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Phase diagram of antiferromagnetic Potts model on the kagome lattice

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

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

E-mail: sheikh77@mail.ru

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Using the method of computer simulation, phase transitions 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 were carried out. The studies were carried out for the magnitude of the exchange interaction of second neighbors in the range $0 \leq J_2 \leq 1$. A phase diagram of the dependence of the critical temperature on the magnitude of interactions of second neighbors was constructed. An analysis of the nature of phase transitions was carried out. It was found that for values $J_2 = 0$ and 0.1 there is no phase transition in this model. It is shown that in the range $0.2 \leq J_2 \leq 1$ a second-order phase transition is observed.

Keywords: frustrations, phase transitions, Monte Carlo method, Potts model.

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1. Introduction

The study of phase transitions (PTs), critical, magnetic and thermodynamic properties of compounds having a kagome lattice attracted much attention. This is due to the fact that in antiferromagnetic compounds having the kagome lattice, frustration may occur due to the special geometry of the lattice. Frustration effects play an important role in magnetic systems. Experimental, theoretical and numerical studies made it possible to establish that magnetic systems with frustrations in many ways exhibit properties different from the corresponding non-frustrated systems, which causes increased interest in the study of frustration phenomena in magnetic systems [1–3]. Spin lattice models are widely used to study the physical properties of such systems.

One of the spin lattice models that recently received increased interest is the Potts model. The interest in this model is caused by the fact, that Potts model serves as a basis for the theoretical description of a wide range of physical properties in the physics of condensed matter. These include some classes of adsorbed gases on graphite, complex anisotropic ferromagnets of cubic structure, various multilayer magnetic systems, spin glasses, multicomponent alloys, etc. [1,4,5]. As an example of substances described by the Potts model and having a hexagonal lattice structure, we can provide adsorbed films: adsorbed hydrogen atoms $(2 \times 2)-2H/Ni(111)$ on the surface of nickel Ni(111) are placed at the nodes of the hexagonal lattice [6]. In such adsorbed structures PTs are described by the universality class of two-dimensional Potts models with $q = 4$ [7].

In recent years, a significant number of papers [4,8–16] was devoted to the study of spin systems described by the Potts model, in papers it was 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 second neighbors and the geometry of the lattice. Analysis of the data obtained in these papers shows that, depending on the number of spin states q and the spatial dimension, the Potts model demonstrates PT of the first or second kind. The two-dimensional Potts model with the number of spin states $q = 4$ is quite unique and is still poorly understood. This model is also interesting because the value $q = 4$ is the boundary value of the interval $2 \leq q \leq 4$, 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 the present paper we studiedy of 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 J_2. This model at $J_2 = 0$ is frustrated model. Consideration of ferromagnetic interactions of second neighbors in this model can lead to the appearance of different phases and PTs, and also affect its physical properties. The study of the influence of the magnitude of the ferromagnetic interaction of second neighbors on PT in the model under consideration is practically absent the literature. In connection with this, in this paper we study PT of this model in a wide range of values of the magnitude of the interaction of second neighbors.

2. Model and method of study

A Hamiltonian of a Potts model with the number of spin states $q = 4$ taking into consideration interactions of

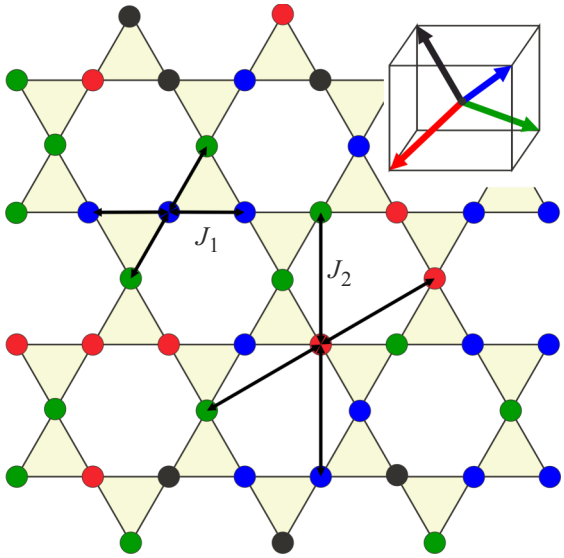

Figure 1. Potts model with the number of spin states $q = 4$ on Kagome lattice. The insert shows the corresponding color representation for each of the four possible spin directions.

the first and second nearest neighbors, can be written as follows [17,18]:

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

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

where J_1 and J_2 — parameters of exchange antiferromagnetic ($J_1 < 0$) and ferromagnetic ($J_2 > 0$) interactions, respectively, for the first and second neighbors, $\theta_{i,j}$, $\theta_{i,k}$ — angles between interacting spins $S_i - S_j$ and $S_i - S_k$. This paper considers the range of values $0 \leq J_2 \leq 1$ with a step of 0.1.

