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Calculation of relative dispersions of magnetization, heat capacity and susceptibility in a two-dimensional weakly diluted 3-state Potts model

© G.Y. Ataeva[1], A.B. Babaev[1,2], A.K. Murtazaev[1]

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

E-mail: ataeva20102014@mail.ru

Received April 6, 2023
Revised June 1, 2023
Accepted June 3, 2023

Using the Monte Carlo method, the relative dispersions of magnetization R_m, heat capacity R_c and susceptibility R_χ are calculated for a weakly diluted 3-state Potts model on a square lattice at a spin concentration $p = 0.90$. It is revealed that the introduction of disorder in the form of nonmagnetic impurities into the two-dimensional Potts model leads to non-zero values for R_m, R_c, R_χ at the critical point. It is found that these values decrease markedly for systems with linear dimensions $L > 40$.

Keywords: nonmagnetic impurities, dispersion, Potts model, Monte Carlo method, phase transition.

DOI: 10.61011/PSS.2023.07.56414.55

1. Introduction

The main problem of condensed matter physics is still the influence of nonmagnetic order on various thermal and magnetic characteristics of the studied system. This is due to the fact that real systems always have various defects, impurities or other imperfections that impair the system uniformity, and their consideration is essential [1–5] for the analysis of various physical properties. In addition, it can be reasonable expected that critical parameters of the studied system may depend on the disordering method. In particular, [6,7] found that disorder provided by a canonical method (fixed fraction of magnetic nodes) gave results which were different from the case when disorder was implemented by a grand canonical method (fraction of magnetic nodes in each impurity configuration fluctuated). Later, [8] used a renormalization group to explain such behavior by the difference of finite-size effects in these two types of dilution.

As of today, these problems have not been investigated sufficiently. Features in terms of the Potts lattice models attract great theoretical and experimental interest. For the Potts models, features of thermodynamic parameter distribution over the corresponding assembly depending on sizes L of the studied systems. Rigorous study of such behavior is possible in the nearest future only on the basis of numerical experiment data and is virtually impossible by other methods.

Therefore, this study uses the Monte Carlo method to investigate self-averaging of thermodynamic critical parameters of a two-dimensional weakly diluted 3-state Potts model depending on the sizes of the studied systems. Note that the Potts models can be used to check the effecy of impurities on the phase transitions (PT) and to determine their role as a stabilizing factor in case of second-order PT. On the other hand, in accordance with the Harris criterion [9], for the two-dimensional Potts models with $q = 3$ or $q = 4$, impurities shall also influence the critical behavior, because for these models in undiluted state $\alpha = 1/3$ and $\alpha = 2/3$, respectively.

2. Three-dimensional impurity Potts model on the square lattice

Here we provide a three-dimensional impurity Potts square-lattice model used to describe a wide range of objects and phenomena in condensed matter physics. In this model, impurities are canonically distributed [2]. For building such model, the following aspects shall be taken into account:

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

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

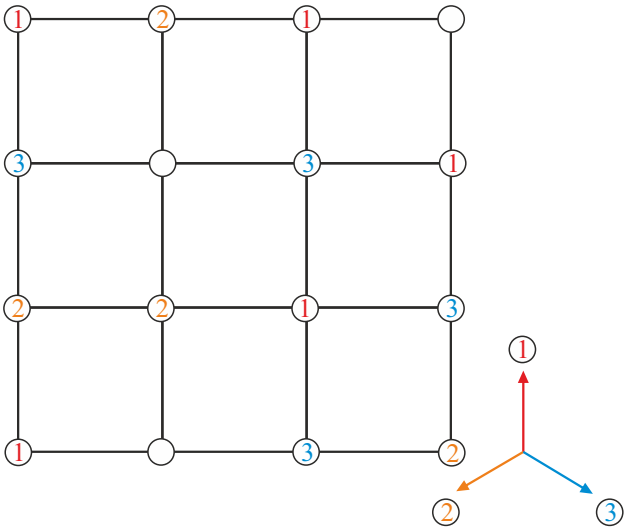

Figure 1. Standard two-dimensional 3-state weakly diluted Potts square-lattice model.

