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Ising model on a body-centered cubic lattice with competing exchange interactions in strong magnetic fields

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The effect of an external magnetic field on phase transitions, magnetic and thermodynamic properties of the antiferromagnetic Ising model on a body-centered cubic lattice with competing exchange interactions was studied using the replica algorithm of the Monte Carlo method. It is shown that a second-order phase transition is observed in the range of magnetic field values $7.0 \le H \le 10.0$, and a first-order phase transition is observed in the range $11.0 \le H \le 13.0$. A further increase in the magnetic field strength leads to the suppression of the phase transition.

Keywords: phase transition, Ising model, magnetic field, Monte Carlo method.

1. Introduction

In condensed matter physics, studies of phase transitions (PT), magnetic, critical, and thermodynamic properties of spin systems with competing exchange interactions are of great interest. The competing exchanges can lead to the appearance of frustrations. The physical properties of frustrated spin systems are very different from ordinary ones. Frustrated spin systems have a rich variety of phases and PT's due to a high degree of degeneracy and high sensitivity of such systems to external factors, including a magnetic field. The effect of a magnetic field can play an important role in the behavior of spin systems with competing exchange interactions [1–6].

In this paper, we study the effect of a magnetic field on the character of PT, the magnetic and thermodynamic properties of the antiferromagnetic Ising model on a body-centered cubic (bcc) lattice with competing exchange interactions.

The Ising model, including competing exchange interactions, for various types of lattices was theoretically and numerically studied in [7–13]. The magnetic structures of the ground state and the phase diagram of the dependence of the critical temperature on the magnitude of the interaction between the next-nearest neighbors were obtained in [6] by the Monte Carlo (MC) method for the Ising model on a bcc lattice. The regions of the first- and second-order phase transitions in the phase diagram were also determined in this work. Theoretical studies [7] and their results are in good agreement with the data of numerical simulation [6] and show that for the Ising model on a bcc lattice there is a PT of the second-order. In [8], this model was analyzed from the point of view of the influence of a magnetic field in the range of strengths $0.0 \le H \le 6.0$ on the thermodynamic and magnetic properties of the system. It was revealed that the PT is of the second order in the indicated range of the magnetic field strength. Studies of the three-dimensional antiferromagnetic Ising model on a triangular layered lattice under the action of an external magnetic field ($0.0 \le H \le 6.0$) also revealed a second-order phase transition [9]. It was shown that the further increase in the magnetic field value lifts the degeneracy of the ground state and smears PT in the system.

Analysis of the literature data shows that an external magnetic field affects most of the physical properties of spin systems with competing exchange interactions [8, 9]. In this connection in the present paper, we have studied an influence of a strong magnetic field on the order of PT, the magnetic and thermodynamic properties of the antiferromagnetic Ising model on a bcc lattice. The interest in the considered model is attracted by the fact that comprehensive studies of the external magnetic field effect on the PT, the magnetic and thermodynamic properties of this model have not yet been carried out on the basis of modern methods. The main attention for such systems was paid to models based on a square, triangular and hexagonal lattices [14–23]. The study of the considered model using modern methods and ideas will provide an answer to a number of questions related to the type of PT, magnetic and thermodynamic properties of spin systems with competing exchange interactions, as well as the influence on them of an external magnetic field.

2. Model and method of investigation

The Hamiltonian of the antiferromagnetic Ising model on a bcc lattice with allowance for the interactions of nearest and next-nearest neighbors has the following form:

$$\mathrm{H} = -J_1 \sum_{\langle i,j\rangle} S_i \cdot S_j - J_2 \sum_{\langle i,l\rangle} S_i \cdot S_l - H \sum_{\langle i\rangle} S_i, \qquad (1)$$

where J_1 and J_2 are the exchange constants of the antiferromagnetic type interaction of nearest ($J_1 = -1$) and next-nearest ($J_2 = -1$) neighbor spins, $S_i = \pm 1$ are Ising spins, H is an external magnetic field with strength in units $|J_1|$. The normalized magnitude of the magnetic field was varied in the range $0.7 \le H \le 14$. The paper presents the case $r = |J_2|/|J_1| = 1.0$.

