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Phase Transitions of the Mixed-Spin Ising Model on the Square Lattice

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The mixed-spin Ising model $S = (1/2, 1)$ on a square lattice has been investigated using a highly efficient replica exchange Monte Carlo algorithm. The system was studied with fixed exchange interaction and anisotropy parameters: $J_1 = -1$ (between spins in sublattices A and B), $J_2 = -0.5$ (between spins in sublattice B), and $D = 1.0$ (anisotropy for spins in sublattice B). Temperature and field dependencies of the main thermodynamic characteristics (energy, specific heat, entropy, magnetization) were calculated. Ground state structures were visualized. The existence of two successive phase transitions was revealed: at $T_{C1} = 0.285$ a transition to a partially disordered state occurs, and at $T_{C2} = 0.35$ — a transition to a paramagnetic state. A detailed analysis of the field dependencies reveals a complex, multi-step magnetization curve, indicating multiple field-induced phase transitions. We identify a series of magnetization plateaus, determine the corresponding magnetic structure for each, and calculate the critical field values for the transitions between these phases, leading to a comprehensive understanding of the system's phase diagram and its response to external perturbations.

Keywords: Mixed-spin Ising model, ground state structure, phase transitions, replica exchange algorithm, Monte Carlo method.

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1. Introduction

Analysis of the magnetic properties of low-dimensional spin systems remains one of the central objectives of the condensed matter physics. These systems not only demonstrate an enhanced diversity of critical phenomena and phase transitions, but are also of great interest for the applied areas, such as spintronics, information storage and development of new magnetic materials [1–3]. Among multiple theoretical models used to describe such systems, the Ising's model plays a special part due to its conceptual simplicity and simultaneously the ability to describe the complex physical phenomena, including cooperative behavior, long-range order occurrence and disorder effect [4,5]. Despite the existence of precise solutions for a unidimensional and a two-dimensional case of a homogeneous model, more complex modifications, such as models with the mixed spin, still remain an unsolved and a relevant problem.

Ising's models with a mixed spin are of a special interest in this context, with their crystal lattice consisting of two or more sublattices with different spin values [4–18]. Such systems are natural models to describe ferrimagnetics, where the compensation of magnetic torques results in apperance of unique thermodynamic characteristics, such as a compensation point. Combinations of integral and semi-integral spins, for example, $S = (1/2, 1)$ and $S = (3/2, 2)$, are especially interesting, since they combine effects of quantum and classic nature, which results in a complex competitive behavior between the exchange interactions, anisotropy and external fields [9–11].

Many papers were dedicated to analysis of the mixed spin models using various theoretical and computational approaches, including the middle field method, effective field theory and Monte Carlo method (MCM) [12–16]. In particular, for system $S = (1/2, 1)$ a phase diagram and critical behavior were studied on a square lattice [12,13]. It was shown that the introduction of the exchange interaction (J_2) following the closest neighbor and single-ion anisotropy (D) may lead to appearance of new phases, including partially ordered states, and influence the sequence of phase transitions [14,15].

Despite a significant progress in the study of the mixed spin models, their phase behavior and, in particular, fine effects related to the sequence of phase transitions, require further in-depth study. Application of the modern computational methods, in particular, highly efficient Monte Carlo algorithms, opens new capabilities for the detailed analysis of such systems, making it possible to overcome the limitations related to their complex energy landscape and strong fluctuations.

Our previous paper [18] used a replica exchange algorithm to study the Ising's model with the mixed spin $S = (1/2, 1)$ on a square lattice. The study conducted for the system of linear dimension $L = 10$ made it possible to identify four different magnetic phases (AF, $B{-}AF$, *0I* and *0II*) and build the common phase diagram depending on the parameters of exchange and anisotropy. Temperature dependences of key thermodynamic parameters were calculated for each of the identified phases.

Subsequent, more detailed calculations on the systems with the enlarged linear dimensions ($L = 20$, 40 and 100) in general confirmed the previously established pattern. However, a key difference and the main subject of this study was the behavior of the system in phase *0I*. It was found that at $L > 20$ this phase demonstrates not one, but two subsequent phase transitions, which were not identified previously. As the temperature increased, the system undergoes a transition from the ordered phase *0I* to the intermediate partially disordered phase, and then — to the paramagnetic state.

