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Phase Transitions in an Antiferromagnetic Ising Model with Competitive Exchange Interactions in a Magnetic Field

K. Sh. Murtazaev[a, *], A. K. Murtazaev[b], M. K. Ramazanov[a, b], and M. A. Magomedov[a, b]

[a] *Amirkhanov Institute of Physics, Dagestan Federal Research Center, Russian Academy of Sciences, Makhachkala, 367003 Russia*

[b] *Dagestan Federal Research Center, Russian Academy of Sciences, Makhachkala, 367000 Russia*

**e-mail: 5kurban@mail.ru*

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Abstract—A highly efficient replica Monte Carlo algorithm is used to study the antiferromagnetic Ising model for a body-centered cubic lattice with competing exchange interactions in an external magnetic field. Phase transitions are analyzed. A strong magnetic field is shown to suppress phase transitions.

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INTRODUCTION

Studies of phase transitions (PTs) and the magnetic and thermodynamic properties of model spin systems with competing exchange interactions are currently of great interest in the physics of condensed matter. Competition between exchange interactions in magnetic spin systems can result in frustrations. Properties and parameters of the frustrated spin systems differ considerably from those of many phases and phase transitions. This variety of PTs is due to the strong degeneracy of these systems and their high sensitivity to various external factors. An external magnetic field can result in new physical phenomena in the behavior of frustrated and spin systems with competing exchange interactions [1–6].

In this work, we studied a 3D antiferromagnetic Ising–body centered cubic (BCC) lattice with competing exchange spin interactions. The effect an external magnetic field has on the magnetic and thermodynamic properties of the considered model and the nature of the PT is examined.

Ising models with competition between exchange spin interactions have been used to investigate different types of lattices. Results from calculations and theoretical studies of the considered model were reported in [6–9]. The authors of [6] obtained sublattice structures in the ground state for a 3D antiferromagnetic Ising model on a BCC lattice using the Wang–Landau algorithm for Monte Carlo (MC) studies. They discovered phase diagram regions where first- and second-order phase transitions occur. Theoretical studies presented in [7] showed that a second-order PT occurs in the Ising BCC lattice. This result agrees with the data obtained in [6]. The effect a magnetic field has on the order of the phase transition and thermodynamic properties was examined in [8] for the considered Ising model with a magnetic field of $0.0 \le H \le 6.0$. It was found that a second-order PT is observed in the considered H range. The study in [9] of the antiferromagnetic Ising model on a layered triangular lattice showed that a second-order PT is observed for a magnetic field of $0.0 \le H \le 6.0$. It was discovered that strong magnetic fields eliminate degeneracy of the ground state and result in blurring of the PT.

Analysis of the literature data shows that many physical properties of spin systems with competition between exchange spin interactions depend on the presence or absence of an external magnetic field [10–12]. We therefore performed numerical calculations to investigate PTs and the thermodynamic properties of a 3D antiferromagnetic Ising model on a BCC lattice in strong magnetic fields. These studies are also of interest because most similar works are devoted to models on hexagonal triangle and square lattices [13–23]. Examining this spin system using efficient state-of-the-art algorithms provides answers to a number of questions related to the effect a magnetic field has on the thermodynamic properties of and phase transitions in spin lattice systems with competing exchange interactions. Studies of the effect magnetic fields have on PTs are also of importance, since the effect external factors have on the behavior of devices and electronic items cannot be ignored in modern microelectronics and spintronics. Modern microelectronics have been miniaturized to the extent that factors considered unimportant earlier cannot be disregarded today.

MODEL AND INVESTIGATIVE TECHNIQUE

The Hamiltonian that describes the given spin system has the form

$$H = -J_1\sum_{\langle i,j\rangle} S_iS_j - J_2\sum_{\langle\langle i,l\rangle\rangle} S_iS_l - H\sum_i S_i, \quad (1)$$

where J_1 and J_2 are constant values (constants) of spin exchange interaction between first ($J_1 = -1$) and second ($J_2 = -1$) nearest neighbors (spins), $S_i = \pm 1$ is the Ising spin, and H is the strength of the magnetic field (measured in units of $|J_1|$). The magnetic field was varied in the range of $7.0 \le H \le 14.0$.

Spin systems with competition between spin exchange interactions described by microscopic Hamiltonians have been investigated using the Monte Carlo (MC) technique [9, 11, 24–33]. Calculations are now performed using many versions of Monte Carlo algorithms. A technique that is one of the most efficient and accurate ways of exploring and calculating such spin systems is the MC replica exchange algorithm [34], and we therefore use it in our studies.

