

Frustrations and phase transitions in the Ising model on square lattice

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Abstract. The phase transitions in two-dimensional antiferromagnetic Ising model are studied on a square lattice by taking the interactions of next-nearest neighbors into account. The model is investigated on basis of the replica Monte Carlo algorithm and the histogrammic analysis of data. The diagram of the critical temperature dependence on an interaction value of next-nearest neighbors is plotted. The studied model reveals the phase transition of second order and the frustration points depending on relative interaction values and magnetic field. A effect, heat capacity splitting near the frustration points, is found.

Introduction

The modern physics of condensed state uses different lattice models for quantitative description of phase transitions (PTs) and critical properties (CP). Theoretical methods used on simple lattice models could solve very limited number of tasks. One of such models is a two-dimensional Ising model. The Ising model with interaction of nearest neighbors has been well studied by different methods and approaches [1-4]. The same model on a square lattice with ferromagnetic interactions of first and second neighbors has been accurately solved. However the taking into account of antiferromagnetic interactions of second nearest neighbors in classical two-dimensional Ising model is attended by quenching of the main state and appearing of different phases and phase transitions. Furthermore, accounting for interactions of next-nearest neighbors can influence on a critical behavior of the model, in particular, the various anomalies of critical properties appear [5].

First renormalization group calculations and numerical simulation by the Monte Carlo (MC) method for two-dimensional antiferromagnetic Ising model on a square lattice with interactions of next-nearest neighbors were carried out in works [6, 7] by the end of the 1970s. Authors supposed the presence of a phase transition of second order, estimated the temperature of the phase transition, and calculated critical exponents.

In works [8-10], authors reported the second order PTs in antiferromagnetic Ising model on a square lattice with interactions of next-nearest neighbors. Also this model could possess “anomalous” critical exponents. Additionally, the dependence of critical exponents on correlation J_{NNN} / J_{NN} (J_{NN} and J_{NNN} denote the constants of exchange interactions of nearest and next-nearest neighbors, correspondingly) was determined. But the scenario of a continuous phase transition was doubted after calculations by the mean-field theory which recognized the phase transition of first order [11].



According to works [12-14] the first order PTs were observed for Ising model on a square lattice with ferromagnetic interactions of nearest neighbors and with antiferromagnetic interactions of next-nearest neighbors in value intervals $J_{NNN} / J_{NN} = 0.5 \div 1.2$ in the system. In our previous work [15] we estimated the antiferromagnetic Ising model on a square lattice with taking into account the interactions of next-nearest neighbors for $J_{NNN} / J_{NN} = 1$ and determined the second order phase transition.

The main goal of the present work is to provide the accurate determination of a PT order of antiferromagnetic Ising model on a square lattice with taking into account next-nearest neighbors within value intervals $0.1 \leq J_{NNN} / J_{NN} < 1$ on basis of the replica Monte Carlo algorithm using a reliable and verified scheme and a unified technique.

Model and method

The antiferromagnetic Ising model on a square lattice taking into account interactions of second nearest neighbors is described by Hamiltonian [15]:

$$H = -J_{NN} \sum_{\langle i,j \rangle} (S_i \cdot S_j) - J_{NNN} \sum_{\langle i,j \rangle} (S_i \cdot S_j) - h \sum_i s_i \quad (1)$$

where $S_{i,j} = \pm 1$ is the Ising spin. The first term in the Equation (1) accounts for the exchange interaction of nearest neighbors by the value of $J_{NN} < 0$, and the second term considers next-nearest neighbors by $J_{NNN} < 0$, h is the external magnetic field.

The investigation of phase transitions in frustrated spin systems by traditional theoretical, experimental, and numerical methods faces with complex problems. This is connected with the inherent in such models problems of multiple valleys of local energy minima. Such systems can be rigorously and sequentially studied by the Monte Carlo methods on basis of microscopic Hamiltonians [16-19] but the standard Monte Carlo methods fail to solve these problems. Therefore, in recent time many new versions of Monte Carlo algorithms are developed for solution of these problems. The most powerful and effective algorithms for estimation of PTs and CPs in frustrated systems proved to be the replica Monte Carlo algorithms [20].