This paper studied in detail the two-stage mechanism of phase transition in phase *0I*, which appears only in the correct accounting of the finite-dimensional effects using rather big systems.

This article is dedicated to the comprehensive analysis of this complex phenomenon. We focus on the set of parameters ($J_1 = -1$, $J_2 = -0.5$, $D = 1.0$), corresponding to phase *0I*, with the purpose to establish the physical nature of each of two phase transitions and to characterize the properties of the occurring intermediate partially disordered phase. We used the calculations of the thermodynamic values and visualization of spin configurations to provide a microscopic description of the process of magnetic order destruction by heating.

2. Model and method of study

The Ising's model with the mixed spin S=(1/2, 1) may be specified by the following Hamiltonian [6–11,18]:

$$H = -J_1 \sum_{\langle i,j\rangle} \sigma_i S_j - J_2 \sum_{\langle i,j\rangle \in B} S_i S_j + D \sum_{j\in B} S_j^2 - h \sum_{i\in A} \sigma_i - h \sum_{i\in B} S_i,$$

$$\sigma_i = \pm 1/2, \quad S_i = 0, \pm 1, \tag{1}$$

where the first sum takes into account the exchange interaction between the spins in the sublattice A and sublattice B, the second sum — exchange only between the spins in the sublattice B, the third one — single-ion anisotropy of spins in the sublattice B, the fourth and the fifth one — effect of the external magnetic field.

The lattice with the spins in the nodes, the legend for various spin states and exchange interactions between the spins are provided in Figure 1. The square lattice is broken into two sublattices A and B, each also dividing into two sublattices $A1$, $A2$, $B1$ and $B2$. Figure 1 for some nodes also specifies the corresponding sublattices.

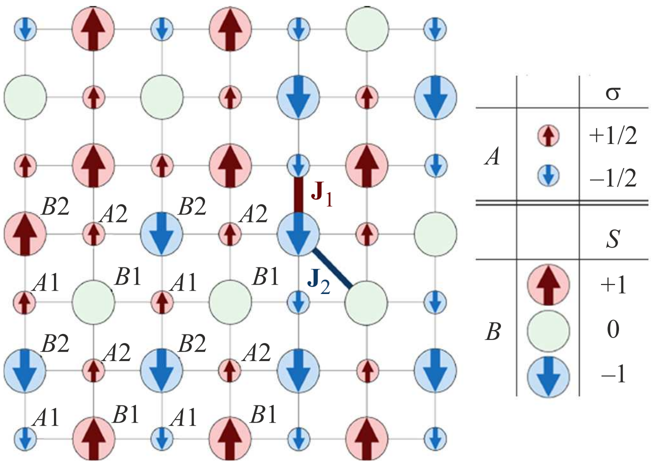

Figure 1. Ising's model with the mixed spin.

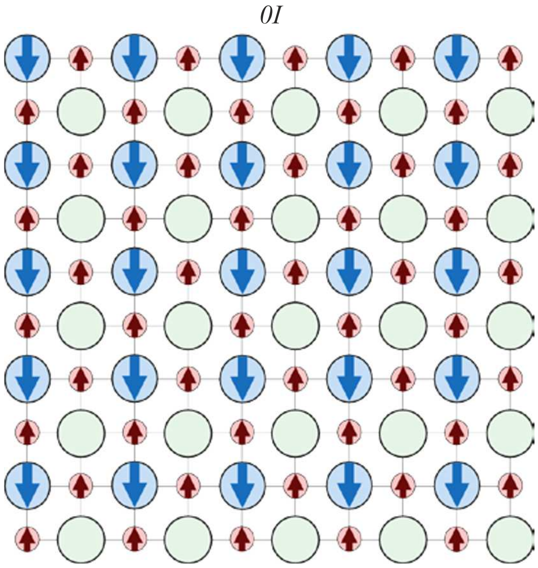

Figure 2. Magnetic structure of the ground state at $J_1 = -1$, $J_2 = -0.5$, $D = 1.0$.

