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ORDER, DISORDER AND PHASE TRANSITIONS IN CONDENSED MEDIA

STUDY OF PHASE TRANSITIONS AND THERMODYNAMIC PROPERTIES OF THE POTTS MODEL WITH FRUSTRATIONS ON THE KAGOME LATTICE

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Abstract. The Monte Carlo method was used to study phase transitions and thermodynamic properties of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the kagome lattice with interactions of the first J_1 and second J_2 neighbors. The studies were carried out for the magnitude of the interaction of second neighbors in the interval $0 \leqslant r=|J_2/J_1| \leqslant 1$. It was found that at $r = 0$ the system exhibits disorder and strong degeneracy of the ground state. It is shown that taking into account ferromagnetic interactions of second neighbors will remove the degeneracy of the ground state. An analysis of the nature of phase transitions in the considered interval r was carried out. It is shown that in the range $0.2 \leqslant r \leqslant 1$ a second-order phase transition is observed.

Keywords: *Monte Carlo method*, *phase transitions*, *Potts model*, *antiferromagnetic*, *frustrations*

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1. INTRODUCTION

The study of phase transitions (PT) and thermodynamic properties of compounds having a kagome lattice attracts a lot of attention. This is due to the fact that frustrations can occur in such compounds due to the special geometry of the lattice. In antiferromagnetic compounds having a kagome lattice, frustrations are observed when taking into account the exchange interactions of the nearest neighbors. In kagome lattice ferromagnets with antiferromagnetic interactions of the second neighbors, frustrations arise due to the competition of exchange interactions between the first and second neighbors. Frustration effects play an important role in magnetic spin systems. Frustrated magnets exhibit properties different from the corresponding non-frustrated magnetic systems, which causes increased interest in studying the phenomena of frustration in magnetic systems [1 – 3]. The models of Ising, Heisenberg, Potts, etc. are widely used to study the physical properties of such magnets. These models describe a large class of real physical systems: layered magnets, liquid helium films, superconducting films, adsorbed films, etc. [1, 4, 5]. To date, the classical Ising and Heisenberg models have been studied quite well and many of their properties are known [6 – 10]. Unlike the Ising and Heisenberg models, there are very few reliably established facts for the Potts model. In recent years, a significant number of papers have been devoted to the study of spin systems described by the Potts model [4, 11- 16], in which many questions were answered. It has been shown that the physical properties of the Potts model depend on the spatial dimension of the lattice, the number of spin states q, the magnitude of the interaction of the second neighbors and the geometry of the lattice [11 –19]. Most of the available results are obtained for the Potts model with the number of spin states $q = 2$ and $q = 3$ [11, 12, 13]. Depending on the number of spin states q spatial dimension, the Potts model demonstrates PT of the first or second kind. The two-dimensional Potts model with the number of spin states is $q = 4$ quite unique and has so far been little studied. This model can be used to describe the behavior of some classes of adsorbed gases on graphite [20]. This model is also interesting

because the value $q = 4$ is the boundary value of the interval $2 \leqslant q \leqslant 4$, where PT of the second kind is observed and the range of values $q > 4$ in which PT occurs as a transition of the first kind [4]. In this paper, we study the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the Kagome lattice, taking into account the ferromagnetic exchange interactions of the second neighbors. This model, even without taking into account the interactions of the second neighbors, is frustrated due to the special geometry of the lattice. Taking into account the ferromagnetic interactions of the second neighbors in this model can lead to a change in the degeneracy of the ground state, the appearance of various phases and OP, as well as affect its thermodynamic and magnetic properties. The study of the effect of the magnitude of the ferromagnetic interaction of the second neighbors on the PT and thermodynamic properties of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the Kagome lattice is practically not found in the literature. In this regard, in this paper we conduct a study of the PT and thermodynamic properties of this model in a wide range of values of the interaction of the second neighbors. The study of the considered model based on modern methods and ideas will provide an answer to a number of questions related to the physics of frustrated spin systems and systems with competing exchange interactions.

