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Energy analysis of magnetic structures of the ground state of the Potts model with competing exchange interactions

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Based on the Wang–Landau algorithm, the Monte Carlo method was used to study the magnetic structures of the ground state and the thermodynamic properties of the two-dimensional Potts model with the number of spin states $q = 4$ on a triangular lattice, taking into account the exchange interactions of the first J_1 and second J_2 nearest neighbors. The studies were carried out for the value of the interaction of the second nearest neighbors in the range $-2.0 \leq J_2 \leq 0.0$. The magnetic structures of the ground state are constructed in the interval considered. An energy analysis of the magnetic structures of the ground state has been carried out. A phase diagram of the dependence of the critical temperature on the value of J_2 is constructed. It is shown that taking into account the interactions of the second nearest neighbors leads to the appearance of frustrations and violation of the magnetic ordering.

Keywords: Frustrations, magnetic structures, Monte Carlo method, Potts model.

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1. Introduction

Low-dimensional lattice models describe a large class of real physical systems: multilayer magnetics, liquid helium films, superconducting films, adsorbed films etc. Frustrations can arise in these systems due to the competition exchange interactions, geometric or energy limitations. Magnetic materials having a triangular lattice are heavily frustrated due to a specific geometry. As temperature decreases, the ordering process in such systems is much slower as compared to even the standard frustrated systems. This behavior is due to the fact that systems with a smaller coordination number can have not only states with non-trivial global degeneracy, but also locally degenerated states [1–4].

Most studies of spin systems with frustrations were up to now restricted to the Ising model, XY and Heisenberg models. Very few reliably established facts exist for a frustrated Potts model. Most available results were obtained for a two-dimensional Potts model with the number of spin states $q = 2$ and $q = 3$ [5–11]. The physical properties of a Potts model differ greatly depending on q, type and lattice spatial dimension [11–13].

In the present paper we study a two-dimensional Potts model on a triangular lattice with the number of spin states $q = 4$. This model is rather unique and still poorly studied. A Potts model can be used to describe the behavior of certain classes of adsorbed gases on graphite [14]. 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 second-order phase transitions (PT) are observed, and the range of $q > 4$, where a first-order PT takes place [12]. An analysis of the obtained results of the study of a two-dimensional Potts model with the number of spin states $q = 4$ on triangular [15], hexagonal [16,17] and trihexagonal lattices [18], shows that this model displays a transition having the features of a first-order PT.

Almost no studies of a two-dimensional Potts model with the number of spin states $q = 4$ on a triangular lattice with competing exchange interactions of the first and second nearest neighbors were published. Competition of exchange interaction in this model may cause a frustration, degeneracy of the ground state, formation of new magnetic structures of the ground state, as well as affect its thermodynamic properties. In this connection, we have attempted at using the Wang–Landau algorithm of the Monte-Carlo (MC) method to perform an energy analysis of magnetic structure of the ground state of a two-dimensional Potts model with the number of spin states $q = 4$ on a triangular lattice with ferromagnetic interaction of the first nearest neighbors and antiferromagnetic interaction of the second nearest neighbors. It is known that at the value of $q = 3$ a Kosterlitz–Thouless transition is observed for a mixed ferro-antiferromagnetic Potts model [19–21].

Since the Potts model behavior depends on quantity q, it is particularly interesting to study the magnetic and thermodynamic properties for $q = 4$ at different correlations of the magnitude of antiferromagnetic interaction of the second nearest neighbors. The currently available data does not allow for unambiguous determination of the regularities of change of the thermodynamic behavior of a frustrated Potts model with the number of spin states $q = 4$ and these issues still remain open. Studies are conducted using the modern methods and ideas which makes it possible to answer a number of questions related to the physics of frustrated spin systems.

2. Model and method of study

A Hamiltonian of a Potts model with the number of spin states $q = 4$, taking into consideration interactions of the first and second nearest neighbors, can be written as follows:

$$H = -J_1 \sum_{\langle i,j\rangle, i\neq j} \delta_{i,j} - J_2 \sum_{\langle i,k\rangle, i\neq k} \delta_{i,k}, \qquad (1)$$

where $\delta_{i,j} = \begin{cases} 1 & \text{if } S_i = S_j \\ 0 & \text{if } S_i \neq S_j \end{cases}$ (delta function), $S_i = 1, 2, 3, 4$, J_1 and J_2 — parameters of exchange ferro- ($J_1 > 0$) and antiferromagnetic ($J_2 < 0$) interaction respectively for the first and second nearest neighbors. In the present study, the magnitude of interaction of the second nearest neighbors varies in the range of $-2.0 \leq J_2 \leq 0.0$, while $J_1 = 1$.