Presently, spin systems with competing exchange interactions, which are specified by microscopic Hamiltonians, are being successfully investigated on the basis of the MC method [9, 11, 24–28]. Recently, many new variants of MC algorithms have been developed. One of the most effective before them is the replica exchange MC algorithm [29]. That is why we use this algorithm in this study.

We used a replica exchange algorithm in the following form:

(1) Simultaneously N replicas X_1, X_2,… X_N with temperatures T_1, T_2,… T_N are modeled.

(2) After performing one MC-step/spin for all replicas, data exchange between neighboring replicas X_i and X_{i+1} is carried out according to the Metropolis scheme with a 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 $\Delta = (U_i - U_{i+1})(1/T_i - 1/T_{i+1})$, U_i and U_{i+1} are internal replica energies.

The main advantage of the method is a priory known probability of exchange, while for other algorithms the determination of the probability is often a rather time-consuming procedure.

The calculation was carried out for systems with periodic boundary conditions and linear dimensions of the bcc lattice $L = 12$–60 and the total number of spins $N = 2\times L\times L\times L$. For the analysis of the nature and character of the PT, the histogram method and the Binder cumulant method were used. To bring the system into a thermodynamically equilibrium state, the initial segment of length $\tau_0 = 4\cdot 10^5$ of MC-steps/spin was discarded, which is several times longer then the non-equilibrium one. The average thermodynamic parameters were calculated along the Markov chain up to $\tau = 500\tau_0$ MC-steps/spin.

3. Results of simulation

The following expressions were used to plot the temperature dependences of the susceptibility χ and the heat capacity C:

$$\chi = \begin{cases} (NK)\left(\langle m^2\rangle - \langle m\rangle^2\right), & T < T_N, \\ (NK)\langle m^2\rangle, & T \ge T_N, \end{cases} \qquad (2)$$

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

where $K = |J_1|/k_B T$, U is the normalized internal energy, m is the normalized order parameter, and T_N is the critical temperature.

The order parameter of the system was calculated using the formula:

$$m = 3m_1 - m_2 - m_3 - m_4, \qquad (4)$$

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

The following expression was used to calculate the magnetization of the system:

$$M = \frac{1}{N} \sum_{\langle i\rangle} S_i. \qquad (5)$$

Determination of an order of the PT and a value of the critical temperature T_N was carried out using the method of fourth-order Binder cumulants U_L.

$$U_L = 1 - \frac{\langle m^4\rangle_L}{3\langle m^2\rangle_L^2}. \qquad (6)$$

With Ex. (6) the critical temperature T_N can be determined for a second-order PT with high accuracy [10].

The temperature dependences of the heat capacity and magnetic susceptibility for the case $L = 24$ at some values of the magnetic field strength are shown in Figs. 1 and 2. It can be seen from these plots that with an increase of the magnetic field strength in the range $7.0 \le H \le 10.0$, the maxima of heat capacity and susceptibility shift towards lower temperatures. Simultaneously an increase in the absolute values of the peaks is observed. In the range of magnetic field strengths $11.0 \le H \le 13.0$, the peaks of heat capacity and susceptibility become sharper, as shown in Figs. 1 and 2. This allows assuming that the first-order phase transition

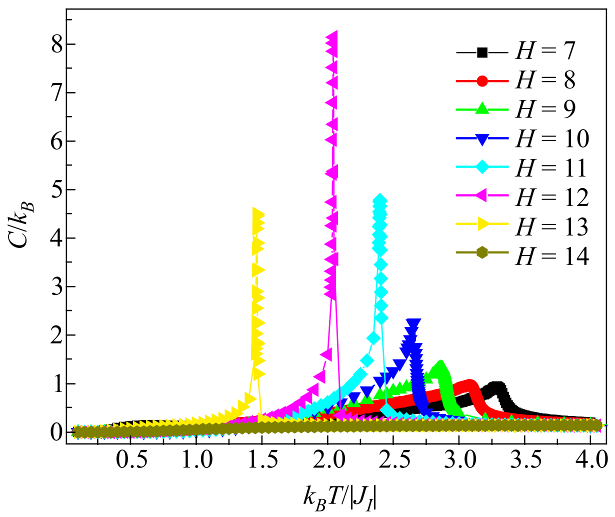

Fig. 1. Dependence of heat capacity C/k_B on temperature $k_BT/|J_1|$.

