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ORDER, DISORDER, AND PHASE TRANSITION IN CONDENSED SYSTEM

Simulation of a Four-Component Potts Model on a Hexagonal Lattice by the Wang–Landau Method with Controlled Accuracy

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Abstract—The critical behavior of a four-component Potts model on a hexagonal lattice is investigated numerically. A modified Wang–Landau method is used with controlled accuracy of estimating the density of states (DOS). The finite-dimensional analysis of the results confirms the presence of a second-order phase transition with critical exponents corresponding to the universality class of the two-dimensional four-component Potts model.

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1. INTRODUCTION

The theory of second-order phase transitions provides a classification of statistical physics models with ferromagnetic interaction over a set of features such as the spatial dimension of the system, the dimension of the order parameter, and the symmetry of the ground state (see, for example, [1]). The universality hypothesis is a consequence of the approach to critical phenomena—a renormalization group theory in which the details of the Hamiltonian do not affect the critical exponents and scaling transformations of functions [2]. The results obtained with this theory were confirmed within general theories such as conformal field theory [3, 4] and the stochastic Schramm–Loewner evolution theory [5, 6]. There are a large number of numerical studies that sufficiently reliably reproduce the critical exponents and do not contradict the universality hypothesis. Moreover, the results of the study of nonequilibrium systems are also formulated in terms of universality [7]. Thus, numerous systems with various details of the Hamiltonian and small-scale differences are well classified by a set of critical exponents that depends only on the global properties of the Hamiltonian. Technically, this can be expressed in such a way that the amplitude of the correlation length depends on local properties, but its decrease at large distances in the neighborhood of a phase transition does not depend on local properties, and the behavior at large distances is described by a universal function.

It should be noted that not all quantities are universal. For example, the values of the critical amplitudes of universal functions are not universal in and of themselves, and only some of their combinations are independent of the details of the Hamiltonian [1]. One should also carefully interpret universality in reduced dimension systems in which the finiteness of a system in one direction can give explicit dependence on both the size of the system and the type of boundary conditions. Of course, these phenomena are also a consequence of global effects, because the size of the system and the type of boundary conditions limit the divergence of the correlation length, whereby the dependence on the size of the system becomes explicit. A remarkable example is given by the expression for the correlation length in the Ising model on an infinite strip of finite width L with free boundary conditions at the edges of the strip, $\xi(L) \propto L/\pi$, which was obtained in [8] with the help of conformal field theory [3] with explicit dependence of the correlation length on the width of the strip. This dependence is universal given the width of the strip and the type of boundary conditions.

One more refinement of universality comes from the anisotropy of the system [9]. For example, for the Ising model on a triangular lattice with the spin–spin interaction constant J' along one of the lattice directions and the interaction constant J along the two other directions, the Binder cumulant, which is a kind of universal combination of critical amplitudes, explicitly depends on the anisotropy parameter—the ratio of the interaction constants $q = J'/J$ [10]. Note, however, that the interaction anisotropy is a global characteristic of the Hamiltonian.

Note also that in some cases even the introduction of impurities may not change the class of universality. This can be seen in the example of the two-dimensional Ising model, well studied analytically and numerically, in which the correlation length acquires an additive logarithmic correction due to impurities [11], which leads to logarithmic corrections to thermodynamic observables; however, the dependence of these corrections on the correlation length remains the same function as that in the case of the absence of impurities. At the same time, the universality of the ratio of critical amplitudes is also preserved; their numerical values also characterize the universality class [12]. Thus, a relatively low concentration of impurities does not violate the global properties, and the model exhibits behavior in the universality class of the two-dimensional Ising model. This approach also shows that a change in the universal behavior in this model can occur only in the neighborhood of the percolation phase transition point: a high impurity concentration may lead to a percolation geometric cluster, which changes the critical properties of the system, and, at an impurity concentration of more than 10 percent, the system exhibits a deviation from the universal behavior of the Ising model due to the mixing of the effects of two critical regions [12]. This is also a manifestation of the global characteristic—geometric percolation—which is described by a different set of critical exponents and a different functional dependence of the correlation length.

