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Study of the influence of weak magnetic fields on phase transitions of the four-component antiferromagnetic Potts model

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Using the computer simulation method, phase transitions and thermodynamic properties of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on a hexagonal lattice in weak magnetic fields have been studied. The studies were carried out for the magnetic field range $0.0 \leq h \leq 5.0$ with a step of 0.5. It has been established that in the field range $0.0 \leq h \leq 3.0$ a first-order phase transition is observed. It was found that in the interval $3.5 \leq h \leq 5.0$ the system becomes frustrated.

Keywords: Frustration, Phase transitions, Monte Carlo method, Potts model.

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1. Introduction

In condensed matter physics, there is an increased interest in the study of phase transitions (PTs) and related critical phenomena. In all condensed matters, under certain conditions, one or more PTs occur. The study of factors influencing PT in condensed matter is of particular interest. Such factors include the external magnetic field, the interaction of next nearest neighbors, impurities, thermal and quantum fluctuations, etc. At present, the question of the influence of external disturbing factors on PT in magnetic spin systems is of fundamental importance. The inclusion of these perturbing factors can lead to a wide variety of phases and PTs in such systems, as well as completely new physical behavior [1–5].

In this study, we investigate the influence of an external magnetic field on the nature of PT and the thermodynamic properties of magnetic spin systems. Various lattice models, such as Ising, Potts, Heisenberg models, etc. [6–11] are used to solve this type of tasks. Despite the successes achieved in this area, the Potts model is still insufficiently studied. The interest in this model is caused by the fact, that Potts model serves as a basis for the theoretical description of a wide range of physical properties and phenomena in the physics of condensed matter. These include complex anisotropic ferromagnetics, spin glasses, multicomponent alloys and liquid mixtures. Based on the Potts model with different number of spin states q, structural PTs can be described in many materials [2,4,11]. As an example of substances described by the Potts model and having a hexagonal lattice structure, we can provide adsorbed films: adsorbed hydrogen atoms (2×2) — 2H—Ni(111) on the surface of nickel Ni(111) are placed at the nodes of the hexagonal lattice [12]. In such adsorbed structures PTs are described by the universality class of two-dimensional Potts models with $q = 4$ [13]. There are practically no studies studying the influence of the external magnetic field as a perturbing factor on PT and the thermodynamic properties of the antiferromagnetic Potts model, and this question still remains open and insufficiently studied.

To that end, in this paper we used Monte-Carlo (MC) method to study the impact of weak magnetic fields on PTs and thermodynamic properties of two-dimensional Potts model with a number of spin states $q = 4$ on a hexagonal lattice, taking into account exchange interactions between the first and second nearest neighbors. This model is also interesting because the value $q = 4$ is a limit value, above which PT of the first kind shall be observed [10].

In recent years, when studying this model, attention was mainly paid to ferromagnetic systems [14–19]. These papers showed that the magnitude of the next nearest neighbors interaction, as well as the external magnetic field can radically affect PT and the thermodynamic behavior of the ferromagnetic Potts model. PT nature and the features of the thermodynamic behavior of the Potts model for the antiferromagnetic case on hexagonal lattice practically were not studied.

2. Model and method of study

The Hamiltonian of the Potts model, taking into account the interaction of the first and second neighbors, as well as the external magnetic field, has the following form:

$$\begin{aligned}\mathscr{H} &= -J_1 \sum_{i,j(i\neq j)} \mathbf{S}_i\mathbf{S}_j - J_2 \sum_{i,k(i\neq k)} \mathbf{S}_i\mathbf{S}_k - h\sum_i \mathbf{S}_i \\ &= -J_1 \sum_{i,j(i\neq j)} \cos\theta_{i,j} - J_2 \sum_{i,k(i\neq k)} \cos\theta_{i,k} - h\sum_i \mathbf{S}_i,\end{aligned} \tag{1}$$

where J_1 and J_2 — parameters of exchange antiferromagnetic ($J_1 < 0$ and $J_2 < 0$) interactions, respectively, for