2. MODEL AND METHOD OF STUDY

The Hamiltonian of the Potts model with a number of states $q = 4$ taking into account the interactions of the first and second neighbors, can be represented in the following form [21, 22]:

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

where J_1 and J_2 are the parameters of the exchange antiferromagnetic ($J_1 < 0$) and ferromagnetic ($J_2 > 0$) interactions, respectively, for the first and second neighbors, $r = | J_2/J_1 |$ the magnitude of the interaction of the second neighbors, $\theta_{i,j}$, $\theta_{i,k}$ — the angles between the interacting spins $S_i - S_j$ and $S_i - S_k$. In this paper, we consider the interval of values in $0 \leqslant r \leqslant 1$ at 0.1 increments. The summation in equation (1) is performed for each pair of adjacent spins.

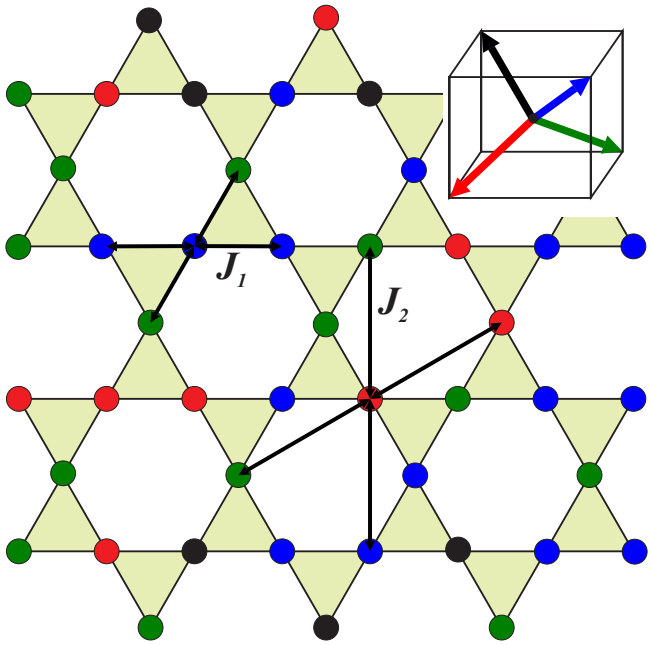

Fig. 1. The Potts model with the number of spin states $q = 4$ on the kagome lattice. The inset shows a corresponding color representation for each of the four possible spin directions

In this model, each spin has four nearest neighbors, so the summation $4N$ was performed once. $N = L \times L$ — the number of spins in the system, $L = 12$ –72, where L is measured in the size of the unit cell. The same procedure is carried out for the next nearest neighbors. A schematic description of the model under study is shown in Fig. 1. As you can see in the figure, each spin has four nearest (J_1) and four next-to-nearest (J_2) neighbors. The backs, marked with circles of the same color, have the same direction. The inset to the drawing shows a corresponding color representation for each of the four possible spin directions. The directions of the spins are set in such a way that the equality is satisfied

$$\theta_{i,j} = \begin{cases} 0, & \text{if } S_i = S_j; \\ 109.47^\circ, & \text{if } S_i \neq S_j. \end{cases}$$

or

$$\cos\theta_{i,j} = \begin{cases} 1, & \text{if } S_i = S_j; \\ -1/3, & \text{if } S_i \neq S_j. \end{cases} \quad (2)$$

According to condition (2) for two spins, S_i and S_j, the energy of the pair exchange interaction $E_{i,j} = -J_1$ if $S_i = S_j$. In the case when $S_i \neq S_j$,

energy $E_{i,j} = J_1/3$. Thus, the energy of the paired interaction of the spins is equal to one value with their identical direction and takes on a different value when the directions of the spins do not match. For the Potts c model $q = 4$ in three-dimensional space, this is possible only with the orientation of the spins, as shown in the box in Fig. 1. Currently, one of the most effective algorithms for studying such systems is the Wang–Landau algorithm of the Monte Carlo method [23], especially in the low-temperature region. Therefore, we used this algorithm in this study. This algorithm is an implementation of the entropy modeling method and allows you to calculate the density function of the system states. The Wang–Landau algorithm is based on the fact that by making a random walk in the energy space with probabilities inversely proportional to the density of states $g(E)$, we get a uniform distribution of energies. By selecting the transition probabilities such that the visit to all energy states would become uniform, one can obtain an initially unknown density of states $g(E)$, knowing which, one can calculate the values of the necessary thermodynamic parameters at any temperature. Since the density of states increases $g(E)$very rapidly with the increase in the size of the studied systems, the value is used for the convenience of storing and processing large numbers $\ln g(E)$. The Wang–Landau algorithm is described in more detail in [13]. By determining the density of the system states, it is possible to calculate the values of thermodynamic parameters at any temperature. In particular, internal energy U, free energy F, heat capacity C and entropy S can be calculated using the following expressions:

$$U(T) = \frac{\sum_E Eg(E)e^{-E/k_BT}}{\sum_E g(E)e^{-E/k_BT}} \equiv \langle E \rangle_T, \quad (3)$$

$$F(T) = -k_BT \ln\left(\sum_E g(E)e^{-E/k_BT}\right), \quad (4)$$

$$C = N\left(|J_1| / k_BT\right)^2 \cdot \left(\left\langle U^2 \right\rangle - \left\langle U \right\rangle^2\right), \quad (5)$$

$$S(T) = \frac{U(T) - F(T)}{T}, \quad (6)$$

where $K = |J_1|/k_BT$, N is the number of particles, T s the temperature (hereafter the temperature is given in units $|J_1|/k_B$), U is a normalized value. Calculations were performed for systems with periodic boundary conditions (CCGT).

3. SIMULATION RESULTS

Figure 2 shows the temperature dependences of the heat capacity C for different values r obtained for a system with a linear size $L = 24$ (hereinafter, the statistical error does not exceed the size of the symbols used to construct the dependencies). As can be seen in the figure, there is $r = 0.1$ no sharp peak for the value on the temperature dependence of the

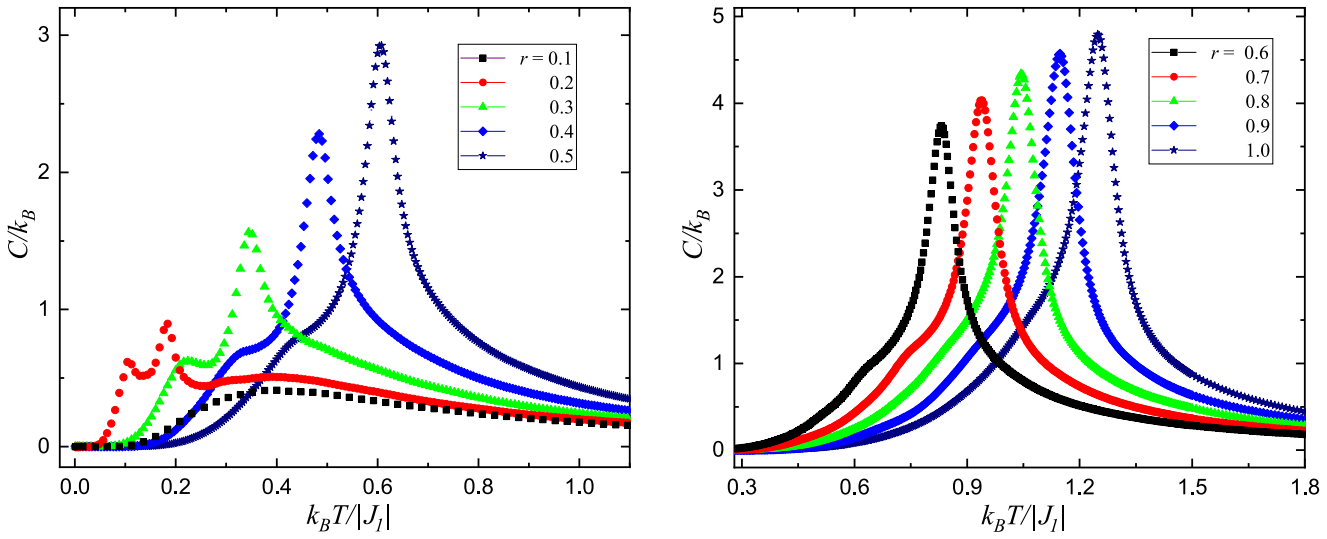

Fig. 2. Temperature dependences of heat capacity C

heat capacity, but a smoothed peak is observed. The absence of a pronounced peak in heat capacity is explained by the fact that at $r \leqslant 0.1$ there is no order in this model. For the values $r = 0.2$ and the $r = 0.3$ splitting of the heat capacity is observed. There are two peaks and one smooth "hump". As the value increases, the r smooth hump and the low-temperature peak disappear and one pronounced peak remains on the temperature dependence of the heat capacity. The presence of a hump indicates the low dimensionality of the system, and splitting of the heat capacity is usually observed for frustrated spin systems [2, 24]. For the model we are investigating, the splitting of the heat capacity is due to the fact that taking into account the exchange interactions of the second neighbors leads to the appearance of a partially ordered magnetic state. The r growth is accompanied by a shift of maxima towards high temperatures and an increase in the value of maxima. The increase in the absolute values of the heat capacity maxima occurs due to an increase in the contribution of the exchange interactions of the second neighbors.