A schematic and symbolic representation of the model is shown in Fig. 1. The inset shows a symbolic representation for each of the four spin values. The figure also shows the interactions between the first J_1 and second J_2 nearest neighbors.

At present, such systems based on microscopic Hamiltonians are being successfully studied based on the MC method [22–29]. Many new variants of MC method algorithms have been developed recently. The Wang–Landau algorithm is one of the most efficient for studying such systems [30,31], particularly in the low-temperature region.

We made additions to the standard Wang–Landau algorithm which make it possible to reveal the magnetic structure of the system's ground state. This algorithm is an implementation of the entropy modeling method and allows for calculating the system's density of states function. The Wang–Landau algorithm is based on the following: we obtain a uniform energy distribution by making a random walk in the space of energies with probabilities inversely proportional to the state density $g(E)$. By selecting such transition probabilities that visiting of all energy states becomes uniform, we can obtain an initially unknown state density $g(E)$, which can be determined in order to calculate the values of the necessary thermodynamic parameters at any temperature. Since state density $g(E)$ increases very quickly with an increase of the sizes of the systems under study, quantity $\ln g(E)$ is used for convenient storage and processing of large numbers.

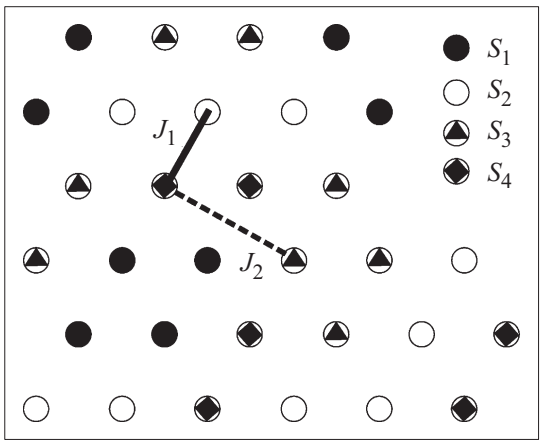

Figure 1. Schematic representation of Potts model.

We used the Wang–Landau algorithm in the following form.

A random initial spin configuration is set. The starting values of state density are $g(E) = 1$, energy distribution histograms are $H(E) = 0$, starting modification factor is $f = f_0 = e^1 \approx 2.71828$. We make multiple steps in the phase space until we obtain a relatively flat histogram $H(E)$ (i.e. until all possible system energy states are visited approximately the same number of times). Thereat, probability of transition from a state with energy E_1 into a state with energy E_2 is determined using the formula $p = g(E_1)/g(E_2)$. If a transition to a state with energy E_2 occurred, then $g(E_2) \to f \times g(E_2)$, $H(E_2) \to H(E_2) + 1$ otherwise $g(E_1) \to f \times g(E_1)$, $H(E_1) \to H(E_1) + 1$. If the histogram became „flat" we zero out the histogram $H(E) \to 0$, reduce the modification factor $f \to \sqrt{f}$, and continue again until $f \geq f_{\min}$. In our case $f_{\min} = 1.0000000001$. A histogram is considered relatively flat if its value for all the possible energy states is taken equal to minimum 90% of the total average value. We made additions to the standard Wang–Landau algorithm which make it possible to determine the magnetic structure of the system's ground state. When the state with the minimum energy is reached (presumably, the system's ground state), the magnetic structure is memorized as a line containing the values of all spins. Having determined the system's state density, we can calculate the values of thermodynamic parameters at any temperature. In particular, internal energy U, free energy F, specific heat capacity C and entropy S can be calculated using the following expressions:

$$U(T) = \frac{\sum\limits_E Eg(E)e^{-E/k_BT}}{\sum\limits_E g(E)e^{-E/k_BT}} \equiv \langle E\rangle_T, \qquad (2)$$

