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Phase transitions in the diluted 2D three-state Potts model on a square lattice

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The computer simulation method was used to study phase transitions in a two-dimensional site-diluted 3-state Potts model. Systems with linear dimensions $L \times L = N$, $L = 10 \div 160$ at a spin concentration $p = 1.00$, 0.80 are considered. The numerical data obtained indicate that in a pure 3-state Potts model on a square lattice, a phase transition of the second order is observed in accordance with the theory. The introduction of disorder in the form of non-magnetic impurities ($p = 0.80$) in the 3-state Potts model preserves the phase transition of the second order.

Keywords: Potts model, Monte Carlo method, thermodynamic parameters, disorder.

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1. Introduction

The computer technologies and computational study methods have developed to their prevalence over the theoretical and experimental methods in studying the unordered magnetic systems. This is due to the fact that real systems always have complicating factors, which impede use of theoretical and experimental procedures [1–5]. Many of the known theoretical arrangements within a theory & field renormalization & group method becomes inoperative if applied to systems with disorder (see reviews [4,5]). In modern experimental studies big difficulties are encountered when studying thermodynamic and critical properties of the spin systems with in-frozen disorder. Today's experimental results do not make it possible to form a complete and consistent picture of critical behavior of impurity systems. It is not just the situation when the results of experimental studies largely depend a method and a specific sample, but on a sample preparation method as well. Moreover, in practice there is no experimental studies to be carried out based on a single approach on series of same-type samples with strictly-controlled content of an impurity quantity. Almost all the experimental studies still have a serious unresolved problem of getting to an asymptotic critical mode [2,4]. This background presents promising results and possibilities of studying the impurity systems by means of MC methods.

By now, it is known that structure flaws realized as non-magnetic impurities affect thermal and magnetic characteristics of the spin systems and may affect phase transitions (PT), if the so-called Harris criterion is met [6]. According to this criterion, the impurities are substantial, if a respective critical index of heat capacity α of a pure system is positive, i.e. the heat capacity diverges, and, therefore, this criterion can be applied to the three-dimensional Ising model, for which $\alpha > 0$. During recent thirty years, the study of critical properties of the unordered Ising model with in-frozen disorder has been reflected in a significant number of papers (see reviews [4,5] and [7,8]) and has got a substantial progress in understanding features of impact of the non-magnetic impurities on this model. At the same time, the Harris criterion is not applied for the two-dimensional Ising model, as $\alpha = 0$. Detailed examination of this case [9] allowed concluding that impurity impact affects only the heat capacity behavior, whereas other thermodynamic and correlation functions do not change their behavior.

On the other hand, in case of the spin systems, homogeneously undergoing phase transitions of the first order the impurities can affect a kind of phase transitions [10]. A recent paper [11] has also indicated a stabilizing role of the non-magnetic impurities when implementing the phase transitions of the second order by applying the theoretical methods. To study this case, the Potts model suits well. On the one hand, it is related to the fact, that the Potts model has the evident phase transition of the first order when $q > 4$ and the evident phase transition of the second order when $q \leq 4$. On the other hand, the Potts model is a theoretical tool to be applied to study a wide class of phenomena in the condensed matter physics [12]. It is obvious that the

lattice structure of this model is isomorphic for a big number of such systems as: a lamellar magnetic material, aerogels, liquid helium films, superconductive films, etc. [13].

Thus, the Potts models can be used to check the specifics of impurity impact on the phase transitions and to determine their role as a stabilizing factor in case of the phase transitions of the second order. Moreover, in accordance with the Harris criterion, [6] for the two-dimensional Potts models with $q = 3$ or with $q = 4$ the impurities must also affect the critical behavior as for these models $\alpha = 1/3$ and $\alpha = 2/3$, respectively. The paper [14] has studied a four-component ($q = 4$) impurity Potts model and demonstrated that the phase transition and the critical behavior of this model are affected by disorder implemented as non-magnetic impurities. At the same time, for the Potts mode with $q = 3$ the literature has almost zero information as to influence of the in-frozen disorder on the phase transition and its critical behavior, in particular, when the disorder is canonically implemented as the non-magnetic impurities. Values of the critical temperatures are not determined and one has not revealed the specifics of disorder impact on the thermodynamic parameters such as magnetization m, susceptibility χ, energy E, heat capacity C and Binder cumulants U_L and V_L.

