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Phase transitions in a three-dimensional ferromagnetic Potts model on a layered hexagonal lattice

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A Monte Carlo study was conducted of the phase transitions and magnetic and thermodynamic properties of a three-dimensional ferromagnetic Potts model with $q = 3$ spin states on a layered hexagonal lattice with nearest-neighbor interactions. Temperature dependences of energy, heat capacity, magnetization, and susceptibility were constructed. The nature of the phase transition was analyzed using a histogram data analysis method and the fourth-order Binder cumulant method. It was shown that a first-order phase transition is observed in the model under study.

Keywords: Energy, Magnetization, Susceptibility, Heat capacity.

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1. Introduction

The study of phase transitions (FT), magnetic and thermodynamic properties of magnetic spin systems is a relevant problem of condensed matter physics [1–5]. Various lattice models are successfully used to study the features of thermodynamic behavior and the nature of PT. A slew of interesting data was obtained on their basis. Lattice spin models make it possible to describe a number of real magnetic materials. Complex spin lattice models based on microscopic Hamiltonians are successfully determined by theoretical physics methods [6,7].

One of the spin lattice models used to describe real physical systems is the Potts model. The Potts model is a generalization of the Ising model, obtained by changing the number of spin states q. Phase transitions in Potts model exhibit more diverse properties than in Ising model, since the number of spin states q is related to the symmetry of the order parameter. One of the interesting Potts model's features is the dependence of the phase transition type on q: in the two-dimensional case, at $q > 4$, the system demonstrates a first-order PT, while at $q \leq 4$, the transition is continuous [8,9].

The Potts ferromagnetic model has been well studied in the two-dimensional case [8–11]. Despite the successes achieved, there are still unexplored issues related to the Potts model's physical properties versus spatial dimension of the lattice, number of spin states q, amount of interaction of the second neighbors, external magnetic field, lattice geometry and other factors [9–16]. Potts model is also of interest because it describes a large class of real physical systems: layered magnets, liquid helium films, superconducting films, adsorbed films, etc. [8,17]. For example, structural PT in materials such as $SrTiO_3$ or $Pb_3(PO_4)_2$ [18] are well described by the two-dimensional Potts model with the number of spin states $q = 3$, and PT in pyrochlore KOs_2O_6 — can be described by a 3D ferromagnetic Potts model with the number of spin states $q = 4$ [19].

In this paper, we study the Potts ferromagnetic model with the number of spin states $q = 3$ on a layered hexagonal lattice. There are very few papers devoted to the phase transitions, magnetic, and thermodynamic properties of the three-component Potts model on a layered hexagonal lattice. The data from analytical methods for the three-dimensional Potts model in case of $q > 3$ indicates the presence of the first-order PT, but there is no any rigorous argument to prove or disprove this fact. The data obtained by Monte Carlo method (MC) demonstrate that in the 3D ferromagnetic Potts model with the number of spin states $q = 4$, a first-order phase transition is observed on the layered hexagonal lattice [20] and on Kagome lattice [21]. The results of studies using renormalization and ε-expansion indicate that 3D Potts model with $q = 3$ uses the first-order PT [22,23]. At the same time, a nonperturbative renormalization group study of this model shows that the method of renormalization and ε-expansion may fail [24,25].

In this regard, based on the replica exchange algorithm of MC method, we conducted a study of the phase transitions, magnetic and thermodynamic properties of the ferromagnetic Potts model with the number of spin states $q = 3$ on a layered hexagonal lattice. This model is studied on the basis of modern methods and ideas dealing with a number of issues related to the thermodynamic properties of 3D spin lattice systems.

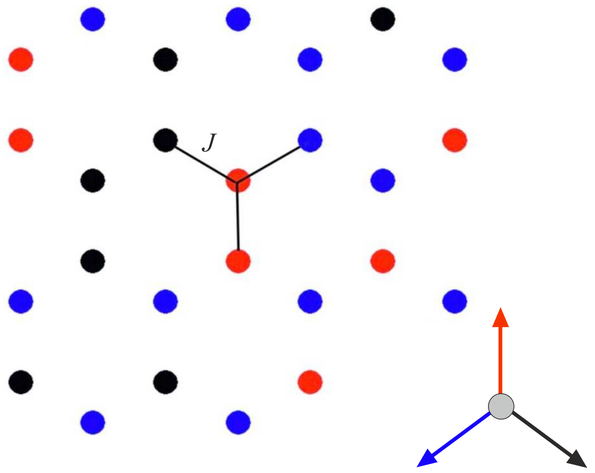

Figure 1. Potts model with the number of spin states $q = 3$ on hexagonal lattice.