A schematic description of model under study is presented in Figure 1. As can be seen in the Figure, each spin has four nearest (J_1) and four next nearest (J_2) neighbors. 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 possible spin directions. Spin directions were defined in such a way that the following equality is valid

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

According to condition (2), for two spins S_i and S_j the energy of the pair exchange interaction is $E_{i,j} = -J_1$ if $S_i = S_j$. If $S_i \neq S_j$, the energy is $E_{i,j} = J_1/3$. Thus, the energy of the pair interaction of 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 with $q = 4$ in three-dimensional space, this is only possible if the spins are oriented as shown in the insert Figure 1.

Currently one of the most effective algorithms for studying such systems is the Wang–Landau algorithm of Monte Carlo method [19], especially in the low-temperature region. Therefore, we used this algorithm in this study. This algorithm allows you to calculate the density function of states of the system and produces spin configurations in the system. The Wang–Landau algorithm is described in more detail in the paper [10]. Having determined the density of states of system $g(E)$, we can 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:

$$U(T) = \frac{\sum\limits_E E g(E) e^{-E/k_B T}}{\sum\limits_E g(E) e^{-E/k_B T}} \equiv \langle E \rangle_T, \qquad (3)$$

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

$$C = \left(\frac{(|J_1|/k_B T)^2}{N}\right)\left(\langle U^2\rangle - \langle U\rangle^2\right) \qquad (5)$$

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

where $K = |J_1|/k_B T$, N — number of particles, T — temperature (hereinafter the temperature is given in units $|J_1|/k_B$), (U is a normalized value). Calculations were performed for systems with periodic boundary conditions (PBC) and linear dimensions $L \times L = N$, $L = 12 \div 72$, where L is measured in lattice cell sizes.

3. Simulation results

Figure 2 shows the temperature dependences of entropy S for different vaues J_2 obtained for the system with linear size $L = 24$ (hereinafter the statistical error does not exceed symbol sizes used to plot dependencies). This figure shows that the system entropy with temperature increasing tends to the theoretically predicted value $\ln 4$. For the case $J_2 = 0$ in the low-temperature region the entropy tends to a nonzero value. Moreover, this entropy value differs highly from zero. This behavior of entropy indicates that for $J_2 = 0$ the ground state of the system is highly degenerate. Such behavior of entropy is typical for frustrated spin systems. When the second neighbors are included ($J_2 \geq 0.1$) in the low-temperature region the entropy tends to zero. This means that the exchange interaction of second neighbors in this model removes the degeneracy of the ground state, even at small values J_2.

Temperature dependences of heat capacity C for different values J_2 and linear dimensions L are presented in Figure 3. As can be seen in the Figure, for the value $J_2 = 0.1$ there is no sharp peak in the temperature dependence of the heat

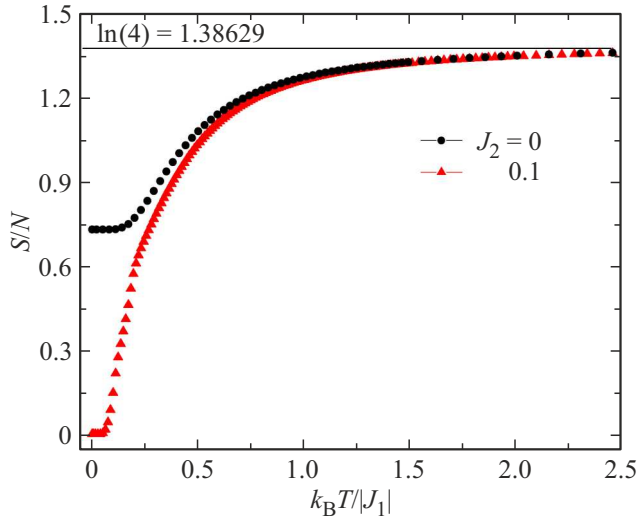

Figure 2. Temperature dependence of entropy S.

