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Critical behavior of the three-component Potts model on a square lattice

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The critical behavior of the three-component Potts model on a square lattice has been studied using the Monte Carlo method. Systems with linear dimensions $L \times L = N$, $L = 10 \div 320$ are considered. Based on the theory of finite-dimensional scaling, static critical indices are calculated: heat capacity α, susceptibility γ, magnetization β and the critical index of the correlation radius ν. It is found that the obtained critical indices for the three-component Potts model on a square lattice coincide quite well with the data for the rigid hexagon model, to which the two-dimensional Potts model with the number of spin states $q = 3$ can be reduced.

Keywords: Potts model, critical indices, scaling hypothesis, Monte Carlo method, thermodynamic parameters.

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1. Introduction

Critical phenomena associated with second-order phase transitions are divided into a limited number of flexibility classes depending on the specific material properties, fundamental system symmetry, spatial size and number of order parameter components [1,2]. The ideas behind the scaling and flexibility hypothesis are fundamental for understanding phase transitions (PT) and critical phenomena (CP) in various systems. Theoretical and experimental investigation methods face a number of problems in calculation of critical parameters, determining the features, nature and mechanisms of critical behavior for complex systems [3,4]. This and some other factors result in the fact that PT and CP in such systems shall be preferably studied by the Monte Carlo (MC) method, which is facilitated by increasing computational capabilities of modern computers and many advanced algorithms.

One of the models used to describe real physical systems is the Potts model. It is obvious that the lattice structure of this model is isomorphic to many systems such as: complex magnetic, ferroelectric materials, multicomponent alloys and liquid mixtures, as well as adsorption of noble gases on graphite type adsorbents. The Potts model is simple, but nontrivial in content and fully meets the fundamental requirement that is used to study phase transitions and multicritical phenomena [5]. Despite the extensive theoretical investigations of spin lattice systems described by various Potts models over the recent thirty years, up to now, this model for $q > 2$ directly has not been solved on various 2D and 3D lattices. Study of magnetic and critical properties of these models is of high fundamental and practical importance. On the one hand, this is because this model has high applied significance. Theoretical studies [6] report that the Potts model will have the first-order PT at $q > 4$ and second-order PT at $q \leq 4$. These findings say nothing about the critical indices at $q \leq 4$ because this model was not solved accurately for an arbitrary temperature. At the same time, this model with $q = 3$ and $q = 4$ may be reduced to other models whose behavior is well known. Therefore, the main objective of the study is to investigate directly the critical behavior of the Potts three-component square-lattice model using the Wolff cluster algorithm of the MC method [7] and to compare the obtained critical data with the existing literature data.

2. Three-component Potts model on a square lattice and the study procedure

Let us formulate the three-component Potts model on a square lattice.

The following aspects shall be taken into account for the purpose of simulation:

1. In sites on the square lattice contain spins S_i which can be oriented in three symmetric directions of the hypertetrahedron in space with dimension $d = q - 1$ so that the angles between any two spin directions are equal (see Figure 1).

2. The bond energy between two sites is equal to zero if they are in different states (no matter which) and to $|J|$ if the interacting sites are in the same states (no matter which).

Taking into account these features, a microscopic Hamiltonian of such system can be written as [8]:

$$H = -\frac{1}{2} J \sum_{i,j} \delta(S_i, S_j), \quad S_i = P_1,\ P_2,\ P_3, \qquad (1)$$

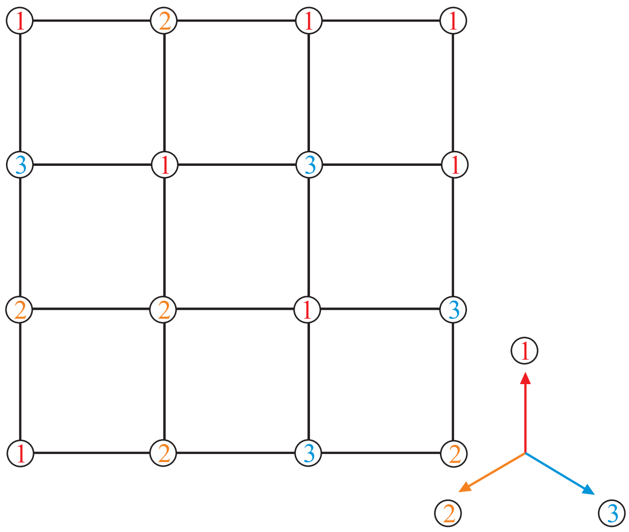

Figure 1. Standard three-component Potts modei on a square-lattice.

where J is the exchange ferromagnetic ($J > 0$) interaction parameter, P_i is the symbol of site states with No. i,

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

Systems with linear dimensions $L \times L = N$, $L = 10 \div 320$ were studied. 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. For each chain, averaging was carried out on the Markov chain segment with a length up to $\tau = 100\tau_0$. For the largest system, $L = 320$, $\tau_0 = 1.8 \cdot 10^3$ MC steps per spin. In addition, to improve the accuracy of calculations, averaging was carried out over 10 different initial configurations.