2. Model and method of study

Taking into account interactions of the nearest neighbors, a Hamiltonian of the Potts model with the number of the spin states $q = 3$ can be written as follows:

$$H = -J \sum_{\langle i,j\rangle, i\neq j} S_i S_j = -J \sum_{\langle i,j\rangle, i\neq j} \cos\theta_{i,j}, \qquad (1)$$

where J — is a parameter of exchange ferromagnetic ($J > 0$) interaction of the nearest neighbors, $\theta_{i,j}$ is an angle between the interacting spins$S_i - S_j$.

The lattice consists of hexagonal layers stacked along z axis. The spins are located in the lattice sites. Each spin has five nearest neighbors: three neighbors in the plane and two neighbors in the adjacent layers. Adjacent layers are located parallel to each other, without displacements. The calculations were performed for the systems with periodic boundary conditions (PBC) and linear dimensions $L \times L \times L = N, L = 12 \div 48$, where L is measured in sizes of a unit cell.

A schematic description of the model for the two-dimensional case is shown in Figure 1.

Spins marked with circles of the same color have the same direction. The insert window in the figure shows the corresponding color representation for each of the three possible spin directions. The spin directions are pre-defined in such a way that the following equality is valid:

$$\cos\theta_{i,j} = \begin{cases} 1, & \mathit{if}\ \ S_i = S_j \\ -1/2, & \mathit{if}\ \ S_i \neq S_j \end{cases}. \qquad (2)$$

According to the condition (2), for the two spins S_i and S_j the energy of pair exchange interaction $E_{i,j} = -J$ if $S_i = S_j$. If $S_i \neq S_j$, the energy $E_{i,j} = J/2$. Thus, the energy of pairwise interaction of the 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 $q = 3$ in three-dimensional space, this is only possible if the spins are oriented as shown in the insert Figure 1.

At present, such systems based on microscopic Hamiltonians are being successfully studied using advanced MC method algorithms [10,26–28]. One of the most effective algorithms for studying these systems is the replica exchange algorithm [29]. We used this algorithm in this study. We used the replica exchange algorithm in the following form:

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

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

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

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

3. Study results

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

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

where $K = |J|/k_B T$, U is internal energy.

Figure 2 shows temperature dependences of heat capacity C (hereinafter a statistical error does not exceed sizes of symbols used for plotting the dependences) for the systems with various linear sizes.

In this Figure it is clear that for all the systems near the critical temperature, the dependence of heat capacity on

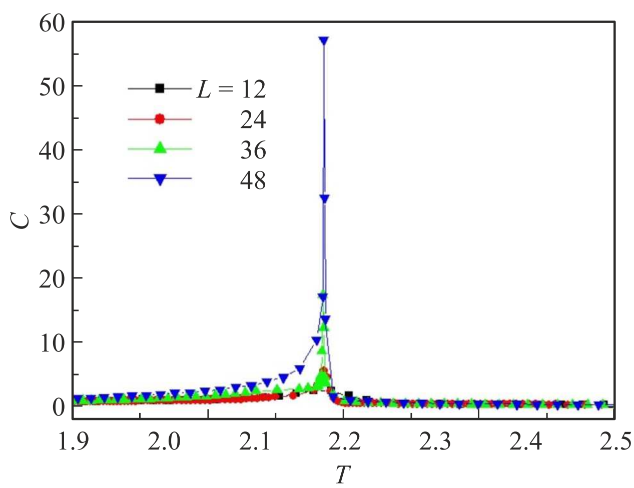

Figure 2. Temperature dependences of heat capacity C.

the temperature exhibits well-pronounced maximums that increase with an increase of the number of the spins in the system, wherein within the limits of an error these maximums fall within the same temperature for all values of L. This indicates, firstly, the high efficiency of the method used to add PBCs, and secondly, the achievement of saturation by N for many of the studied parameters. A drastic increase of the maximum (sharp maximum) of heat capacity with the increase of the linear sizes is typical for the systems, in which the first order phase transition is observed.