By now the replica Monte Carlo algorithms and the finite-size scaling theory become the basic tools for the investigation of critical properties of such complex systems.

To analyze a nature of phase transitions and the peculiarities of thermal characteristics near the critical point is used a histogram method [21]. The histogram analysis allows to estimate the reliability and accuracy of data derived from Binder cumulants calculations by Monte Carlo method and also to determine other important parameters [22].

The histogram method uses a random walk in the energy space and allows to detect accurate estimations for energy state densities $g(U)$. The probability of transition from one state into another is determined by the formula

$$P(U \rightarrow U') = \min[g(U) / g(U'), 1] \quad (2)$$

where U and U' denote the energies before and after spin flip.

The calculations were carried out for the systems with periodic boundary conditions and linear sizes $L \times L = N$, $L = 20 \div 150$. The exchange interaction correlation of next-nearest neighbors and nearest neighbors changed in value intervals $0.1 \leq J_{NNN} / J_{NN} < 1$. The system was brought into a thermodynamic equilibrium state by cut-off $\tau_0 = 4 \times 10^5$ MC step/spin, which is several times larger than the nonequilibrium part, where τ_0 denotes the length of nonequilibrium part of Markovian chain. The thermodynamic properties were averaged along the Markovian chain of length up to $\tau = 100\tau_0$ MC step/spin.

Simulation results

The temperature behavior of heat capacity and susceptibility was determined by the expressions [23]:

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

$$\chi = \begin{cases} (NK) \left(\langle m^2 \rangle - \langle m \rangle^2 \right), & T < T_N \\ (NK) \langle m^2 \rangle, & T \geq T_N \end{cases} \quad (4)$$

where $K = |J|/k_B T$, N is the number of particles, U is the internal energy, m is the order parameter.

The order parameter m was derived from expressions [15]:

$$m_\lambda = \frac{4}{N} \sum_{i \in \lambda} S_i, \quad \text{where } \lambda = 1, 2, 3, 4, \quad (5)$$

$$m^a = [m_1 + m_2 - (m_3 + m_4)]/4, \quad (6)$$

$$m^b = [m_1 + m_4 - (m_2 + m_3)]/4, \quad (7)$$

$$m = \sqrt{(m^a)^2 + (m^b)^2}, \quad (8)$$

where m_1, m_2, m_3, m_4 are the order parameters of sublattices.

Figures 1 and 2 present the temperature dependences of the heat capacity and susceptibility obtained at $L=80$ for different values J_{NNN}/J_{NN} (here and elsewhere a statistic error does not exceed the sizes of symbols used for plotting the curves). Note that decrease of J_{NNN}/J_{NN} in intervals $1 \geq J_{NNN}/J_{NN} \geq 0.6$ is accompanied with maxima shift towards lower temperatures and simultaneously the absolute maxima of heat capacity and susceptibility increases. We interpreted such behavior by the reason that when increasing the interactions of next-nearest neighbors, the contribution of interaction energy increases in modulus what enhances the rigidity of the system, and correspondingly the phase transition temperature arises. The increase in the absolute values of maxima is accounted for competing of nearest neighbors and next-nearest neighbors.