In recent years, publications have appeared in which assertions based on numerical simulation are in contradiction with the above-described universality picture. In particular, in [13], based on the numerical simulation of the four-component Potts model on a hexagonal lattice, the authors argued that the system undergoes a first-order phase transition. It is known that the Potts model with local interaction undergoes a second-order phase transition, which has been demonstrated analytically [14, 15], numerically [16], and, what is especially important, experimentally [17].

In Section 3, we present the results of numerical analysis of a four-component Potts model on a hexagonal lattice by a method of direct estimation of the density of states (DOS), similar to the method used in [13]. The difference lies in that, to estimate the DOS, we used a modification of the direct Wang–Landau method [20], which has higher accuracy of estimating the DOS, rather than the direct Wang–Landau method [18, 19]. In addition, to estimate the convergence rate of the DOS calculations, we used the previously proposed method [21]. We present the results of estimating critical exponents, which show that the four-component Potts model on a hexagonal lattice does not exhibit a deviation from the expected universal behavior in the class of universality of the four-component Potts model. The converse and erroneous assertion of [13] is apparently based on the absence of the convergence of the DOS estimate to the required one due to the known drawbacks of the direct Wang–Landau method, as well as due to the use of a qualitative method of analysis, which does not have proper accuracy.

In Section 2, we give a detailed description of the modified method that we used to carry out a numerical analysis.

2. MODIFIED WANG–LANDAU METHOD WITH CONVERGENCE CONTROL

The Wang–Landau method [18] has become widespread due to the simplicity of its implementation for classical systems with discrete energy spectrum. The method allows direct numerical evaluation of the DOS (more precisely, the formulation of the method shows that it directly evaluates the entropy). It is based on an ingenious heuristic idea of taking the transition between the states of the simulated system proportional to the ratio of the current DOSs depending on the initial and final energies. We call this transition probability the Wang–Landau probability. The partition function of systems with discrete spectrum can be represented as

$$Z = \sum_{k=1}^{N_E} g(E_k) e^{-E_k/k_B T}, \quad (1)$$

where $g(E_k)$ is the number of states (DOS) with energy E_k ($k = 1, 2, ..., N_E$), N_E is the number of energy levels, k_B is the Boltzmann constant, and T is temperature. Notice that the DOS itself does not depend on temperature, but its knowledge makes it possible to obtain the free energy as a function of temperature. The derivatives of the free energy with respect to temperature give thermodynamic observables such as the internal energy of the system and the specific heat. To obtain the free energy as a function of other parameters of the Hamiltonian, for example, the magnetic field, one needs an extended representation of the partition function with the DOS depending also on the magnetic field. The method is sufficiently general. It can also be applied to optimization problems [22] that allow the representation of the objective function in a form similar to expression (1).

2.1. The Wang–Landau Algorithm

The algorithm consists of the following steps: (1) an auxiliary function $H(E_k) = 0$ and a current value of the logarithm of DOS $\log(E_k) = 1$, ($k = 1, 2, ..., N_E$) are initialized, an arbitrary configuration of the system is defined, its energy is calculated, and the initial value of the parameter $f = \exp(1)$ is specified (its meaning will be explained below); (2) by any Monte Carlo method, a possible transition to another state is simulated (most often the Metropolis method is used [19]); (3) transition from a state with energy E_k to a state with

energy E_m is accepted with the Wang–Landau probability

$$P_{WL}(E_k, E_m) = \min\left(1, \frac{\tilde{g}(E_k)}{\tilde{g}(E_m)}\right), \quad (2)$$

where the current estimation of the DOS $\tilde{g}(E_k) = \exp\log(E_k)$ is used and the values of the auxiliary function of the accepted state $H(E_k) = H(E_k) + 1$ and the function $\log(E_k) = \log(E_k) + 1$ are increased; steps 2 and 3 are repeated until the auxiliary function $H(E_k)$ becomes flat with some percent of error, for example 5% [18]; (4) after that, it is recommended [18] to reset the auxiliary function, $H(E_k) = 0$, reduce the current value of the parameter $f = \sqrt{f}$, calibrate the current value of the DOS logarithm $\log(E_k) = f\log(E_k)$, ($k = 1, 2, ..., N_E$), and return to step 2. The process ends when a certain chosen value of the parameter f, for example, $f = \exp(10^{-8})$, is reached.