This model possesses a rather rich pattern of phases, where the system finds itsels depending on values J_1, J_2 and D. In this paper we present the simulation results for the case of the fixed value $J_1 = -1$, $J_2 = -0.5$, $D = 1.0$. At these values of the parameters in the ground state the system is in the phase designated as *0I*, where the spins in the sublattice A are directed upwards, the spins in the sublattice $B1$ take zero values, and the spins in the sublattice $B2$ are directed downwards. In the absence of the external magnetic field, the system ground state is fourfold degenerate. One of the four possible structures of the system ground state is given in Figure 2. The energy of the system ground state at the same time is defined as

$$E_{0I} = \frac{1}{2} J_1 + \frac{1}{4} D = -0.25.$$

Temperature dependences of the Ising's model with the mixed spin $S = (1/2, 1)$ were studied using the Monte Carlo replete exchange algorithm. The selection of this method is justified by its proven effectiveness in the study of the systems with competing interactions and complex energy structure. Details of implementation and justification for the applicability of using the Monte Carlo replete exchange may be found in papers [18–20] and references therein. Calculations were performed simultaneously for 300 replicas with periodic boundary conditions and linear dimensions $L \times L = N$, where L — linear dimension of the lattice ($L = 10$, 20, 40 and 100), N — number of spins in the system. To bring the system into the state of thermodynamic equilibrium, a section with length of $\tau_0 = 2 \cdot 10^4$ 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 $\tau = 50\tau_0$.

The main thermodynamic parameters (energy E, heat capacity C, entropy S, magnetization of the system m and magnetic torques of sublattices m_A and m_B, and also the order parameter q) were calculated using the following formulas:

$$\langle E \rangle = \langle H \rangle, \tag{2}$$

$$C = \frac{1}{Nk_\mathrm{B}T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right), \tag{3}$$

$$S = \int_0^T \frac{C}{T}\,dT, \tag{4}$$

$$m = \frac{1}{N}\left\langle \sum_{i \in A} \sigma_i + \sum_{j \in B} S_j \right\rangle, \tag{5}$$

$$m_A = \frac{1}{N}\left\langle \sum_{j \in A} \sigma_i \right\rangle, \tag{6}$$

$$m_B = \frac{1}{N}\left\langle \sum_{j \in B} S_j \right\rangle, \tag{7}$$

$$q = |m_{B1} - m_{B2}| = \frac{1}{N}\left\langle \left| \sum_{j \in B1} S_j - \sum_{j \in B2} S_j \right| \right\rangle, \tag{8}$$

where E — system energy. Temperature is given in units $|J_1|$.

3. Simulation results

Temperature dependence of the system internal energy for various linear dimensions of the lattice is presented in Figure 3. It should be noted that for the convenience of comparison and generalization the results are presented in dimensionless units normalized to exchange interaction J_1. Such normalization makes it possible to compare the results for the system with different J_1 and find common patterns.

Temperature dependence of heat capacity for the systems with various linear dimensions is given in Figure 4. The analysis of this dependence makes it possible to obtain information on how the system accumulates and releases energy when temperature varies, and on the presence of phase transitions.

Visually the chart shows two maxima of heat capacity — the system contains two phase transitions. The first phase transition occurs in the critical point $T_{C1} = 0.285$, which corresponds to the first maximum of heat capacity. Besides, the system changes from the ordered state (phase *0I*) to the partially disordered state (phase PD). In this state the spins in the sublattice A maintain the order and take values $+1/2$, and the spins in the sublattice B take random values -1 or 0, and the share of the spins with value -1 is equal to the share of the spins with value 0. Therefore, the calculation of the sublattice magnetization values provides no information on the phase transition. To detect this phase transition, it is necessary to use the order parameter q, specified by formula (8). When temperature $T_{C2} = 0.35$ is achieved, the second phase transition takes place: the system from the partially disordered phase changes to paramagnetic state (phase PM).