capacity, but a smoothed peak is observed. The absence of a pronounced peak in heat capacity is explained by the fact that at $J_2 \leq 0.1$ there is no order in this model. For the values $J_2 = 0.2$ and $J_2 = 0.3$ the splitting of the heat capacity is observed. The graph shows two peaks and one smooth „hump“ (Figure 3, *a*). The presence of „hump“ indicates that the system is low-dimensional, and the heat capacity splitting is usually observed for frustrated spin systems [2,20]. For the model we are studying, the heat capacity splitting is due to the fact that consideration of the exchange interactions of second neighbors leads to the appearance of a partially ordered magnetic state. With value J_2 increasing the smooth „hump“ and the low-temperature peak disappear, and one pronounced peak remains (Figure 3, *b*). This Figure shows that dependence of the heat capacity C on temperature for all systems near the critical temperature shows well-defined maxima, which increase with increase in number of spins in the system, and these maxima, within the limits of error, 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 PBC, and secondly, the achievement of saturation by N for many parameters we studied.

To analyze the character of PT and to determine the critical temperature T_N we used the method of fourth-order Binder cumulants [21]:

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} \tag{7}$$

where U_L — magnetic cumulant.

The parameter of system order m was calculated by the formula:

$$m = \frac{1}{N}\left(\frac{4N_{\max} - N_1 - N_2 - N_3 - N_4}{3}\right) \tag{8}$$

where N_1, N_2, N_3, N_4 — number of spins corresponding to one of 4 spin directions, respectively.

Expression (7) allows to define the critical temperature T_N more accurately for PT of second kind. Also, the use of Binder cumulants allows good testing the type of PT in a system. In case of PT of the second kind the temperature dependency curves of Binder cumulants U_L have a clearly defined point of intersection [21].

Figure 4 shows typical dependence of U_L on temperature for $J_2 = 0.5$ at different values L. It can be seen from the graph that in the critical region the temperature dependencies U_L intersect each other in a single point ($T_N = 0.662$). This supports the assumption of PT of the second kind presence in this model. Similar picture is observed for all values in the range of $0.2 \leq J_2 \leq 1.0$.

Figure 5 shows the phase diagram of critical temperature vs. magnitude of interaction of the next to nearest neighbors. The diagram shows that for the values $J_2 = 0.0$ and 0.1 the critical temperature is zero, and there is no PT. This is explained by the absence of magnetic ordering in this model at $J_2 \leq 0.1$. The increase in the contribution of the influence of exchange interaction of next to nearest neighbors in this model leads to PT occurrence.

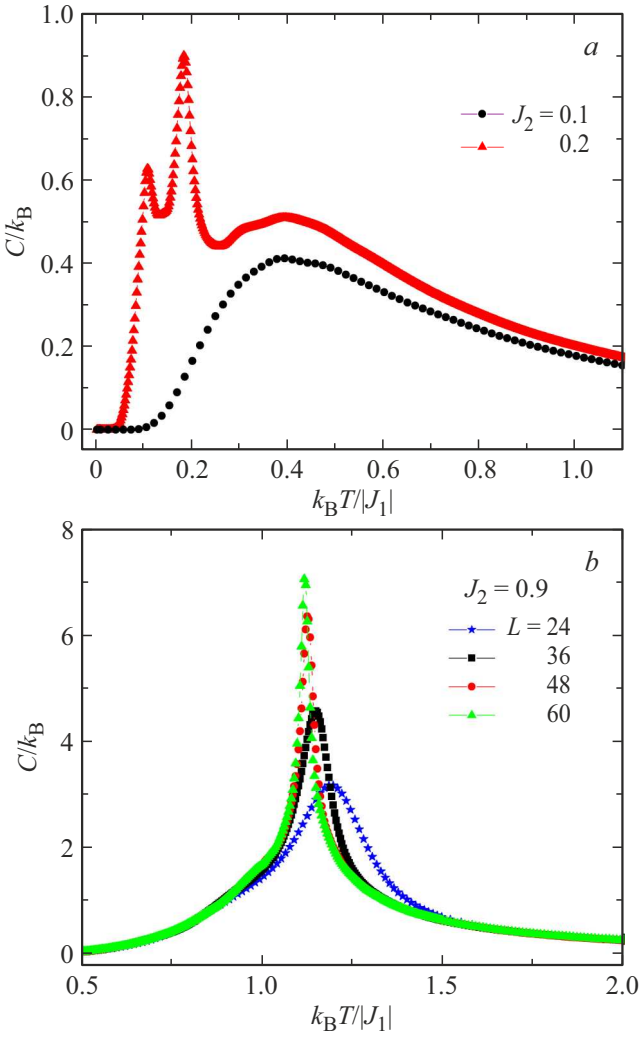

Figure 3. Temperature dependencies of heat capacity C.

