13,07,05

Phase transitions in a three-dimensional ferromagnetic Potts model on a kagome lattice

© M.K. Ramazanov[1,2], A.K. Murtazaev[1,2], T.R. Rizvanova[1], M.R. Dzhamaludinov[1], M.A. Magomedov[1,2]

[1] Institute of Physics of the Dagestan Federal Research Center of the Russian Academy of Sciences, Makhachkala, Dagestan Republic, Russia
[2] Dagestan State University, Makhachkala, Dagestan Republic, Russia

E-mail: sheikh77@mail.ru

Received May 13, 2025
Revised August 20, 2025
Accepted August 26, 2025

The Monte Carlo method was used to study phase transitions and thermodynamic properties of the three-dimensional ferromagnetic Potts model with the number of spin states $q = 4$ on the kagome lattice with nearest neighbor interactions. Temperature dependences of energy and heat capacity were constructed. The nature of the phase transition was analyzed using the fourth-order Binder cumulants method and the histogram method. It was found that the first-order phase transition is observed in this model.

Keywords: Monte Carlo method, Binder cumulants, spin interactions, heat capacity.

DOI: 10.61011/PSS.2025.09.62364.117-25

1. Introduction

Investigation of phase transitions (PT) and thermodynamic properties of spin lattice models still attracts a large attention of specialists [1–5]. When studying the phase transitions and critical phenomena, the most fruitful were ideas laid down in a hypothesis of scaling, universality and in a renormalization group theory [6]. In recent years, the phase transitions in the spin systems are successfully studied by a Kramers–Wannier transfer-matrix method [7,8]. It is extremely difficult to investigate the spin lattice models based on microscopic Hamiltonians by theoretical physics methods. It resulted in investigation of the phase transitions and the critical phenomena by numerical experiment methods [6,9].

One of the spin lattice model that now receives increased interest is the Potts model. The interest in this model is caused by the fact that the Potts model serves as a basis for theoretical description of a wide range of physical properties in the condensed matter physics. These include some classes of adsorbed gases on graphite, complex anisotropic ferromagnetics of a cubic structure, various multilayer magnetic systems, spin glasses, multicomponent alloys, etc. [10–12]. As an example of substances described by the Potts model, we can provide adsorbed films: adsorbed hydrogen atoms (2×2) — 2H—Ni(111) on the surface of nickel Ni(111) are arranged at lattice sites [13]. In these adsorbed structures, the phase transitions are described by a universality class of two-dimensional Potts models when $q = 4$ [14].

Physical properties of the Potts model depend on a spatial dimension of the lattice, a number of the spin states q and a geometry of the lattice [10,15–23]. Depending on the number of the spin states q and the spatial dimension, the Potts model demonstrates the first- or second-order phase transition. The ferromagnetic Potts model is quite well studied in a two-dimensional case [10,24]: when $q > 4$ the system demonstrates the first-order phase transition, whereas when $q \leq 4$ the transition is continuous. It is known for the three-dimensional case that when $q > 3$ the system exhibits the first-order phase transition. Behavior of an antiferromagnetic Potts model is considered to be more complicated. In the three-dimensional antiferromagnetic Potts model, for $q = 3$ and 4, the simple cubic lattice exhibits the second-order phase transition, whereas for $q = 5$ a zero temperature transition is observed, and for $q = 6$ the order is absent at any temperatures [25].

Unlike the ferromagnetic two-dimensional Potts model that is quite well studied due to its universality, the three-dimensional model still has open issues related to investigation of a nature and a character of the phase transition, the influence of external disturbing factors on critical and thermodynamic properties, etc.

In this regard, in the present study, based on a replica algorithm of the Monte Carlo method we have attempted to study the phase transition and thermodynamic properties of the ferromagnetic three-dimensional Potts with the number of the spin states $q = 4$ on the kagome lattice with interaction of the nearest neighbors.

2. Model and method of study

Taking into account interactions of the nearest neighbors, a Hamiltonian of the Potts model with the number of the

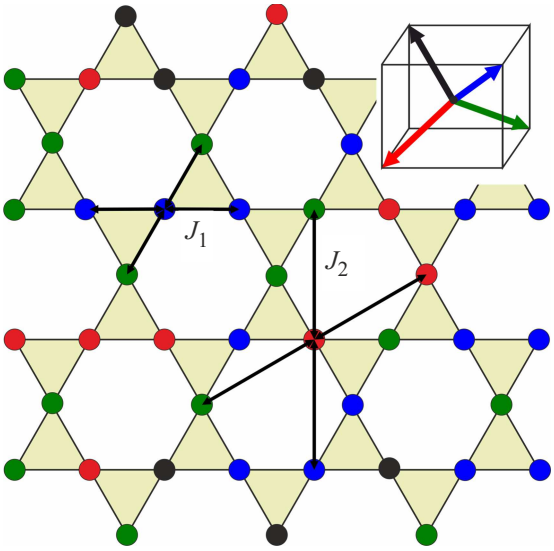

Figure 1. Potts model with the number of the spin states $q = 4$ on the kagome lattice.