is realized in this range. The shift of the maxima of the heat capacity and susceptibility towards lower temperatures can be explained by the weakening of the exchange interaction between the spins caused by the action of the magnetic field. As seen in Fig. 1 at the value of the magnetic field $H = 14$ there is no peak on the temperature dependence of the heat capacity. This fact indicates the suppression of the PT in stronger magnetic fields.

Figure 3 shows typical dependences of the magnetic order parameter m on the temperature at different values of the magnetic field H. It can be seen that with an increase in the magnetic field, the abrupt step of the magnetic order parameter dependence shifts towards low temperatures. This can be explained by the weakening of the exchange interactions of the spins caused by the application of a magnetic field. In the range of magnetic field values $11.0 \leq H \leq 13.0$, the observed decrease of the order parameter becomes sharper. Such behavior is typical for a first-order phase transition.

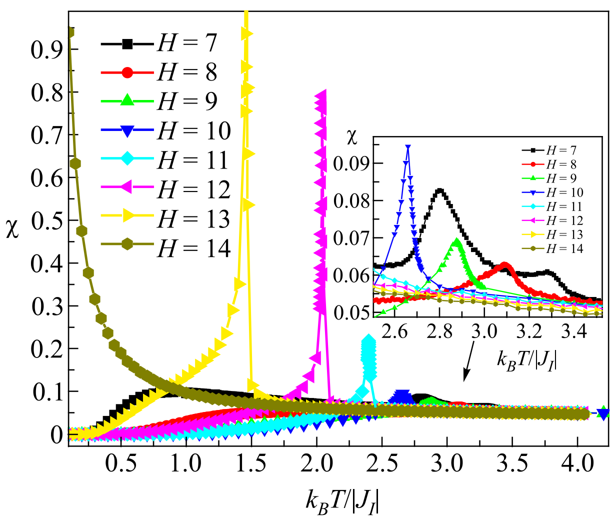

Fig. 2. Dependence of magnetic susceptibility χ on temperature $k_BT/|J_1|$.

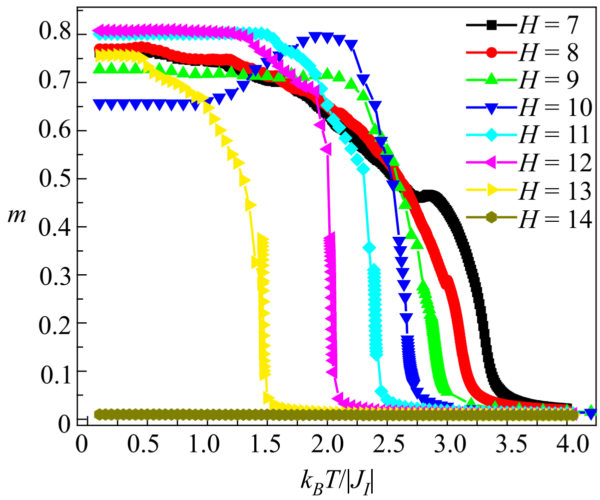

Fig. 3. Dependence of magnetic order parameter m on temperature $k_BT/|J_1|$.

Dependencies of magnetization M on the temperature at the given values of the magnetic field H are shown in Fig. 4. One can see that the system magnetization increases with the magnetic field H. From the dependences shown in the figure, it can be concluded that in the range of magnetic field values $7.0 \leq H \leq 10.0$, the magnetization first decreases monotonically to a certain temperature preceding the phase transition, and then, up to the phase transition temperature, slightly increases. After that, a slow decrease begins due to thermal fluctuations. On the contrary, in the range of magnetic field values $11.0 \leq H \leq 13.0$, the magnetization increases with a positive derivative up to the PT temperature. Further dependence is similar to that described above. At the value of the magnetic field $H = 14$, the magnetization decreases monotonously with the increasing temperature in the entire range.