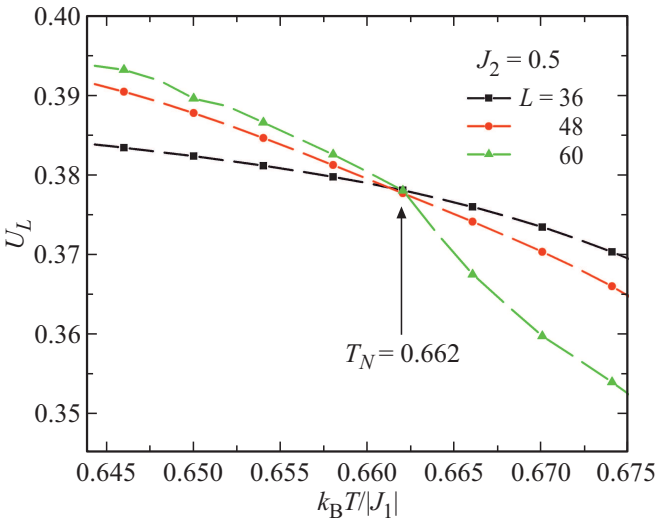

Figure 4. Temperature dependencies of Binder magnetic cumulant U_L.

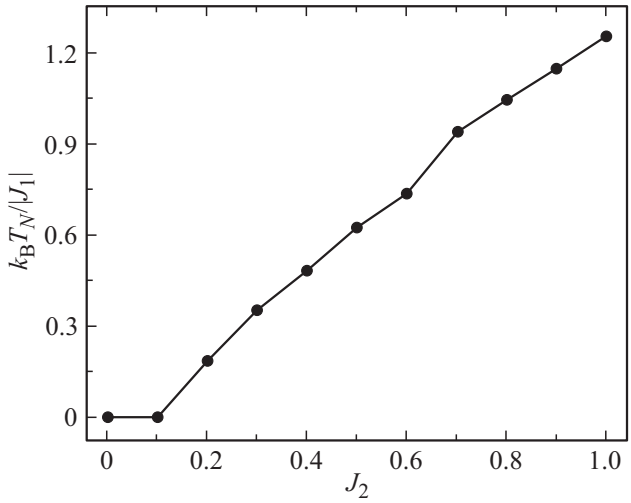

Figure 5. Phase diagram of critical temperature vs. magnitude of interaction of the next to nearest neighbors.

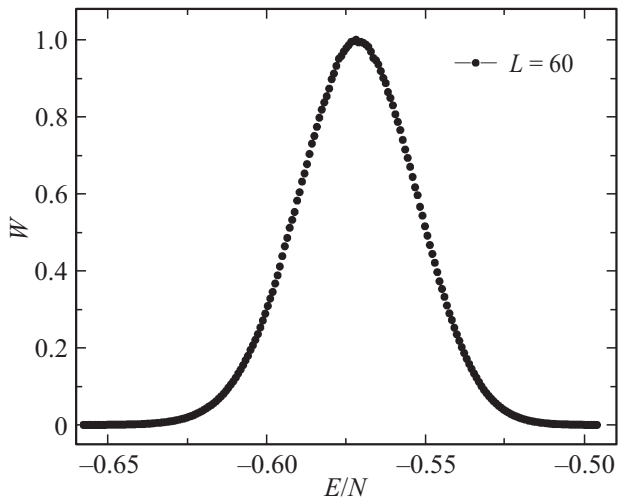

Figure 6. Histograms of the energy distribution for $J_2 = 0.5$.

To determine PT kind, we used histogram data analysis of MC method [19,22]. This method allows for reliable determination of PT kind. PT order calculation procedure by this method is described in detail in [23,24]. The results obtained on the basis of histogram data analysis show that PT of the second kind is observed in this model in range $0.2 \leq J_2 \leq 1.0$. This is demonstrated in Figure 6. This Figure shows the histogram of the energy distribution for system with linear size $L = 60$ for the value $J_2 = 0.5$. The graph is plotted for temperature close to the critical temperature ($T_N = 0.622$). It can be seen from the Figure that in the dependence of the probability W on energy one maximum is observed, which indicates PT of second kind. The presence of the one maximum in energy distribution histograms is a sufficient condition for the PT of the second kind. Note, that one maximum in the distribution histograms for the model under study are observed for values J_2 in the range $0.2 \leq J_2 \leq 1.0$. This allows us to state that in this range of values J_2 PTs of the second kind are observed.