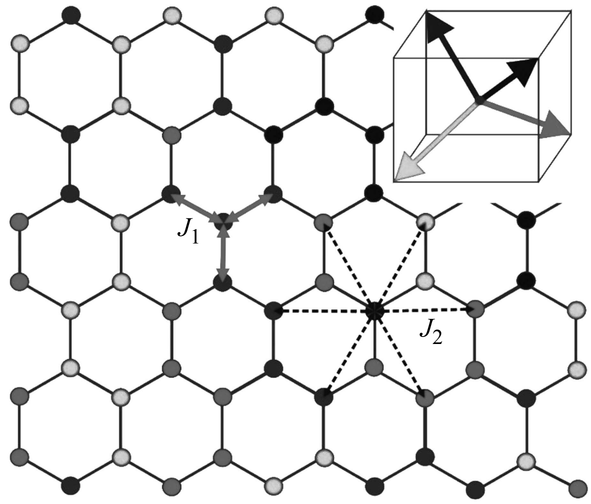

Figure 1. Potts model with the number of spin states $q = 4$ on hexagonal lattice. The insert shows the corresponding representation for each of the four possible spin directions.

nearest and next nearest neighbors, $\theta_{i,j}$, $\theta_{i,k}$ — angles between interacting spins $\mathbf{S}_i$–$\mathbf{S}_j$ and $\mathbf{S}_i$–$\mathbf{S}_k$, h — magnitude of the magnetic field (given in units $|J_1|$). This study considers the case when $J_1/J_2 = 1$. The external magnetic field varied in the range of $0.0 \le h \le 5.0$ with a step of 0.5. The magnetic field is directed along one of spin directions.

A schematic description of model under study is presented in Figure 1. As it can be seen in the Figure, each spin has three nearest (solid lines) and six next nearest (dashed lines) neighbors. The insert in the Figure shows the corresponding representation for each of the four possible spin directions.

Spin directions were defined in such a way that the following equality is valid

$$\cos\theta_{i,j} = \begin{cases} 1, & \text{if } \mathbf{S}_i = \mathbf{S}_j \\ -\frac{1}{3}, & \text{if } \mathbf{S}_i \neq \mathbf{S}_j \end{cases}. \tag{2}$$

According to condition (2), for two spins $\mathbf{S}_i$and $\mathbf{S}_j$the energy of the pair exchange interaction is $E_{i,j} = -J_1$ if $\mathbf{S}_i = \mathbf{S}_j$. If $\mathbf{S}_i \neq \mathbf{S}_j$, the energy is $E_{i,j} = J_1/3$. Thus, the energy of the pair interaction of spins is equal to one value when their directions are the same, and takes another value when the directions of the spins do not coincide. For the Potts model with $q = 4$ in three-dimensional space, this is only possible if the spins are oriented as shown in the insert Figure 1.

Such systems based on microscopic Hamiltonians are successfully studied on the basis of the MC [18–23] method. In recent year many new MC algorithms were developed. One of the most effective algorithm for studying similar systems is the replica-exchange algorithm [24].

We used the replica-exchange algorithm in the following form:

1. simultaneously N replicas $X_1, X_2, \ldots, X_N$ with temperatures $T_1, T_2, \ldots, T_N$ are simulated;

2. after performing one MC step/spin for all replicas, data is exchanged between a pair of neighboring replicas X_i and X_{i+1} in accordance with the Metropolis scheme with probability

$$w(X_i \to X_{i+1}) = \begin{cases} 1, & \text{for } \Delta \ge 0 \\ \exp(-\Delta), & \text{for } \Delta > 0 \end{cases},$$

where $\Delta = (U_i - U_{i+1})(1/T_i - 1/T_{i+1})$, U_i and U_{i+1} — internal energies of the replicas.

To bring the system into the state of thermodynamic equilibrium, a section with length of $\tau_0 = 4 \cdot 10^5$ MC steps per spin was cut off, which is several times greater than the length of the non-equilibrium section. The thermodynamic parameters were averaged along a Markov chain with a length up to $\tau = 100\tau_0$ MC-steps per spin. Calculations were performed for systems with periodic boundary conditions and linear dimensions $L \times L = N$, $L = 12$–60, where L — linear lattice size, N — number of spins in the system.

3. Simulation results

To observe the temperature behavior of the heat capacity C we used the following expression [25]:

$$C = (NK^2)\big(\langle U^2\rangle - \langle U\rangle^2\big), \tag{3}$$

where $K = |J_1|/(k_\mathrm{B}T)$, U — internal energy.

Figure 2 shows temperature dependencies of heat capacity C for different values of magnetic field h at $L = 48$. It can be seen from the Figure, that in the range of $0.0 \le h \le 3.0$ well-defined maxima of heat capacity are observed near the critical region. Note that with magnetic field increasing, the maximum heat capacity shifts towards low temperatures. Such behavior of heat capacity is explained by the fact, that the increase in magnetic field strength results in quick ordering of the system, and decrease in fluctuations and, hence, decrease in PT temperature. As can be seen in the Figure, for the field value $h = 3.5$ the smooth dome-shaped maximum is observed. This shows that the magnetic field leads to PT suppression in the system. It may be assumed that this behavior of heat capacity is related to a change in the magnetic ordering. Further growth of the field ($h = 4.5$ and 5.0) leads to the heat capacity splitting. Heat capacity splitting is a special property inherent in frustrated models. This behavior of the heat capacity allows us to say that for field values $h \ge 3.5$ frustrations arise in this model.