The temperature dependences of the Binder cumulant U_L at $H = 8$ for different values of L are shown in Fig. 5. Here a clearly defined intersection point ($T_N = 3.120$)

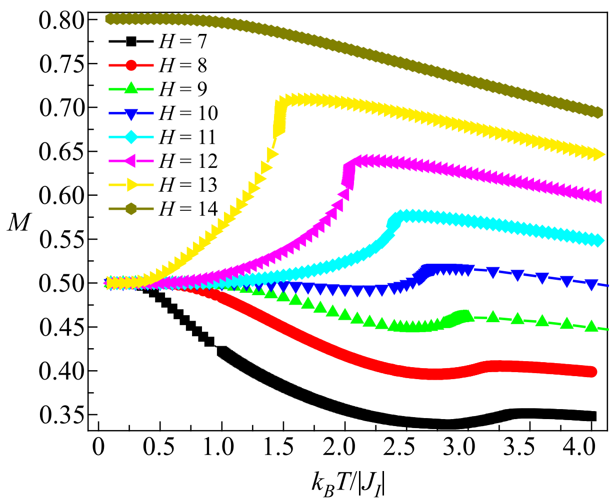

Fig. 4. Dependence of magnetization on temperature $k_BT/|J_1|$.

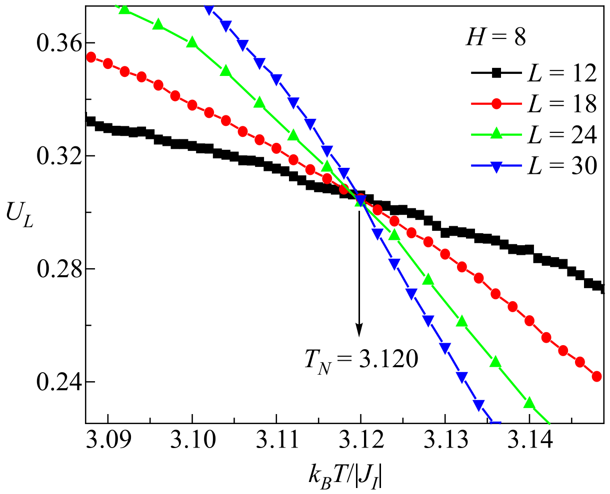

Fig. 5. Dependence of Binder cumulant U_L on temperature $k_BT/|J_1|$ at different L and at $H = 8$.

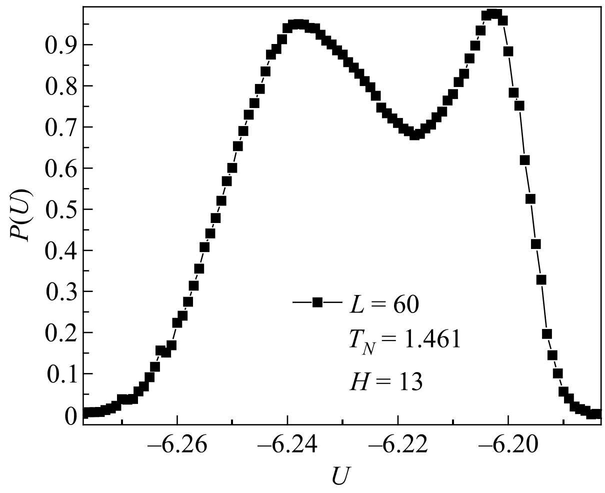

Fig. 7. Histogram of energy distribution at $H = 13.0$.

is seen, which indicates a second-order PT and is a critical temperature. Similar dependences of the Binder cumulants were calculated for all values of the magnetic field in the range $7.0 \le H \le 14.0$. Analysis of the results has shown that a second-order phase transition is observed in the range $7.0 \le H \le 10.0$. There are no clearly defined intersection points on the temperature dependences of the Binder cumulants U_L for the stronger fields $11.0 \le H \le 14.0$.

