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Phase transitions in a two-dimensional antiferromagnetic Potts model on a kagome lattice

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The phase transitions and thermodynamic properties of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the kagome lattice are studied by the Monte Carlo method, taking into account the exchange interactions of the first J_1 and second J_2 nearest neighbors. The studies were carried out for the value of the interaction of the second nearest neighbors in the interval $-1.0 \leq J_2 \leq 0.0$. An analysis of the character of phase transitions has been carried out. It is shown that in the interval $-1.0 \leq J_2 \leq -0.1$, a second-order phase transition is observed, while at $J_2 = 0.0$, frustrations disturb the order in the system and lead to the disappearance of the phase transition

Keywords: Frustration, phase transition, Monte Carlo method, Potts model.

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1. Introduction

Currently, of great scientific interest are studies of phase transitions (PT), critical, magnetic and thermodynamic properties of magnets described by two-dimensional lattice Ising models and Potts [1–3]. These models describe a large class of real physical systems: layered magnets, liquid helium films, superconducting films, adsorbed films, etc. [1,4,5]. Unlike the Ising model, there are very few reliably established facts for the two-dimensional Potts model with a different number of spin q states. Most available results were obtained for a two-dimensional Potts model with the number of spin states $q = 2$ and $q = 3$ [6–8]. Depending on the number of spin states q and the spatial dimension, the Potts model demonstrates the first or second kind of PT. The two-dimensional Potts model with the number of spin states $q = 4$ is almost unique and still little studied. A Potts model can be used to describe the behavior of certain classes of adsorbed gases on graphite [9]. This model is also interesting because the value of $q = 4$ is the boundary value of the interval $2 \leq q \leq 4$, where the second kind of PT is observed, and the range of values $q > 4$, in which the PT occurs as a transition of the first kind [4].

The results of studies of the two-dimensional ferromagnetic Potts model with competing exchange interactions on triangular [10] and hexagonal [11,12] lattices and on the Kagome lattice [13] by the Monte Carlo (MC) method show that the nature of the PT and the thermodynamic behavior of this model depend on type of lattice. This is due to the fact that the degree of degeneration of the ground state of the system and the point of frustration depend on the type of lattice.

The study of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the Kagome lattice, taking into account the exchange interactions of the first and second nearest neighbors, is practically not found in the literature. This model, even without taking into account the interactions of the second nearest neighbors, is frustrated due to the special geometry. Taking into account the antiferromagnetic interactions of the second nearest neighbors in this model can lead to a change in the degree of degeneracy of the ground state and the appearance of various phases and PT, as well as affect the description of its thermodynamic and magnetic properties.

In the study [14], unique electronic and quantum properties were discovered in the study of compounds having a Kagome lattice. The authors associate this behavior with a feature of the structure of the Kagome lattice. For example, layered vanadium antimonides AV_3Sb_5 ($A = \mathrm{K, Rb, Cs}$), which are a family of topological metals with a Kagome lattice, exhibit a number of strongly correlated electronic phases, including charge order and superconductivity. A schematic representation of such a lattice is presented in Fig. 1.

In this regard, in this paper we have attempted, based on the MC method, to study of PT and thermodynamic properties of the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the Kagome lattice with the interaction of the first (J_1) and the second nearest (J_2) neighbors. Since the behavior of the Potts model depends on the magnitude of J_2, it is of particular interest to study the nature of the PT for this model at different ratios of the magnitude of the antiferromagnetic interaction of the second nearest neighbors. From the data obtained to date, it is impossible to unambiguously deter-

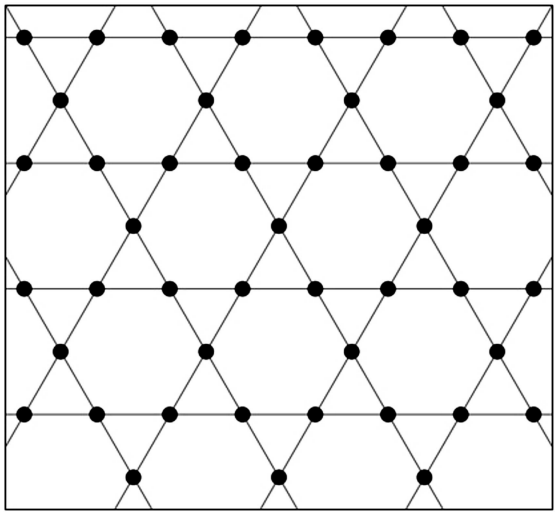

Figure 1. Schematic representation of the kagome lattice.

mine the nature of the PT and the patterns of changes in the thermodynamic behavior of the frustrated Potts model on the Kagome lattice with the number of spin states $q = 4$, and these questions still remain open. The study is performed on the basis of modern methods and ideas that allows answering a number of questions related to the character and nature of PT of frustrated spin systems.