$$F(T) = -k_BT \ln\left(\sum_E g(E)e^{-E/k_BT}\right), \qquad (3)$$

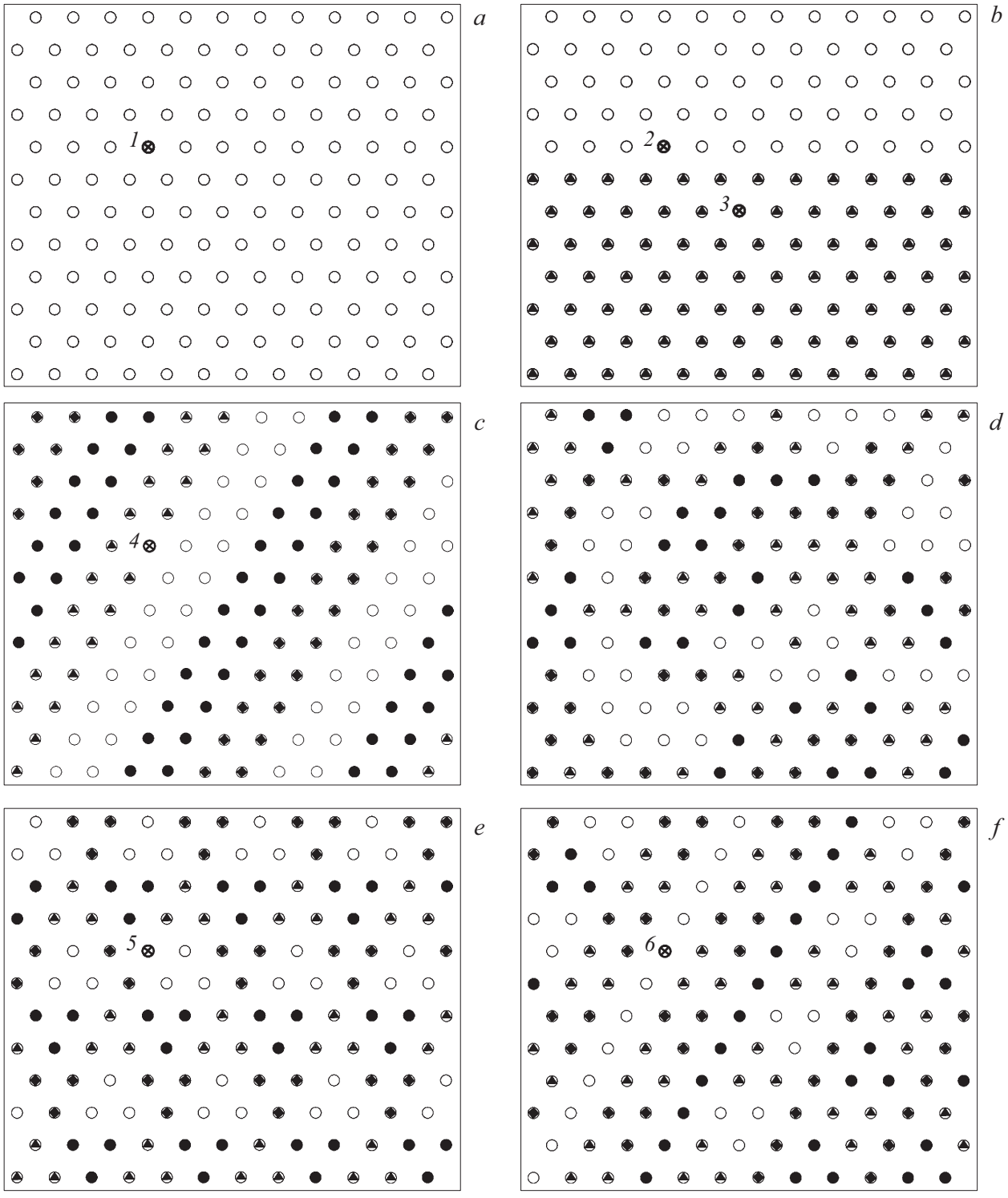

Figure 2. Spin configuration in one of the ground states implemented in the system at $J_1 = 1$ and different J_2: (a) $-0.5 \leq J_2$, (b) $J_2 = -0.5$, (c) $-1 < J_2 < -0.5$, (d) $J_2 = -1$, (e) and (f) $J_2 \leq -1$.

$$C = \left(\frac{(|J_1|/k_\mathrm{B}T)^2}{N}\right)\left(\langle U^2\rangle - \langle U\rangle^2\right), \qquad (4)$$

$$S(T) = \frac{U(T) - F(T)}{T}, \qquad (5)$$

where N is particle count, T — temperature (hereinafter temperature is given in $|J_1|/k_\mathrm{B}$ units). The calculations were performed for systems with periodic boundary conditions and linear dimensions $L \times L = N$, $L = 12 \div 120$ in the range of $-2.0 \leq J_2 \leq 0.0$.