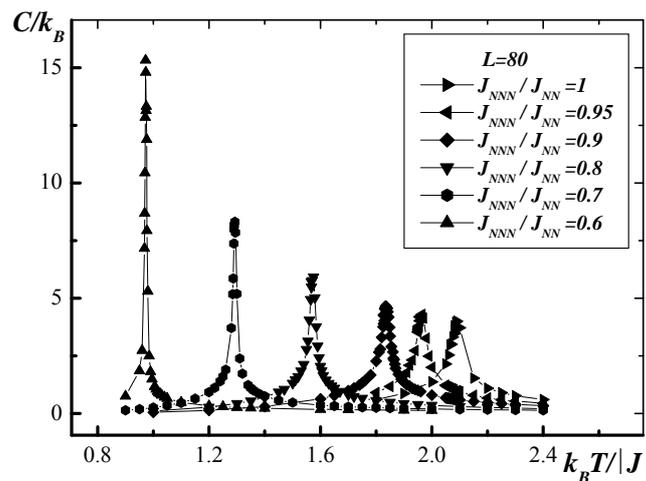


Figure 1. The dependence of heat capacity C/k_B on the temperature $k_B T/|J|$ for different J_{NNN}/J_{NN} .

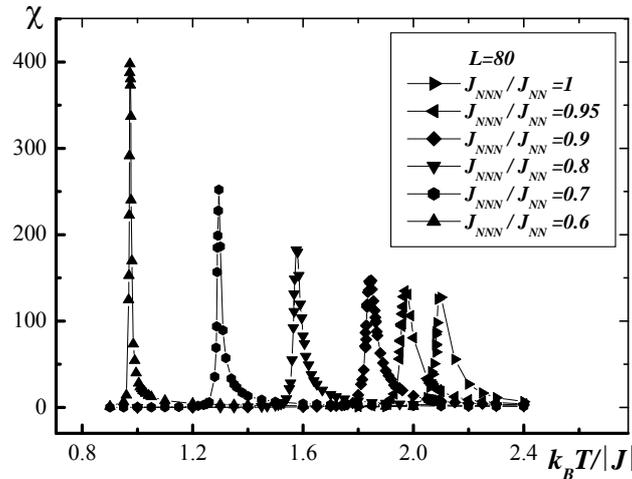


Figure 2. The dependence of susceptibility χ on the temperature $k_B T/|J|$ for different J_{NNN}/J_{NN} .

Figures 3 and 4 show the temperature curves of the heat capacity and susceptibility in intervals $0.1 \leq J_{NNN}/J_{NN} \leq 0.4$. It is notable that well-marked maxima are observed in all temperature curves of heat capacity C and susceptibility χ for all r near the critical temperature. We observe opposite behavior in the case when $0.1 \leq J_{NNN}/J_{NN} \leq 0.4$. The phase transition temperature shifts towards higher temperatures at the decrease of r from 0.4 to 0.1.

We determined the critical temperatures T_N using the method of forth-order Binder cumulants [24, 25]:

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3 \langle m^2 \rangle_L^2}, \quad (9)$$

$$V_L = 1 - \frac{\langle U^4 \rangle_L}{3 \langle U^2 \rangle_L^2}, \quad (10)$$

where U_L is the cumulant in magnetization, V_L is the cumulant in energy.

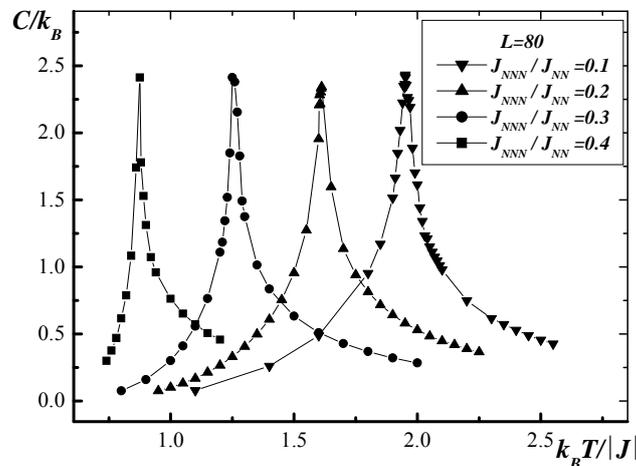


Figure 3. The dependence of heat capacity C/k_B on the temperature $k_B T/|J|$ for different J_{NNN}/J_{NN} .