2.2. Modification: The 1/t Algorithm

For most spin models with discrete energy spectrum, such a procedure leads to a good estimate of the DOS, and therefore the algorithm has been used in a large number of studies.[1] Nevertheless, even in the early applications of the method, the authors noted that it leads to an error of a few percent in estimating the DOS [23]. Accordingly, the results for the thermodynamic functions for relatively large systems may have significant errors, including errors in the critical region.

A method to overcome such a drawback—the $1/t$ algorithm—was proposed later by Belardinelli and Pereyra [20]. Theoretical justification of the convergence of the $1/t$ algorithm was obtained by Liang et al. [22] on the basis of stochastic approximation theory.

A modification with the use of the $1/t$ algorithm is based on changing the behavior of the calibration coefficient f from the square root law to the law of inverse proportionality to the computation time, $f \propto 1/t$, measured in Monte Carlo steps. The coefficient of proportionality is chosen from the continuity of matching the two laws after a certain number of steps 2–3–4 of the original Wang–Landau algorithm.

2.3. Convergence Criterion of the DOS

The modified Wang–Landau method makes it possible in principle to estimate the DOS with arbitrary accuracy. However, this requires an astronomical amount of computation, since the convergence of the estimate to the expected value is logarithmically slow. Moreover, the convergence estimate of the DOS is not known a priori.

The solution to this problem was proposed in our article [21]. We introduced an additional matrix $T(E_k, E_m)$ with elements $T(E_k, E_m)$ equal to the frequency of transitions between states with energies E_k and E_m. To estimate this matrix, a counter of the number of transitions $\tilde{T}(E_k, E_m)$ between states with energies E_k and E_m is added at each step of the basic Wang–Landau algorithm. The result of [22] suggests that $\tilde{T}(E_k, E_m)$ asymptotically approximates $T(E_k, E_m)$. This assumption was verified by numerical simulation of Potts models with 2, 3, and 4 components and the XY model in lattice dimensions 1, 2, and 3 and by comparing with the exact results in a number of cases, as well as with the results of accurate numerical experiments with the use of other Monte Carlo methods. For the one-dimensional Ising model, the matrix was calculated exactly [21].

In all cases of analytical and numerical investigations, it was noted that the sought matrix $T(E_k, E_m)$ is doubly stochastic. Its largest eigenvalue is equal to one. Thus, the deviation of the modulus of the difference of the largest eigenvalue of the matrix $\tilde{T}(E_k, E_m)$ from unity can be used as a criterion of approximation to the desired DOS. The question of the uniqueness of this value of the DOS remains open. However, the startling fact that the initial stage of the original Wang–Landau method for systems with discrete spectrum leads to a good initial estimate of the DOS and the proven fact that in this case the $1/t$ algorithm leads to the desired DOS suggest that such a method of controlling the accuracy of the DOS estimation is sufficiently reliable. Moreover, in the appendix of [21] we proved that if the estimated matrix $\tilde{T}(E_k, E_m)$ is close to a stochastic matrix, then the estimated DOS is close to the desired one. The proof is based on the fact that, at step 2 of the Wang–Landau algorithm, we generate a random walk in the configuration space that satisfies the detailed balance condition. In this case, each element of the transition matrix $T(E_k, E_m)$ is a product of the Wang–Landau probability multiplied by the probability of a random walk in the configuration space from state with energy E_k to state with energy E_m (formula (2) in [21]). In addition, in [21], by an example of the one-dimensional Ising model we have shown analytically that if one uses exact values of the DOS when constructing the matrix $\tilde{T}(E_k, E_m)$, then the transition matrix is doubly stochastic.