3. Simulation results

Fig. 2, *a* shows the magnetic structure of the ground state for $J_2 = 0$. The ground state is a ferromagnetic one, where all spins are oriented along one of the four directions — the system has four-fold degeneracy. Such a situation is observed in the range of $-0.4 \le J_2 \le 0$. Fig. 2, *b* shows the magnetic structures of the ground state for the case of $J_2 = -0.5$. As seen from the figure, the ferromagnetic ordering is disrupted. Band structures of different widths are observed. Fig. 2, *c* shows the magnetic structures of the ground state for the case of $J_2 = -0.7$. Band structures having different band directions are observed in the figure. Such a situation is observed in the range of $-1 \le J_2 < -0.5$. The number of states is $\ln(N_{GS}) \propto L$. Disruption of the magnetic ordering of the band structure type is observed for the case of $J_2 = -1$ (Fig. 2, *d*). Regions with triplet ordering arise in the system on the background of the band structures. The degree of degeneracy of the ground state in this case is $\ln(N_{GS}) \propto L^2$. Triplet and stripe-triplet structures occur in the system in the range of $-2.0 \le J_2 \le -1$ (Fig. 2, *e,f*). The number of states is $\ln(N_{GS}) \propto L$.

To perform an energy analysis of the magnetic structures of the ground state, we marked nodes on a lattice sized 12×12 which is shown in Fig. 2. Each node has 6 nearest neighbors and 6 next nearest neighbors. The energy contribution of node i is determined as

$$E_i = -\frac{J_1}{2}\sum_j \delta_{i,j} - \frac{J_2}{2}\sum_k \delta_{i,k} = -\frac{J_1}{2}n - \frac{J_2}{2}m, \qquad (6)$$

where n — number of the nearest neighbors having the same value that the given spin, m — number of the next nearest neighbors having the same value.

Depending on structure and spin position on the lattice, the following variants shown in Fig. 2 are possible.

1. All spin neighbors have the same value ($n = 6$ and $m = 6$).

2. The spin is on the boundary of two wide bands ($n = 4$ and $m = 3$).

3. The spin is on the second line from the boundary of two wide bands ($n = 6$ and $m = 5$).

4. The spin is in a stripe structure with the width of 2 bands ($n = 4$ and $m = 2$).

5. Any of the nodes on a triplet structure ($n = 2$ and $m = 0$).

6. Any of the nodes on a triplet structure ($n = 2$ and $m = 0$).

7. Spins on a lattice with frustrations have a random number n and m.

The dependence of energy of these nodes on J_2 is shown in Fig. 3 (hereinafter the statistical error does not exceed the sizes of the symbols used for dependence plotting). Depending on structure of the ground state, a system may contain a different number of nodes of type 1–7. The structures shown in Fig. 2 for a 12×12 lattice contain:

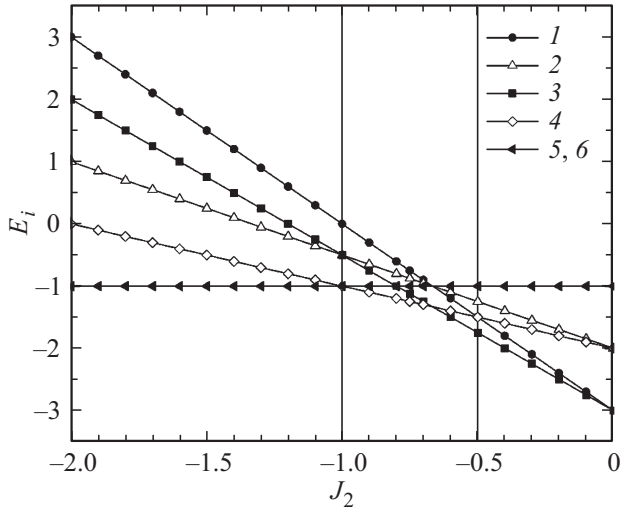

Figure 3. Energy analysis of magnetic structures of the ground state.

a) all 144 spins of type 1;

b) 96 spins of type 1, 24 spins of type 2, 24 spins of type 3. When a system contains several bands, this spin correlation can vary, and the condition of equality of the number of type 2 and type 3 nodes is always met;

c) all 144 spins of type 4;

d) all 144 spins of type 7. A frustrated unordered state;

e) all 144 spins of type 5;

f) all 144 spins of type 5 or 6.