spin states $q = 4$ can be written as follows:

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

where J_1 is a parameter of exchange ferromagnetic ($J_1 > 0$) interaction of the nearest neighbors, $\theta_{i,j}$ is an angle between the interacting spins $S_i - S_j$.

The Potts model on the kagome lattice is schematically described in Figure 1 for the two-dimensional case.

The present article considers the lattice that consists of such two-dimensional layers folded along the orthogonal axis. As it is clear in the figure, each spin in each layer has four nearest (J_1) and four second (J_2) neighbors. In the three-dimensional case, interactions of two other spins in the nearest layers are added. Thus, the number of the nearest spins in the model in question is six. The present study does not take into account interaction of the second neighbors ($J_2 = 0$).

Spins marked with circles of the same color have the same direction. The insert in the figure shows the corresponding color representation for each of the four possilbe spin directions. The spin directions are pre-defined in such a way that the following equality is valid:

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

According to the condition (2), for the two spins S_i and S_j the energy of pair exchange interaction $E_{i,j} = -J_1$ if $S_i = S_j$. In case when $S_i \neq S_j$, the energy is $E_{i,j} = J_1/3$. Thus, the energy of pair interaction of the spins is equal to one value when their directions are the same, and takes another value when the directions of the spins do not coincide. For the Potts model when $q = 4$ in the three-dimensional space, this is only possible if the spins are oriented as shown in the insert in Figure 1.

At present, such systems based on the microscopic Hamiltonians are being successfully studied based on the MC [26–29]. Many new variants of the MC algorithms have been developed recently. One of the most effective algorithms for studying these systems is the replica exchange algorithm [30]. The replica exchange algorithm is effective for studying the systems with large linear sizes and in a critical area. Therefore, we used this algorithm in the present study. We used the replica exchange algorithm in the following form:

1. Simultaneously, N replicas $X_1, X_2, \ldots, X_N$ with the temperatures $T_1, T_2, \ldots, T_N$ are simulated.

2. After performing one MC step/spin for all the replicas, data is exchanged between a pair of adjacent replicas X_i and X_{i+1} in accordance with the Metropolis scheme with probability

3.

$$w(X_i \to X_{i+1}) = \begin{cases} 1, & \text{for } \Delta \leq 0, \\ \exp(-\Delta), & \text{for } \Delta > 0, \end{cases}$$

where $\Delta = -(U_i - U_{i+1}) \cdot (1/T_i - 1/T_{i+1})$, U_i and U_{i+1} are internal energies of the replicas.

The main advantage of this algorithm is that probability of exchange is *a priori* known, whereas for other algorithms determination of probability is a quite long procedure and takes much time. For each replica, the replica exchange algorithm implements random wandering across a „temperature interval“, which in turn stimulates random wandering in the field of potential energy. It helps to solve a problem of „sticking“ of the system in many states with a local minimum energy, which is typical for the spin system with frustrations.

The calculations were performed for the systems with periodic boundary conditions (PBC) and linear dimensions $L \times L \times L = N$, $L = 12-96$, where L is measured in lattice cell sizes.

3. Simulation results

To observe a temperature behavior of heat capacity C we used the following expression [31]

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

where $K = |J_1|/(k_B T)$, U is internal energy.

Figure 2 shows temperature dependences of heat capacity C (hereinafter a statistical error does not exceed sizes of symbols used for plotting the dependences) for the systems with various linear sizes. It is clear that for all the systems near the critical temperature, the dependence of heat capacity on the temperature exhibits well-pronounced maximums that increase with an increase of the number of the spins in the system, wherein within the limits of