In connection therewith, the purpose of this study is to study impact of non-magnetic impurities on the phase transitions and the thermodynamic behavior of the three-component ($q = 3$) two-dimensional Potts model on a square lattice.

2. Two-dimensional impurity Potts model with $q = 3$ on the square lattice

Here we include formulation of the two-dimensional standard impurity Potts model with a number of spin states $q = 3$, which is used to describe a big number of objects and phenomena in the condensed matter physics. In the model under our consideration the impurities are canonically distributed [4]. When building such a model the following features shall be taken into account:

1. The square lattice sites have spins S_i, which can be oriented in 3 symmetric directions in the space with a dimension $q - 1$, so that the angles between any two spin directions are equal and the non-magnetic impurities (vacancies) (see Fig. 1). The non-magnetic impurities are randomly distributed and fixed on various lattice sites (quenched disorder).

2. The bond energy between the two sites is zero, if they are in different states (no matter in which exactly) or, if at least one site contains a non-magnetic atom, and is equal to J, if the interacting sites are in the identical states (again, no matter in which exactly).

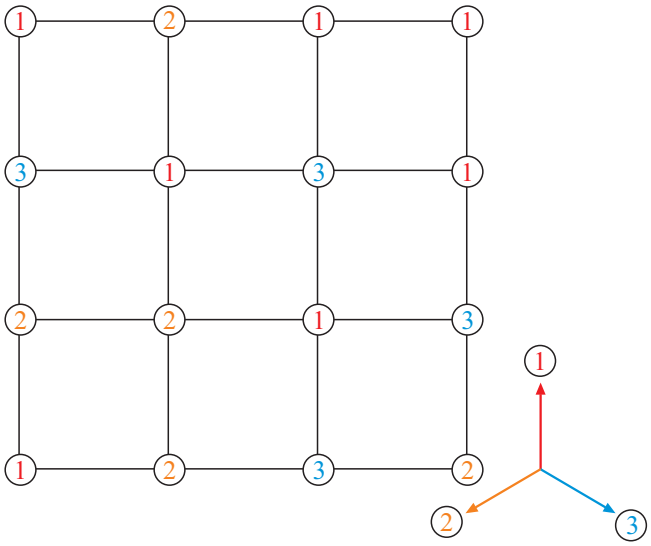

Figure 1. Standard two-dimensional Potts model with the number of the spin states $q = 3$ on the square lattice.

Taking into account these features, a microscopic Hamiltonian of such a system can be presented as follows [13]:

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

where

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

and

$$\rho_i = \begin{cases} 1, & \text{if the site has a spin} \\ 0, & \text{if the site has a non-magnetic impurity.} \end{cases}$$

A concentration of the magnetic spins is determined by the expression:

$$p = \frac{1}{L^2} \sum_{i=1}^{L^2} \rho_i \delta(S_i, q). \qquad (2)$$

Then the value $p = 1$ corresponds to the pure Potts model, while $p = 0$ — the empty, purely-impurity lattice.

3. Research procedure

Presently, as selected from all the options of cluster algorithms of the Monte-Carlo method, the Wolff algorithm is the most effective [15]. The procedure of its realization is detailed in the papers [8,16]. In this paper, we have used that algorithm as follows.

1. Two random numbers specify coordinates i, j of the site on the lattice. If this site has a non-magnetic impurity, then new random numbers are generated until the coordinates of the magnetic spin S_i are generated.

2. All the nearest neighbors S_j of this spin S_i are considered. If the adjacent site is occupied with the magnetic spin, then with the probability

$$P = 1 - \exp(-K), \tag{3}$$

where $K = J/k_B T$, k_B — Boltzmann constant, T — temperature, the bond between S_i and S_j is activated, if S_i and S_j have identical values when $J > 0$. Note that for the Potts model, in order to express the probability of spin inclusion in the cluster (2), the exponent 2, which is typical for the corresponding probability of the Ising model, disappears. Thus, it can be affirmed that the Potts model with the spin state $q = 2$ is equivalent to the Ising model with accuracy of a number factor 2 in the exchange constant J.

3. If the bond between the spins S_i and S_j is activated, then the spin in the site j is included in the cluster. It should be noted that, as for the Ising model with the impurities, the same spin can be included in the cluster only once, whereas it can be checked for cluster inclusion several times.

