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Investigation of the influence of weak magnetic fields on thermodynamic properties of the Potts model with the number of spin states $q = 4$ on a hexagonal lattice

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The replica exchange algorithm of the Monte Carlo method was used to study phase transitions and thermodynamic properties of the two-dimensional Potts model with the number of spin states $q = 4$ on a hexagonal lattice in weak magnetic fields. The studies were carried out for the interval of the magnetic field value $0.0 \leq H \leq 3.0$ with a step of 1.0. It is found that a first-order phase transition is observed in the considered range of field values.

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

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1. Introduction

In recent years in the physics of condensed state there is an increased interest in research of impact of different disturbing factors on the phase transitions (PTs), magnetic structures of the ground state, critical, magnetic, and thermodynamic properties of spin systems. Today the issue of impact of external magnetic field, the second nearest neighbors interactions, non-magnetic impurities and quantum fluctuations is of fundamental importance. Inclusion of these disturbing factors may result in a large variety of phases and PTs in magnetic spin systems [1–7]. The study of external factors impact on frustrated spin systems is of special interest. It is related to the fact that properties of frustrated spin systems are different of those of correspondent non-frustrated systems. Frustrated system are highly sensitive to external disturbing factors. Introduction of external disturbances in these systems may result in completely new physical behavior. To that end, in this study we consider the impact of weak magnetic fields on the character of PT and thermodynamic properties of frustrated spin systems. Various lattice models, such as Potts model, Ising model, Heisenberg model, etc. are used to solve this type of tasks.

By now, the impact of external disturbing factors, including magnetic field in Ising and Heisenberg models, is studied well enough [8–13]. The situation with Potts model is completely different. The Potts model is poorly 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 with cubic structure, spin glasses, multicomponent alloys and liquid mixtures. Based on the Potts model with different number of spin states structural PTs can be described in many materials [13]. There are few or no works devoted to the research of the external magnetic field impact as a disturbing factor on PTs and thermodynamic properties of the Potts model, and this issue is still open and poorly studied.

To that end, in this work we used Monte-Carlo method (MC) 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 in that the value of $q = 4$ is a limit value for the interval of $2 \leq q \leq 4$, where a PT of the second kind is observed, and the range of $q > 4$, where a PT of the first kind is observed [14]. The study is performed on the basis of modern methods and ideas that allows answering a number of questions related to the character and nature of PTs of frustrated spin systems.

2. Model and method of study

The Hamiltonian in the Potts model taking into account the interaction of the first and second nearest neighbors, as well as external magnetic field can be written as

$$H = -J_1 \sum_{\langle i,j,\rangle, i\neq j} S_i S_j - J_2 \sum_{\langle i,j,\rangle, i\neq k} S_i S_k - H \sum_{\langle i \rangle} S_i$$
$$= -J_1 \sum_{\langle i,j,\rangle, i\neq j} \cos\theta_{i,j} - J_2 \sum_{\langle i,j,\rangle, i\neq k} \cos_{i,k} - H \sum_{\langle i \rangle} S_i \tag{1}$$

where J_1 and J_2 — parameters of exchange ferro- ($J_1 > 0$) and antiferro- magnetic ($J_2 < 0$) interaction for the first and second nearest neighbors, $\theta_{i,j}$, $\theta_{i,k}$ — angles between interacting spins $S_i - S_j$ and $S_i - S_k$, H — magnetic field (given in J_1 units of measure). In study we consider the case when $|J_1| = |J_2| = 1$. The external magnetic field varied in the range of $0.0 \leq H \leq 3.0$ with a step of 1.0. The magnetic field was directed along one of spin directions.

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

$$\theta_{i,j} = \begin{cases} 0 & \text{if } S_i - S_j \\ 109.47^\circ, & \text{if } S_i \neq S_j \end{cases} \Rightarrow \cos\theta_{ij}$$
$$= \begin{cases} 1 & \text{if } S_i = S_j \\ -1/3, & \text{if } S_i \neq S_j. \end{cases} \tag{2}$$

These systems now are successfully studied on the basis of MC method of microscopic Hamiltonians [15–20]. In recent year many new MC algorithms were developed. One of the most effective algorithm for studying similar systems is the replica-exchange algorithm [21].

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

1. N replicas $X_1, X_2, \ldots X_N$ with temperatures of $T_1, T_2, \ldots T_N$ are simulated simultaneously.
2. After one MC-step/spin is fulfilled for all replicas, data exchange is performed between a pair of neighboring replicas X_i and X_{i+1} in accordance with Metropolis algorithm with a probability of

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

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

To analyze the nature and character of PTs, the method of fourth-order Binder cumulants and histogram method of data analysis were used [22–24]. To bring the system into the state of thermodynamic equilibrium, a section was cut off with a length of $\tau_0 = 4 \cdot 10^5$ MC-steps per spin, which is several times greater than the length of non-equilibrium section. The thermodynamic parameters were averaged along a Markov chain with a length of $\tau = 500\tau_0$ MC-steps per spin. Calculations were made for systems with periodic boundary conditions and linear dimensions of $2 \times L \times L \times L = N$, $L = 12 \div 60$, where L — linear dimension of the lattice, 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]:

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

where $K = |J_1|/k_B T$, U — internal energy.

