11

Phase transitions in a two-dimensional weakly diluted 4-state Potts model on a hexagonal lattice

© A.B. Babaev[1,2], A.K. Murtazaev[1]

[1] Amirkhanov Institute of Physics, Dagestan Federal Research Center, Russian Academy of Sciences, Makhachkala, Russia
[2] Dagestan Federal Research Center, Russian Academy of Sciences, Makhachkala, Russia

E-mail: b_albert78@mail.ru

Received March 3, 2023
Revised March 3, 2023
Accepted March 27, 2023

The Monte Carlo method is used to study phase transitions in a two-dimensional weakly diluted 4-state Potts model on a hexagonal lattice. Systems with linear dimensions $L = 21 \div 336$ at spin concentrations $p = 1.00$, 0.90 are considered. The use of the fourth-order binder cumulants method and histogram data analysis showed that the introduction of nonmagnetic impurities has a stabilizing role in the implementation of the second-order phase transition in the Potts model under study on a hexagonal lattice.

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

DOI: 10.21883/PSS.2023.05.56056.29

1. Introduction

Analysis of models that have nontrivial behavior during first and second order phase transition (PT) is essential for theoretical study of PT and at the same time allows to calculate accurately a partition function. Such models usually seldom ensure indirect comparison with the experiment, but are very useful for understanding of PT physics [1]. By now, there are several solvable models, including — the two-dimensional Ising square-lattice model [2]. The Potts model with $q = 2$ is isomorphic to the Ising model for which the exact solution was obtained on a hexagonal lattice more than seventy years ago [3]. However, in attempts to calculate critical parameters for the 4-state $(q = 4)$ Potts model on various lattices, analytical methods face insuperable difficulties. This resulted in the development of some hypotheses allowing to assess approximately the critical points according to polynomial expressions whose validity is not proved [4,5].

For the Potts models on various lattices, there is still no exact solution. Study of magnetic and thermal properties of these models on various two-dimensional lattices is of high fundamental and practical importance. This is associated with the fact that many objects and phenomena observed in condensed matter physics, in particular, intercalation of alkali metal atoms into the graphite lattice as well as inert gas adsorption on graphite type adsorbents are described by low-dimensional Potts hexagonal-lattice models [1,4] and their study is of great current interest. Thus, the interest in the Potts hexagonal-lattice model [4,5] is associated with the variety of its structural properties. Substances with a hexagonal lattice structure may be illustrated on adsorbed films: adsorbed hydrogen atoms (2×2) — 2H/Ni(111) on Ni(111) surface are located in hexagonal lattice points [6]. Phase transitions in such adsorbed structures are described by the class of versatility of the two-dimensional Potts models with $q = 4$ [7]. Moreover, it should be noted that the Potts models may be used to check the aspects of impacts induced by impurities on phase transitions and to determine their role in implementation of a certain type of PT. In accordance with the Harris criterion [8], for the two-dimensional Potts models with $q = 3$ or $q = 4$, the impurities shall also influence their critical behavior, because for these models in pure conditions $\alpha = 1/3$ and $\alpha = 2/3$, respectively. In [9], for 4-state $(q = 4)$ standard model, and in [10] — for Potts vertex model — with impurity concentration $c = 0.1$ $(c = 1 - p)$, a square lattice was used to show that critical behavior of this model is slightly exposed to weak disorder in the form of nonmagnetic impurities. At the same time, for the Potts hexagonal-lattice model with $q = 4$, there are almost no literature data describing the way how the frozen disorder impacts phase transitions and its critical behavior. Critical temperatures were not determined and the aspects of impact induced by disorder on thermodynamic properties such as magnetization m, susceptibility χ, energy E, thermal capacity C and Binder cumulants U_L and V_L, depending on the linear dimensions L of the studied systems.

Therefore, the main goal of this study is to investigate the influence of nonmagnetic impurities on phase transitions and various thermodynamic properties in a standard two-dimensional Potts hexagonal-lattice model depending on L.

2. Two-dimensional weakly diluted 4-state Potts model

A two-dimensional standard weakly diluted 4-state Potts model used to describe a wide range of objects and

phenomena in the condensed matter physics will be defined here. In the model under consideration, the impurities are distributed in a canonical way [11]. When building such model, the following aspects shall be taken into account:

1. Spins S_i are present in the hexagonal lattice points, which can be oriented in 4 symmetric directions of the hypertetrahedron in space with dimension $q-1$ so that the angles between any two spin directions are equal (see Fig. 1). The nonmagnetic impurities are randomly distributed and fixed on various lattice points (quenched disorder).