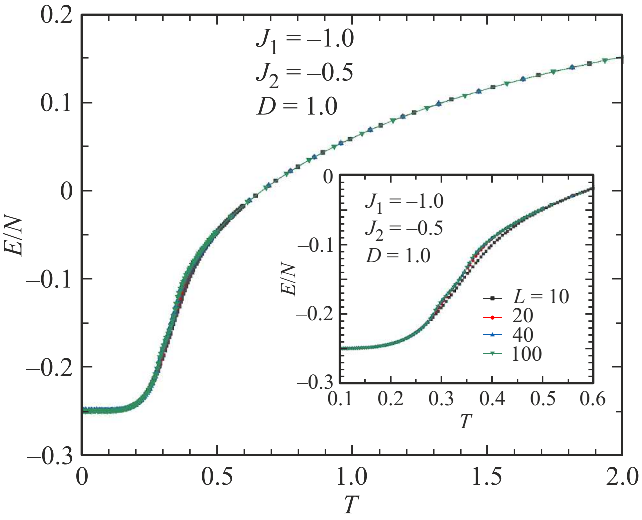

Figure 3. Temperature dependence of system internal energy E.

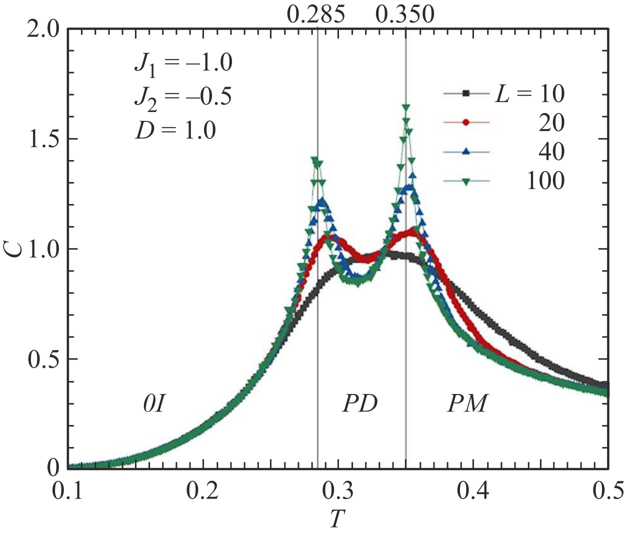

Figure 4. Temperature dependence of system heat capacity C.

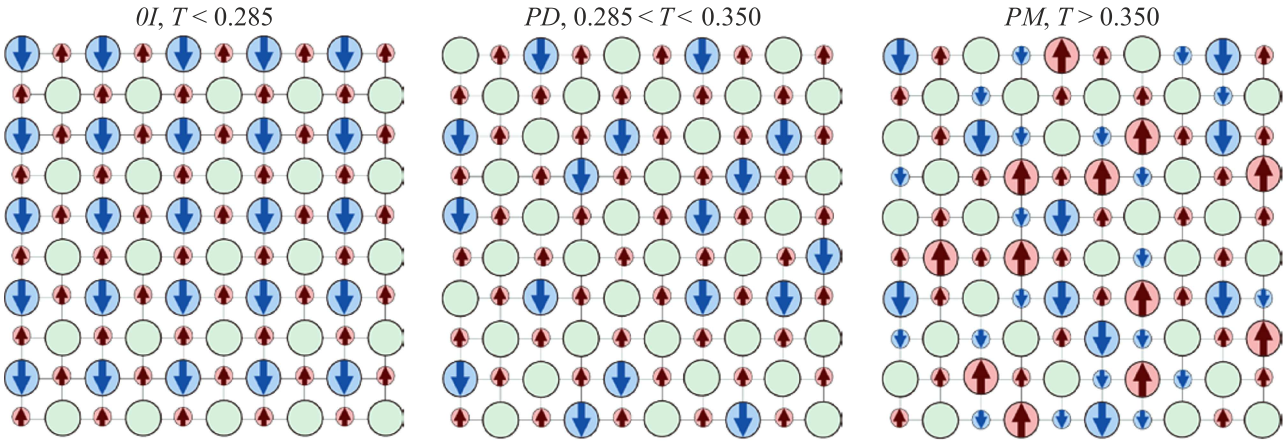

Figure 5. Magnetic structures of the system at different temperatures.