4. After checking all the nearest neighbors of the selected spin i, the first cluster-included spin becomes „a central one"to start the process of activation of bonds of this spin with the nearest neighbors. This process continues until checking all the nearest neighbors of all the cluster-included spins or reaching system boundaries.

5. All the spins as bonded therebetween form „a cluster".

6. The cluster produced is turned with the probability 1. For the Potts model, the cluster turn means that a new value of the spin S_i', as different from the old value S_i, will be assigned to all the cluster-included spins, with equal probability among all of its states q. Then we pass to the item 2.

The efficiency of the single-cluster Wolff algorithm as applied to the Potts model can be judged by a critical index z, which characterizes the efficiency of the algorithm being used. In particular, the study of the clean two-dimensional Potts model with $q = 3$ based on the single-cluster Wolff algorithm has demonstrated that the critical index $z = 0.60 \pm 0.02$, while using the Metropolis classic algorithm provided the value $z \approx 2$ [17]. According to the above-mentioned Wolff algorithm [14], the Markov process has been realized for the systems with periodic boundary conditions. The calculations have been carried out for the systems with periodic boundary conditions, for the systems with linear dimensions $L = 10 \div 160$ and a number of the sites $p \times L \times L = N$. Originally, configurations were specified so that all the spins were ordered along one of the axes X, Y or Z. In order to bring the system to an equilibrium, a nonequilibrium section of the length τ_0 was cut off for the system with the linear dimensions L. This nonequilibrium section was discarded. Each chain had average done across a section of the Markov chain of the length $\tau = 150\tau_0$. For the biggest system $L = 160$, $\tau_0 = 1.8 \cdot 10^3$ MC steps/spin.

4. Simulation results

The computer simulation included calculation of the thermodynamic characteristics of a single sample by the following formulas [12,18]:

$$U = [\langle U \rangle] = \frac{1}{N}[\langle H \rangle], \tag{4}$$

$$m_F = \frac{\left[q\left(\frac{N_{\max}}{N}\right) - 1\right]}{q - 1}, \tag{5}$$

$$C = (NK^2)\left[\langle U^2 \rangle - \langle U \rangle^2\right], \tag{6}$$

$$\chi = (NK)\left[\langle m^2 \rangle - \langle m \rangle^2\right], \tag{7}$$

where $K = |J|/k_B T$, $N_{\max} = \max\{N_1, N_2, N_3\}$, N_i — a number of the spins in a state with $q = i$, $N = pL^2$ — a number of the magnetic points; the angle brackets mean thermodynamic averaging, while the square brackets mean averaging across the impurity configurations.

The Figures 2 and 3 show typical magnetization dependences for the pure ($p = 1.00$) and diluted ($p = 0.80$) Potts model on the temperature, respectively. Here and below, all the figures include a data error, which does not exceed dimensions of symbols used for plotting. As it is clear from these figures, all the considered systems have evident behavior, which is typical for the phase transition of the second order.

The Figures 4 and 5 show the temperature dependences for susceptibility χ and heat capacity C, for the systems with different linear dimensions L at the spin concentration $p = 1.0$, while in the Figures 6 and 7 — at $p = 0.8$. As it is clear from these figures, the spin systems with quite big linear dimensions L have prominent maximums in the critical area and these maximums fall into the same temperature within the error.

A method of the Binder cumulants of the fourth order has shown good results for analysis of the PT nature [19]:

$$V_L(T, p) = 1 - \frac{\left\langle E^4(T, p; L)\right\rangle_L}{3\left\langle E^2(T, p; L)\right\rangle_L^2}, \tag{8}$$

$$U_L(T, p) = 1 - \frac{\left\langle m^4(T, p; L)\right\rangle_L}{3\left\langle m^2(T, p; L)\right\rangle_L^2}, \tag{9}$$

where E — energy and m — a parameter of the system order with the linear dimension L. The expressions (8) and (9) allow determining the temperature $T_l(p)$ with a high accuracy in the phase transitions of the first and second order, respectively. It should be noted that the use of the Binder cumulants also allows good determination of the PT order in the system. The phase transitions of the second order are characterized by the following features [20]: the averaged value $V_L(T, p)$ tends to a definite value V^* as per the expression:

$$V(T, p) = V^* + bL^{-d} \tag{10}$$

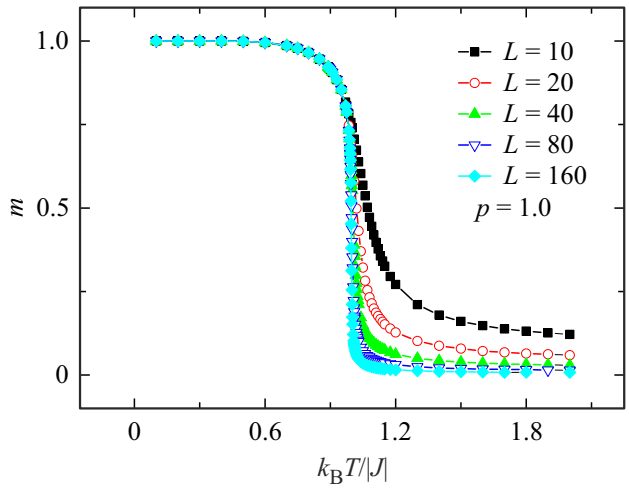

Figure 2. Temperature magnetization dependence for the pure Potts model.

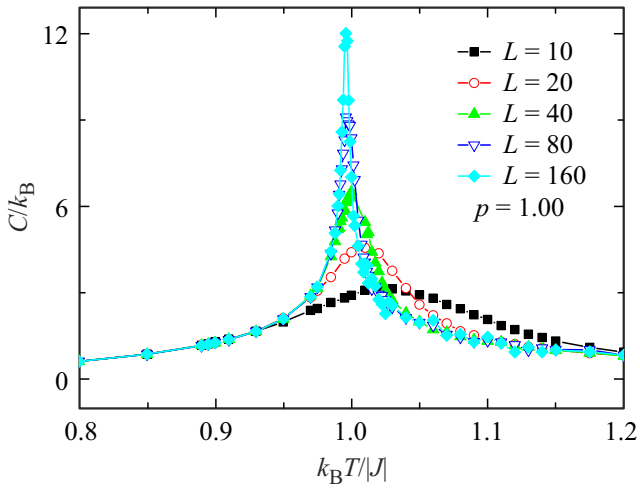

Figure 5. Temperature heat capacity dependence for the pure Potts model.

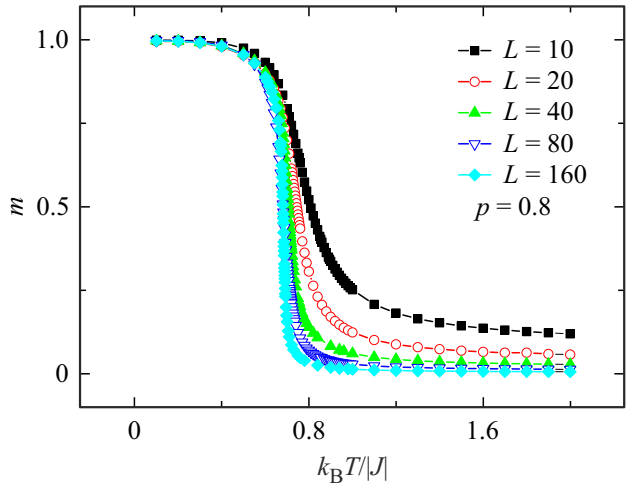

Figure 3. Temperature magnetization dependence for the diluted Potts model.

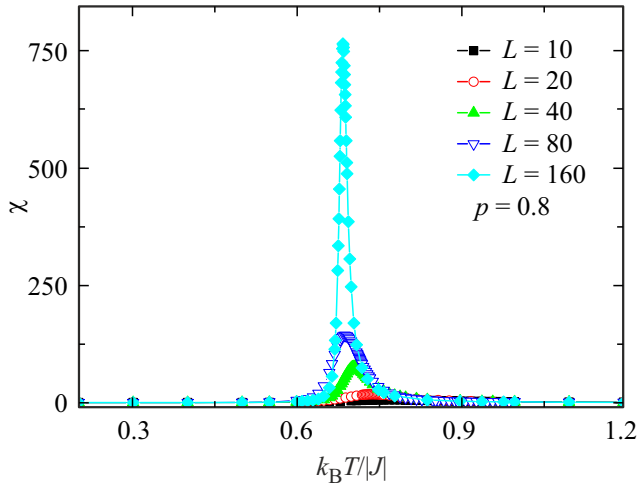

Figure 6. Temperature susceptibility dependence for the diluted Potts model.