Figure 3 shows the temperature dependences of the total energy of the spin system E for different values of the magnetic field. The figure shows that in the interval $0.0 \le h \le 3.0$ near the critical region the energy changes abruptly. This energy behavior is characteristic of the PT of first kind. For field values in the interval $3.5 \le h \le 5.0$ near the critical region, the energy of the system changes smoothly. It can be assumed that the FP nature changed.

To analyze PT kind, we used histogram data analysis of MC method [26,27]. This method allows for reliable

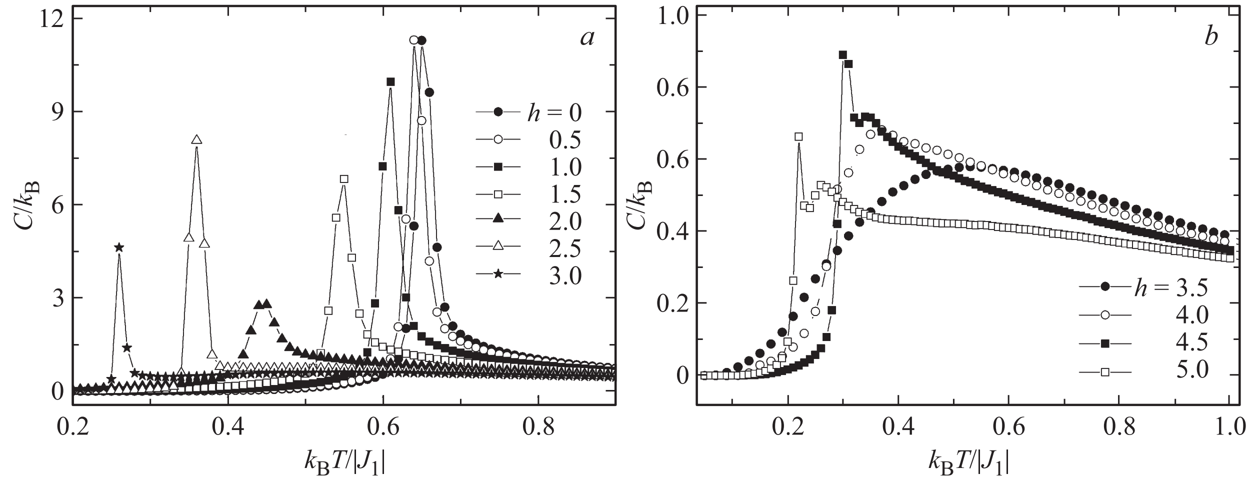

Figure 2. Temperature dependences of heat capacity.

