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Computer simulation of phase transitions in low-dimensional Potts models

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The Monte Carlo method is used to study phase transitions in the two-dimensional Potts model with the number of states spin $q = 3$ on square and hexagonal lattices. Considered systems with linear dimensions $L \times L = N$, $L = 21 \div 102$. The obtained numerical data indicate that in the considered In the Potts model, a second-order phase transition is observed in accordance with the analytical theory. The Binder cumulants method of the fourth order determines the values of the critical points of the Potts model on different lattices.

Keywords: Phase transitions, Potts model, Monte Carlo, thermodynamic parameters, critical temperature.

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1. Introduction

In statistical physics, the Potts model is one of the widely used in describing various objects and phenomena. This model was proposed in 1952 by Domb [1] is still a theoretical tool used to study a wide class of phenomena and objects in condensed matter physics.

By now, it is known that in the Potts model with the number of spin states $q > q_c(D)$, where D- is the dimension of the system, there is a PT of the first order, and a PT of the second order in the case of $q < q_c(d)$ [2,3]. For the 2D-Potts model the value is $q_c = 4$, while for the 3D-model it is $q_c = 2.45$ [1,3]. Moreover, for $q_c(d = 2) = 4$, a PT of the second order is observed, and for $q_c(d = 3) = 2.45$ — a weakly expressed PT of the first order. In addition, for two-dimensional Potts models with the number of spin states q, from considerations of the duality of square, triangular, and hexagonal lattices, simple polynomial expressions were obtained that allow one to determine the critical point [4,5]

$$v = \sqrt{q}, \tag{1}$$

$$v^3 + 3v^2 = q, \tag{2}$$

$$q^2 + 3qv = v^3, \tag{3}$$

where $v = e^{J/k_BT} - 1$. The validity of these expressions has been rigorously established only for ferromagnetic Potts models with $q \geq 4$ and $q = 2$ [5].

Of particular interest is the Potts model on a hexagonal lattice [6] associated with the variety of its structural properties. As an example of substances with a hexagonal lattice structure, one can provide adsorbed films, in particular, adsorbed hydrogen atoms (2×2) — 2H/Ni (111) on the nickel surface Ni (111) are located at nodes of hexagonal lattice [6]. Phase transitions in such adsorbed structures are described by the universality class of the two-dimensional Potts model with $q = 4$.

The Potts model for $q = 2$ turns into the Ising model for which the exact solution was obtained on a hexagonal lattice more than fifty years ago [7]. At the same time, when trying to calculate the critical parameters for the Potts model, analytical methods encounter insurmountable difficulties, in particular, the validity of expression (3) for this model at $q = 3$ on a hexagonal lattice has not yet been proved [5]. It is of great interest to determine the value of the critical points by the Monte Carlo (MC) method and compare them with the theoretical values arising from the expressions (1)–(3).

In this regard, the purpose of this article is to study the thermodynamic properties of the Potts model with the number of spin states $q = 3$ on hexagonal and square lattices, determine their critical points and compare the obtained data with the data of analytical methods, where possible.

2. Two-dimensional Potts model with $q = 3$ spin states on a hexagonal lattice

The ferromagnetic (FM) Potts model is a natural generalization of the Ising model. In the Ising model, there are N discrete objects, called lattice nodes, each of which can be in one of two states. In the Potts model, each node can already be in one of the $q \geq 2$-states. Therefore, when constructing a two-dimensional ferromagnetic Potts

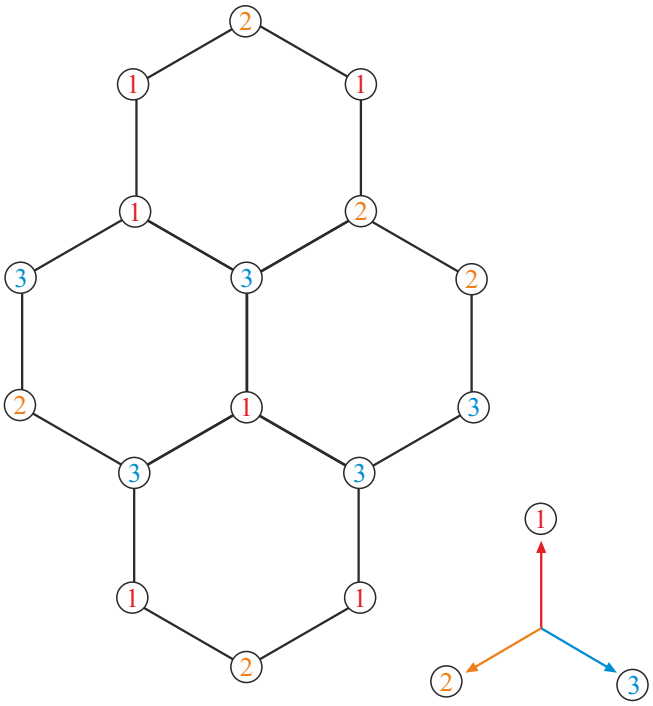

Figure 1. Two-dimensional Potts model with $q = 3$ spin states on a hexagonal lattice.

model with the number of spin states $q = 3$, in particular on a hexagonal lattice, it is necessary to keep in mind the following features [1].