For a more detailed analysis of the nature of the PT, we used the histogram method of data analysis. In Figs. 6 and 7, histograms of energy distribution for a system with linear size $L = 60$ are shown at field values $H = 8.0$ and 13.0, respectively. The graphs are plotted for temperatures close to critical. As can be seen, one well-pronounced maximum is observed on the dependence of the probability P on the energy U at the value of the applied magnetic field $H = 8.0$. The presence of one maximum on the histogram testifies in favor of the second-order PT. A similar picture is observed for field values in the range $7.0 \le H \le 10.0$.

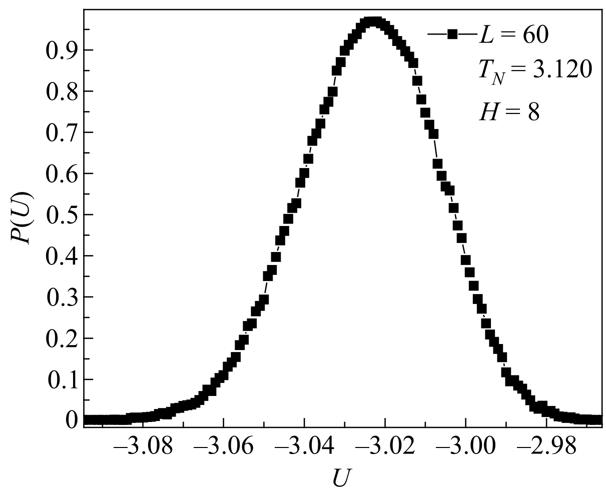

Fig. 6. Histogram of energy distribution at $H = 8.0$.

For a magnetic field $H = 13.0$, the histogram exhibits two maxima (bimodality), which is evidence in favor of the first-order PT. The presence of a double peak on the histogram is a sufficient condition for the FP to be of the first order. Bimodality was observed for the range of magnetic field values $11.0 \le H \le 13.0$. Thus, our results show that in the range of magnetic field values of $7.0 \le H \le 10.0$, the antiferromagnetic ordering occurs as a second-order PT, and in the range $11.0 \le H \le 13.0$, as the first-order one.

4. Conclusion

The study of the antiferromagnetic Ising model on a body-centered cubic lattice with competing exchange interactions in an external magnetic field was carried out using the replica algorithm of the Monte Carlo method. The range of values of the magnetic field strength $7.0 \le H \le 14.0$ is considered. It is shown that a second-order phase transition occurs in the range of magnetic field values $7.0 \le H \le 10.0$, and a first-order one occurs in the range $11.0 \le H \le 13.0$. It was found that a further increase in the magnetic field strength leads to the suppression of the phase transition.

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1. R. S. Gekht, *Sov. Phys. Usp.* **32**, 871 (1989).
2. A. Z. Patashinsky and V. L. Pokrovsky, *Fluctuation Theory of Phase Transitions*, Nauka, Moskow (1982) [in Russian].
3. K. Katsumata, H. Aruga Katori, S. Kimura, Y. Narumi, M. Hagiwara, and K. Kindo, *Phys. Rev. B* **82**, 104402 (2010).
4. Shang-keng Ma, *Modern Theory of Critical Phenomena*, Westview Press (1976).
5. A. K. Murtazaev, M. K. Ramazanov, D. R. Kurbanova, and M. K. Badiev, *Phys. Solid State* **60**, 1173 (2018).