Taking into account these features, a microscopic Hamiltonian of such system can be written as [12]:

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

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

$$\rho_i = \begin{cases} 1, & \text{if there is a spin in the node} \\ 0, & \text{if a non-magnetic impurity} \\ & \text{is located in the node} \end{cases},$$

P_q is the spin state with number i, J is the exchange ferromagnetic interaction parameter.

The concentration of magnetic spins is defined by expression

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

Then $p = 1$ corresponds to the Potts model and $p = 0$ — to an empty purely impurity lattice.

3. Investigation procedure

Wolff cluster algorithm of the Monte Carlo method is currently the most effective algorithm [13,14]. The algorithm procedure is addressed in detail in [15,16]. This study uses the algorithm as follows.

1. A random lattice site is chosen. If this site contains a nonmagnetic impurity, then a site is randomly chosen again until a site with S_i is chosen.

2. All the nearest neighbors S_j of this spin S_i are considered. If the adjacent site is occupied by a spin co-directional with this unflipped spin S_i, then with probability $p = 1 - \exp(-K)$, where $K = J/k_B T$, this spin is also flipped and its coordinated are stored in the stack. Then the nearest neighbors of the last spin with which the bond was established are reviewed. This process lasts until the system boundaries are achieved.

3. All bonded spins form „a cluster".

4. The spin flip procedure ends when the stack is empty. This process is called a cluster flip.

Calculations were performed for the systems with periodic boundary conditions at spin concentrations $p = 1.0, 0.9$. Systems with linear sizes $L \times L = N$, $L = 20-160$ were studied. The initial configurations were set in such a way that all spins were in the same states. In order to bring the system to equilibrium, a non-equilibrium section τ_0 in length was separated for the system with the linear dimensions L. This nonequilibrium section was discarded. Then,averaging was carried out for a Markov chain section $\tau = 400\tau_0$ in length. For the largest system, $L = 160$, $\tau_0 = 2 \cdot 10^3$ MC steps per spin. Moreover, averaging over various initial configurations was carried out. For $p = 1.0$, 10 initial configurations were used for averaging. For systems with concentration $p = 0.90$, configuration averaging over 1000 various configurations was performed.

4. Simulation results

Fluctuation relations [17] were used to observe the temperature behavior of susceptibility and heat capacity:

$$\chi = \overline{(NK)(\langle m^2 \rangle - \langle m \rangle^2)}, \qquad (3)$$

$$C = \overline{(NK^2)(\langle U^2 \rangle - \langle U \rangle^2)}, \qquad (4)$$

where $K = J/k_B T$, $(J > 0)$, $N = pL^2$ is the number of magnetic nodes, m is the system magnetization, angle brackets denote thermodynamic averaging, the top bar denotes averaging over the canonical assembly with various disordering.

To calculate magnetization in a two-dimensional weakly diluted Potts model, the following relation was used:

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

Figure 2 shows susceptibility values χ_j for various impurity configurations j of the two-dimensional 3-state Potts model in the weakly diluted mode with $p = 0.90$, $T = T_c(p)$, $0 \leq j \leq N_s$, N_s is the total number of impurity configurations. Averaged values of $\overline{\chi_j}$ are also given herein for the corresponding assembly with various distribution of nonmagnetic impurities for the systems with linear size $L = 160$. As shown in the illustration, the number of

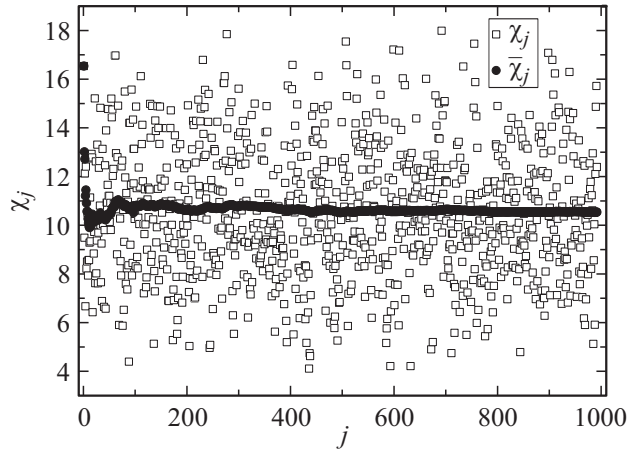

Figure 2. Susceptibility distribution over the canonical assembly with various distribution of nonmagnetic impurities for the system with $p = 0.90$, $T = T_c$ and linear size $L = 160$.

impurity configurations N_s used for averaging allows to achieve the asymptotic critical mode.