Figure 3 shows temperature dependences of the energy E for the system with the various linear sizes L. As it is clear in the figure, a drastic surge of the energy is observed for all L in the critical area. This behavior is typical for the first-order phase transition. Thus, the temperature dependences of heat capacity and energy are an evidence of the first-order phase transition.

The system magnetization m was found by the formula:

$$m = \frac{1}{N}\sum_{i=1}^{N} S_i, \tag{4}$$

where S_i — a three-component unit vector $S_i = (S_i^x, S_i^y, S_i^z)$.

Figure 4 shows graphs of magnetization m versus temperature for different values of L. The Figure shows that in the low-temperature region, the magnetization value is equal to one, which is typical for the ferromagnetic model. As the temperature rises near the critical region, a drastic decrease in magnetization is observed. While with the rise of L the magnetization starts to decline in a more abrupt way. This magnetization behavior is characteristic of the first-order phase transition.

Magnetic susceptibility was found by the formula:

$$\chi = \begin{cases} (NK)\left(\langle m^2\rangle - \langle |m|\rangle^2\right), & T < T_C \\ (NK)\langle m^2\rangle, & T \geq T_C \end{cases}, \tag{5}$$

where T_C — critical temperature.

Figure 5 shows graphs of magnetization χ versus temperature for different values of L. It is clear from the Figure that for all the systems near the critical temperature, the dependence of susceptibility on temperature exhibits the well-pronounced maximums that rise with an increase in the number of spins in the system, wherein within the limits of an error these maximums fall within the same temperature even for the systems with the lowest value of L. An abrupt rise of the maximum (sharp maximum) of susceptibility as the linear sizes grow is typical for the systems where the first-order phase transition is observed.

In order to analyze the phase transition character and to determine the critical temperature T_C, we used a method of fourth-order Binder cumulants [7]:

$$V_L = 1 - \frac{\langle U^4\rangle_L}{3\langle U^2\rangle_L^2}, \tag{6}$$

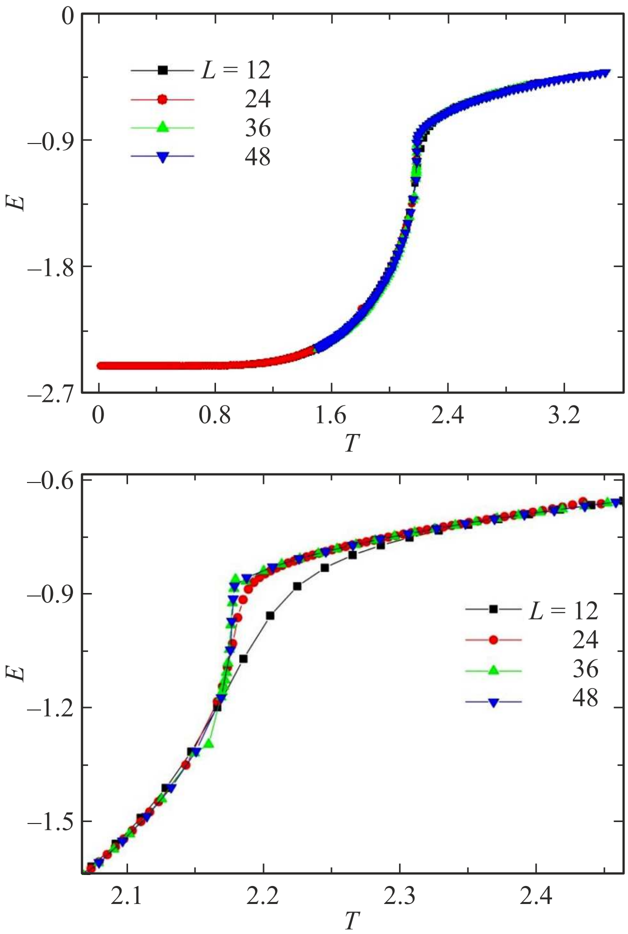

Figure 3. Temperature dependence of energy E.