2. The bond energy between two points is equal to zero, if they are in different states (whichever) or, if at least one point contains a nonmagnetic atom, and is equal to J, if the interacting points are in the identical states (again, whichever).

Taking into account these features, a microscopic Hamiltonian of such system can be written as [4]:

$$H = -\frac{1}{2} J \sum_{i,j} \rho_i \rho_j \delta(S_i, S_j), \quad S_i = P_1, P_2, P_3, P_4, \quad (1)$$

where summation covers all nearest neighbors, J is the exchange interaction parameter ($J > 0$), P_q is the number of various states of a selected spin S_i, $\rho_i = 1$, if point i is occupied by a magnetic atom, and $\rho_i = 0$, if point i contains a nonmagnetic impurity,

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

A concentration of the magnetic spins is determined using the expression

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

Then $p = 1$ corresponds to the pure Potts model, while $p = 0$ corresponds to an empty, entirely impurity lattice.

3. Research procedure

Wolff algorithm — is currently one of the most effective cluster algorithms within the Monte Carlo (MC) method [12]. The algorithm procedure is addressed in detail in [13,14]. Herein, this algorithm is used as follows.

1. Two random numbers define coordinates i, j of the hexagonal lattice point. If this point contains a nonmagnetic impurity, then new random numbers are generated until magnetic spin coordinates S_i are generated.

2. All the nearest neighborsS_j of this spin S_i are considered. If an adjacent point is occupied by a magnetic spin, then with probability

$$P = 1 - \exp(-K), \quad (3)$$

where $K = J/k_B T$, k_B is the Boltzmann constant, T is the temperature, a bond is activated between S_i and S_j,

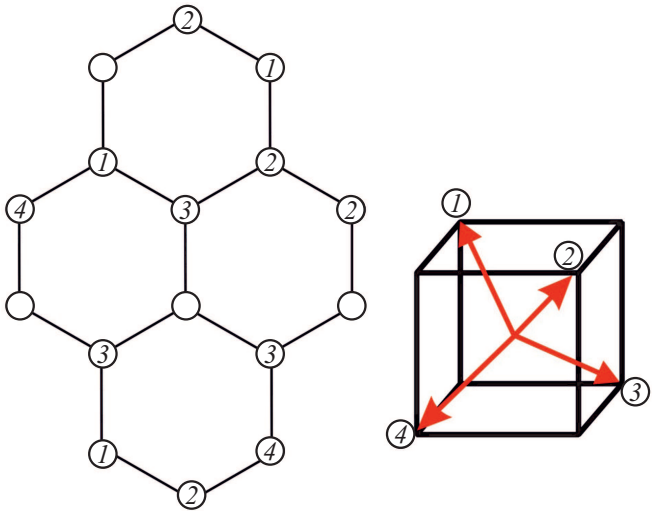

Figure 1. Two-dimensional standard 4-state wekly diluted Potts model on a hexagonal lattice.

if S_i and S_j are equal at $J > 0$. Note that for the Potts model, in order to express the probability of spin inclusion in the cluster (3), exponent 2, which is typical of the corresponding probability of the Ising model, disappears. Thus, it can be claimed that the Potts model with spin state $q = 2$ is equivalent to the Ising model with accuracy of number factor 2 in the exchange constant J.

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

4. After all nearest neighbors of the selected spin$i$ have been checked, the first spin included in the cluster becomes „central“ and the process of bond activation between this spin and its nearest neighbors starts. This process continues until all nearest neighbors of all spins included in the cluster are checked or the system boundaries are achieved.

5. All bonded spins form „a cluster“.

6. The resulting cluster is flipped with probability equal to 1. For the Potts model, cluster flip means that a new spin value S_i' other than the old value S_i, will be assigned to all spins included in the cluster, with equal probability among all of its states q. Then proceed the step 2.

The efficiency of the single-cluster Wolff algorithm applicable to the Potts model can be assessed by critical index z, which characterizes the efficiency of the algorithm. In particular, the study of the clean two-dimensional Potts model with $q = 4$ based on the single-cluster Wolff algorithm has demonstrated that critical index $z = 0.60 \pm 0.02$, while the traditional Metropolis algorithm gives $z \approx 2$ [15]. According to the above-mentioned Wolff algorithm [12], the Markov process was implemented for the systems with periodic boundary conditions. The calculations were carried out for the systems with linear dimensions $L = 21 \div 336$ and number of spins $N = 2 \times p \times L \times L/3$. Configurations were

initially specified in such a way that all spins were ordered along one of the axes X, Y or Z. For system equilibration, a nonequilibrium section with length τ_0 was cut off for the system with linear dimension L. This nonequilibrium section was discarded. For each chain, averaging was carried out for a Markov chain section with length $\tau = 360\tau_0$. For the largest system $L = 336$, $\tau_0 = 2 \cdot 10^3$ MC-steps/spin. In addition, configurational averaging was carried out or 1000 various impurity configurations.