The magnetization of the system m was calculated using the formula

$$m = \frac{1}{N}\sum_{i=1}^{N} S_i, \tag{7}$$

where is a three S_i— component unit vector $S_i = \left(S_i^x, S_i^y, S_i^z\right)$. It can take one of the four directions shown in the box in Fig. 1.

Figure 3 shows graphs of the dependence of magnetization $m$on temperature for different values r. In the absence of interactions of the second neighbors, there is no order in the system and the magnetization value is close to zero. When taking into account the interactions of the second neighbors, a partial ordering is observed in the system and the magnetization in the low-temperature region has values other than zero. This is explained by the fact that the interaction of the second neighbors leads to a change in the magnetic structure of the ground state, and a partial order arises in the system. The figure shows that $r \geqslant 0.1$ with increasing temperature, the magnetization m gradually decreases, which indicates in favor of the second kind of PT.

The dependences of entropy S on temperature are shown in Fig. 4. As can be seen in the figure, for the entire considered range of r values with an increase of temperature entropy tends to a theoretically predicted value $\ln 4$. For the case $r = 0$ in the low-temperature region, the entropy tends to a value other than zero. At the same time, this entropy value is very different from zero. This behavior of entropy indicates that at $r = 0$ the basic state of the system is highly degenerate. In addition, it is known that in systems with frustrations, entropy S at low temperatures should tend to a value other than zero. In the range $0.1 \leqslant r \leqslant 1$ in the low-temperature region, the entropy tends to zero. This means that there is r no degeneration of the ground state in this range. Thus, we see that taking into account the ferromagnetic interactions of the second neighbors leads to the removal of the degeneracy of the ground state, even at small values r.

To determine the type of PT, we used a histogram analysis of the MC method data [23, 25]. This method allows you to reliably determine the type of PT. The method of determining the type of PT by this method is described in detail in [26, 27]. The results obtained on the basis of histogram data analysis show that in this mode $0.2 \leqslant r \leqslant 1.0$ of the second kind is observed in the interval. This is demonstrated in Figure 5. This figure shows the histograms of the energy distribution for systems with different linear dimensions for the value $r = 0.5$. Graphs are plotted for temperatures close to critical ($T = 0.718$). The figure shows that, depending on the probability W of energy, there is one maximum for all values L, which indicates a second-kind PT. The presence of one maximum on the histograms of the energy distribution is a sufficient condition for PT of the second kind. In addition, the figure shows that as the linear dimensions of the system increase, the width of the histogram decreases, which is typical for PT of the second kind. Note that one maximum on the histograms of the distribution for the studied model is observed for values r in the interval $0.2 \leqslant r \leqslant 1.0$. This allows us to assert that PT of the second kind is observed in this range of values.

4. CONCLUSION

The study of phase transitions and thermodynamic properties of the two–dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the Kagome lattice, taking into account the ferromagnetic interactions of the second neighbors, was performed using the Wang-Landau algorithm