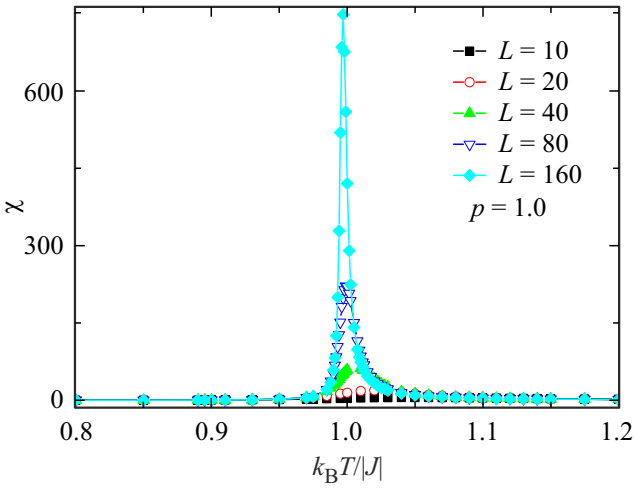

Figure 4. Temperature susceptibility dependence of the pure Potts model.

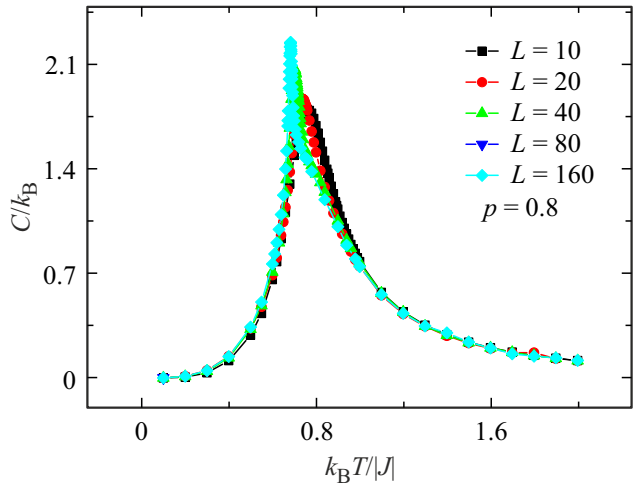

Figure 7. Temperature heat capacity dependence for the diluted Potts model.

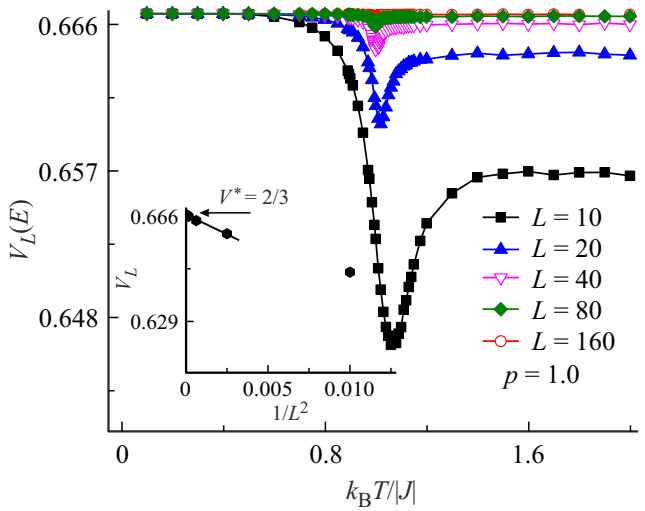

Figure 8. Temperature dependence of the Binder cumulants $V_L(T)$ for the two-dimensional pure Potts model with the number of the spin states $q = 3$.

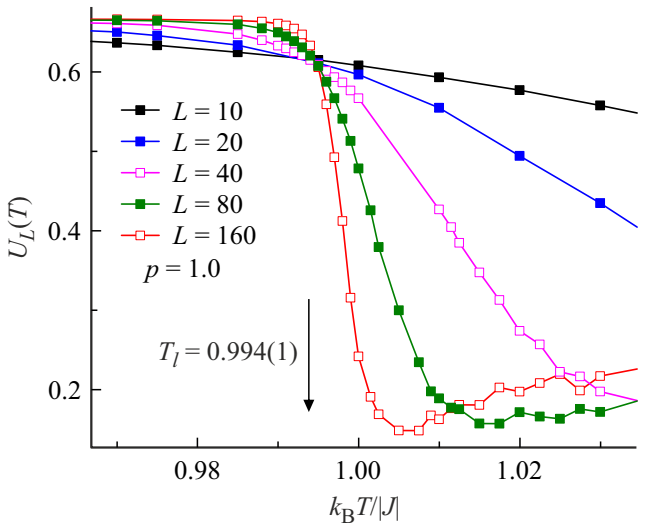

Figure 9. Temperature dependence of the Binder cumulants $U_L(T)$ for the two-dimensional pure Potts model with the number of the spin states $q = 3$.

