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Thermodynamic behavior of a two-dimensional clock model with $q = 5$ spin states

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The Monte Carlo method was used to study the thermodynamic properties and phase transitions in a two-dimensional ferromagnetic clock model with $q = 5$ spin states on a triangular lattice. Systems with linear dimensions $L \times L = N$, $L = 24 \div 120$ are considered. Two maxima are found on the temperature dependence of the heat capacity, which indicate the presence in the model under study of two phase transitions of the Berezinsky–Kosterlitz–Thouless type.

Keywords: Monte Carlo method, phase transitions, clock model, thermodynamic parameters, ferromagnets.

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1. Introduction

In recent years, the study of phase transitions (PT), critical and thermodynamic properties in magnetic systems has been successfully carried out using Monte Carlo (MC) methods [1–3]. This is due to the fact that these methods allow us to study realistic models that take into account the factors present in real materials. The increase in computing capabilities of modern computers, the emergence of new algorithms specially designed to solve a wide range of problems has led to the fact that the MC method has proven itself as a powerful tool for studying the PT and thermodynamic properties of models of magnetic systems [4–6].

One of the models used to describe real physical systems is the clock model with the number of spin states q. Many physical properties of this model depend on the value of q. In the case when $q = 2$, 3, 4 this model has an exact solution. The hourly model is reduced to the Ising model and the Z_3 Potts model at $q = 2$ and 3, respectively. This model at $q = 4$ is equivalent to two copies of the Ising model. It is established that for these three cases, a second kind of PT is observed in the system from a high-temperature paramagnetic phase to a low-temperature ferromagnetic ordered phase. When $q \to \infty$ this model is reduced to the standard XY model. In this case, spontaneous symmetry breaking is not observed, but PT occurs from the low-temperature Berezinsky–Kosterlitz–Thouless (BCT) phase into the high-temperature paramagnetic phase. For a clock model with the number of spin states $q = 5$, there are very few precisely established facts. By the present time, the question remains open about the genus of PT at the value of $q = 5$.

In this paper we study a two-dimensional clock model on a triangular lattice with $q = 5$ to get an answer to this question. Practically no studies of this model on a triangular lattice have been found in the literature. In this regard, in this paper we have attempted to study the PT and thermodynamic properties of this model on a triangular lattice.

2. Model and method of study

The Hamiltonian for a clock model with q-states, which is a discretized spin XY model, can be written as follows:

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \qquad (1)$$

where the spin states q at the node i are denoted by a flat angle $\theta_i = 2\pi k_i/q$, $k_i = 1, \ldots, q$, J — parameter of the ferromagnetic exchange interaction.

In recent decades, the clock model with q-state has been widely studied both analytically [7–13] and numerically [14–25]. However, the nature of the PT is still unclear for small q, such as $q = 5$ and 6. At a value of $q = 2$, this model reduces to the classical Ising model with up-down spin symmetry, and in the limiting case, at $q \to \infty$ — XY models where the spin orientations are continuous inside the plane. In the case of a two-dimensional XY — model ($q \to \infty$), there is no far-ordered phase at finite temperatures, as stated by Mermin's theorem–Wagner [26]. Instead, the system undergoes a BCT transition of infinite order from the paramagnetic phase to the BCT phase.

In this study, we consider the case with $q = 5$ on a triangular lattice. A schematic description of this model is presented in Fig. 1. The directions for each of the 5 spin states are shown in the box. Each spin has six nearest neighbors as it is seen in the picture.

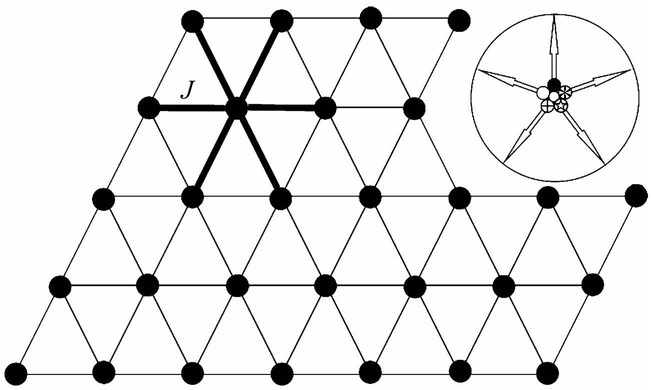

Figure 1. Schematic representation of the clock model with $q = 5$.

Lattice magnetic systems based on microscopic Hamiltonians are successfully studied on the basis of the MC [27–32] method. Recently, many new variants of algorithms have been developed for the study of such systems. One of the most effective algorithms for studying such systems is the Wang–Landau [33] algorithm, especially in the low-temperature region.