Phase transitions in the three-component Potts model on a square lattice in various dilution modes were carefully investigated in [9]. This study [9] quite accurately defined the critical temperature T_c using the Binder fourth-order cumulants method. It should be noted that the PT temperature $T_c = 0.994(1)$ obtained for the given Potts model agrees fairly well with an analytical value as obtained by Potts [10] as follows

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

3. Simulation results

This study used the finite-size scaling theory [11] to calculate the static critical indices (CI) of: heat capacity α, susceptibility γ, magnetization β and critical index ν of the correlation radius. According to this theory, the free energy for a quite large system with PBC at temperature T close to critical temperature T_c of an infinitely large system may be written as [11]:

$$F(T, L) \propto L^{-d} F_0(tL^{1/\nu}), \tag{2}$$

where $t = |T - T_c|/T_c$, $T_c = T_c(L = \infty)$ and ν is the static critical correlation radius index of the infinite system $(L = \infty)$.

Equation (2) results in the equivalent equations for heat capacity, susceptibility and spontaneous magnetization corresponding to one spin.

$$C(T, L) \propto L^{\alpha/\nu} C_0(tL^{1/\nu}), \tag{3}$$

$$\chi(T, L) \propto L^{\gamma/\nu} \chi_0(tL^{1/\nu}), \tag{4}$$

$$m(T, L) \propto L^{-\beta/\nu} \chi_0(tL^{1/\nu}), \tag{5}$$

where α, γ, β is the static critical indices for the system with $L = \infty$ associated with the hyperscaling relation $2 - \alpha = d\nu = 2\beta + \gamma$ [12,13].

In addition, a number of methods for determining the critical correlation radius index ν was proposed using the finite-size scaling theory [14]. In accordance with this theory, the following relation is satisfied in the phase transition point

$$V_n = L^{1/\nu} g_{V_n}, \tag{6}$$

where g_{V_n}-is some constant and the following expressions may serve as V_n

$$V_i = \frac{\langle m^i E\rangle}{\langle m^i\rangle} - \langle E\rangle, \quad (i = 1,\ 2), \tag{7}$$

$$V_3 = \frac{dU_L}{d\beta} = \frac{1}{3\langle m^2\rangle^2}\left[\langle m^4\rangle\langle E\rangle - 2\frac{\langle m^4\rangle\langle m^2 E\rangle}{\langle m^2\rangle^2} + \langle m^4 E\rangle\right], \tag{8}$$

where $\beta = 1/T$, T is the temperature.

It follows from relations (4)–(5) that in a system with $L \times L$ at $T = T_c$ and fairly high L, susceptibility and magnetization satisfy the following analytical expressions

$$\chi \sim L^{\gamma/\nu}, \tag{9}$$

$$m \sim L^{-\beta/\nu}. \tag{10}$$

These relations were used to determine γ and β. A similar expression for heat capacity does not describe the practical findings which was demonstrated in [14,15]. For approximation of the temperature dependence of heat capacity on L, other expressions are usually used, for example [16]:

$$C_{\max}(L) = C_{\max}(L = \infty) - AL^{\alpha/\nu}, \tag{11}$$

where A is some coefficient.

To calculate CI α, β, γ and ν, dependences of C, m, χ and V_n on L at $T = T_c$ were built. Data review performed using the nonlinear least-square method determined the values of α/ν, β/ν, γ/ν and $1/\nu$. Then, the averaged values of ν at

Critical indices

Method	$k_B T_c/J$	ν	α	γ	β	$\alpha + 2\beta + \gamma = 2$
Theory [6,17]		5/6	1/3	13/9	1/9	2.00
		0.833	0.333	1.444	0.111	
Square lattice (our data)	0.994(2)	0.82(1)	0.36	1.44	0.10	2.00
Hexagonal lattice, MC method [18]	0.621(2)	0.84	0.33	1.44	0.11	1.99

$n = 1$, 2 and 3 determined herein were used to determine the indices α, β and γ.