Figures 1 and 2 demonstrate the parameter f and the convergence criterion $\delta = |1 - \lambda_1|$ as a function of the Monte Carlo step t for two lattice sizes. At the first stage, the parameter f decreases by the exponential law of the Wang–Landau method [18, 19], which is then followed by the power-law decay according to the law $1/t$ [20]. The convergence criterion δ also decreases by

[1] The wide popularity of the Wang–Landau method is shown, for example, by the fact that by the time this article is written the official website of APS publishers contained a list of citations from more than 2140 articles.

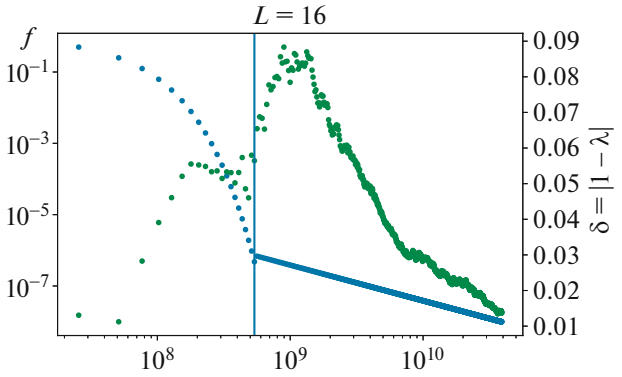

Fig. 1. Parameter f and the accuracy criterion $\delta = |1 - \lambda_1|$ as a function of the Monte Carlo step t for calculating the four-component Potts model on a hexagonal lattice with a linear size of $L = 16$. The blue color corresponds to the values of the parameter f, and the green color, to the values of the accuracy criterion δ.

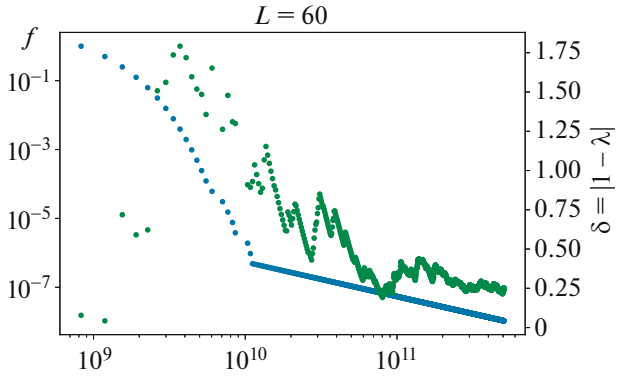

Fig. 2. Parameter f and the accuracy criterion $\delta = |1 - \lambda_1|$ as a function of the Monte Carlo step t for calculating the four-component Potts model on a hexagonal lattice with a linear size of $L = 60$. The blue color corresponds to the values of the parameter f, and the green color, to the values of the accuracy criterion δ.

the power law at the final stage of computation, though not always uniformly.

2.4. Estimates of the Characteristic Times of the Algorithm: Tunneling Time and Mixing Time

The characteristic times of the Wang–Landau algorithm are the tunneling time and the mixing time.

The tunneling time is associated with the initial stage of the algorithm and characterizes the typical time when using the histogram flatness criterion. Formally, it can be defined as the time of the first visit of one end of the energy spectrum when the simulation starts at the other end of the spectrum [24]. This time is also called the first passage time [25]. Actually, the Wang–Landau algorithm is based on a random walk on the energy spectrum. If we did not use the Wang–Landau probability P_{WL} (see expression (2)) for accepting each transition, then we would have a random walk on the energy spectrum, i.e., on a one-dimensional lattice with the number of sites L^2. In this case, the time to reach the opposite end of the spectrum (the tunneling time) would be proportional to the square of the number of energy levels, which grows proportionally to L^2 on the two-dimensional lattice. In other words, a free random walk on the energy spectrum of our model yields a tunneling time proportional to the fourth power of the lattice size, L^4. In our case, the difference of the Wang–Landau probability P_{WL} from unity leads to a more pronounced increase in the tunneling time, and the numerical estimates lead to a still faster increase in the tunneling time with an increase in the lattice size, and for the two-dimensional Ising model we have $t_{\text{tun}} \propto L^{4.8(4)}$.