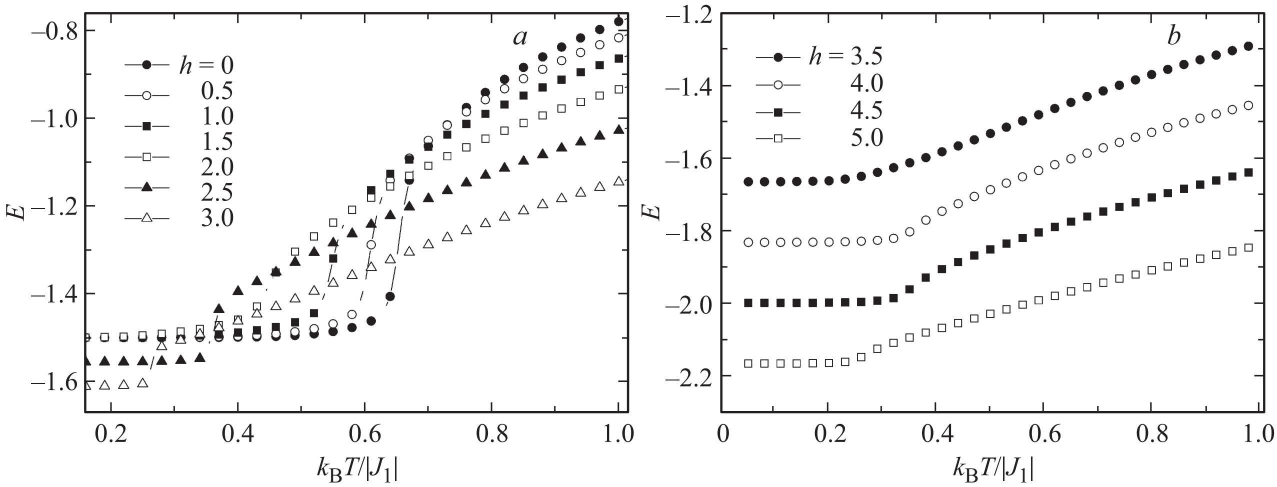

Figure 3. Temperature dependences of energy.

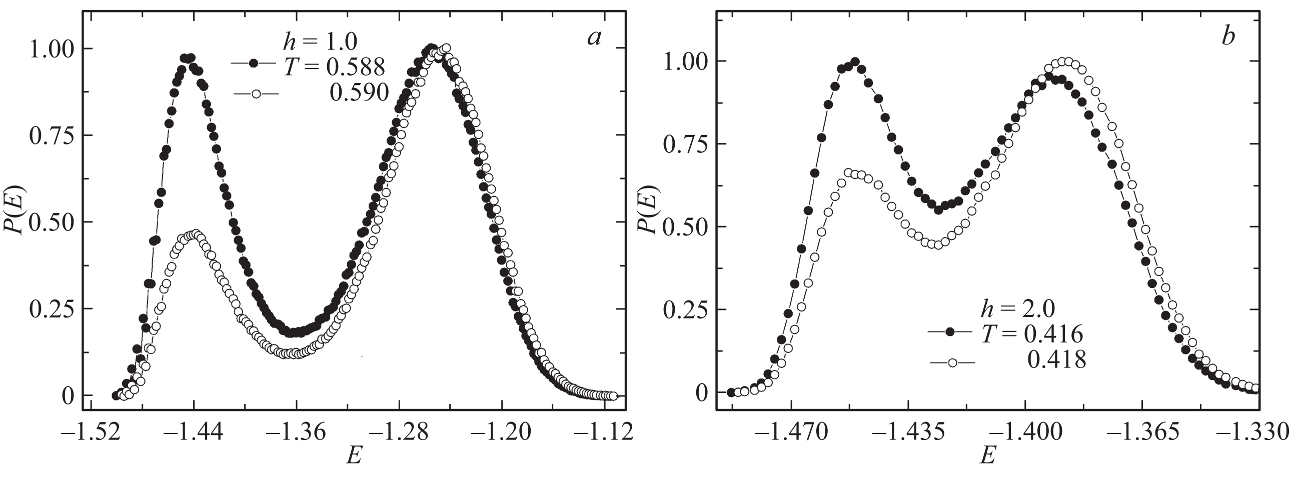

Figure 4. Energy distribution histograms.

determination of PT kind. The procedure determining PT kind by this method is described in detail in [16].

The results obtained on the basis of histogram data analysis show that PT of the first kind is observed in this model. This is demonstrated in Figure 4, where the energy distribution histograms are provided for a system with linear dimensions $L = 60$ for $h = 1.0$ and 2.0. The graphs are plotted for temperatures close to the critical temperature. It can be seen from the Figure that the dependence of probability P on energy E for all temperatures and fields has two peaks, which give an evidence for the PT of the first kind. The presence of the double peak in energy distribution histograms is a sufficient condition for the PT of the first kind. Note, that double peaks in the distribution histograms for the model under study are observed for field values in the range $0.0 \le h \le 3.0$. This let us state that in this interval of values h PTs of the first kind are observed. Results of this study show that weak external magnetic field does not lead to PT change, but leads to frustrations in the model under study. For the Potts ferromagnetic model with $q = 4$ it was found that weak external magnetic field changes PT of first-kind to second kind [16]. The study of PT of the antiferromagnetic model in a wide range of values h is not found in the literature.

4. Conclusion

The impact of weak external magnetic field on phase transitions and Potts thermodynamic models with a number of spin states $q = 4$ on the hexagonal lattice with interactions of the first and second neighbors was studied using the replica-exchange algorithm of Monte Carlo method. The nature of phase transitions is analyzed on the basis of histogram method. It is shown, that in the range of values $0.0 \le h \le 3.0$ the phase transition of the first kind is observed. It was found that in the interval $3.5 \le h \le 5.0$ the system becomes frustrated.

Conflict of interest

The authors declare that they have no conflict of interest.

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