In the MC replica exchange algorithm we employ, several instances (copies) Q of system $X_1, X_2, \ldots, X_Q$ with temperatures $T_1, T_2, \ldots, T_Q$ modeled concurrently. To eliminate the critical slowing down of the system after the execution of one MC step/spin, configurations (data) are exchanged for all copies between a pair of neighboring replicas X_i and X_{i+1} with probability

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

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

Calculations were performed using periodic boundary conditions. Linear dimensions of the system were $2 \times L \times L \times L = N$, $L = 12$–60, where N is the number of spins in the system and L is the lattice size. To study the type of the PT and determine the critical temperature, we used histograms for data analysis and the fourth-order Binder cumulant approach [35, 36]. To reach thermodynamic equilibrium in the system, we allocated a segment containing $\tau_0 = 4 \times 10^5$ MC steps per spin, the size of which was several times larger than that of the nonequilibrium segment. Thermodynamic parameters were averaged along a Markov chain up to $\tau = 500\,\tau_0$ MC steps per spin long.

COMPUTER MODELING RESULTS

Temperature dependence of thermal capacity C was calculated using the formula

$$C = (NK^2)(\langle H^2\rangle - \langle H\rangle^2), \quad (2)$$

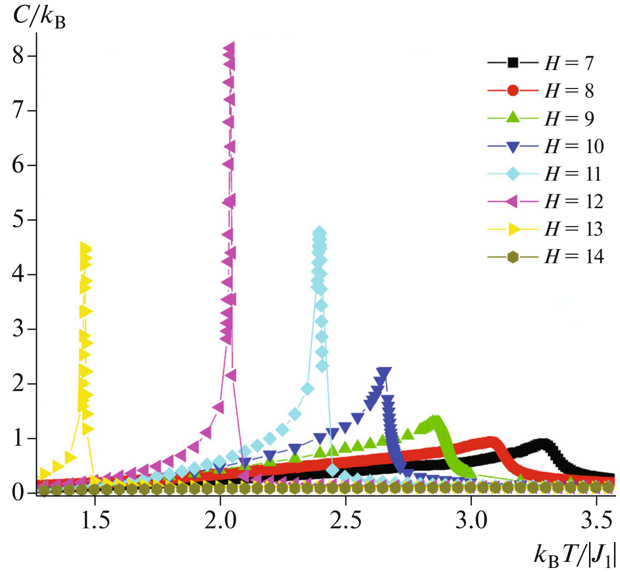

Fig. 1. Thermal capacity C/k_B as a function of temperature $k_BT/|J_1|$.

where

$$K = |J_1|/k_BT$$

and T is the inverse temperature, N is the number of particles, and H is the onian operator.

The order parameter of this system was calculated as [37]:

$$m = 3m_1 - m_2 - m_3 - m_4, \quad (3)$$

where m_1, m_2, m_3, m_4 are the sublattice order parameters.

This system contains four sublattices. A more detailed description of the sublattice structures was presented in [6].

Magnetization was calculated using the formula

$$M = \frac{1}{N}\sum_i S_i. \quad (4)$$

Fourth-order Binder cumulant U_L was used to determine the type of PT:

$$U_L = 1 - \frac{\langle m^4\rangle_L}{\langle 3m^2\rangle_L^2}. \quad (5)$$

Equation (5) allows us to determine with high accuracy critical temperature T_N if a second-order phase transition occurs in the system [10].

Figure 1 shows temperature dependences of the thermal capacity at $L = 24$ for different strengths of the magnetic field. We can see in the figure that if magnetic field H grows in the range of $7.0 \le H \le 10.0$, thermal capacity maxima shift to lower temperatures. An increase in the thermal capacity maxima can also be noted in the plot. If the strength of the magnetic field

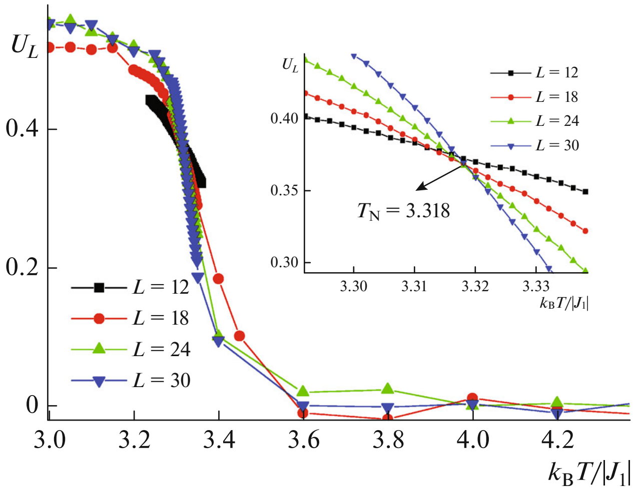

Fig. 2. Binder cumulant U_L as a function of temperature $k_BT/|J_1|$ for different L at $H = 7.0$.

is in the range of $11.0 \leq H \leq 13.0$, sharper peaks are observed in the critical region. We may hypothesize that a first-order PT occurs in this range. We assume the magnetic field enhances competing spin interaction between the first and second nearest neighbors, due to which the maxima of thermal capacity shift to lower temperatures. Figure 1 shows that no peak of thermal capacity is observed for magnetic field $H = 14$. This indicates that a subsequent increase in the magnetic field suppresses the PT.