The energy analysis of different spin configurations of ground states at $J_1 = 1$ and different J_2 is shown in Fig. 4. Thus, the following is energetically profitable, depending on quantity J_2

$-0.5 \le J_2$	*a*,
$J_2 = -0.5$	*a, b, c*,
$-1 \le J_2 \le -0.5$	*c*,
$J_2 = -1$	*c, d, e, f*,
$J_2 \le -1$	*e, f*.

Fig. 5 shows the temperature dependences of entropy S/N for different values of exchange interaction J_2. It can be seen from the figure that, with a temperature increase, entropy for all systems tends to the theoretically predicted value $\ln 4$. At low temperatures close to the absolute zero, entropy for certain values of J_2 tends to a non-zero value of S_0. A non-zero residual entropy is due to degeneracy of the ground state. The dependence of quantity S_0 for different values of exchange interaction J_2 is shown in Fig. 6. As seen from the figure, entropy S_0 in the range of $-0.4 \le J_2 \le 0.0$ at low temperatures tends to a zero value. The system in this range is not degenerate and order is maintained. Entropy at low temperatures in the ranges of $-0.9 \le J_2 \le -0.5$ and $-2.0 \le J_2 \le -1.2$ tends to a non-zero value. This is related to weak degeneracy of the ground state. This behavior is related to a partial ordering

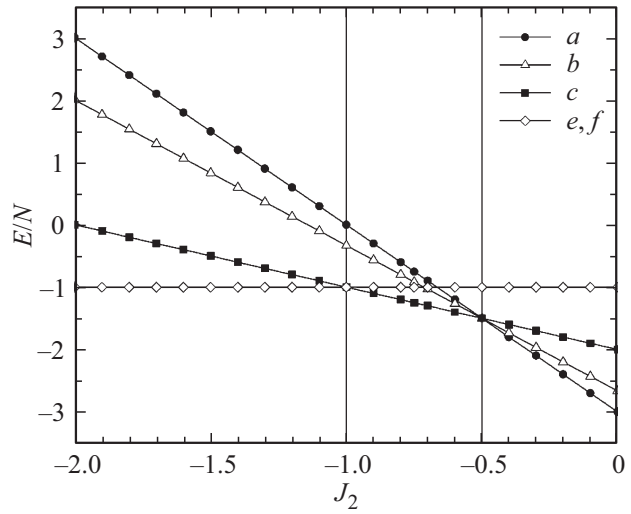

Figure 4. Energy analysis of different spin configurations of the ground state.

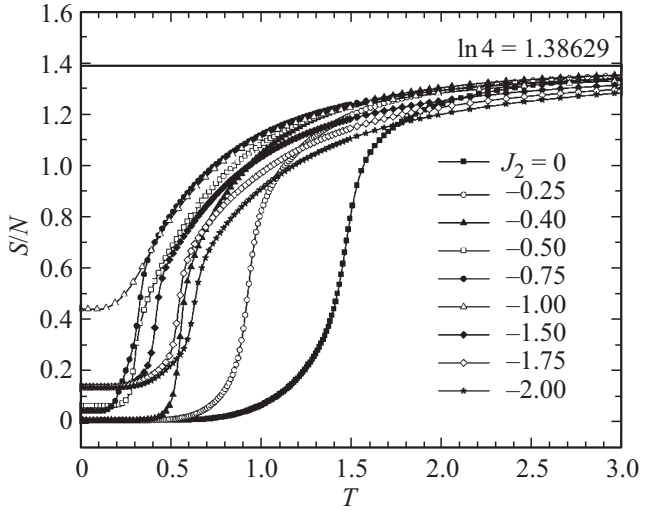

Figure 5. Temperature dependences of entropy S/N for different magnitudes of exchange interaction J_2.

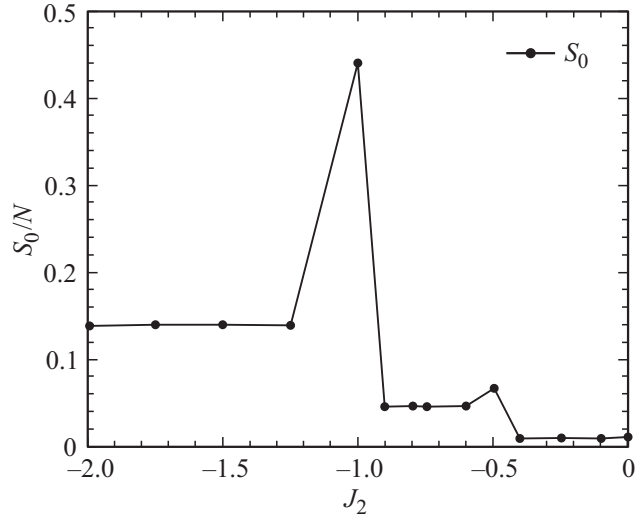

Figure 6. Dependences of entropy S_0 for different magnitudes of exchange interaction J_2.