1) Spins S_i are located at the hexagonal lattice nodes, which can orient themselves in 3-x symmetric directions of the hypertetrahedron in space of dimension $q - 1$, so that the angles between any two directions of the spins are equal (see Fig. 1). Note that a hexagonal lattice is a triangular lattice with one third of the nodes removed in a regular manner.

2) The binding energy between two nodes is equal to zero if they are in different states (it doesn't matter which ones) and equals J if the interacting nodes are in the same states (again, it doesn't matter which states).

Taking into account these features, a microscopic Hamiltonian of such a system can be presented as follows [5]:

$$H = -\frac{1}{2} J \sum_{i,j} \delta(S_i, S_j), \qquad S_i = 1,\ 2,\ 3, \tag{4}$$

where

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

In computer simulation, we used the Wolf cluster algorithm of the Monte Carlo method [8]. At the same time, at each Monte Carlo step, a cluster is first built, then it is turned over. This algorithm is considered in more detail in [9]. The initial configurations were set in such a way that all spins were in the same states. To bring the system to an equilibrium state, the relaxation time τ_0 was calculated for all systems with linear dimensions L. This nonequilibrium section was discarded. Then the averaging was carried out over a section of the Markov chain with the length $\tau = 160\tau_0$. For the biggest system $L = 102$, $\tau_0 = 2 \times 10^8$ MK steps/spin. In addition, to improve the accuracy of calculations, averaging was carried out over 15 different initial configurations. Then these data were used to calculate the average values of thermodynamic parameters.

3. Results of the numerical experiment

Fluctuation relations [10] were used to observe the temperature behavior of the heat capacity and susceptibility:

$$C = \left(NK^2\right)\left(\langle U^2\rangle - \langle U\rangle^2\right), \tag{5}$$

$$\chi = (NK)\left(\langle m_F^2\rangle - \langle m_F\rangle^2\right), \tag{6}$$

where $K = |J|/k_B T$, $N = 0.75 \cdot L^2$ is the number of magnetic nodes on the hexagonal lattice and $N = L^2$ is the number of magnetic nodes on a square lattice, U-internal energy, m_F is system order parameter, angle brackets denote ensemble averaging. The following expression was used as the magnetization (m_F) for FM Potts model [11,12]:

$$m_F = \frac{\left[q\left(\frac{N_{\max}}{N}\right) - 1\right]}{q - 1}, \tag{7}$$

where, $N_{\max} = \max\{N_1, N_2, N_3\}$, N_1 is the number of spins in the state with $q = 1$, N_2 is the number of spins in the state with $q = 2$, N_3 is the number of spins in the state with $q = 3$, angle brackets mean thermodynamic averaging.

Figures 2 and 3 show the temperature dependences for the susceptibility χ and heat capacity C for the two-dimensional FM Potts model on hexagonal and square

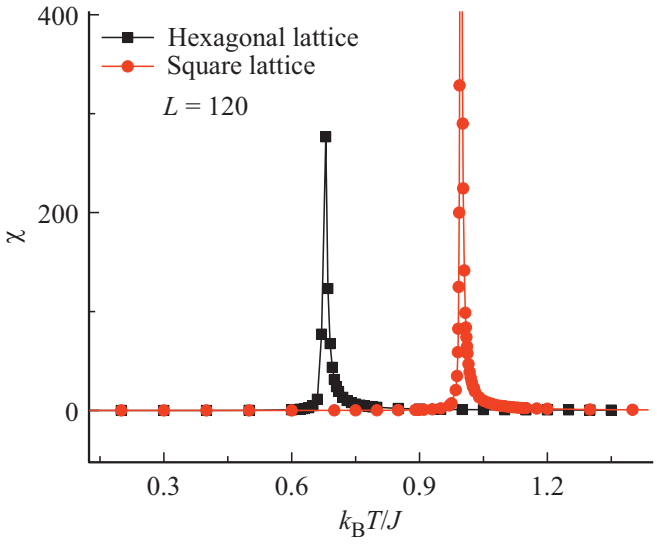

Figure 2. Temperature dependence of the susceptibility χ for the two-dimensional Potts model with $q = 3$ on various lattices.