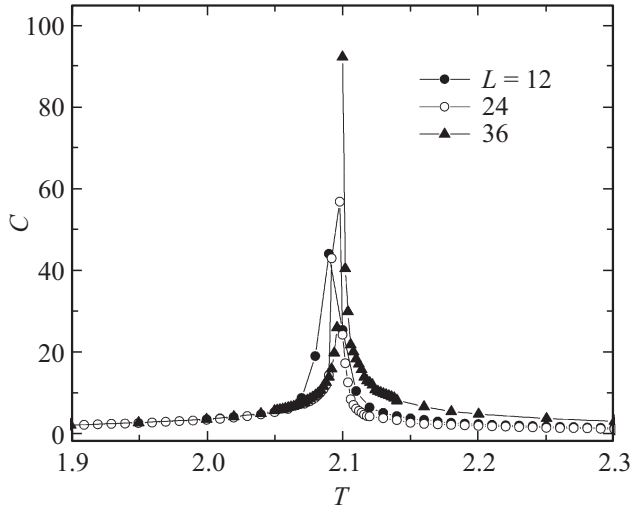

Figure 2. Temperature dependences of heat capacity C.

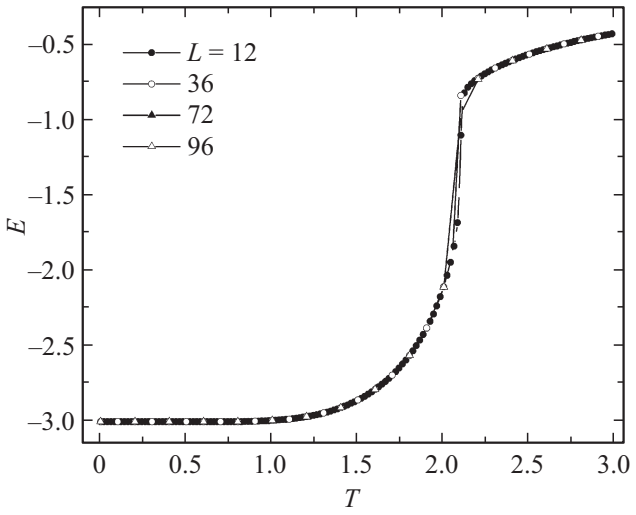

Figure 3. Temperature dependence of energy E.

an error these maximums fall within the same temperature even for the systems with the least value of L. This indicates, firstly, the high efficiency of the method used to add PBCs, and secondly, the achievement of saturation by N for many parameters studied by us. An abrupt increase of the maximum (the sharp maximum) of heat capacity with the increase of the linear sizes is typical for the systems, in which the first-order phase transition is observed.

Figure 3 shows temperature dependences of the energy E for the system with the various L. As it is clear in the figure, a sharp jump of the energy is observed for all L in the critical area. This behavior is typical for the first-order phase transition. Thus, the temperature dependences of heat capacity and the energy support the first-order phase transition.

In order to analyze the phase transition character and to determine the critical temperature T_C, we used a method of fourth-order Binder cumulants [9]:

$$V_L = 1 - \frac{\langle U^4 \rangle_L}{3\langle U^2 \rangle_L^2} \tag{4}$$

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} \tag{5}$$

where V_L is an energy cumulant, U_L is a magnetic cumulant.

The expressions (4) and (5) allow determining the critical temperature T_C with high accuracy for the first- and second-order phase transitions, respectively. Also, the use of the Binder cumulants allows good testing of the phase transition type in the system. It is known that the first-order phase transitions are characterized by the fact that the magnitude V_L tends to some non-trivial value V^* according to the expression

$$V_L = V^* + bL^{-d} \tag{6}$$

when $L \to \infty$ and $T = T_C(L)$, where the value of V^* is different from 2/3, and the minimum magnitude $U_{L\,\min}(T = T_{\min})$ diverges: $U_{L\,\min}(T = T_{\min}) \to \infty$ when $L \to \infty$.

In case of the second-order phase transition, curves of the temperature dependence of the Binder cumulants U_L have a clearly defined point of intersection [9]. Our data are analyzed to show that the typical dependences U_L on the temperature do not intersect in the same point in the critical area at the various values of L. This supports the first-order phase transition in this model. The temperature dependence of the energy cumulant V_L is shown in Figure 4 at the various values of L. As it is clear from the graph, the value of V_L does not tend to 2/3, while the value of V^* is 2/3, which is typical for the first-order phase transition. This value is calculated using the expression (6).

In order to more exactly determine the phase transition order, we used MC data histogram analysis [32,33]. This method allows for reliable determination of the phase transition order. A procedure of determination of the phase transition order by this method is described in detail in the studies [34,35]. The results that are obtained based on the data histogram analysis show that the first-order phase transition is observed in this model. It is demonstrated in Figure 5. This figure shows energy distribution histograms for the system with the various linear sizes. The graph is plotted for the temperature that is close to the critical temperature. It is clear from the figure that the dependence of probability W on the energy exhibits two maximums, which indicate the first-order phase transition. The presence of the two maximums on the energy distribution histograms is a sufficient condition for the first-order phase transition.