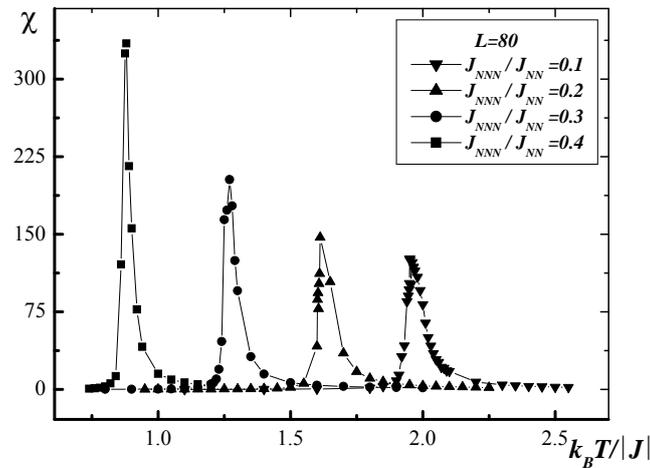


Figure 4. The dependence of susceptibility χ on the temperature $k_B T/|J|$ for different J_{NNN}/J_{NN} .

From Expressions (9) and (10) the critical temperature can be detected to a high accuracy. It should be noted that Binder cumulants provide good testing of PTs type in the system. It is common knowledge that the temperature curves of Binder cumulants U_L have a well-marked cross point at second order PTs [25].

Figure 5 presents the U_L temperature curve at $J_{NNN}/J_{NN} = 0.7$ for different values of L . This figure shows the accuracy in the detection of critical temperature. As is evident from insert, the well-marked cross point observed in the critical region (here and elsewhere the temperature is expressed in the unit of $|J|/k_B$) indicates the second order PTs. The critical temperatures for other J_{NNN}/J_{NN} values were determined in a similar way.

The temperature dependence of cumulants in energy V_L at $J_{NNN}/J_{NN} = 0.7$ for different L is shown in Figures 6. As is obvious from the figure, the minimum magnitude of V_L disappears at increase in L and the value of V_L tends to $2/3$ at $T \rightarrow 0$ what also is typical for second order PTs. By a diagram form in Figures 6 one can predict a type of the phase transition in the system. A detail description is reported in our previous work [24].

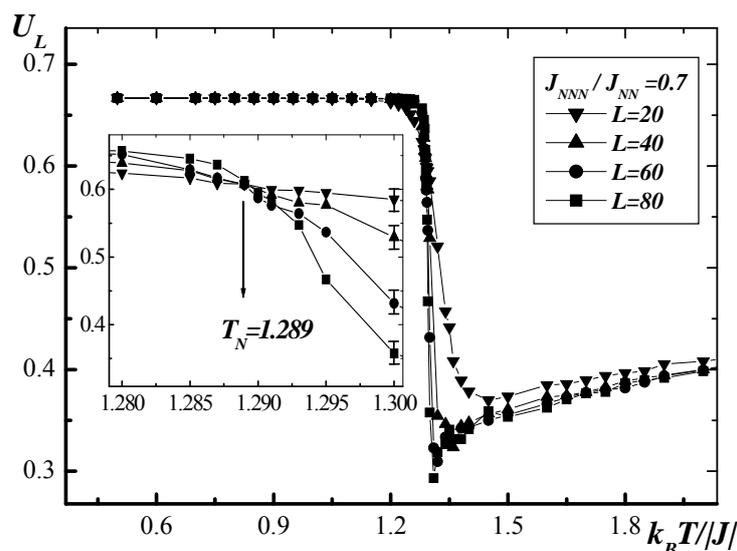


Figure 5. The dependences of Binder cumulant U_L on the temperature $k_B T/|J|$ for $J_{NNN}/J_{NN} = 0.7$.