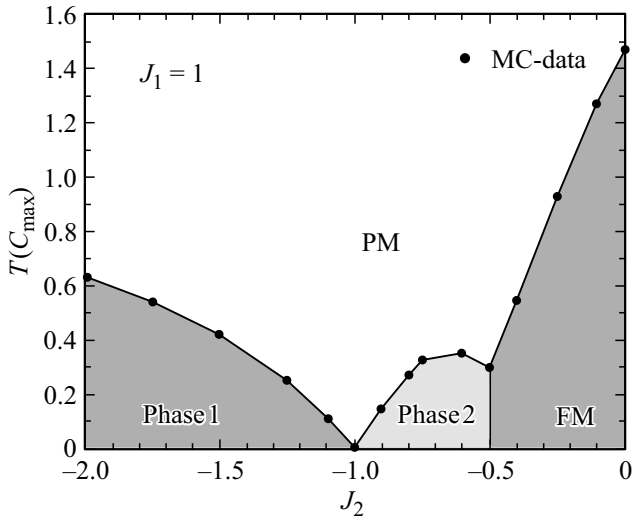

Figure 7. Phase diagram of dependence of the critical temperature on magnitude of interaction of the second nearest neighbors.

of the system. It should be noted that entropy in the low-temperature region for the value of $J_2 = -1.0$ takes on a larger value due to a strong degeneracy of the ground state. Such a situation is usually observed for frustrated spin systems [32]. It can be assumed that the system becomes heavily frustrated at the value of $J_2 = -1.0$.

The phase diagram of dependence of the critical temperature on magnitude of interaction of the second nearest neighbors is shown in Fig. 7. In order to plot a phase diagram, we plotted temperature dependences of heat capacity at different values of the magnitude of exchange interaction of the second nearest neighbors in the range of $-2.0 \le J_2 \le 0.0$. We determined temperature $T(C_{\max})$, at which heat capacity is the maximum, for each value of J_2. The temperature, which corresponds to the maximum heat capacity, can be considered close to the critical temperature. It can be seen from the figure that temperature $T(C_{\max})$ varies with change of the value of J_2. Several different phases are observed in the diagram: ferromagnetic (FM), paramagnetic (PM), Phase 1 (stripe-triplet) and Phase 2 (stripe). The critical temperature at the value of $J_2 = -1.0$ is equal to zero and there is not PT. This is due to the fact that competition of exchange interactions of the first and second nearest neighbors for a given value of J_2 results in total frustration. Frustrations disrupt the system order and cause disappearance of the PT.

Occurrence of different phases in the diagram is due to a change of the magnetic structure of the ground state. Each phase corresponds to different magnetic structures.

1. The ordered ferromagnetic phase $(J_2 < -0.5)$ corresponds to the magnetic structure shown in Fig. 2, *a*.

2. The stripe phase $(-1 < J_2 \le -0.5)$ — to the magnetic structures shown in Fig. 2, *b, c*.

3. The frustrated unordered phase $(J_2 = -1)$ — to the magnetic structure shown in Fig. 2, *d*.

4. The stripe-triplet phase ($-2.0 \leq J_2 \leq -1$) — to the magnetic structures shown in Fig. 2,*f*.

4. Conclusion

The study of magnetic structures of the ground state and thermodynamic properties of a two-dimensional Potts model with the number of spin states $q = 4$ on a triangular lattice while considering the interactions of the first and second nearest neighbors was conducted using the Wang–Landau algorithm of the Monte-Carlo method. We have determined the magnetic structures of the ground state at different values of the magnitude of interaction of the second nearest neighbors. It was found that a change in the magnitude of interaction of the second nearest neighbors in the given model results in a change of magnetic ordering. An energy analysis of magnetic structures of the ground state has been performed. A phase diagram of dependence of the critical temperature on magnitude of exchange interaction of the second nearest neighbors has been plotted. It is shown that strong frustration effects are observed at the value of $J_2 = -1$, which disrupt the magnetic ordering.

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Conflict of interest

The authors declare that they have no conflict of interest.

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