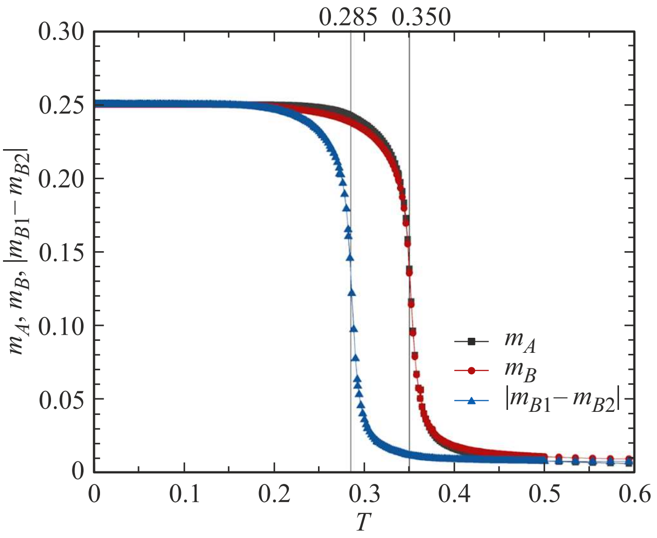

Figure 6. Temperature dependences of magnetic torques of m_A, m_B sublattices and order parameter $q = |m_{B1} - m_{B2}|$.

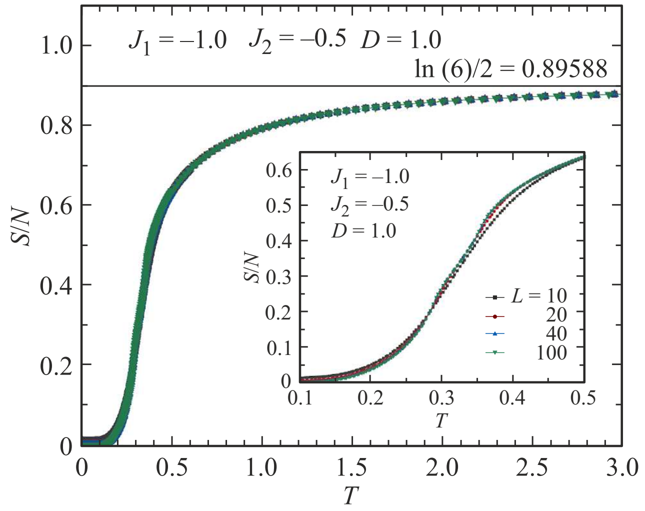

Figure 7. Temperature dependence of S system entropy.

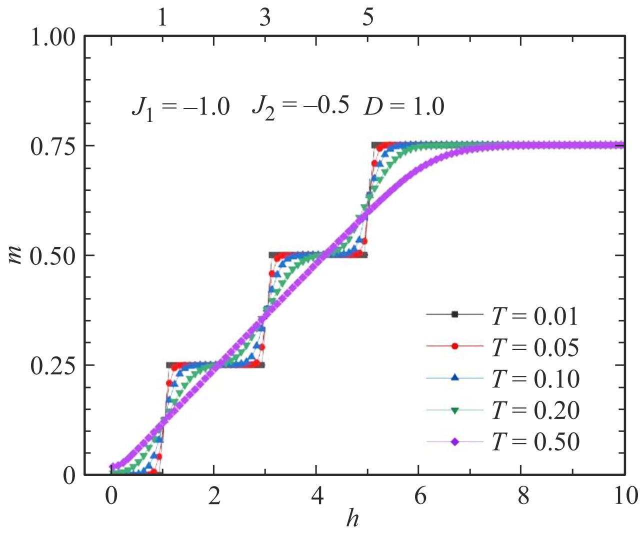

Figure 8. Field dependence of magnetization m.