4. Simulation results

With numerical study of phase transitions, thermodynamic properties U, m, C, χ were calculated for an individual sample using the following equations [1,16]:

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

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

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

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

where $K = J/k_B T$, $N_{\max} = \max\{N_1, N_2, N_3, N_4\}$, N_i is the number of spins in state with $q = i$, $N = (2/3)pL^2$ is the number of magnetic atoms; angle brackets mean thermodynamic averaging, while square brackets mean averaging over the impurity configurations.

Figures 2 and 3 show typical magnetization dependences for the pure ($p = 1.00$) and weakly diluted ($p = 0.90$) Potts model on the temperature, respectively. Hereinafter, data error in all Figures does not exceed the dimensions of symbols used for plotting diagrams. These Figures show that, for all considered systems, behavior typical for second order PT is observed.

A Binder second-order cumulant method is proven to be the most efficient for PT analysis [17]:

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

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

where E is the energy and m is the magnetization of a system with linear dimension L. Expressions (8) and (9) ensure high-accuracy calculation of PT temperature $T_l(p)$ for first- and second-order PT, respectively. It should be noted that the Binder cumulants also ensure reliable calculation of PT order in the spin system in question. Second-order phase transitions are characterized by the following features [18]: averaged $V_L(T, p)$ tends to nontrivial value V^* according to

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

with $L \to \infty$ and $T = T_l(L)$, where $V^* = 2/3$, and temperature dependence curves of Binder cumulants $U_L(T, p)$ in the

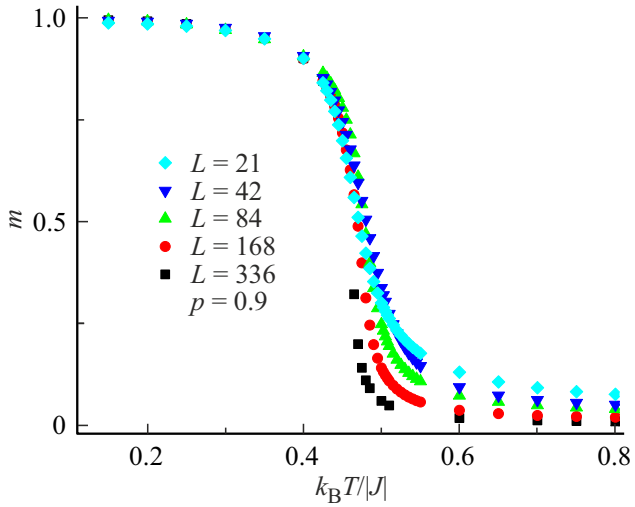

Figure 2. Temperature dependence of magnetization m for the weakly diluted 4-state Potts model with spin concentration $p = 0.90$ on hexagonal lattice.

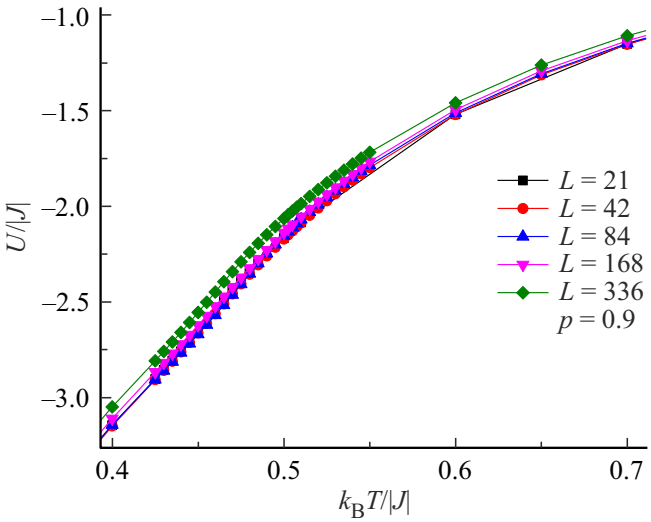

Figure 3. Temperature dependence of energy $U/|J|$ for the weakly diluted 4-state Potts model with spin concentration $p = 0.90$.

critical region have a clearly pronounced point of intersection. The listed features for fourth-order Binder cumulants $V_L(T, p)$ and $U_L(T, p)$ are demonstrated in Figures 4 and 5, respectively, for ferromagnetic weakly diluted Potts model with $q = 4$ on hexagonal lattice with spin concentration $p = 0.90$. PT order calculation procedure by this method is described in detail in [9,10].