The second characteristic time, the mixing time, is important at the final stage of the algorithm when approximating to the sought DOS. It is defined as the difference between the first and second eigenvalues of the transition matrix $T(E_k, E_m)$ [26],

$$t_{\text{mix}} \propto \frac{1}{|\lambda_2 - \lambda_1|}, \tag{3}$$

i.e., as a spectral gap.

Numerical experiment shows that, for the two-dimensional Ising model, the mixing time increases with the lattice size L according to the power law $t_{\text{mix}} \propto L^{4.28(4)}$.

These estimates show that the Wang–Landau method requires a huge number of Monte Carlo steps to achieve the required result, which can be seen from the scales of the horizontal axis in the convergence criterion graphs given above in Figs. 1 and 2. Preliminary estimates of the characteristic times for the model under study do not strongly differ from the times for the Ising model. It is important that the characteristic times increase faster than the fourth power of the linear size L of the lattice.

2.5. Details of the Numerical Experiment

Calculation of eigenvalues λ_1 and λ_2 of the random walk transition matrix with the Wang–Landau probability $T(E_n, E_m)$ were carried out with the help of the dgeev() function from the Intel® one API Math Kernel Library LAPACK [27].

For a random choice of spin at step 2 of the algorithm, we used an MT19937 pseudorandom number generator from the library of [28].

The number of steps between the tests of the histogram $H(E)$ on the uniformity of filling is 10^6.

Each $1/t$-th step of the algorithm was run until at least $N_E \times 10^8 \approx 10^8 \times L^2$ steps are made at the third step of the algorithm.

The thermodynamic functions (see expressions (5)–(8)) were calculated by the Mathematica software.

3. RESULTS OF SIMULATION

The Hamiltonian of the Potts model has the form

$$H = -\frac{1}{2}\sum_{nn}\delta_{\sigma_i,\sigma_j}, \tag{4}$$

where the summation is over all nearest neighbors, the coefficient 1/2 takes into account that each pair of spins appears twice in the sum, and δ is the Kronecker delta. In our case, σ_i takes four possible values.

The density of states $g(E_K)$ ($k = 1, 2, ..., N_E$) was calculated on hexagonal lattices with linear number of sites $L = 6$, 8, 12, 16, 24, 30, 36, 48, 54, 60, 62, and 72 (see Fig. 3), on which energy values from $-3/2L^2$ to zero are implemented.

The application of the method described in Section 2 resulted in a set of numerical data for the DOS $g(E_k)$ of the four-component Potts model on a hexagonal lattice. These data were used to calculate the energy E, specific heat C, and the Binder cumulant B_E [29] as a function of inverse temperature $\beta = 1/k_B T$ by the formulas

$$E(\beta) = \langle E\rangle = \frac{\sum_{i=0}^{N_E} E_i g(E_i) e^{-\beta E_i}}{\sum_{i=0}^{N_E} g(E_i) e^{-\beta E_i}}, \tag{5}$$

$$\langle E^2\rangle = \frac{\sum_{i=0}^{N_E} E_i^2 g(E_i) e^{-\beta E_i}}{\sum_{i=0}^{N_E} g(E_i) e^{-\beta E_i}}, \tag{6}$$

$$C(\beta) = \beta^2(\langle E^2\rangle - \langle E\rangle^2), \tag{7}$$

$$B(\beta) = 1 - \frac{\langle E^4\rangle}{3\langle E^2\rangle^2}. \tag{8}$$

The graphs of energy E/N and specific heat C/N per site, as well as the graphs of the Binder cumulant, are given in Figs. 4, 5, and 6, respectively. The number of sites is $N = L^2$.