at $L \to \infty$ and $T = T_l(L)$, where $V^* = 2/3$, and the curves of the temperature dependence of the Binder cumulants $U_L(T, p)$ will have a distinct intersection point. The said features for the Binder cumulants of the fourth order $V_L(T, p)$ and $U_L(T, p)$ are shown in the Figures 8 and 9, respectively, for the ferromagnetic Potts model with the $q = 3$ on the square lattice with no structural disorder $p = 1.00$. The similar picture is also observed when adding a non-magnetic disorder of the concentration $c = 0.2$, $c = 1 - p$ (see the Figures 10 and 11). The procedure to determine a PT order by this method is described in detail in the papers [21–23]. It should be noted that the PT temperature $T_l = 0.994(1)$ obtained for the pure spin system at $p = 1.0$ agrees fairly well with an analytical value as obtained by Baxter [12] by the formula:

$$\frac{k_B T_l}{|J|} = \frac{1}{\ln(1+\sqrt{3})} = 0.99497\ldots.$$

Regardless of the method of Binder cumulants of the fourth order, we have also carried out a histogram data analysis for the two-dimensional Potts model with the number of the spin states $q = 3$ on the square lattice. The histogram data analysis includes the following probability of the system under consideration having the energy U and the

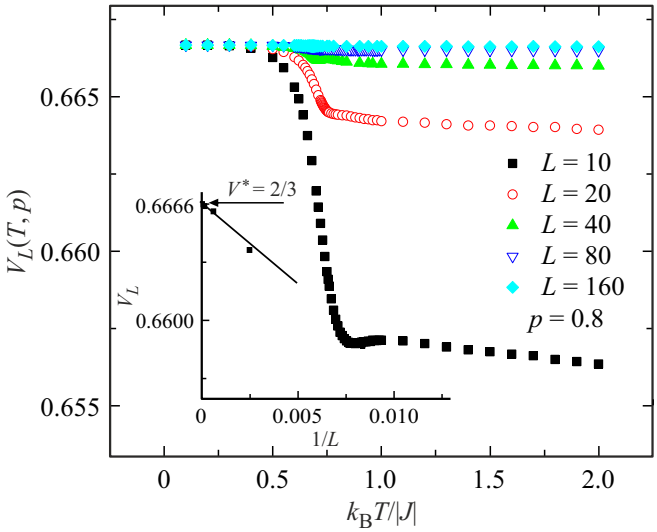

Figure 10. Temperature dependence of the Binder cumulants $V_L(T)$ for the two-dimensional diluted Potts model with the number of the spin states $q = 3$.

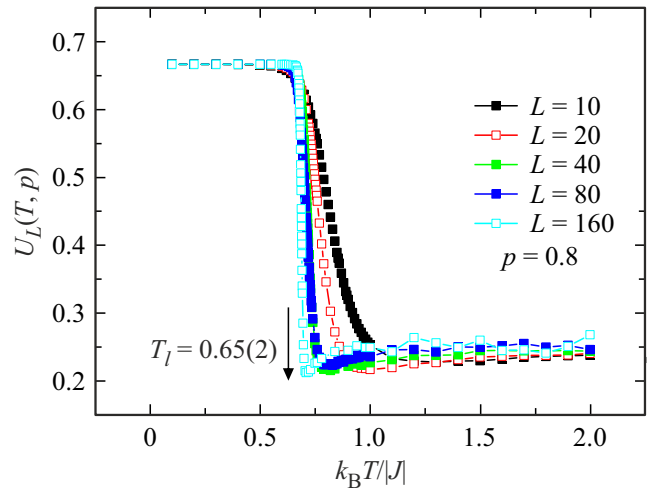

Figure 11. Temperature dependence of the Binder cumulants $U_L(T)$ for the two-dimensional diluted Potts model with the number of the spin states $q = 3$.