Bar diagram data analysis carried out for the two-dimensional weakly diluted 4-state Potts model on hexagonal lattice with $p = 0.90$ also proves the second-order PT is present. It is shown in Figure 6 for the spin system with the linear dimension $L = 336$. This Figure shows energy distribution bar diagrams for spin systems with three various temperatures in vicinity of the critical

temperature T_c (Curie temperature). Figure 6 shows that dependences of probability P on system energy E for three various temperatures in vicinity of T_c have one well pronounced maximum. Such behavior is also typical of the second order PT.

Analysis of data calculated using the MC method cluster algorithm for the 4-state pure Potts model on square lattice [14] and on hexagonal lattice [19] has demonstrated the second-order PT. At the same time, the study of this model on hexagonal lattice by direct Wang–Landau method in [20] has detected the first-order PT. Later, using a modified version of the Wang–Landau method in [21], inaccuracy of statements made in [20] was demonstrated and importance of accuracy control for system state density assessment was shown. The modified version of the Wang–Landau method allowed the authors of [21] to achieve the results identical to [19,22], that were obtained using the cluster algorithms within the MC method.

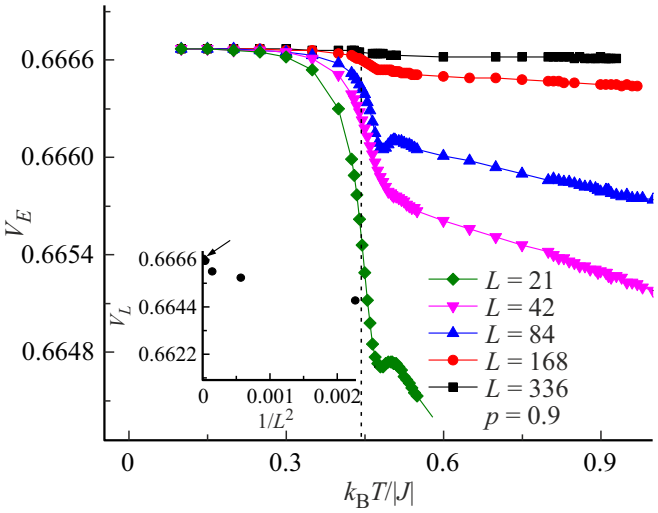

Figure 4. Temperature dependence of Binder cumulants $V_L(T)$ for the weakly diluted 4-state Potts model with spin concentration $p = 0.90$.

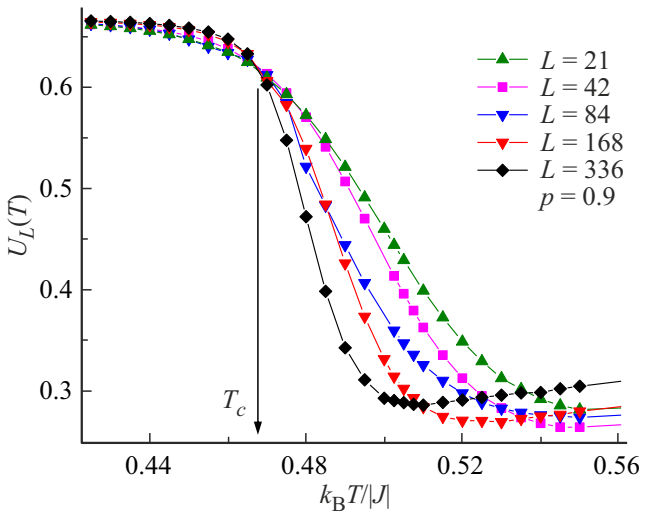

Figure 5. Temperature dependence of Binder cumulants $U_L(T)$ for the weakly diluted 4-state Potts model with spin concentration $p = 0.90$.