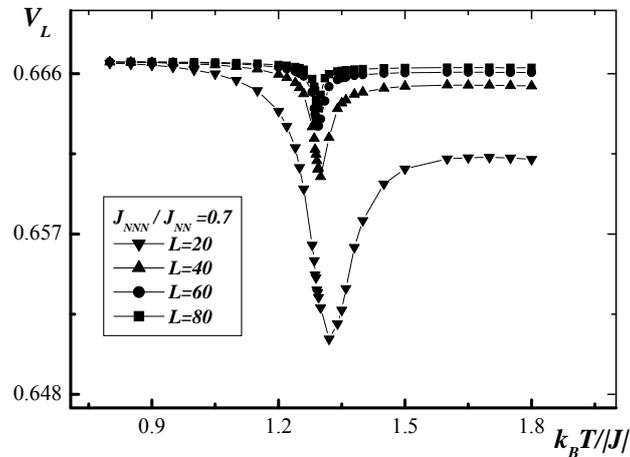


Figure 6. The dependences of Binder cumulant V_L on the temperature $k_B T / |J|$ for $J_{NNN} / J_{NN} = 0.7$.

Figure 7 presents the dependence of critical temperature on an interaction value of next-nearest neighbors. As is evident from the diagram, the different phases cross at a point $J_{NNN} / J_{NN} = 0.5$: 1) ferromagnetic, 2) paramagnetic, and 3) super antiferromagnetic lines. The figure demonstrates that the critical temperature $T_N = 0$ and phase transition are lack for the value $J_{NNN} / J_{NN} = 0.5$. This comes from the similarity in the interactions of nearest neighbors and next-nearest neighbors at $J_{NNN} / J_{NN} = 0.5$ and the whole system frustrates. It disorders the system and results in a disappearance of phase transition. It can be inferred by Figure 8 where the heat capacity temperature curve at $J_{NNN} / J_{NN} = 0.5$ for big size lattices (150) has not an abrupt jump but changes smoothly. A similar behavior of the heat capacity temperature curve is observed for $J_{NNN} / J_{NN} = 0.49$ and $J_{NNN} / J_{NN} = 0.495$ which are below the value $J_{NNN} / J_{NN} = 0.5$. For two-dimensional case in all frustration points, the temperature dependence of the heat capacity is of smooth maximum form. When moving away from the frustration point, a sharp lambda-shaped peak appears in the heat capacity and the smooth maximum is slightly decreasing (heat capacity splitting). At further moving away from the frustration point the smooth maximum vanishes and the sharp peak remains only. This is demonstrated in Figure 9. Also the figure exhibits the well-marked maxima near the critical temperature for values $J_{NNN} / J_{NN} = 0.505$ and $J_{NNN} / J_{NN} = 0.51$, which are above the value $J_{NNN} / J_{NN} = 0.5$.

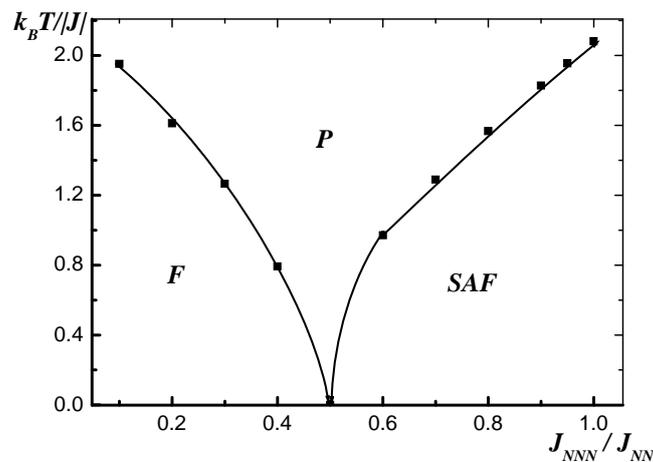


Figure 7. The phase diagram of dependence critical temperature on the interaction value of next-nearest neighbors, where *F* – ferromagnetic phase, *P* – paramagnetic phase, *SAF* – super antiferromagnetic phase.