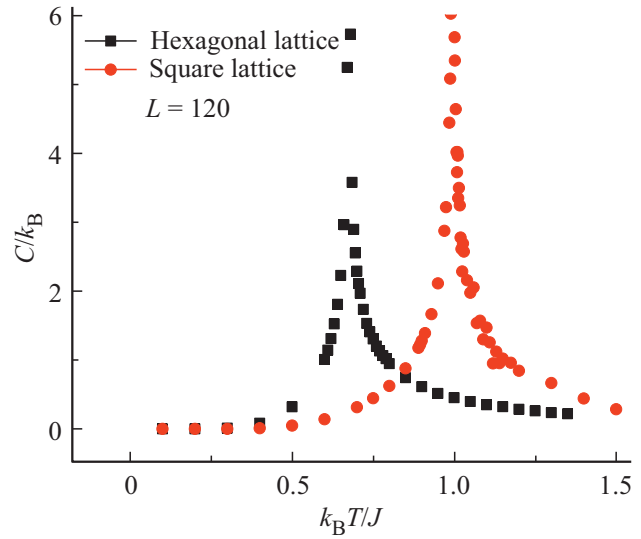

Figure 3. Temperature dependence of the heat capacity C for the two-dimensional Potts model with $q = 3$ on various lattices.

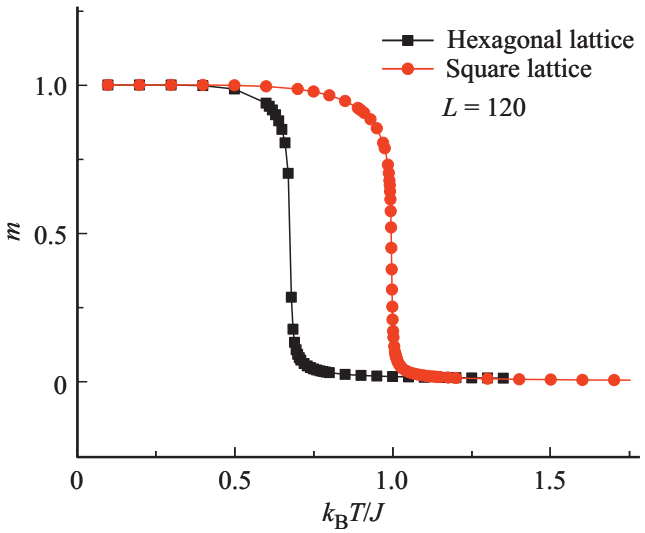

Figure 4. Temperature dependence of the magnetization m_F for the two-dimensional Potts model with $q = 3$ on various lattices.

lattices for systems with linear dimensions $L = 120$. Here and below, all the figures include a data error, which does not exceed dimensions of symbols used for plotting. Note that the dependences of the susceptibility χ and heat capacity C on temperature for all the systems under study exhibit clearly pronounced maxima characteristic of phase transitions. Figure 4 shows the dependences of the magnetization m_F on temperature T for the considered Potts model on various lattices. As can be seen in Fig. 4, there is a monotonic decrease in the value of m_F with increasing temperature and a noticeable decrease in high-temperature „tails".

To determine the critical temperatures and analyze the nature of the phase transition, we used the fourth-order Binder cumulant method [13]:

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

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

where E is the energy and m is the order parameter of the system with linear dimensions L. Expressions (8) and (9) enable to determine with good accuracy the phase transition temperature T_l during phase transitions of the first and second order, respectively. The technique for determining critical points by this method is given in the articles [14,15].

It should be noted that the use of the Binder cumulants also allows good determination of the phase transition order in the system. In case of PT of the second order the temperature dependency curves of Binder cumulants $U_L(T)$ have a clearly defined point of intersection. The characteristic temperature dependences of the Binder cumulants $U_L(T)$ for the 2D ferromagnetic Potts model with $q = 3$ on a hexagonal lattice for systems with different linear dimensions L are shown in Fig. 5. As can be seen from Fig. 5, a clearly defined intersection point is observed in the critical region, which indicates a phase transition of the second order. Figure 6 shows the temperature dependences of $V_L(T)$. As can be seen in the inset in this figure, in the critical region $V_L(T)$ tends to 2/3 with increasing linear size of the system L, which is also characteristic of a PT of the second order. A similar behavior was observed for fourth-order Binder cumulants in the case of the Potts model with $q = 3$ on a square lattice. This model was partially studied by us in the article [16].