Figure 1 shows temperature dependencies of heat capacity C for different values of magnetic field at $L = 24$. It can be seen from the figure, that in the range of $0.0 \leq H \leq 3.0$ well-defined peaks are observed near the critical region. When a weak magnetic field ($H = 1.0$) is turned on, the peak of heat capacity shifts towards high temperatures. Further increase in field strength results in shift of the heat capacity peak 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, decrease in fluctuations and, hence, decrease in PT temperature. For a field strength of $H = 2.0$, the peak of heat capacity becomes smoother. It may be assumed that this behavior of heat capacity is related to a change in the magnetic ordering.

To analyze the character of PT and to determine the critical temperature TC, we used the method of fourth-order Binder cumulants [22]:

$$V_L = 1 - \frac{\langle U^4 \rangle_L}{3\langle U^2 \rangle_L^2} \tag{4}$$

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} \tag{5}$$

where V_L — energy cumulant, U_L — magnetic cumulant.

The parameter of system order m was calculated by the following formula:

$$m = \frac{1}{N}\left(\frac{4N_{\max} - N_1 - N_2 - N_3 - N_4}{3}\right), \tag{6}$$

where N_1, N_2, N_3, N_4 — number of spins corresponding to one of 4 spin directions, respectively.

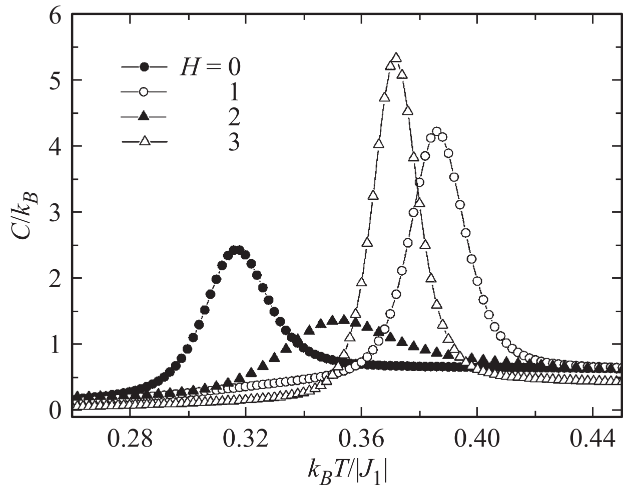

Figure 1. Temperature dependencies of heat capacity C/k_B.

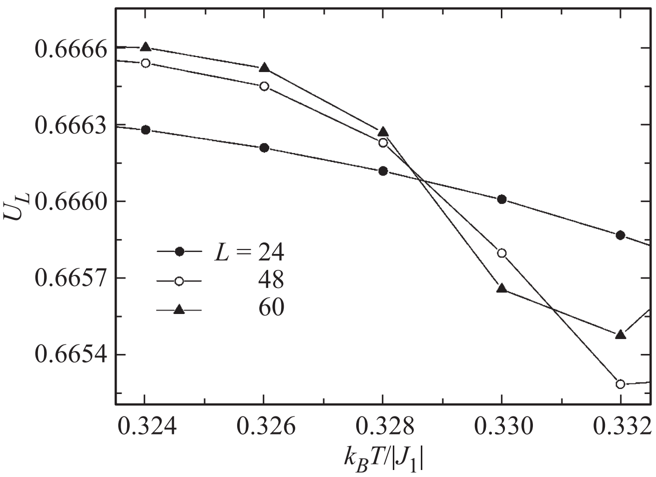

Figure 2. Temperature dependencies of Binder magnetic cumulant U_L.

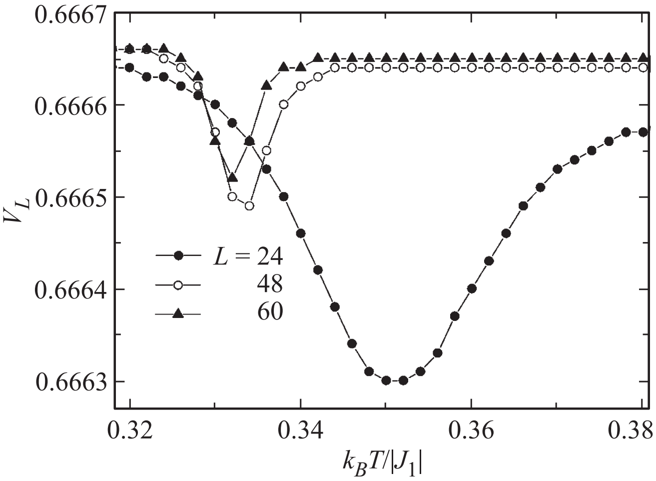

Figure 3. Temperature dependencies of Binder energy cumulant V_L.