Figures 2–5 shows typical log-log scale dependences of susceptibility, magnetization, heat capacity and V_n for

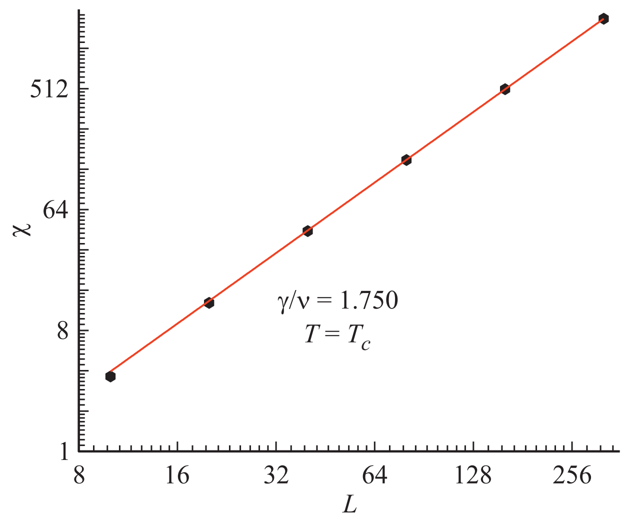

Figure 2. Typical dependence of susceptibility χ on linear lattice dimensions L at $T = T_c$.

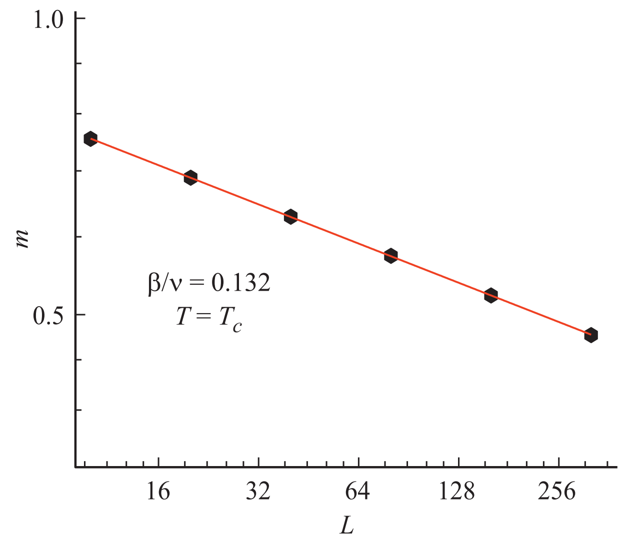

Figure 3. Typical dependence of magnetization m on linear lattice dimensions L at $T = T_c$.

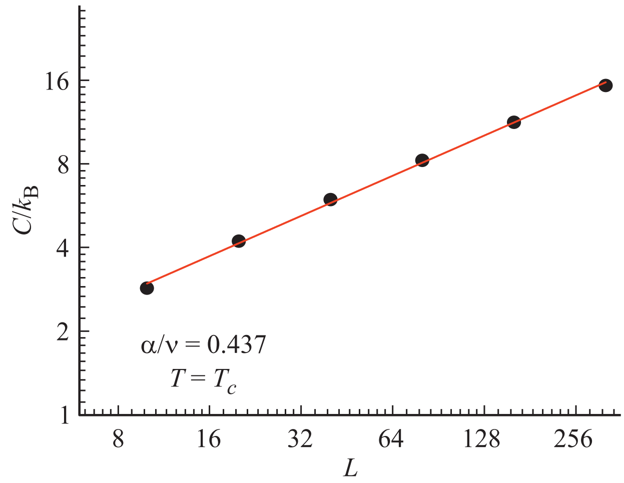

Figure 4. Typical dependence of heat capacity C on linear lattice dimensions L at $T = T_c$.

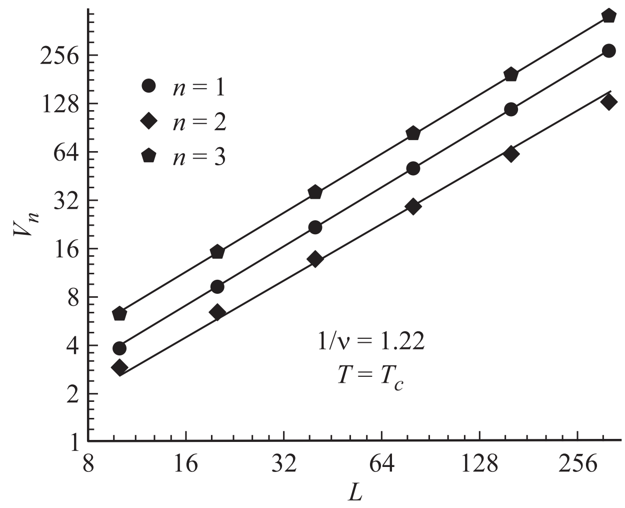

Figure 5. Typical dependence of V_n on linear lattice dimensions L at $T = T_c$.