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. This 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 such transition probabilities that visiting of all energy states becomes uniform, we can obtain an initially unknown state density $g(E)$, which can be determined in order to calculate the values of the necessary thermodynamic parameters at any temperature. In particular, internal energy U, free energy F, specific heat C and entropy S. Since the density of states $g(E)$ grows very rapidly with the increase in the size of the systems under study, the value $\ln g(E)$ is used for the convenience of storing and processing large numbers.

Calculations were performed for systems with periodic boundary conditions and linear dimensions $L \times L = N$, $L = 24 \div 120$, where L — linear lattice size, N — number of spins in the system.

3. Simulation results

Wang−Landau algorithm is an effective method for calculating the energy state density. The advantage of the algorithm is that the density of states $g(E)$ in the system does not depend on temperature. Knowing the density of the states of the system, it is possible to calculate the temperature dependence of any thermodynamic parameter of interest to us. Figure 2 shows the densities of states $g(E)$ for different linear dimensions of the system (here and further on the graphs, the statistical error does not exceed the sizes of symbols used to construct dependencies). The density of states has a domed shape. The density of states $g(E)$ increases significantly with an increase in the linear dimensions of the system due to the degeneracy of the ground state.

Figure 3 shows the characteristic dependences of the heat capacity C on the temperature for systems with different linear dimensions L.

Note that on the dependences of the heat capacity C on the temperature for all systems near the critical temperature, two well-pronounced maxima are observed, which within the error range fall on the same temperature even for systems with the lowest value L. This indicates, firstly, the high efficiency of the method used to add periodic boundary conditions, and secondly, the achievement of saturation by N for the parameters we studied. The presence of two maxima on the temperature relationship of the heat capacity allows speaking about two consecutive PT in this model. A similar result was obtained in [23,34], where a clock model with $q = 5$ on a square lattice was investigated.

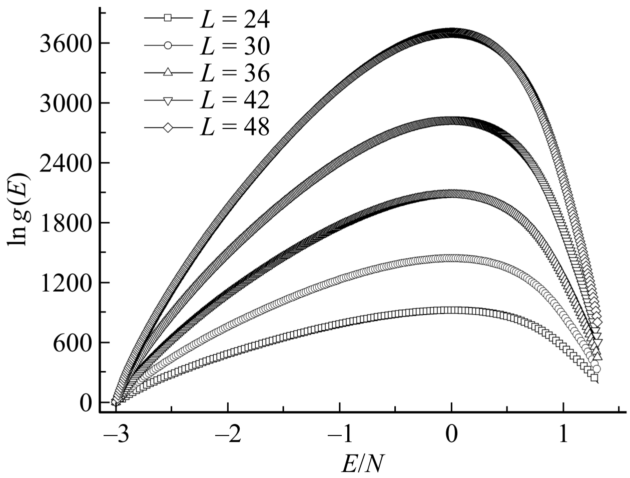

Figure 2. Density of states $g(E)$ at various linear dimensions L.

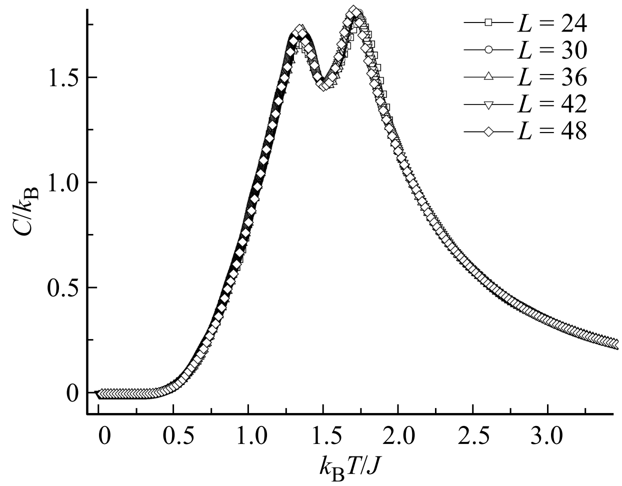

Figure 3. Dependence of heat capacity C/k_B on temperature $k_BT/|J|$ for different L.

Figure 4 shows the temperature dependence of the total energy of the spin system E for different linear lattice sizes. The figure shows that near the critical temperature, the energy changes continuously. This energy behavior is characteristic of the second kind of PT.

Figure 5 shows the temperature dependences of entropy S for systems with different linear dimensions L. The figure shows that with increasing temperature, the entropy for all systems tends to the theoretically predicted value $\ln 5$. At low temperatures close to absolute zero, entropy tends to zero for all values L. Zero residual entropy indicates the absence of degeneracy of the ground state.