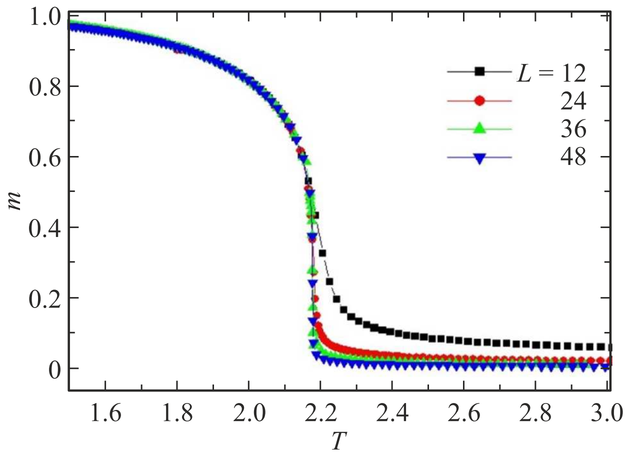

Figure 4. Temperature dependences of magnetization m.

$$U_L = 1 - \frac{\langle m^4\rangle_L}{3\langle m^2\rangle_L^2}, \tag{7}$$

where V_L — is the cumulant for energy, U_L — is the cumulant for magnetization.

The expressions (6) and (7) allow determining the critical temperature T_C with high accuracy for the first- and second-order phase transitions, respectively. Also, the use of the Binder cumulants allows good testing of the phase transition type in the system. In case of the second-order phase transition, curves of the temperature dependence of the Binder cumulants U_L have a clearly defined point of intersection [7]. Our data are analyzed to show that typical

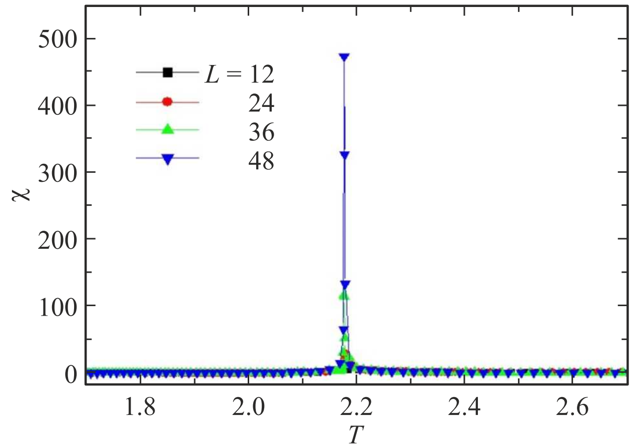

Figure 5. Temperature dependences of susceptibility χ.

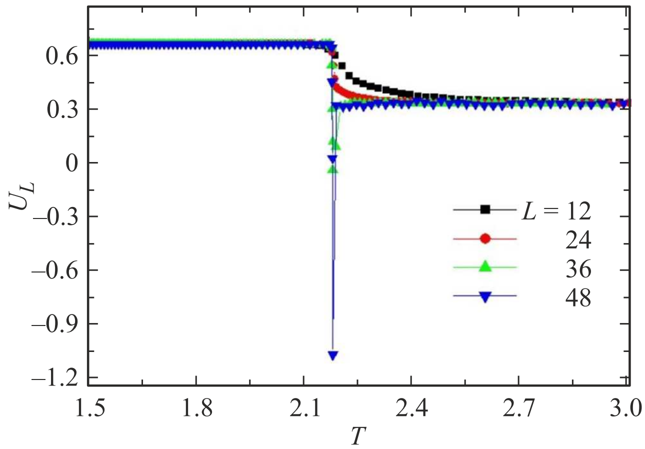

Figure 6. Temperature dependencies of Binder cumulant U_L.

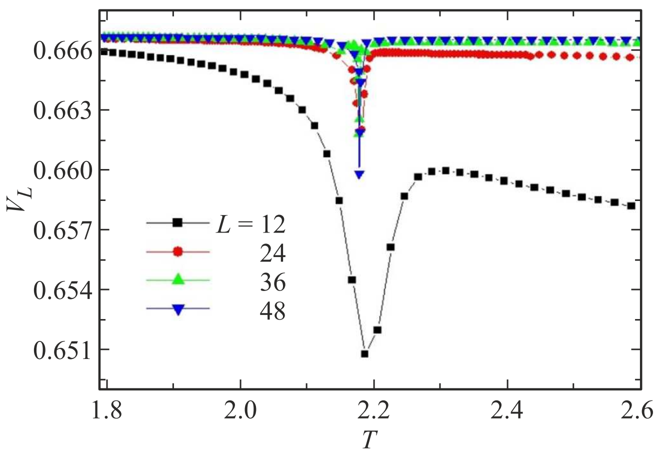

Figure 7. Temperature dependencies of Binder cumulant V_L.