Figure 6 shows the energy distribution histograms for the system with the linear sizes $L = 24$. The graphs are plotted at the various temperatures that are close to the critical temperature. It is clear from the figure that for all the temperatures the dependence of probability W on the energy E exhibits two maximums that indicate the first-order phase transition.

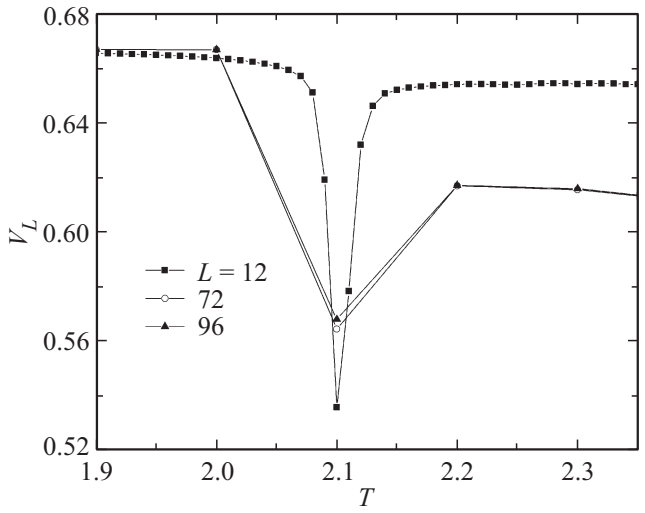

Figure 4. Temperature dependencies of the Binder energy cumulant V_L.

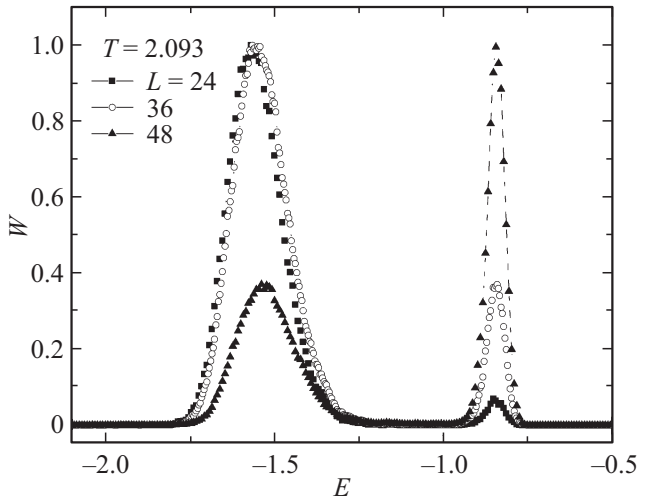

Figure 5. Histograms of distribution of the energy for the various L.

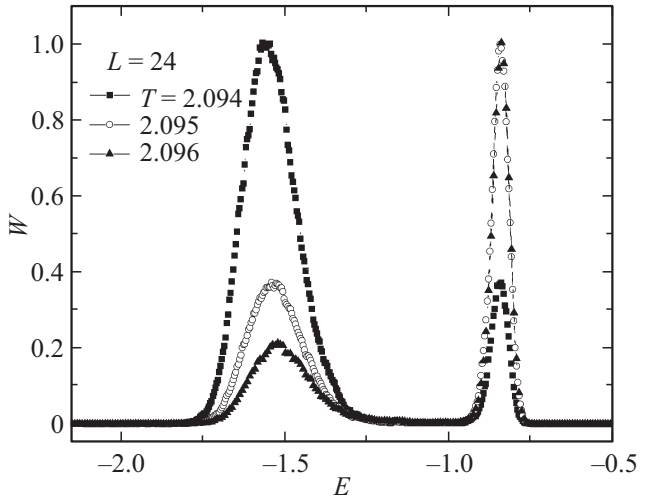

Figure 6. Histograms of distribution of the energy for the various T.

4. Conclusion

The phase transitions in the ferromagnetic three-dimensional Potts model with the number of the spin states $q = 4$ on the kagome lattice have been studied taking into account interactions of the nearest neighbors using the replica algorithm of the Monte Carlo method. The character of the phase transitions is analyzed based on the Binder cumulant method and the data histogram analysis. It is shown that the first-order phase transition is observed in the model in question.