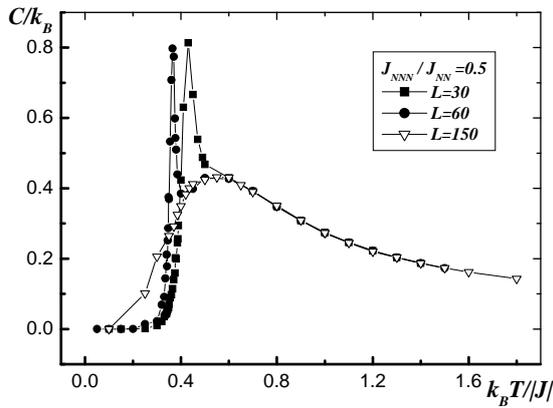


Figure 8. The dependence of heat capacity C/k_B on the temperature $k_B T/|J|$ for $J_{NNN}/J_{NN} = 0.5$.

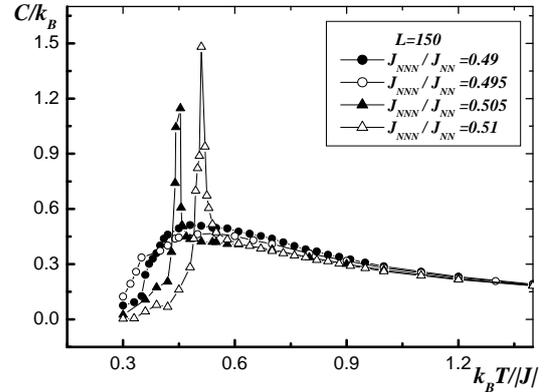


Figure 9. The dependence of heat capacity C/k_B on the temperature $k_B T/|J|$ for $L = 150$.

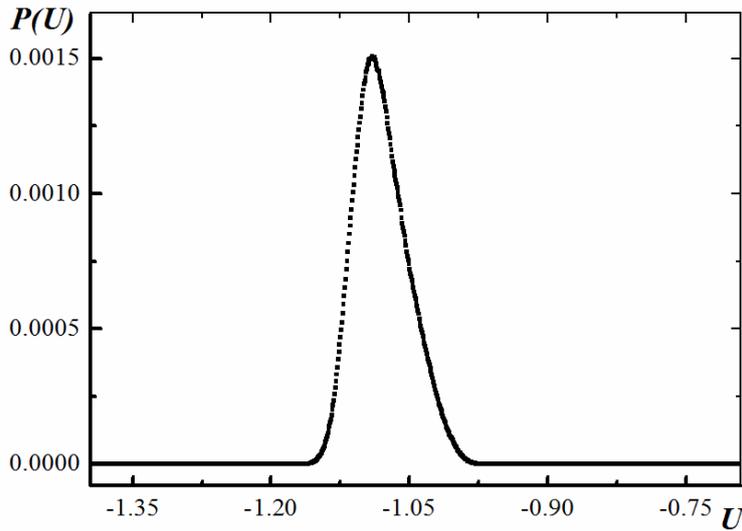


Figure 10. The histogram of energy distribution for $J_{NNN}/J_{NN} = 0.7$.

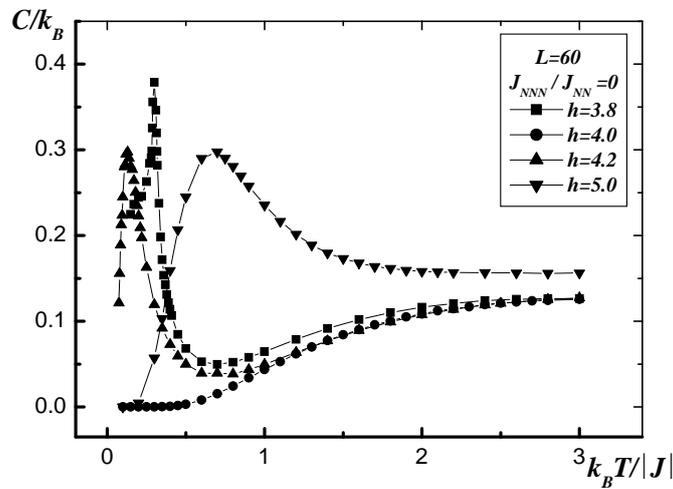


Figure 11. The dependence of heat capacity C/k_B on the temperature $k_B T/|J|$ for different h .