2. Model and method of study

The Hamiltonian of the Potts model, considering the interactions of the first and second nearest neighbors, can be represented in the following form,

$$H = -J_1 \sum_{\langle i,j\rangle, i\neq j} S_i S_j - J_2 \sum_{\langle i,k\rangle, i\neq k} S_i S_k$$

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

where J_1 and J_2 — parameters of exchange antiferromagnetic interactions ($J_1 < 0$, $J_2 < 0$), respectively, for the first and second nearest neighbors, $\theta_{i,j}, \theta_{i,k}$ — the angles between the interacting spins $S_i - S_j$ and $S_i - S_k$. The magnitude of the interaction of the second nearest neighbors varied in the range $-1.0 \leq J_2 \leq 0.0$.

The directions of the vectors are set in such a way that the equality holds

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

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

Such systems based on microscopic Hamiltonians are successfully studied on the basis of the MC [15–21]. In recent years, many new variants of algorithms of the MC method have been developed. The Wang–Landau algorithm is one of the most efficient for studying such systems [22,23], particularly in the low-temperature area. Therefore, we used this algorithm in this study. The Wang−Landau algorithm is an implementation of the entropy modeling method and allows you to calculate the density function of the states of the system. The Wang−Landau algorithm was used by us in the following form:

– an arbitrary initial configuration of spins is given, the starting values of the density of states $g(E) = 1$, histograms of energy distributions $H(E) = 0$, the starting modification factor $f = f_0 = e_1 \approx 2.71828$;

– we repeatedly perform steps in phase space until we get a relatively flat histogram $H(E)$ (i.e. until all possible energy states of the system are visited approximately the same number of times). In this case, the probability of transition from a state with energy E_1 to a state with energy E_2 is determined by the formula $p = g(E_1)/g(E_2)$. If the transition to a state with energy E_2 has taken place, then the value of the density of states $g(E_2)$ with energy E_2 is multiplied by the factor f and the histogram with this energy $H(E_2)$ increases by 1 ($g(E_2) := fg(E_2)$, $H(E_2) := H(E_2) + 1$). Otherwise, all this is done for energy E_1 ($g(E_1) := fg(E_1)$, $H(E_1) := H(E_1) + 1$);

– if the histogram has become „flat“, then we reset the histogram ($H(E) := 0$), reduce the modification factor ($f := \sqrt{f}$) and continue again, while $f \geq f_{\min}$. In our case $f_{\min} = 1.0000000001$;

– having determined the density of the states of the system, it is possible to calculate the values of thermodynamic parameters at any temperature — in particular, the internal energy U, free energy F, specific heat C and entropy S can be calculated using the following expressions:

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

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

$$C = \frac{(|J_1|k_BT)^2}{N}(\langle U^2\rangle - \langle U\rangle^2), \qquad (5)$$

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

where N — number of particles, k_B — Boltzmann constant, T — temperature (hereafter the temperature is given in units of $|J_1|/k_B$).

Calculations were performed for systems with periodic boundary conditions and linear dimensions $L \times L = N$, $L = 12-96$ (L is measured in unit cell sizes) in the range $-1.0 \leq J_2 \leq 0.0$.

3. Simulation results

Fig. 2 shows the temperature dependences of the energy E for different values of the exchange interaction J_2. The figure shows that in the low-temperature area $E = 0$ for all values of J_2. This is due to the lack of order in the system in the ground state. With an increase in temperature, we observe that the nature of the change in the energy of the system depends on the magnitude of J_2. With an increase in temperature for systems with a large value of J_2, the energy growth occurs faster (a sharper jump is observed).