Among the computational physics method used to determine the phase transition temperature $T_l(p)$, the fourth-order Binder cumulant method is widely recognized [18,19]:

$$V_L(T, p) = 1 - \frac{\langle E^4 \rangle_L}{3\langle E^2 \rangle_L^2}, \tag{6}$$

$$U_L(T, p) = 1 - \frac{\langle m^4(T, p; L) \rangle_L}{3\langle m^2(T, p; L) \rangle_L^2}, \tag{7}$$

where E is the energy and m is the magnetization of a system with linear dimension L. Equations (6) and (7) allow to determine $T_l(p)$ with the highest accuracy in the first- and second-order phase transitions, respectively. This method is also well proven for determining the kind of phase transition.

Peculiarities of this method when used to determine the temperature and kind of phase transition are described in [20]. Second-order PT has the following distinguishing features [19]:

– Averaged Binder cumulant with respect to energy $V_L(T, p)$ tends to trivial V^* according to

$$V(T, p) = V^* + bL^{-d}, \tag{8}$$

with $L \to \infty$ and $T = T_l(L)$, where V^* is equal to 2/3;

– Binder cumulant curves with respect to magnetization in a critical region have a strongly pronounced crossover point.

Typical dependences of Binder cumulants $V_L(T, p)$ and $U_L(T, p)$ on temperature for systems with different linear sizes at $p = 0.90$ are shown in Figure 3 and 4, respectively. As shown in Figure 4, critical point $T_c = 0.842(1)$ in units J/k_B.

To calculate relative dispersions (squared variation coefficients) of magnetization R_m, susceptibility R_χ and heat capacity R_c at $T = T_c$ depending on linear sizes L of the system, the following expressions were used

$$R_m = \frac{\overline{m^2(L)} - \overline{m(L)}^2}{\overline{m(L)}^2}, \tag{9}$$

$$R_\chi = \frac{\overline{\chi^2(L)} - \overline{\chi(L)}^2}{\overline{\chi(L)}^2}, \tag{10}$$

$$R_C = \frac{\overline{C^2(L)} - \overline{C(L)}^2}{\overline{C(L)}^2}. \tag{11}$$

By numerical data in the critical point T_c calculated using (9)–(11), self-averaging behavior of thermodynamic parameters and their error depending on L can be inferred. Corresponding values of R_m, R_χ and R_c depending on L with spin concentrations $p = 0.90$are shown in the Table.

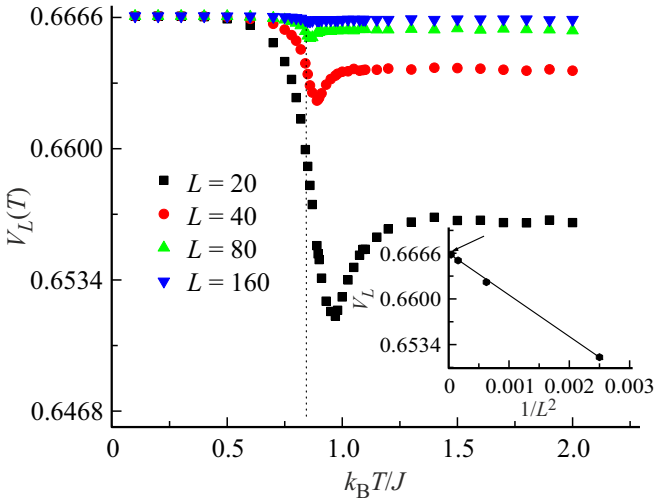

Figure 3. Temperature dependence of Binder cumulants $V_L(T)$ for the weakly diluted 3-state Potts model with $p = 0.90$.