The results obtained allowed us to estimate the values of critical amplitudes. Figure 7 demonstrates the maximum specific heat as a function of the linear size L.

It is well known that the models in this universality class demonstrate multiplicative logarithmic corrections to specific heat [30]. Finite-dimensional analysis

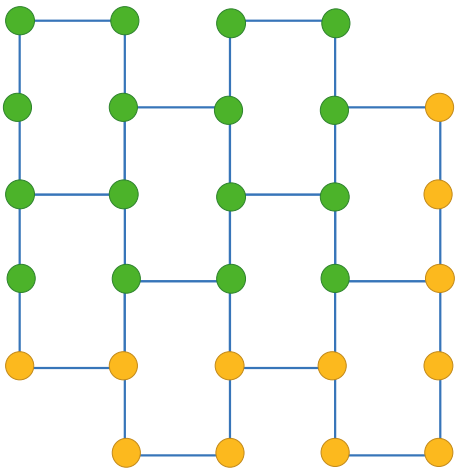

Fig. 3. Example of a hexagonal lattice with a linear size of $L = 4$ used in simulation. The yellow color indicates additional sites to demonstrate the organization of periodic boundary conditions.

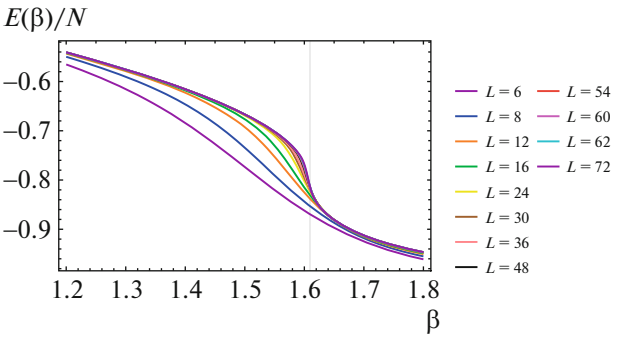

Fig. 4. Temperature dependence of the specific energy for several lattice sizes.

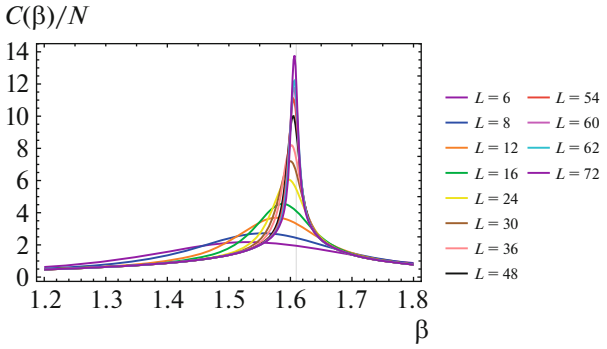

Fig. 5. Temperature dependence of the specific heat for several lattice sizes.

[31] points to the following dependence of the maximum specific heat on the size L of the system:

$$C_{\max} \propto \frac{L^b}{(\ln L)^{3/2}}[1 + ...] \tag{9}$$

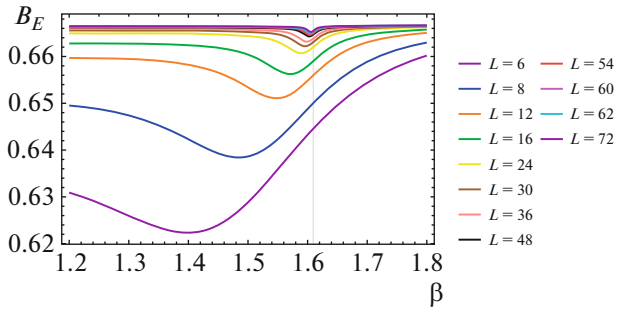

Fig. 6. Temperature dependence of the Binder cumulant for several lattice sizes.