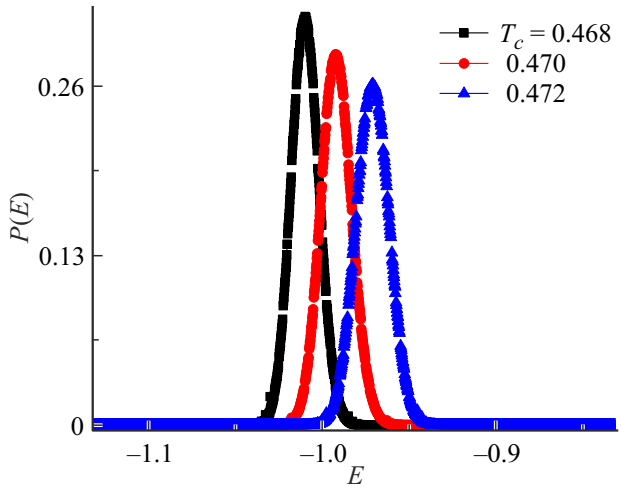

Figure 6. Energy distribution bar diagram for two-dimensional weakly diluted 4-state Potts model on hexagonal lattice.

Thus, introduction of disorder in the form of nonmagnetic impurities into the spin lattice system described by the 4-state Potts model on hexagonal lattice results in stabilization of the second-order PT. In addition, the study of critical behavior of a disordered model on hexagonal lattice is of great interest and will the addressed separately.

5. Conclusion

The cluster algorithm within the Monte Carlo method was used herein to study phase transitions in a two-dimensional 4-state ferromagnetic Potts model in a weakly diluted mode on hexagonal lattice. The findings of our investigations carried out using the fourth-order Binder cumulant method and bar diagram data analysis show that the weakly disordered 4-state Potts model on hexagonal lattice and pure Potts model with $q = 4$ have the second-order PT [10,17]. Introduction of nonmagnetic impurities into the Potts model in question results in stabilization of the second-order PT.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] R. Baxter. Tochno reshaemye modeli v statisticheskoy mekhanike, Mir, M. (1985). 488 p. (in Russian).
[2] L. Onsager. Phys. Rev. **65**, *3–4*, 117 (1944).
[3] R.M.F. Houtappel. Physica **16**, *5*, 425 (1950).
[4] F.Y. Wu. Rev. Mod. Phys. **54**, *1*, 235 (1982).
[5] F.Y. Wu. Exactly Solved Models: A Journey in Statistical Mechanics. World Scientific, London (2009).

[6] L. Schwenger, K. Budde, C. Voges, H. Pfnur. Phys. Rev. Lett. **73**, *2*, 296 (1994).
[7] K. Budde, L. Schwenger, C. Voges, H. Pfnur. Phys. Rev. B **52**, *13*, 9275 (1995).
[8] A.B. Harris. J. Phys. C **7**, *9*, 1671 (1974).
[9] A.B. Babaev, A.K. Murtazaev. Phys. Solid State **62**, *5*, 851 (2020).
[10] A.B. Babaev, A.K. Murtazaev. J. Phys.: Conf. Ser. **1389**, *1*, 01210 (2019).
[11] R. Folk, Yu. Holovatch, T. Yavorskii. Phys. Usp. **46**, *2*, 169 (2003).
[12] U. Wolff. Phys. Rev. Lett. **62**, *4*, 361 (1989).
[13] A.K. Murtazaev, A.B. Babaev, G.Ya. Ataeva. Phys. Solid State **64**, *5*, 264 (2022).
[14] A.K. Murtazaev, A.B. Babaev, G.Ya. Ataeva, M.A. Magomedov. JETP **135**, *3*, 347 (2022).
[15] G.T. Barkema, M.E.J. Newman. https://doi.org/10.48550/arXiv.cond-mat/9703179
[16] P. Peczac, A.M. Ferrenberg, D.P. Landau. Phys. Rev. B **43**, *7*, 6087 (1991).
[17] D.P. Landau, K. Binder. A Guide to Monte Carlo Simulations in Statistical Physics. Cambridge University Press (2014).
[18] D. Loison, K.D. Schotte. Eur. Phys. J. B **5**, *3*, 735 (1998).
[19] A.K. Murtazaev, A.B. Babaev. JETP **134**, *6*, 720 (2022).
[20] A.K. Murtazaev, M.K. Ramazanov, M.K. Mazagaeva, M.A. Magomedov. JETP **129**, *3*, 421 (2019).
[21] M.A. Fadeeva, L.N. Shchur. JETP **135**, *6*, 869 (2022).
[22] J.S. Salas, A.D. Sokal. J. Statistic. Phys. **88**, *3−4*, 567 (1996).

Translated by E.Ilyinskaya