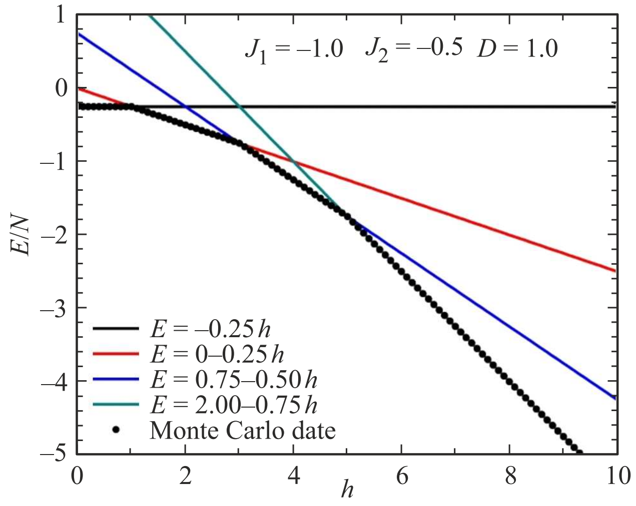

Figure 9. Field dependence of E system energy.

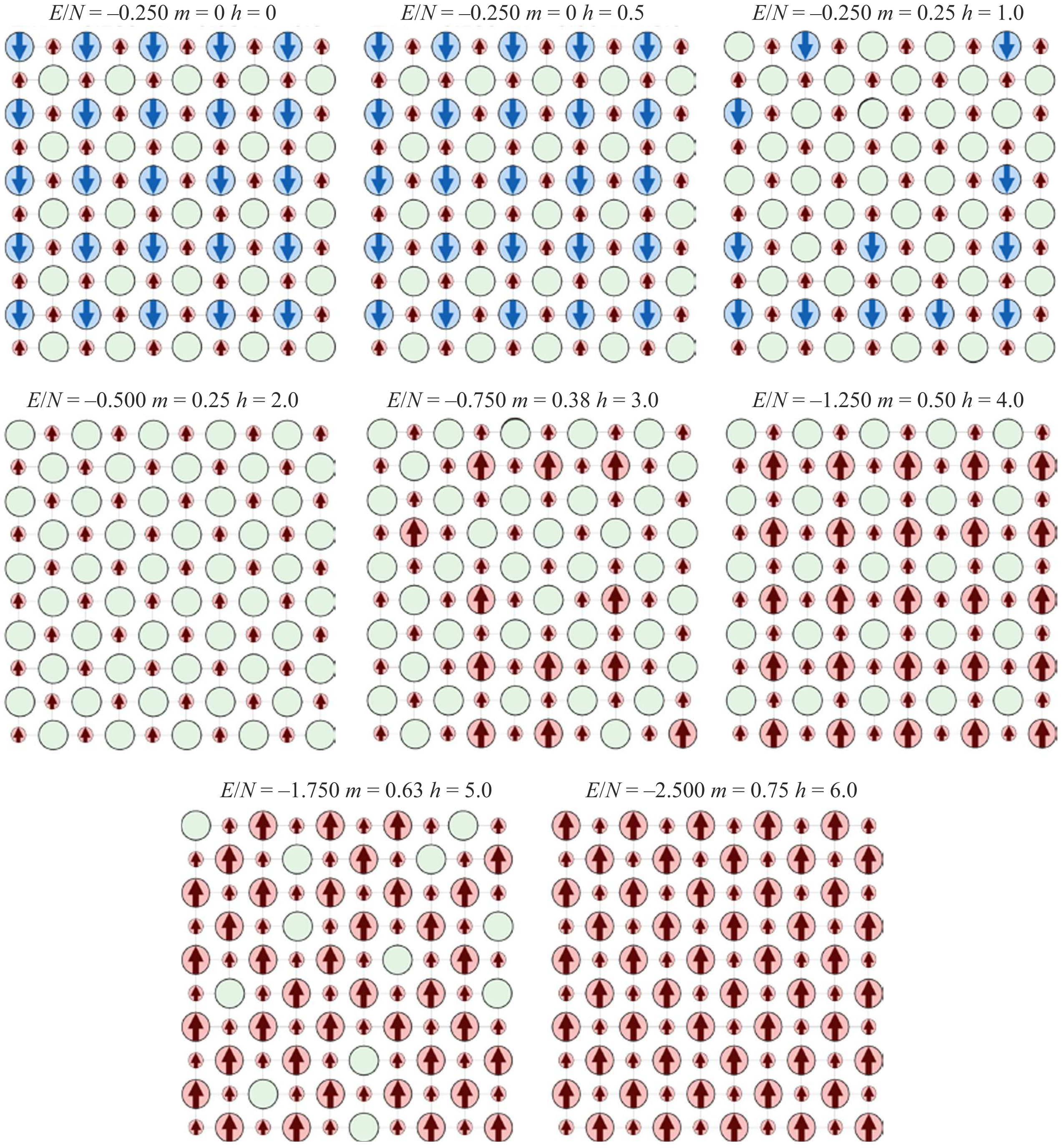

Figure 10. Magnetic structures of the ground state at different values of magnetic field h (at $T = 0.01$).

This process is better visualized in Figure 5, which shows the typical magnetic structures at $T < T_{C1}$, $T_{C1} < T < T_{C2}$ and $T > T_{C2}$.

Figure 6 shows temperature dependences of magnetic torques of sublattices m_A, m_B and order parameter $q = |m_{B1} - m_{B2}|$. For clarity the figure shows the data only for the systems with linear dimensions $L = 100$. As you can see from the figure, values m_A, m_B describe well the phase transition from the partially disordered state to the paramagnetic state at $T_{C2} = 0.35$, whereas the order parameter q is sensitive to the phase transition from the ordered state to the partially disordered state at $T_{C1} = 0.285$.

Figure 7 shows temperature dependence of entropy S for the systems with different linear dimensions. As temperature decreases, entropy tends to value $\ln(4)/N$, which is related to the four-fold degeneracy of the ground state. As the temperature increases, entropy gradually increases, tending towards the theoretical limit $\ln(6)/2 \approx 0.89588$.

This value corresponds to the maximum possible disorder for the system, taking into account available spin configurations. As you can see from the figure, size effects mostly appear near the phase transitions.

The study of the system behavior in the external magnetic field is also of considerable fundamental interest. Field dependences of magnetization at different temperatures are shown in Figure 8. As you can see from the figure, as the magnetic field grows, several magnetization jumps occur. When the value of the magnetic field $h = 1$ is achieved, the system from phase *0I* changes to ferrimagnetic state with magnetization $m = 0.25$. The next jump of magnetization to the value of $m = 0.5$ happens at $h = 3$. Finally, when the magnetic field reaches the value $h = 5$, the system changes to the fully ordered state (field-induced ferromagnetic state). The stepwise nature of magnetization is the effect of competition between the Zeeman energy (trying to build spins along the field) and exchange interaction and anisotropy energies (trying to maintain the antiferromagnetic order). The system changes to a new state, when the energy win from interaction with the field starts exceeding the energy necessary for a „flip“ of another spin group.