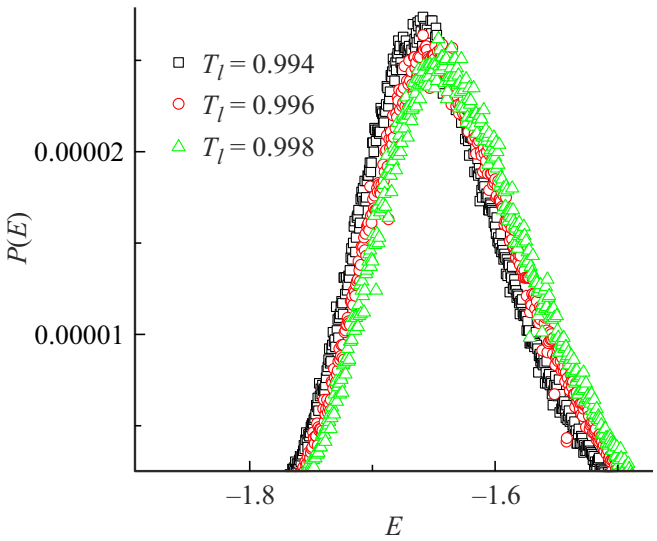

Figure 12. Energy distribution histogram for the two-dimensional pure Potts model with the number of the spin states $q = 3$ on the square lattice at $T = T_l$.

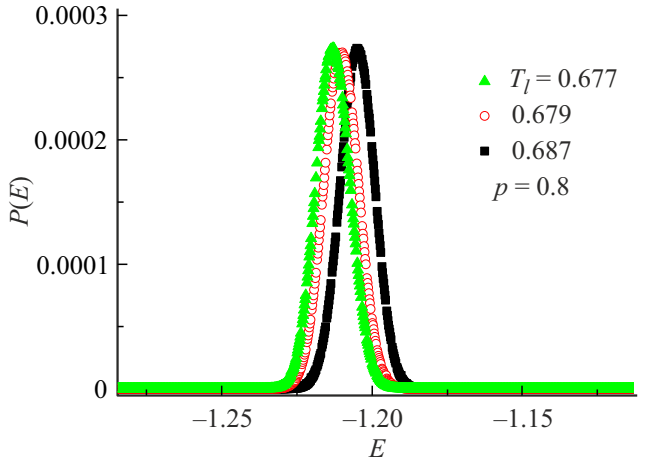

Figure 13. Energy distribution histogram for the two-dimensional diluted Potts model with the number of the spin states $q = 3$ on the square lattice at $T = T_l$.

magnetization m is [24]

$$\overline{P(U,m)} = \frac{1}{Z(K)} W(U,m) \exp[KU], \qquad (11)$$

where $Z(K)$ — an energy distribution function of the whole system, and K — reverse temperature, $W(U,m)$ — a number of configurations with energy U and the order parameter m.

The histogram data analysis, which we have carried out for the two-dimensional ferromagnetic Potts model with the number of the spin states $q = 3$ in the pure at $(p = 1.00)$ and diluted mode at $p = 0.80$ on the square lattice, also means the presence of the phase transition of the second order. It is shown in the Figures 12 and 13 for the spin system with the linear dimension $L = 160$. These figures show the energy distribution histograms for the three different temperature values near T_l for the pure and diluted Potts model with the number of the spin states $q = 3$. As it is clear from these figures, for all the considered systems the dependences of probability P on the system energy U have a prominent maximum for all the considered temperature values. This behavior is also typical for the PT of the second order.

Thus, the paper in question has shown that the order of the phase transition is not affected by the presence of the non-magnetic disorder in the spin system under consideration, which is described by the Potts model with the number of the spin states $q = 3$.

5. Conclusion

By following a single procedure based on the Monte-Carlo method, the present paper has studied the phase transitions in the two-dimensional ferromagnetic Potts model with the number of the spin states $q = 3$ on the square lattice. The data obtained from our studies confirm that in the Potts model under consideration the square lattice has the phase transition of the second order in accordance with the predictions of the analytic theories [10,11]. Addition of the non-magnetic impurities stabilizes the phase transition of the second order in the Potts model under consideration.

Conflict of interest

The authors declare that they have no conflict of interest.

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