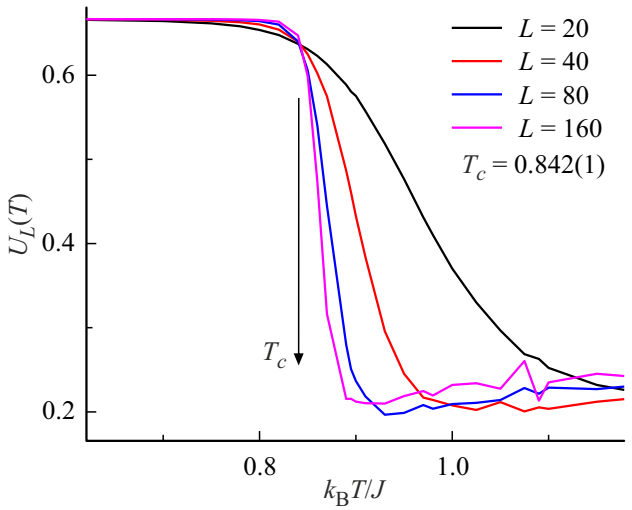

Figure 4. Temperature dependence of Binder cumulants $U_L(T)$ for the weakly diluted 3-state Potts model with $p = 0.90$.

Values of relative susceptibility, magnetization and heat capacity dispersions for two-dimensional 3-state weakly diluted Potts model

L	R_χ	R_m	R_c
10	0.03121	0.00125	0.00542
20	0.02217	0.00114	0.00535
40	0.01504	0.00112	0.00477
80	0.01163	0.00108	0.00307
160	0.00789	0.00101	0.00247

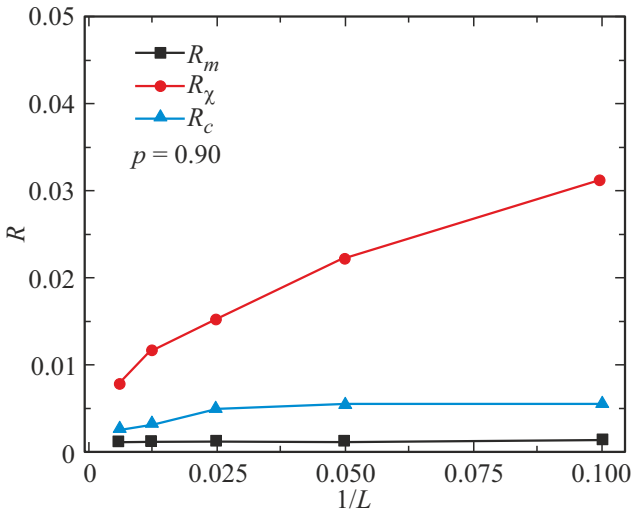

Figure 5. Dependence of relative dispersions of magnetization R_m, heat capacity R_c and susceptibility R_χ on inverse sizes $1/L$ at $p = 0.90$ and $T = T_c$.

As shown in the table, introduction of weak disorder into the two-dimensional 3-state Potts model results in non-zero values of R_m, R_χ and R_c. This data allows to estimate the errors associated with the sizes of the studied systems. Figure 5 shows dispersions of R_m, R_c, R_χ depending on $1/L$. It can be seen that with the increase in the linear sizes, values of R_m, R_c, R_χ decrease considerably.

Thus, from the obtained data R_m, R_c, R_χ, it follows that systems with linear sizes $L > 80$ shall be studied for unambiguous determination of PT kind, critical parameters and other features of a weakly dulited 3-state Potts model.

5. Conclusion

This study for the first time uses a common procedure based on the Monte Carlo cluster algorithm to calculate relative dispersions of magnetization R_m, susceptibility R_χ and heat capacity R_c in the weakly dulited Potts model at spin concentration $p = 0.90$. The obtained data prove the following.

1. Introduction of a weak disorder in the form of nonmagnetic impurities into the two-dimensional 3-state Potts square-lattice model results in non-zero values for R_m, R_χ and R_c indicating bad self-averaging for the studied thermodynamic parameters.

2. For the weakly diluted systems described by the 3-state Potts model, it has been found that distinctive decrease of R_m, R_χ, R_c occurs only at $L > 40$. To obtain valid characteristics for this model, spin systems with $L > 40$ shall be studied.

Conflict of interest

The authors declare that they have no conflict of interest.

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