determining the critical correlation radius index ν on linear lattice dimensions L for the Potts three-component square-lattice model. It shall be emphasized that all obtained data do not deviate from the straight line even at low L. It is obvious that the number of various initial configurations used or averaging and dimensions $L \geq 10$ of the given systems make it possible to achieve the asymptotic critical condition.

It is very important that ν was calculated directly from the numerical experiment data under this study, while in many other studies this index was derived from various scaling ratios.

Critical indices determined from out studies are shown in the table. The table shows that the measured numerical CI values for magnetization β, susceptibility γ and critical correlation radius index ν quite well match the theoretical values in [6,17] based on the considerations in favor of the fact that the Potts model with $q = 3$ and the rigid hexagon model shall be applicable to the same flexibility class. Note that CI α were calculated using expression (11). Moreover, the table shows the CI values calculated in [18] for the Potts model with $q = 3$ on hexagonal lattice.

As shown in this table, CI for the three-component Potts model on various 2D lattices are described by one flexibility class typical for 2D Potts model with $q = 3$.

4. Conclusion

This study used a single procedure to investigate critical behavior of the three-component Potts model on a square lattice. The main set of critical indices for the given Potts model was determined using the finite-size scaling theory. Analysis of the obtained CI for the three-component Potts model on a square lattice has shown that the critical indices for this model agree well with the data for the rigid hexagon model [17] to which the 2D Potts model with $q = 3$ and data obtained on the hexagon lattice may be reduced [18,19]. It is shown that critical behavior of the three-component Potts model on a square lattice is described by the flexibility class specific to the 2D Potts model with $q = 3$.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] L.N. Shchur. UFN **182**, *7*, 787 (2012). (in Russian).
[2] O. Vasilyev, B. Berche, M. Dudka, Yu. Holovatch. Phys. Rev. E **92**, 042118 (2015).
[3] V.S. Dotsenko. UFN **165**, 481 (1995). (in Russian).
[4] I.K. Kamilov, A.K. Murtazaev, Kh.K. Aliev. UFN, **169**, 773 (1999). (in Russian).
[5] A.N. Ermilov. Fisika elementarnykh chastits i atomnogo yadra, **20**, *6*, 1379 (1989). (in Russian).
[6] R. Bekster. Tochno reshaemye modeli v statisticheskoy mekhanike, Mir, M., (1985). (in Russian).
[7] U. Wolff. Phys. Lett. **62**, 361 (1989).
[8] F.Y. Wu. Rev. Mod. Phys. **54**, 235 (1982).
[9] A.K. Murtazaev, A.B. Babaev, G.Ya. Ataeva, M.A. Babaev. FTT **64**, *6*, 639 (2022). (in Russian).
[10] F.Y. Wu. Exactly Solved Models: A Journey In Statistical Mechanics. World Scientific (2009).
[11] M.E. Fisher, M.N. Barber. Phys. Rev. Lett. **28**, 1516 (1972).
[12] Sh. Ma. Sovremennaya teoriya kriticheskikh yavleniy. Mir, M., (1980). (in Russian).
[13] A.Z. Patashinskiy, V.L. Pokrovskiy. Fluktuatsionnaya teoriya fazovykh perekhodov. Nauka, M. (1982). (in Russian).
[14] A. Mailhot, M.L. Plumer, A. Caille. Phys. Rev. B **50**, 6854 (1994).
[15] A.K. Murtazaev, I.K.Kamilov, A.K. Magomedov. ZhETF **120**, *6* (12), 1535 (2001). (in Russian).
[16] P. Peczac, A.M. Ferrenberg, D.P. Landau. Phys. Rev. B **43**, 6087 (1991).
[17] S. Alexander. Phys. Lett. A **54**, 353 (1975).
[18] A.B. Babaev, A.K. Murtazaev. FMM **124**, *7*, 577 (2023). (in Russian).
[19] A.K. Murtazaev, A.B. Babaev. Vychislitel'naya fizika i problemy fazovykh perekhodov. Fizmatlit, M. 2023). (in Russian).

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