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Calculation of relative dispersions of magnetization, susceptibility, and heat capacity in a two-dimensional weakly diluted Potts model based on computer simulation methods

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The Monte Carlo method was used to calculate the relative dispersions of the magnetization R_m, susceptibility R_χ, and heat capacity R_C for a weakly diluted impurity Potts model with the number of spin states $q = 4$. It is shown that the introduction of disorder in the form of nonmagnetic impurities into the two-dimensional Potts model with $q = 4$ on square lattice leads to nonzero values for R_m, R_χ, and R_C at the critical point.

Keywords: Monte Carlo method, Potts model, dispersion of the magnetization, susceptibility and heat capacity.

Introduction

Investigations of real magnetic systems have shown that systems in a pure homogeneous state are rarely found, there are always nonideal features such as impurities and structural defects that affect the magnetic and thermal properties in magnetic structures [1–5]. It should also be borne in mind that in some works the dependence of the thermodynamic parameters on the way of realizing the disorder in the model under study was found. For example, in [6, 7] it was found that the disorder realized by the canonical method (fixing the fraction of magnetic nodes) leads to results that differ from the case when the disorder was realized by the method of the grand canonical type (the fraction of magnetic nodes in each impurity configuration fluctuates). Although the study [8], carried out by the renormalization group methods, explained this behavior by the difference in finite-size effects in these two types of dilution. A rigorous study of such regularities in the near future is possible only based on numerical experiment data and is practically impossible by other methods. Note that the behavior of the thermodynamic critical parameters of disordered models for various realizations of disorder in the form of nonmagnetic impurities in a wide range of changes in the impurity concentration $c_{\text{imp}} = 1 - p$, where p is the spin concentration, has been insufficiently studied with the observance of a unified technique.

The features of the distribution and self-averaging of thermodynamic parameters over the corresponding ensemble have not been clarified. Clarification of these issues in relation to the two-dimensional weakly diluted Potts model with the number of spin states $q = 4$ based on the cluster Monte Carlo (MC) method is the main task of this work.

2. Potts model with quenched-in disorder

A weakly diluted Potts model with the number of spin states $q = 4$ is shown in Fig. 1. In the model under consideration, the disorder is distributed in the form of nonmagnetic impurities in a canonical way (by fixing the fraction of magnetic nodes):

(i) At the sites of a square lattice there are S_i spins, which can be in one of the $q = 4$ states, and nonmagnetic impurities (vacancies). Nonmagnetic impurities are randomly distributed and fixed (see Fig. 1).

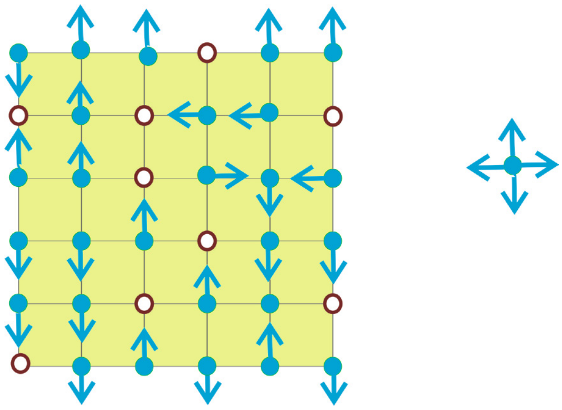

Fig. 1. Two-dimensional weakly diluted Potts model with the number of spin states $q = 4$.

(ii) The binding energy between two neighboring sites is zero if at least one site contains a nonmagnetic atom, and is equal to $|J|$ if both sites are occupied by magnetic atoms.

The Hamiltonian of such a system has the form [9]

$$H = -\frac{1}{2} J \sum_{i,j} \rho_i \rho_j \cos \theta_{i,j}, \quad S_i = 1, 2, 3, 4, \tag{1}$$

where J is the parameter of the exchange interaction of the nearest neighbors ($J < 0$); $\rho_i = 1$ if site i is occupied by a magnetic atom, $\rho_i = 0$ if there is a nonmagnetic impurity in the site; $\theta_{i,j}$ is the angle between the interacting spins $S_i - S_j$. The concentration of magnetic spins p is determined by summing the absolute values of the spin at all lattice sites:

$$p = \frac{1}{L^2} \sum_{i=1}^{L^2} \rho_i |S_i|, \tag{2}$$

where L is the minimum system size.

The value $p = 1$ corresponds to the pure Potts model, $p = 0$ corresponds to an empty purely impurity lattice. The quenched Potts model has a fairly long history. To date, the effect of nonmagnetic impurities in Ising-like models has been well studied [10–15]. At the same time, the problem of the distribution of thermodynamic parameters and their averaging over an ensemble of disordered systems with different realization of disorder has not been studied for all models. It should be noted that, in accordance with the Harris criterion [16], for the two-dimensional Potts model with $q = 4$, the effect of impurities on the magnetic and thermal characteristics should be significant, since the critical heat capacity index $\alpha > 0$ for the pure Potts model with $q = 4$.

The interest in this model is due to the following main reasons.