Expressions (4) and (5) allows determining the critical temperature T_C with a high accuracy for PTs of the first and second kind, respectively. Also, the use of Binder cumulants allows good testing the type of PT in a system. It is known that a PT of the first kind has the characteristic that V_L tends to some non- trivial value V^* according to:

$$V_L = V^* + bL^{-d} \tag{7}$$

at $L \to \infty$ and $T = T_C(L)$, where the value of V^* is different from 2/3, and minimum value of $U_L \min(T = T_{\min})$ diverges ($U_L \min(T = T \min) \to \infty$) at $L \to \infty$.

In case of PT of the second kind the temperature dependency curves of Binder cumulants U_L have a clearly defined point of intersection [22].

Figure 2 shows typical dependence of U_L on temperature for field $H = 3.0$ at different values of L. It can be seen from the graph that in the critical region the temperature dependencies U_L do not intersect each other in a single point. This support the assumption of presence of PT of the first kind in this model. Similar picture is observed for all field values in the range of $0.0 \leq H \leq 3.0$.

The temperature dependence of energy cumulant V_L for the field $H = 3.0$ at different values of L is shown in Fig. 3. As can be seen from the graph, the value of V_L tends to 2/3, while $V^* = 2/3$, which is typical for PTs of the second kind. This value is calculated with the use of expression (7).

To perform a deeper analysis of PT kind, we used histogram data analysis of MC method [23,24]. This method allows for reliable determination of PT kind. The procedure to determine PT kind by this method is described in detail in [17].

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 Fig. 4. This figure represents energy distribution histograms for a system with linear dimensions $L = 60$ for $H = 1.0$ and 2.0. The graphs are plotted for different temperatures close to the critical temperature. It can be seen from the figure that the dependence of probability P on energy E for all

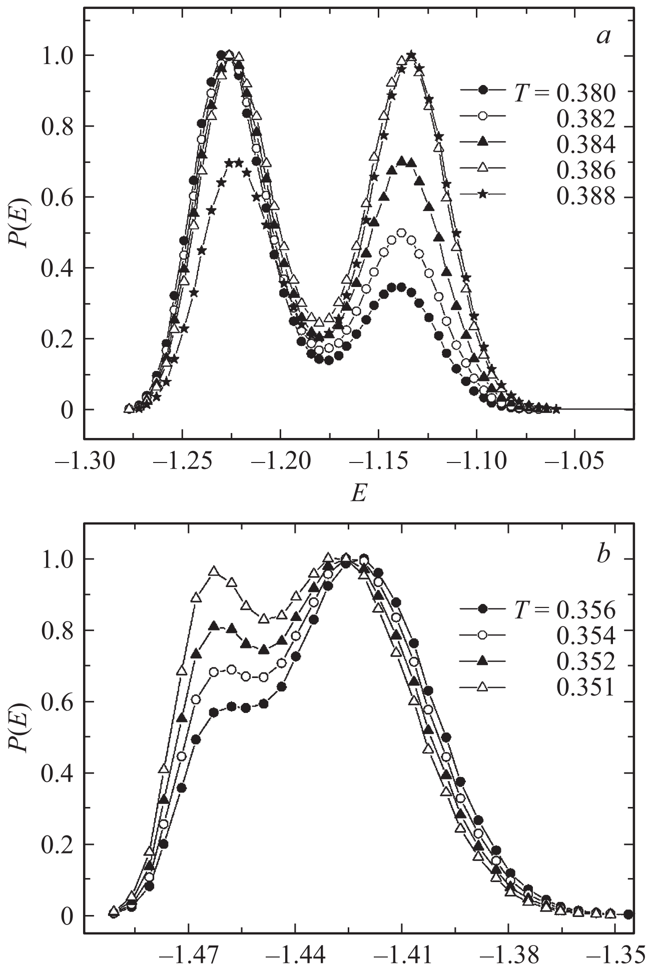

Figure 4. Histograms of energy distribution for $L = 60$ at different temperatures.

temperatures 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 in question are observed for values of H in the range of $0.0 \leq H \leq 3.0$. This let us state that in the considered interval of H values the PT of the first kind is observed.

Results of this study show that weak external magnetic field does not lead to a PT change in the model under examination. In the literature there is no study of PT of this model in a wide interval of H values.

4. Conclusion

The impact of weak external magnetic field on phase transitions and thermodynamic Potts models with a number of spin states $q = 4$ on a hexagonal lattice with interactions of the second nearest neighbors is studied using the replica-exchange algorithm of Monte Carlo method. The character of phase transitions is analyzed in the basis of histogram method and method of Binder cumulants. It is shown, that in the range of $0.0 \leq H \leq 3.0$ a phase transition of the first kind is observed.

Conflict of interest

The authors declare that they have no conflict of interest.

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