4. Conclusion

The study of phase transitions in the two-dimensional antiferromagnetic Potts model with the number of spin states $q = 4$ on the kagome lattice, taking into account ferromagnetic interactions of second neighbors, was carried out using the Wang–Landau algorithm of the Monte Carlo method. The analysis of the nature of phase transitions was carried out in a wide range of values of the interaction between second neighbors J_2. It is shown that in the interval $0.2 \leq J_2 \leq 1$ the phase transition of second kind is observed. For values $J_2 \leq 0.1$ there is no order in the system, and frustrations are observed. It is shown that at the value $J_2 = 0$ the ground state of the system is highly degenerate. Consideration of ferromagnetic interactions of second neighbors leads to the removal of degeneracy of the ground state for values $J_2 \geq 0.1$.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] H.T. Diep. Frustrated Spin Systems. World Scientific Publishing Co. Pte. Ltd., Singapore (2004). P. 624.
[2] F.A. Kassan-Ogly, A.K. Murtazaev, A.K. Zhuravlev, M.K. Ramazanov, A.I. Proshkin. JMMM **384**, 247 (2015).
[3] M.K. Ramazanov, A.K. Murtazaev. FTT **65**, 1455 (2023). (in Russian).
[4] F.Y. Wu. Rev. Mod. Phys. **54**, 235 (1982).
[5] W. Zhang, Y. Deng. Phys. Rev. E **78**, 031103 (2008).
[6] L. Schwenger, K. Budde, C. Voges, H. Pfnur. Phys. Rev. Lett. **73**, 296 (1994).
[7] K. Budde, L. Schwenger, C. Voges, H. Pfnur. Phys. Rev. B **52**, 9275 (1995).

[8] M. Nauenberg, D.J. Scalapino. Phys. Rev. Lett. **44**, 837 (1980).
[9] J.L. Cardy, M. Nauenberg, D.J. Scalapino. Phys. Rev. B **22**, 2560 (1980).
[10] M.K. Ramazanov, A.K. Murtazaev, M.A. Magomedov. Phys. A **521**, 543 (2019).
[11] H. Feldmann, A.J. Guttmann, I. Jensen, R. Shrock, S.-H. Tsai. J. Phys. A **31**, 2287 (1998).
[12] F.A. Kassan-Ogly, A.I. Proshkin. Phys. Solid State. **60**, 1090 (2018).
[13] M.A. Fadeeva, L.N. Schur. ZhETF **162**, 909 (2022). (in Russian).
[14] A.K. Murtazaev, M.K. Ramazanov, M.K. Mazagaeva, M.A. Magomedov. ZhETF **156**, 502 (2019). (in Russian).
[15] D.R. Kurbanova, M.K. Ramazanov, M.A. Magomedov, A.K. Murtazaev. ZhETF **163**, 816 (2023). (in Russian).
[16] M.K. Ramazanov, A.K. Murtazaev, M.A. Magomedov, M.K. Mazagaeva. FMM **124**, 339 (2023). (in Russian).
[17] M.G. Townsend, G. Longworth, E. Roudaut. Phys. Rev. B **33**, 4919 (1986).
[18] Y. Chiaki, O. Yutaka. J. Phys. A **34**, 8781 (2001).
[19] F. Wang, D.P. Landau. Phys. Rev. E **64**, 0561011−1 (2001).
[20] F.A. Kassan-Ogly F.A., B.N. Filippov, A.K. Murtazaev, M.K. Ramazanov, M.K. Badiev. JMMM **24**, 3418 (2012).
[21] K. Binder, D. Heermann. Monte Carlo Simulation in Statistical Physics: An Introduction. Springer, Berlin, Heidelberg (2010).
[22] F. Wang, D.P. Landau. Phys. Rev. Lett. **86**, 2050 (2001).
[23] M. K. Ramazanov, A.K. Murtazaev. Pis'ma v ZhETF **103**, 522 (2016). (in Russian).
[24] A.K. Murtazaev, T.R. Rizvanova, M.K. Ramazanov, M.A. Magomedov. FTT **62**, 1278 (2020). (in Russian).

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