6. A. K. Murtazaev, M. K. Ramazanov, D. R. Kurbanova, M. A. Magomedov, and K. Sh. Murtazaev, *Mater. Lett.* **236**, 669 (2019).
7. A. K. Murtazaev, M. K. Ramazanov, F. A. Kassan-Ogly, and D. R. Kurbanova, *J. Exp. Theor. Phys.* **120**, 110 (2015).
8. A. K. Murtazaev, M. K. Ramazanov, K. Sh. Murtazaev, M. A. Magomedov, and M. K. Badiev, *Phys. Solid State* **62**, 273 (2020).
9. A. K. Murtazaev, M. K. Badiev, M. K. Ramazanov, and M. A. Magomedov, *Physica A* **555**, 124530 (2020).
10. A. K. Murtazaev, M. K. Ramazanov, and M. K. Badiev, *Physica B* **476**, 1 (2015).
11. M. K. Ramazanov, A. K. Murtazaev, and M. A. Magomedov, *Physica A* **521**, 543 (2019).
12. A. K. Murtazaev, M. K. Ramazanov, D. R. Kurbanova, M. K. Badiev, and Ya. K. Abuev, *Phys. Solid State* **59**, 1103 (2017).
13. F. A. Kassan-Ogly and A. I. Proshkin, *Phys. Solid State* **60**, 1090 (2018).
14. A. I. Proshkin and F. A. Kassan-Ogly, *Mater. Sci. Forum* **845**, 93 (2016).
15. H. Kawamura, *J. Phys. Soc. Jpn.* **61**, 1299 (1992).
16. A. Mailhot, M. L. Plumer, and A. Caille, *Phys. Rev. B* **50**, 6854 (1994).
17. L. E. Svistov, A. I. Smirnov, L. A. Prozorova, O. A. Petrenko, A. Ya. Shapiro, and L. N. Dem'yanets, *JETP Lett.* **80**, 204 (2004).
18. A. K. Murtazaev, M. A. Magomedov, and M. K. Ramazanov, *JETP Lett.* **107**, 259 (2018).
19. M. K. Ramazanov and A. K. Murtazaev, *JETP Lett.* **103**, 460 (2016).
20. M. K. Ramazanov and A. K. Murtazaev, *JETP Lett.* **106**, 86 (2017).
21. A. K. Murtazaev, M. K. Ramazanov, and M. K. Badiev, *Physica A* **507**, 210 (2018).
22. F. A. Kassan-Ogly, A. K. Murtazaev, A. K. Zhuravlev, M. K. Ramazanov, and A. I. Proshkin, *J. Magn. Magn. Mater.* **384**, 247 (2015).
23. M. K. Ramazanov, A. K. Murtazaev, and M. A. Magomedov, *Solid State Commun.* **233**, 35 (2016).
24. M. K. Badiev, A. K. Murtazaev, M. K. Ramazanov, and M. A. Magomedov, *Fiz. Nizk. Temp.* **46**, 824 (2020) [*Low Temp. Phys.* **46**, 693 (2020)].
25. A. K. Murtazaev, T. R. Rizvanova, M. K. Ramazanov, and M. A. Magomedov, *Phys. Solid State* **62**, 1434 (2020).
26. A. K. Murtazaev, M. K. Ramazanov, and M. K. Badiev, *Fiz. Nizk. Temp.* **45**, 1493 (2019) [*Low Temp. Phys.* **45**, 1263 (2019)].
27. A. K. Murtazaev, D. R. Kurbanova, and M. K. Ramazanov, *Physica A* **545**, 123548 (2020).
28. R. Masrour, A. Jabar, A. Benyoussef, and M. Hamedoun, *J. Magn. Magn. Mater.* **401**, 695 (2016).
29. F. Wang and D. P. Landau, *Phys. Rev. E* **64**, 056101 (2001).

Модель Ізінга на об'ємно центрованій кубічній ґратці з конкурентними обмінними взаємодіями в сильних магнітних полях

K. S. Murtazaev, A. K. Murtazaev, M. K. Ramazanov, M. A. Magomedov, A. A. Murtazaeva

Вплив зовнішнього магнітного поля на фазові переходи, магнітні та термодинамічні властивості антиферомагнітної моделі Ізінга на об'ємно центровану кубічну гратку з конкурентними обмінними взаємодіями вивчали за допомогою алгоритму реплік методу Монте-Карло. Показано, що фазовий перехід другого роду спостерігається в діапазоні значень магнітного поля $7{,}0 \leq H \leq 10{,}0$, а фазовий перехід першого роду спостерігається в діапазоні $11{,}0 \leq H \leq 13{,}0$. Подальше пригнічення напруженості магнітного поля призводить до заглушення фазового переходу.

Ключові слова: фазовий перехід, модель Ізінга, магнітне поле, метод Монте-Карло.