First, the weakly diluted Potts model with the frozen-in disorder is of practical interest, since it allows, at the level of the simplest model, to include into consideration the macroscopic effects of the disorder, which are always present in real materials.

Second, the study of the effect of quenched disorder on the universal characteristics of critical behavior, in addition to practical, is of great theoretical interest [1, 2].

Third, the first attempts to study this model with a canonical distribution by methods of computational physics were made at a time when the power of computers and the algorithms used by the MC method did not allow calculating the critical parameters with the required degree of accuracy.

3. Research methodology

The research was carried out based on the Metropolis algorithm in combination with the Wolff cluster algorithm of the Monte Carlo method [17]. The method of its implementation is discussed in detail in [18, 19]. In this work, this algorithm is used in the following form:

(i) A node on a lattice is randomly selected. If this site contains a nonmagnetic impurity, then again a site is randomly selected, and so on until a site with a magnetic spin S_i is selected.

(ii) All nearest neighbors S_j of a given spin S_i are considered. If a neighboring site is occupied by a magnetic spin, which is codirectional with the non-inverted spin S_i, then with probability $p = 1 - \exp(-2K)$, where $K = J/(k_B T)$, this spin is also flipped, and its coordinates are stored in the stack. Then the nearest neighbors of the last spin with which the connection was established, are viewed. This process continues until the system boundaries are reached.

(iii) All spins, between which the connection is established, form a "cluster".

(iv) The spins flipped procedure ends when the stack is empty. This process is called cluster flipping.

The calculations were performed for weakly dilute systems with periodic boundary conditions at a spin concentration $p = 0.90$. Systems with linear dimensions $L \times L = N$, $L = 20$ and 120 are considered. The initial configurations were set in such a way that all spins were ordered along one axis. To bring the system to an equilibrium state, the relaxation time τ_0 was calculated for all considered systems, and averaging was carried out for different initial configurations. For systems with a spin concentration $p = 0.90$, configuration averaging was performed over 1000 different configurations.

4. Results of a numerical experiment

The temperature dependence of the susceptibility was calculated according to the fluctuation relation [20]

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

where $K = J/(k_B T)$, J is the ferromagnetic interaction parameter ($J > 0$), $N = pL^2$ is the number of magnetic sites, m is the magnetization of the system, angle brackets denote thermodynamic averaging, the bar above denotes averaging over the canonical ensemble with the different realization of the disorder.

The expression for the magnetization for the two-dimensional weakly diluted Potts model is defined by the following expression [21]:

$$m_F = \left\langle \frac{3}{2} \sum_{\alpha=1}^{4} \left(\frac{N_\alpha}{N} - \frac{1}{3} \right)^2 \right\rangle^{1/2}, \quad (4)$$

where $N_\alpha = \{N_1, N_2, N_3, N_4\}$, N_1, N_2, N_3, and N_4 are the numbers of spins in the states with $q = 1, 2, 3$, and 4, respectively.

The critical temperatures and the order of the phase transition (PT) were determined using the method of fourth-order Binder cumulants [22]. The technique for determining the PT temperature by this method is considered in [23–26]. The critical temperature for the two-dimensional impurity Potts model with the number of spin states $q = 4$ at the spin concentration $p = 0.90$ was determined in [26], $T_c(p) = 0.777(2)$.

Figures 2 show the values of susceptibility χ_j, magnetization m_j, and heat capacity C_j, respectively, for various impurity configurations j of the three-dimensional Potts model in a weakly diluted mode at $p = 0.90$, $T = T_c(p)$, $0 \le j \le N_s$, N_s is the total number of impurity configurations. Here also presented the averaged values $[X_j]$, $[m_j]$, and $[C_j]$ over the corresponding canonical ensemble with the different distribution of nonmagnetic impurities for systems with a linear size $L = 20$. As can be seen, the number of impurity configurations N_s used for averaging makes it possible to achieve an asymptotic critical regime for all the considered thermodynamic parameters in a weakly diluted region. This behavior is due to the fact that, in contrast to works [1, 2], in which the quenched-in disorder is realized in a large canonical way, nonmagnetic impurities in our work were distributed over the system in a canonical way, i.e., by fixing the fraction of magnetic nodes in each disordered configuration with a different realization of disorder, in which fluctuations in the impurity distribution are much smaller than in the case of the grand canonical type.

To calculate the relative dispersion (squares of the coefficients of variation) of the magnetization R_m, susceptibility R_χ, and the heat capacity R_C depending on the linear dimensions L of the system under study, we used the expressions

$$R_m = \frac{\overline{m^2(L)} - \overline{m(L)}^2}{\overline{m(L)}^2}, \quad (5)$$

$$R_\chi = \frac{\overline{\chi^2(L)} - \overline{\chi(L)}^2}{\overline{\chi(L)}^2}, \quad (6)$$

$$R_C = \frac{\overline{C^2(L)} - \overline{C(L)}^2}{\overline{C(L)}^2}. \quad (7)$$