Figure 2 shows the dependences the fourth-order Binder cumulant U_L under magnetic field $H = 7.0$ for different dimensions L of the system. A point of intersection is clearly seen in the plot ($T_N = 3.318$), indicating that a second-order phase transition occurs in the system. The point itself corresponds to the critical temperature. Similar dependences of Binder cumulants were also plotted for the $7.0 \leq H \leq 13.0$ range of magnetic fields. Analysis of the results shows that a second-order PT is observed in the $7.0 \leq H \leq 10.0$ range. No point of intersection is observed on Binder cumulant dependences in the $11.0 \leq H \leq 14.0$ range.

The nature of the PT was analyzed via histogram data analysis. The energy distribution histogram for a spin system with linear size $L = 60$ is plotted for the field $H = 12.0$ in Fig. 3. The plot shows a double maximum (two peaks) on the histogram for field strength $H = 12.0$, which is an indication of a first-order PT. Observing a double peak (bimodality) on energy distribution histograms is a sufficient condition for a first-order PT to occur. Similar behavior is observed in the $11.0 \leq H \leq 13.0$ range of field strengths.

Temperature dependences of magnetic order parameter m for different values of H are presented in Fig. 4. The figure shows that as H increases, the region where the magnetic order parameter diminishes shifts to lower temperatures. This is explained by the magnetic field enhancing the competing spin interaction between the first and second nearest neighbors. The order parameter falls more rapidly if the magnetic field is in the $11.0 \leq H \leq 13.0$ range. Such behavior of the temperature dependence of the magnetic order parameter is characteristic of first-order PTs.

Our results show that in the $7.0 \leq H \leq 10.0$ range of field strengths, the transition from the antiferromagnetic phase to the paramagnetic phase occurs as a second order PT, while a first-order PT is observed in the $11.0 \leq H \leq 13.0$ range. A further increase in the magnetic field suppresses phase transitions.

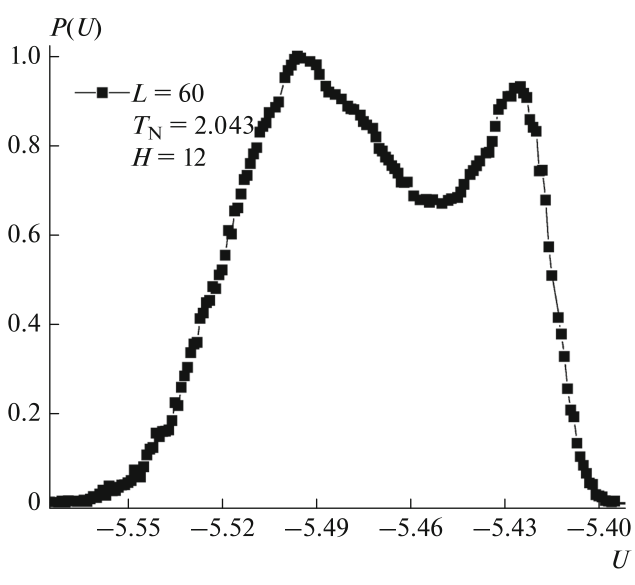

Fig. 3. Energy distribution histogram for $H = 12.0$.

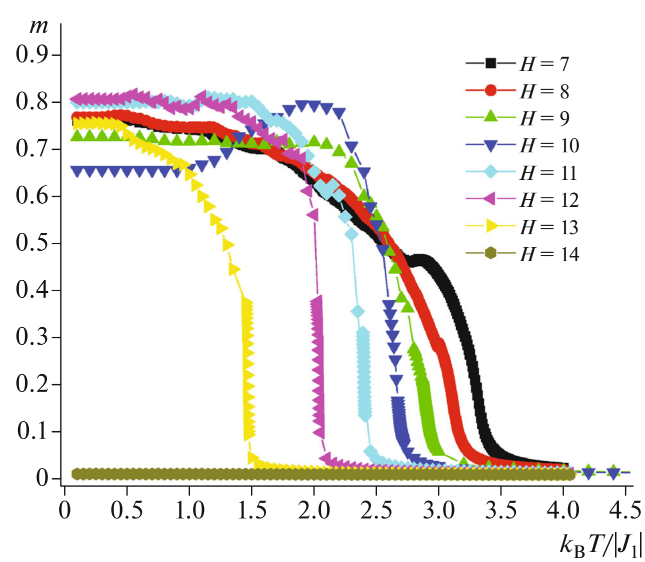

Fig. 4. Order parameter m as a function of temperature $k_BT/|J_1|$.

CONCLUSIONS

An antiferromagnetic Ising model for a body-centered cubic lattice with competing exchange interactions in strong magnetic fields was studied using a replica MC algorithm. The $7.0 \le H \le 14.0$ range of magnetic field strength was considered. It was shown that a second order phase transition occurs in the $7.0 \le H \le 10.0$ range of magnetic field strengths, while the phase transition is of the first order in the $11.0 \le H \le 13.0$ range.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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