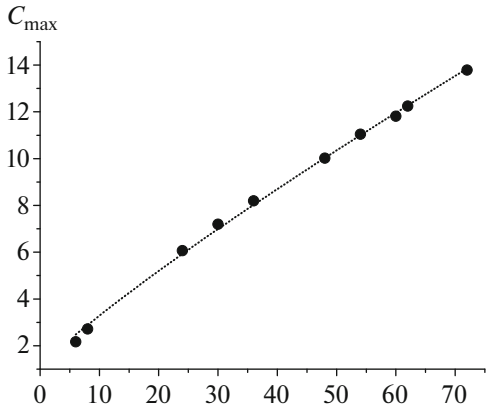

Fig. 7. Maximum specific heat as a function of the size of the system. The dotted line is the approximation of the numerical data.

with the exponent $b = \alpha/\nu = 1$ and a complex combination of logarithmic terms in square brackets.[2] Here α and ν are the critical exponents of the specific heat and the correlation length [1]. The result of approximation of the numerical data by this formula, presented in [31], gives a value of $b = 1.044(8)$ for the exponent in the analysis of the model on a square lattice, which is in good agreement with the analytical value. In our case, similarly, the result of approximation of the maximum specific heat is in good agreement with formula (9) with exponent $b = 1.042(15)$. In [31], the authors also give the result of naive approximation of the data by the power law without logarithmic corrections, which gives an exponent of $b = 0.770(8)$. A similar approximation in our case gives a close value of $b = 0.75(1)$.

In addition, from the specific heat data obtained we can determine the shift of the maximum of the specific heat. It is known that this shift depends on the lattice size [32],

$$\Delta T \propto L^{-1/\nu} \tag{10}$$

and is determined by the correlation length exponent ν. The approximation of the data obtained for the shift of the specific heat maximum by formula (10) gives an estimate of 0.672(11) for the exponent, which is close to the exact value of $\nu = 2/3 \approx 0.667$. A similar result was obtained in [31] from the numerical estimate of the critical exponent of the correlation length.

Thus, the numerical study of the critical behavior of the specific heat of the four-component Potts model on a hexagonal lattice by the modified Wang–Landau method leads to results similar to those of the numerical study of the critical behavior of the four component Potts model on a square lattice by the cluster method [31]. As pointed out in Section 1, this should have been expected.

The position of the minimum of the Binder cumulant can also be used to estimate the correlation length exponent; however, this is complicated by nonsingular corrections to the susceptibility [16].

We also carried out an analysis of the energy distribution function at various temperatures and did not find indications of the coexistence of phases, on the basis of which the authors of [13] made a conclusion about the first-order phase transition in the model under investigation.

4. CONCLUSIONS

We have shown that a modified version of the Wang–Landau method with the estimation of the computation accuracy can be successfully applied to obtain numerical values of the critical exponents in the Potts model with a fourfold degenerate ground state. We have also shown that this model on a hexagonal lattice exhibits critical behavior, similar to the model on the square lattice in the universality class [31], which was previously analyzed in detail numerically.

It is important that, to estimate the density of states, we used two additional ingredients. The first one, the $1/t$ method, makes it possible to avoid distortions in the estimation of the DOS [20]. The second, the method for estimating the degree of deviation of the transition matrix from the stochastic matrix, allows one to control the approximation of the DOS estimate to the expected one [21]. It is also important to take into account logarithmic corrections to the critical behavior [16, 31] in the finite-dimensional analysis of the critical behavior of thermodynamic observables.

After completing our investigations, in the current issue of JETP we found article [33] by the authors of the same group as those of [13], in which, on the basis of the analysis of the same model with the help of the cluster Monte Carlo method, a conclusion was made about a second-order phase transition. However, the results of the previous work [13] with the opposite

[2] We do not present cumbersome expressions in brackets. The details can be found in [31].

conclusion about the first-order phase transition were not discussed.

In contrast to these works, in which the conclusions were made on the basis of a qualitative analysis of energy distribution, we have carried out a numerical evaluation of the critical exponents and compared them with the results of other authors [31]. We have presented and described in detail all the necessary details of the study, which makes it possible to verify the results presented by us.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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