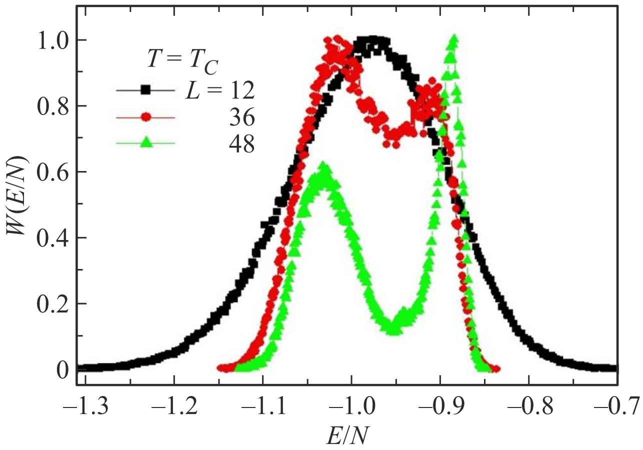

Figure 8. Energy distribution histograms for various L.

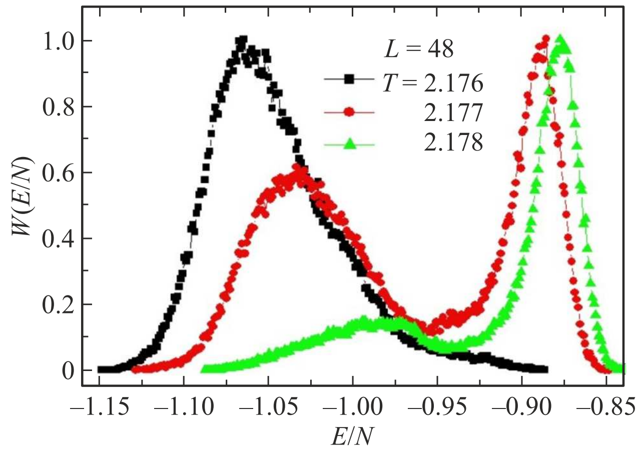

Figure 9. Histograms of distribution of the energy for the various T.

dependences U_L on temperature do not intersect in the same point in the critical area at various L (Figure 6). This supports the first-order phase transition in this model. The temperature dependence of the cumulantV_L is shown in Figure 7 at various L. As can be seen from this figure, the value of V_L in the critical region does not tend to 2/3 with an increase of L, which is typical for the first-order PT.

To determine the order of the PT, we used histogram data analysis of MC method [30,31]. The results that are obtained based on the data histogram analysis show that the first-order phase transition is observed in this model. It is demonstrated in Figure 8. This figure shows energy distribution histograms for the system with the various linear sizes. The graph is plotted for the temperature that is close to the critical temperature. It can be seen from the figure that the dependence of probability W on the energy exhibits two maximums, which indicate the first-order phase transition. The presence of the two maximums on the energy distribution histograms is a sufficient condition for the first-order phase transition.

Figure 9 shows the energy distribution histograms for the system with the linear sizes $L = 24$. The graphs are plotted for different temperatures close to the critical temperature. It is clear from the figure that for all the temperatures the dependence of probability W on the energy E exhibits two maximums that indicate the first-order phase transition. This proves that the first-order PT is observed in this model.

4. Conclusion

The study of phase transitions, magnetic and thermodynamic properties of the ferromagnetic Potts model with the number of spin states $q = 3$ on a layered hexagonal lattice, taking into account the interactions of the nearest neighbors, was performed using a replica algorithm of the Monte Carlo method. The phase transitions behavior was analyzed based on the Binder cumulant method and using the data histogram analysis. It was demonstrated that the first-order phase transition was observed in the studied model.

Conflict of interest

The authors declare no conflict of interest.

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