Figure 9 also shows the field dependence of the full energy of the system made of the energy of exchange interaction and contribution of the spin-field interaction. Fractures in field dependences of full energy correspond to the magnetization jumps.

Figure 10 shows magnetic configurations of the ground state obtained at different values of the external magnetic field and temperature $T = 0.01$, corresponding to various magnetization plateaus in Figure 8.

4. Conclusion

This paper conducted a complex computer simulation of Ising's model with a mixed spin $S = (1/2, 1)$ in a square lattice using highly effective replete exchange algorithm of Monte Carlo method. The study was made for the model that accounts for the exchange interaction between the spins in the sublattice A and B $(J_1 = -1)$, exchange interaction between the spins in the sublattice B $(J_2 = -0.5)$, and also anisotropy for the spins in the sublattice B $(D = 1.0)$.

The computer simulation method was used to determine magnetic structures of the system ground state. Temperature dependences of key thermodynamic characteristics of the system were calculated: energy E, heat capacity C, entropy S, magnetization m. It is shown that two phase transitions happen in the system. At temperature $T_{C1} = 0.285$ the phase transition occurs from the ordered state to the partially disordered state, and when temperature $T_{C2} = 0.35$ is achieved, the transition to the paramagnetic state occurs.

The effect of the external magnetic field on the system magnetic structure is studied. It is shown that there is a stepwise growth of magnetization with the magnetic field rise. Magnetic structures corresponding to each magnetization plateau are determined.

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Conflict of interest

The authors declare that they have no conflict of interest.

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