To analyze the kind of phase transition, we additionally used histograms of the energy distribution. In the case of a phase transition of the first kind, the histogram of the energy distribution at the transition temperature will have two maxima located symmetrically relative to the equilibrium energy value.

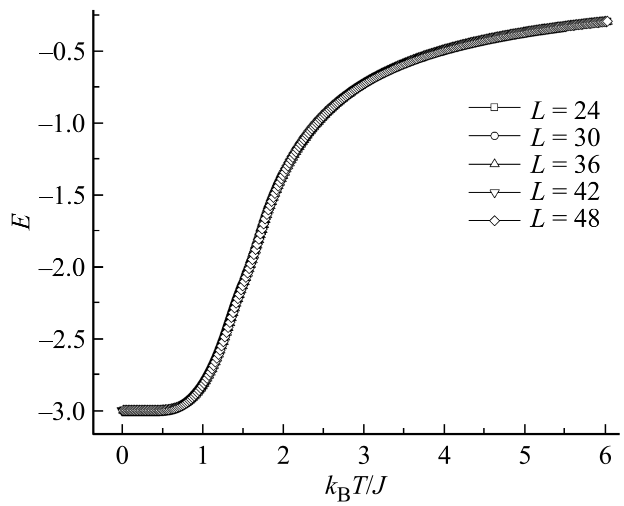

Figure 4. Dependence of energy E on temperature for different L.

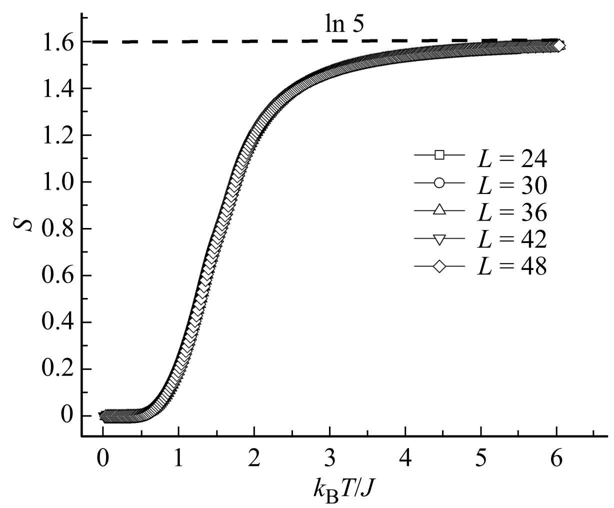

Figure 5. Temperature dependences of entropy S.

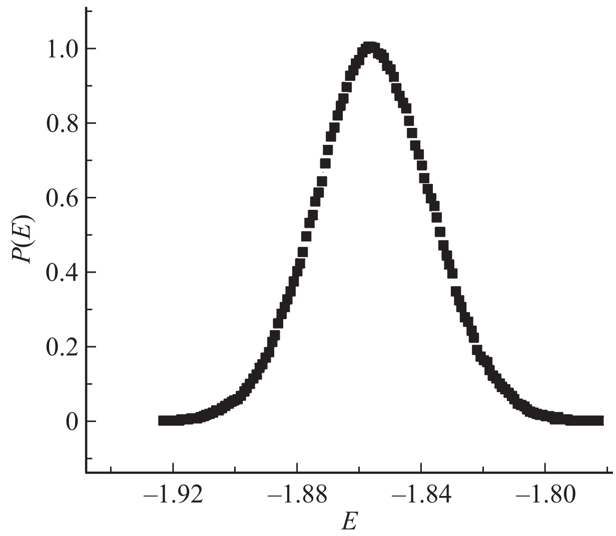

Figure 6. Histogram of energy distribution E.

Figure 6 shows the histograms of the energy distribution for the system $L = 120$. On the graph of the dependence of the probability P on the energy of the system E, one well-expressed maximum is observed. Based on this, it is possible to conclude that the behavior characteristic of a phase transition of the first kind is not observed in the system.

4. Conclusion

The thermodynamic properties of a two-dimensional clock ferromagnetic Potts model on a triangular lattice with the number of spin states $q = 5$ were studied using the Wang–Landau algorithm of the Monte Carlo method. The analysis of the obtained results shows that two maxima are observed on the temperature dependence of the heat capacity. It was found that the system has no degeneracy in the ground state. It was found that two Berezinsky–Kosterlitz–Thouless type phase transitions occur in the system.

Conflict of interest

The authors declare that they have no conflict of interest.

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