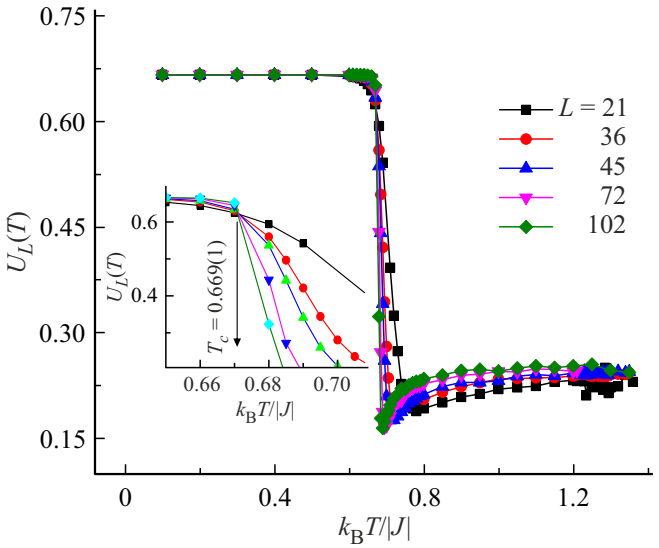

Figure 5. Temperature dependence of the Binder cumulants $U_L(T)$ for the two-dimensional Potts model with $q = 3$ on hexagonal lattice. The inset shows the intersection point of the Binder cumulants $U_L(T)$ corresponding to the critical temperature T_C.

Critical temperature of the 2D ferromagnetic Potts model with the number of spin states $q = 3$ on different lattices, determined by the fourth-order Binder cumulant method

	Method			
	Monte Carlo Model (our data)		Classical hypothesis W_u conjecture[4]	
	square	hexagonal	square	hexagonal
Regular Potts model c $q = 3$	0.994(1)	0.669(1)	$\frac{1}{\ln(1+\sqrt{3})} = 0.9949$	$\frac{1}{\ln(1+3.4114...)} = 0.6737...$

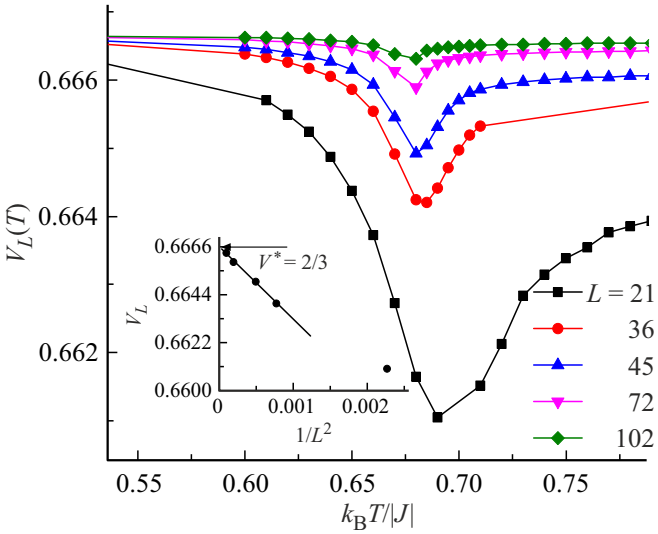

Figure 6. Temperature dependence of the Binder cumulants $V_L(T)$ for the two-dimensional Potts model with $q = 3$ on hexagonal lattice. The inset shows that $V_L(T)$ tends to 2/3 with increasing linear size of the system L in the critical region.

The values of critical temperatures T_c determined by the Binder cumulant method in units of J/k_B for the two-dimensional Potts model with $q = 3$ on square, hexagonal lattices and their comparison with analytical values from the literature are given in the table. As can be seen in the table, the calculated value of T_c by the MC method on a square lattice coincides with the value obtained by Wu [4,5] with greater accuracy than for a hexagonal lattice based on the assumptions of lattice duality.

4. Conclusion

Thus, in this article, we studied the two-dimensional Potts model with the number of spin states $q = 3$. Based on the fourth-order Binder cumulant method, the values of critical points for the Potts model with $q = 3$ on square and hexagonal lattices are determined. It is shown that the value of the critical point obtained by the Monte Carlo method on a square lattice coincides with a high accuracy with the value of the critical point obtained from the consideration of the duality argument [4,5] than for the hexagonal lattice.

Conflict of interest

The authors declare that they have no conflict of interest.

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