The data calculated by expressions (5)–(7) make it possible to judge the self-averaging of thermodynamic quantities and the errors associated with the sizes of the studied systems. The corresponding values of R_m, R_χ, and R_C for systems with $L = 20$ and 120 at the spin concentrations $p = 0.90$ are presented in Table 1. As can be seen, the introduction of weak disorder into the Potts model with $q = 4$ leads to nonzero values of R_m, R_χ, and R_C. Moreover,

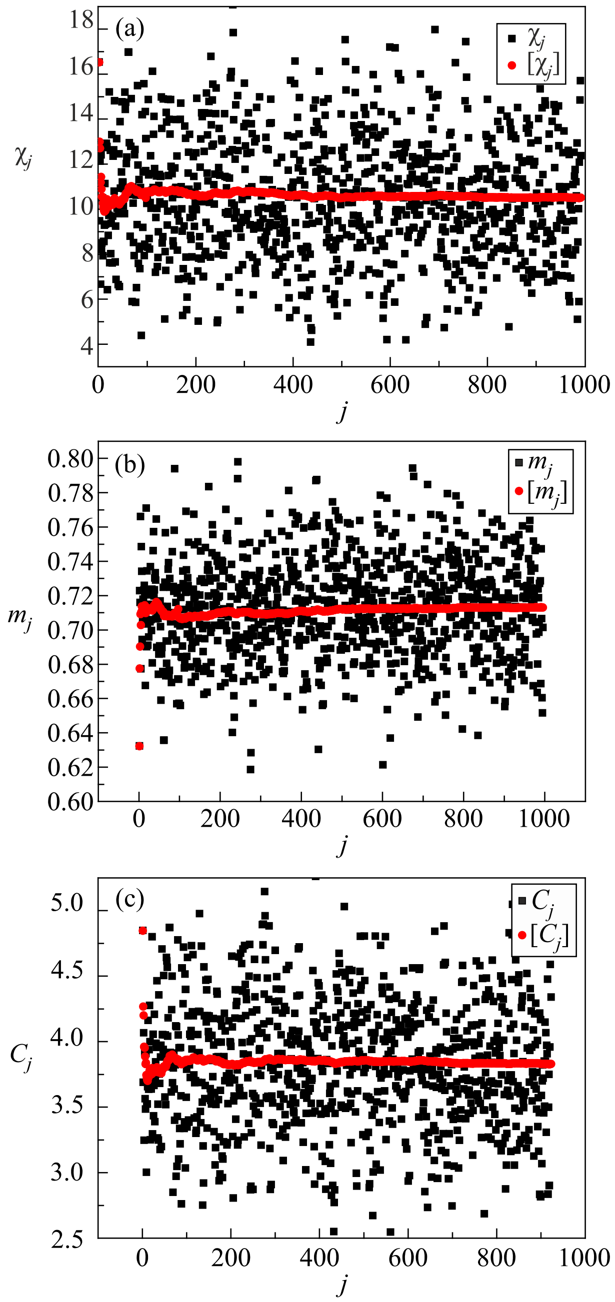

Fig. 2. Distributions of susceptibility (a), magnetization (b), and heat capacity (c) over a canonical ensemble with different distribution of nonmagnetic impurities for a system with $p = 0.90$, $T = T_c(p)$ and linear size $L = 20$.

Table 1. Values of relative dispersions of susceptibility, magnetization, and heat capacity for a weakly diluted Potts model with $q = 4$

L	R_χ	R_m	R_C
20	0.021	0.011	0.012
120	0.018	0.010	0.009

with an increase in the linear size of the system, these data noticeably decrease. This behavior, when the relative variances of R_m, R_χ, and R_C decrease with increasing L corresponds to the case of weak self-averaging (see [2]). Analysis of these data and their scaling in a wide range of dilutions p for spin systems with different L will be the goal of a separate work.

5. Conclusion

First the relative dispersion of the magnetization R_m, susceptibility R_χ, and heat capacity R_C have been calculated for a weakly diluted impurity Potts model with the number of spin states $q = 4$. The calculations were performed for spin systems with linear dimensions $L = 20$ and 120 at a spin concentration $p = 0.90$. It is shown that the introduction of a weak frozen-in disorder in the form of nonmagnetic impurities into the pure Potts model with $q = 4$ on a square lattice leads to nonzero values of R_m, R_χ, and R_C. The obtained data decrease with an increase in the linear size L, which is due to the weak self-averaging of thermodynamic parameters in the considered disordered model.

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Розрахунок відносних дисперсій намагніченості, сприйнятливості та теплоємності у двовимірній слабкорозбавленій моделі Поттса на основі методів комп’ютерного моделювання

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Методом Монте-Карло розраховано відносні дисперсії намагніченості R_m, сприйнятливості R_χ та теплоємності R_C для слабкорозбавленої домішкової моделі Поттса з числом станів спіна $q = 4$. Показано, що внесення безладу у вигляді немагнітних домішок в двовимірну модель Поттса з $q = 4$ на квадратній гратці призводить до відмінних від нуля значень R_m, R_χ та R_C в критичній точці.

Ключові слова: метод Монте-Карло, модель Поттса, дисперсія намагніченості, сприйнятливості та теплоємності.