Fig. 3 shows the temperature dependences of entropy S/N for different values of exchange interaction J_2. As the temperature increases, the entropy for all values of J_2 tends to the theoretically predicted value of $\ln 4$. At low temperatures, the entropy for all values of J_2 tends to a nonzero value of S_0. This behavior of entropy indicates the degeneration of the ground state. It should be noted that for the value $J_2 = 0.0$, the entropy in the low-temperature area takes the largest value $S_0 = 0.73$, which is due to the strong degeneracy of the ground state. With a value of $J_2 = 0.0$, the system is highly frustrated. Taking into account the interactions of the second nearest neighbors leads to a decrease in the value of S_0, which also indicates a decrease in the degeneracy of the ground state. Our data shows that in the entire range $-1.0 \le J_2 \le 0.1$ value $S_0 = 0.33$.

Figures 4 and 5 show the temperature dependences of the heat capacity C for different values of the exchange interaction J_2. The figure shows that for the value $J_2 = 0.0$, the effects of frustration are most pronounced: there is no sharp peak, a smoothed maximum is observed. With the

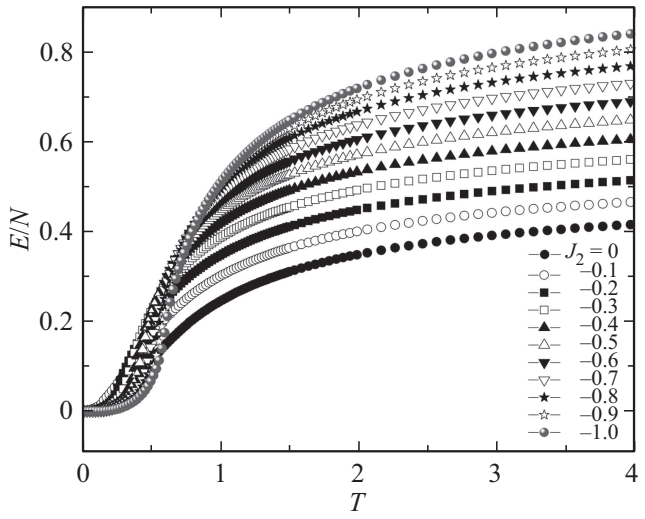

Figure 2. Temperature dependences of energy E for different values J_2.

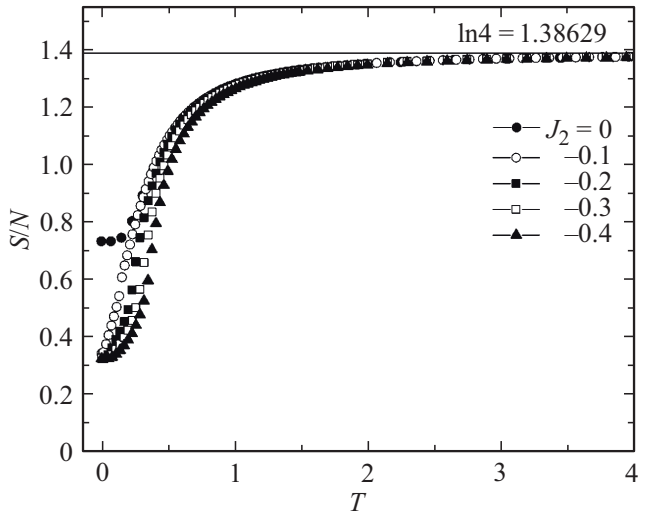

Figure 3. Temperature dependences of entropy S/N for different values J_2.

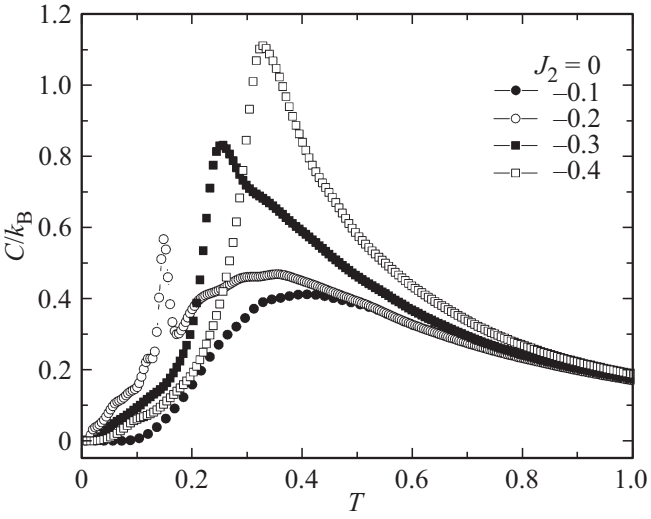

Figure 4. Temperature dependences of heat capacity C for different values J_2.