In work [26], authors reported the phase diagram for phase transition temperature dependence T_N on the ratio of exchange parameters J_{NNN} / J_{NN} for the similar model. They determined that the second order phase transition occurred in value intervals $J_{NNN} / J_{NN} < 0.5$ and $J_{NNN} / J_{NN} \geq 0.948$ and the first order phase transition happened in intervals $0.5 < J_{NNN} / J_{NN} < 0.948$. According to our investigations the second order phase transition took place in intervals $0.5 < J_{NNN} / J_{NN} \leq 1$. This was confirmed by the histogram analysis.

The histogram of energy distribution for $J_{NNN} / J_{NN} = 0.7$ is presented in Figures 10. The diagram is plotted near the critical point for a lattice with $L = 150$. In the Figure, a maximum typical for second order phase transitions is observed [24]. Similar histograms were plotted for other values of J_{NNN} / J_{NN} . According to obtained data the second order phase transitions are observed in all long interval $0.1 \leq J_{NNN} / J_{NN} \leq 1$, except when $J_{NNN} / J_{NN} = 0.5$ where the phase transition fails to take place. The point $J_{NNN} / J_{NN} = 0.5$ is the frustration point.

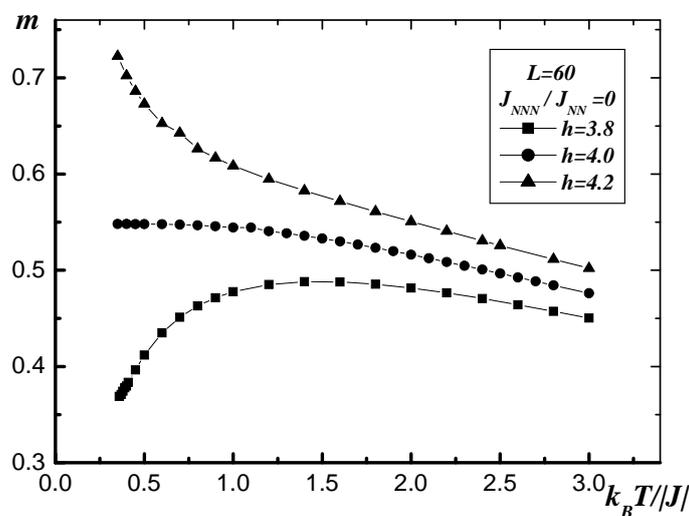


Figure 12. The dependence of order parameter m on the temperature $k_B T / |J|$ for different h .

Figures 11 and 12 present the temperature dependence plots of heat capacity and order parameter on the external magnetic field for a case when accounting the interactions of nearest neighbors only. The plots exhibit the anomalous behavior in the heat capacity and order parameter dependences for the field value $h = 4.0$. This comes from the fact that when the value of external magnetic field is 4.0, the system is frustrated even without considering the interactions of next-nearest neighbors.

Conclusion

The phase transitions in two-dimensional antiferromagnetic Ising model with taking into account of the interactions of next-nearest neighbors are studied using the exact and efficient replica Monte Carlo algorithm. A behavior of phase transitions for different correlations of r of nearest neighbors and next-nearest neighbors is analyzed by the histogram and Binder cumulants methods. The phase diagram of critical temperature dependences on the interaction value of next-nearest neighbors is plotted. The second order phase transition is shown to be happened for all values in intervals $0.1 \leq J_{NNN} / J_{NN} < 1$ except $J_{NNN} / J_{NN} = 0.5$. The value $J_{NNN} / J_{NN} = 0.5$ is detected to be the frustration point for this model. It is shown that this model frustrated in the external field at $h=4.0$ even when taking into account the nearest neighbors only.

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