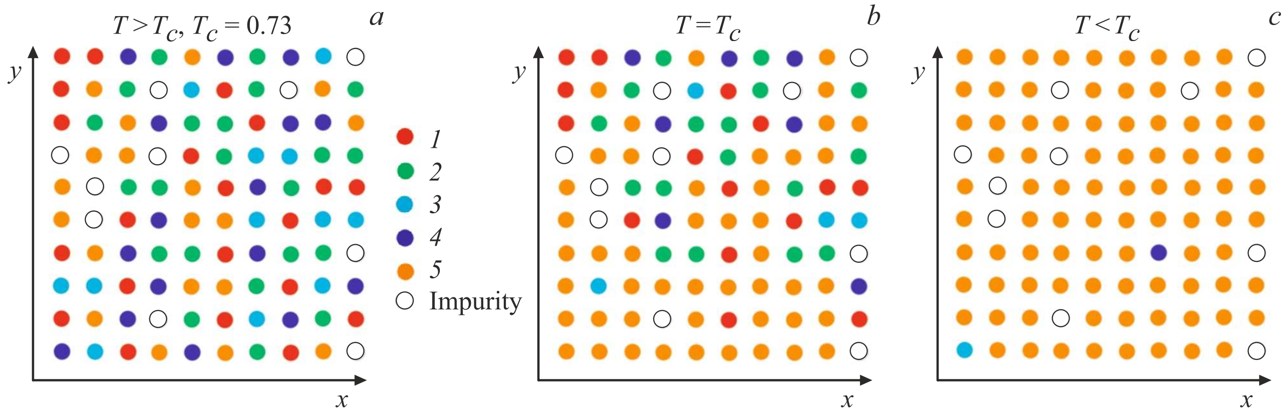

Figure 2. Magnetic structures described by an impurity 5-state Potts model on a square lattice in a weakly diluted mode ($p = 0.90$). With $T = T_c$ (b) a percolation of one of the five possible spin states takes place.

result in a tricritical point p_t. The analysis of spin configurations for this case is presented in [18]

4. Conclusion

Thus, the analysis of magnetic configurations of a two-dimensional weakly diluted Potts model with a number of spin states equal to $q = 5$, for which a first-order PT is observed in the homogeneous state, shows that an insignificant nonmagnetic disorder prevents the coexistence of local phases typical for the first-order PT. The nonmagnetic disorder decreases symmetry of the spin system in question: in the point of phase transition an extended cluster is formed, which is composed of magnetic atoms in only one of five possible spin states (see Fig. 2). Previously, Imry and Ma in their study [5], which has become classic, on the basis of simple energy considerations have forecasted the possible obstacle of the quenched disorder for the macroscopic phase coexistence in systems with a dimension of $d < 2$. Moreover, their argumentations later were extended to weakly diluted systems with an arbitrary small disorder [6]. Validity of these argumentations was strictly proved for systems with $d \leq 2$ in [7]. The results of computational experiment of this study confirm conclusions of the theoretical studies of [5–7].

Conflict of interest

The authors declare that they have no conflict of interest.

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Translated by Y.Alekseev