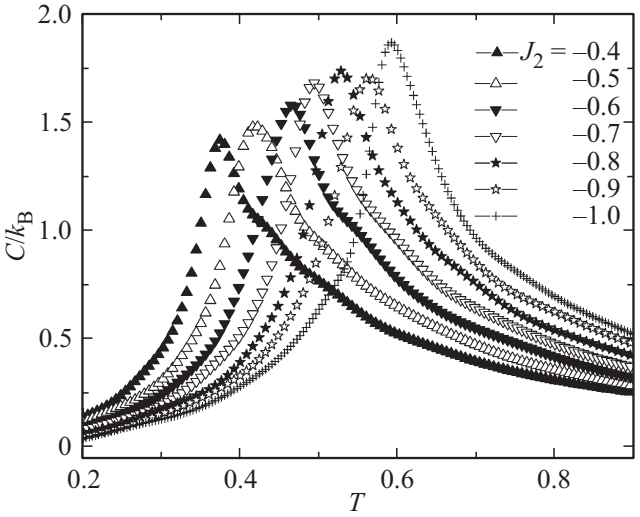

Figure 5. Temperature dependences of heat capacity C for different values J_2.

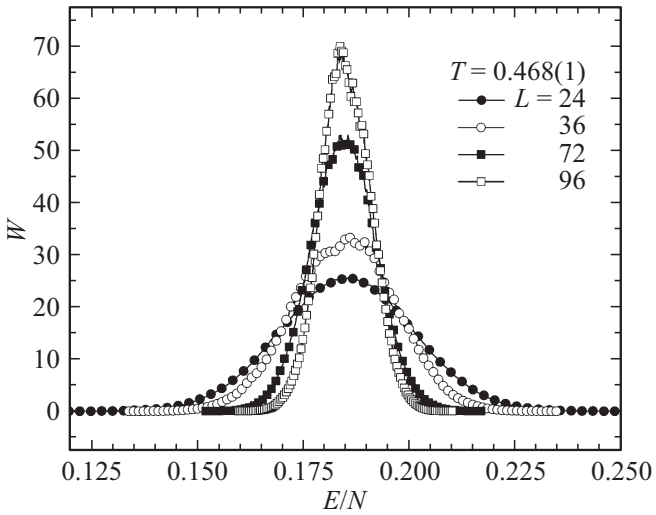

Figure 6. Histograms of the energy distribution for the value $J_2 = -0.5$.

value $J_2 = 0.0$, the system is completely frustrated, and there is no order in the system. When $J_2 = -0.1$ splitting of the heat capacity is observed, which is a characteristic feature of frustrated systems (near the points of frustration there is an acute peak and a domed maximum) [24]. In the range $-1.0 \leq J_2 \leq -0.2$ the heat capacity has an acute peak, the position of which corresponds to a temperature of PT. As can be seen in the figure, this peak increases with an increase in the value of J_2 and shifts towards higher temperatures. To analyze the PT kind, we used a histogram analysis of the data of the MC method [22,23]. Histogram analysis — is one of the most accurate methods to establish the PT kind.

Fig. 6 shows the histograms of the energy distribution for the value $J_2 = -0.5$ for systems with different linear dimensions. The graphs are plotted at a temperature close to critical $(T = 0.4687(1))$. The figure shows that depending on the probability of W on the energy of E/N, one maximum is observed. The presence of one peak on the histograms of the energy distribution is a characteristic feature of the second kind of PT. As can be seen in the figure, as the linear dimensions of the system increase, the histogram narrows, and the peak grows. This behavior is characteristic of the second kind of PT. We note that similar behavior on energy distribution histograms is observed in the range $-1.0 \leq J_2 \leq -0.1$. It can be assumed that in the considered range of values of J_2, there is a second kind of PT, except for the value of $J_2 = 0.0$, where frustrations disrupt the order in the system and lead to the disappearance of the PT.

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 interactions of the first and second nearest neighbors, was performed using the Wang–Landau algorithm of the Monte Carlo method. The nature of phase transitions is analyzed using the histogram method. It is established that in the interval $-1.0 \leq J_2 \leq -0.1$ a phase transition of the second kind is observed. It is shown that for the value $J_2 = 0.0$, strong frustrations are observed in the system, which lead to the disappearance of the phase transition.

Conflict of interest

The authors declare that they have no conflict of interest.

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