Funding

This research was supported by the grant provided by the Russian Science Foundation No. 25-12-20029.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] M. Schmidt, G.L. Kohlrausch, F.M. Zimmer. Physica A **596**, 127126 (2022).
[2] K. Dutta, D. Talukdar. JMMM **556**, 169344 (2022).
[3] D.N. Yasinskaya, V.A. Ulitko, Yu.D. Panov. Phys. Solid State **63**, *10*, 1588 (2021).
[4] A.O. Sorokin. Physica A **602**, 127621 (2022).
[5] A.K. Murtazaev, M.K. Ramazanov. Phys. Solid State **65**, *9*, 1399 (2023).
[6] I.K. Kamilov, A.K. Murtazaev, Kh.K. Aliev. Phys. — Uspekhi **42**, *7*, 689 (1999).
[7] A.V. Zarubin, F.A. Kassan-Ogly, A.I. Proshkin. JMMM **514**, 167144 (2020).
[8] E.S. Tsuvarev, F.A. Kassan-Ogly, A.I. Proshkin. JETP **131**, (2020).
[9] K. Binder, D.W. Heermann. Monte Carlo Simulation in Statistical Physics: An Introduction. Springer, Berlin/Heidelberg (2010).
[10] F.Y. Wu. Rev. Mod. Phys. **54**, *1*, 235 (1982).
[11] H.T. Diep. Frustrated Spin Systems. World Scientific Publishing Co. Pte. Ltd., Singapore (2004). P. 624.
[12] W. Zhang, Y. Deng. Phys. Rev. E **78**, *3*, 031103 (2008).
[13] L. Schwenger, K. Budde, C. Voges, H. Pfnür. Phys. Rev. Lett. **73**, *2*, 296 (1994).
[14] K. Budde, L. Schwenger, C. Voges, H. Pfnür. Phys. Rev. B **52**, *13*, 9275 (1995).
[15] M. Nauenberg, D.J. Scalapino. Phys. Rev. Lett. **44**, *13*, 837 (1980).
[16] J.L. Cardy, M. Nauenberg, D.J. Scalapino. Phys. Rev. B **22**, *5*, 2560 (1980).
[17] M.K. Ramazanov, A.K. Murtazaev, M.A. Magomedov. Physica A **521**, 543 (2019).
[18] H. Feldmann, A.J. Guttmann, I. Jensen, R. Shrock, S.-H. Tsai. J. Phys. A **31**, *10*, 2287 (1998).
[19] H. Duminil-Copin, V. Sidoravicius, V. Tassion. Commun. Math. Phys. **349**, *1*, 47 (2017).
[20] N. Schreiber, R. Cohen, S. Haber. Phys. Rev. E **97**, *3*, 032106 (2018).

[21] F.A. Kassan-Ogly, A.I. Proshkin. Phys. Solid State **60**, 1090 (2018).
[22] M.A. Fadeeva, L.N. Shchur. JETP **135**, *6*, 869 (2022).
[23] M.K. Ramazanov, A.K. Murtazaev, M.A. Magomedov, M.K. Mazagaeva. Phys, Metals. Metallogr. **124**, *5*, 429 (2023).
[24] R.J. Baxter. J. Phys. C **6**, *23*, L445 (1973).
[25] C. Yamaguchi, Y. Okabe. J. Phys. A **34**, *42*, 8781 (2001).
[26] M.K. Ramazanov, A.K. Murtazaev. JETP Lett. **101**, *10*, 714 (2015).
[27] M.K. Ramazanov, A.K. Murtazaev. JETP Lett. **106**, *2*, 86 (2017).
[28] M.K. Ramazanov, A.K. Murtazaev, M.A. Magomedov, M.K. Mazagaeva. Phys. Solid State **62**, *3*, 499 (2020).
[29] M.K. Ramazanov, A.K. Murtazaev. JETP Lett. **109**, *9*, 589 (2019).
[30] A. Mitsutake, Y. Sugita, Y. Okamoto. Biopolymers (Peptide Sci.) **60**, *2*, 96 (2001).
[31] P. Peczak, A.M. Ferrenberg, D.P. Landau. Phys. Rev. B **43**, *7*, 6087 (1991).
[32] F. Wang, D.P. Landau. Phys. Rev. E **64**, *5*, 0561011 (2001).
[33] F. Wang, D.P. Landau. Phys. Rev. Lett. **86**, *10*, 2050 (2001).
[34] M.K. Ramazanov, A.K. Murtazaev. JETP Lett. **103**, *7*, 460 (2016).
[35] A.K. Murtazaev, T.R. Rizvanova, M.K. Ramazanov, M.A. Magomedov. Phys. Solid State **62**, *8*, 1434 (2020).

Translated by M.Shevelev