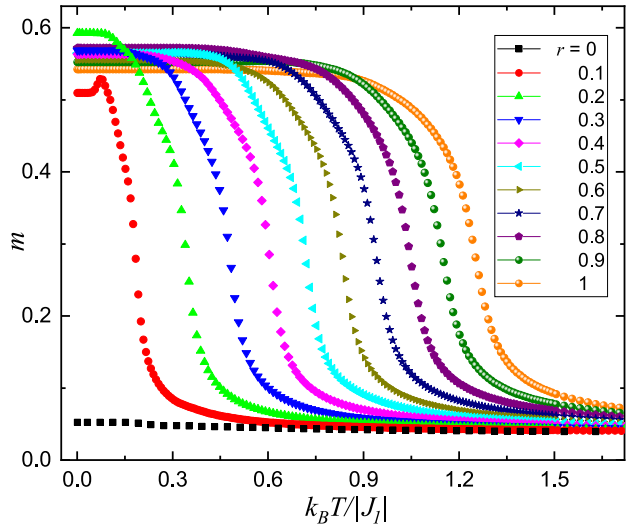

Fig. 3. Temperature dependence of magnetization m

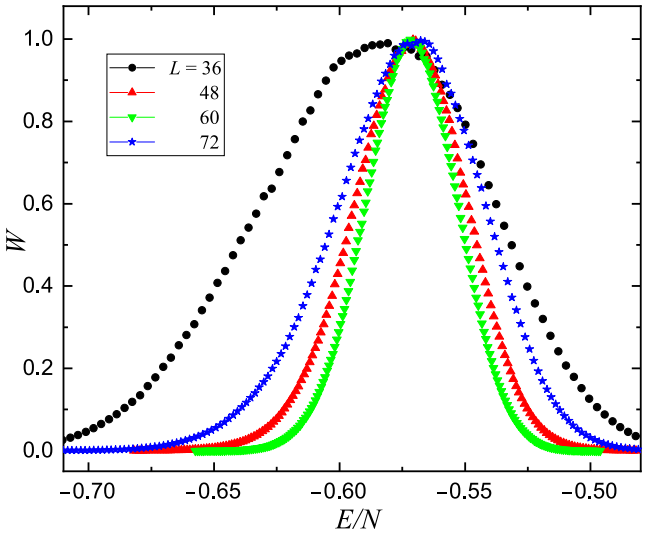

Fig. 5. Histograms of energy distribution for $r = 0.5$ at various L

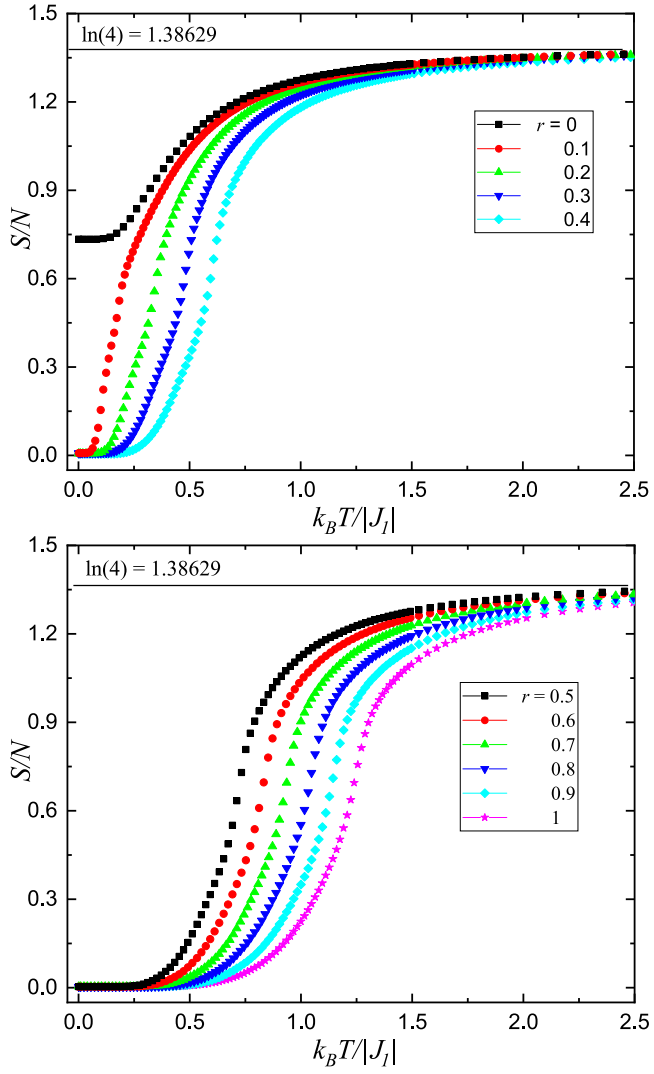

Fig. 4. Temperature dependence of entropy S

of the Monte Carlo method. The analysis of the nature of phase transitions in a wide range of values of the interaction of the second neighbors is carried out r. It is shown that a phase transition of the second kind is observed in the interval $0.2 \leqslant r \leqslant 1$. For the values $r \leqslant 0.1$ there is no order in the system and frustrations are observed. It is shown that at a value of $r = 0$ ground state of the system is strongly degenerate. Taking into account the ferromagnetic interactions of the second neighbors leads to the removal of the degeneracy of the ground state for the values $r \geqslant 0.1$.

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