Critical properties of the three-dimensional frustrated Heisenberg model on a layered-triangular lattice with variable interplane exchange interaction

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The critical properties of three-dimensional (3D) frustrated Heisenberg model on a layered-triangular lattice with variable interplane exchange interaction are investigated by the replica Monte Carlo method. The static magnetic and chiral critical exponents of heat capacity $\alpha=0.26(3)$, susceptibility $\gamma=1.23(4)$, $\gamma_k=0.87(5)$, magnetization $\beta=0.26(1)$, $\beta_k=0.43(2)$, and correlation length $\nu=0.59(2)$, $\nu_k=0.59(2)$, as well as the Fisher exponent $\eta=-0.09(3)$, are calculated by means of the finite-size scaling theory. Another universality class of the critical behavior is shown to be formed by the 3D frustrated Heisenberg model on a layered-triangular lattice. The universality class of the critical behavior of this model is revealed to remain within the limits of values of interplane J' and intraplane J exchange interaction $R=|J'/J|=0.075-1.0$.

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I. INTRODUCTION

The investigation of phase transitions (PT) and critical phenomena (CP) in the frustrated spin systems is one of the difficult and interesting questions of the statistical physics. A modern theory of PT and CP is mainly based on hypothesis of scaling, universality, and the theory of renormalization group.[1,2] The study of frustrated systems (FSs) and spin systems with quenched nonmagnetic disorder shows that most part of results exceeds the bounds of the modern theory of PT and CP.[3]

Success achieved in understanding of PT and CP both in common[4] and in frustrated systems[5–9] are considerably connected with application of the computational physics methods. Obviously, this is connected with serious difficulties at calculation of critical parameters, determination of features, nature, and principles of a critical behavior of such systems using the traditional theoretical and experimental techniques. For these reasons, PT and CP are studied by Monte Carlo (MC) methods.

We study the critical properties of the three-dimensional (3D) frustrated antiferromagnetic Heisenberg model in the layered-triangular lattice with a variable interplane exchange interaction studied by means of the MC method. We choose this model because of the following reasons.

First, the existence of another chiral universality class in the triangular lattice in the FS is still an issue.[5–13] Second, many principle physical properties of FS depend substantially on the lattice geometry. Such a dependence can lead to a decrease in the number of universality classes of the critical behavior. This problem is still not clearly understood. Third, the first attempts to research this model have been done when computers and the algorithms of the MC method were not powerful to calculate the critical parameters with a need accuracy. Fourth, the dependences of the FS critical properties on a value of the interplane exchange interaction are not researched.

The FS critical behavior at a change of interplane exchange interaction parameter cannot be predicted from the data available for today.[7] Moreover, the results in Refs. 4 and 6–10 are contradictory and require more accurate additional researches.

II. MODEL AND METHOD

The antiferromagnetic 3D Heisenberg model on a layered-triangular lattice is the frustrated magnetic system. The Hamiltonian of the system can be written as[7]

$$H=-J\sum_{\langle ij\rangle}(\vec{S}_i\cdot\vec{S}_j)-J'\sum_{\langle ij\rangle}(\vec{S}_i\cdot\vec{S}_j), \quad (1)$$

where $\vec{S}_i$ is a three-component unit vector, $\vec{S}_i=(S_i^x,S_i^y,S_i^z)$ and $J<0$ and $J'>0$ are constants of an exchange interaction. The summation is carried out by the nearest neighbors. The lattice consists of two-dimensional triangular layers stacked parallel along the orthogonal axis. The first term in Eq. (1) represents an antiferromagnetic intraplane interaction of spins, whereas the second term represents the ferromagnetic interplane interactions.[7] Frustrations in this model are caused by the lattice geometry.[7–10]

The magnetic and thermodynamic properties of the model were studied by the MC method in Ref. 7. The second-order PT was shown to be observed in such a system at $T_N=0.954$ (hereafter, the temperature will be given in terms of $|J|/k_B$) and some magnetic static critical exponents (CEs) to be calculated. The direct analysis of the MC data and the determination of exponents from the slopes of the dependences of thermodynamic parameters in diagrams plotted in a logarithmic scale are not convincing, especially for the low MC statistics presented in Ref. 7. In Refs. 8–10, the values of magnetic and chiral CEs α, β, β_k, ν, ν_k, γ, and γ_k are given. The finite-size scaling method chosen for calculations, in our opinion, is not of high accuracy. However, the data obtained in Refs. 7–10 demonstrate that the critical parameters of the 3D frustrated antiferromagnetic Heisenberg model differ from the data characterizing the universality class of the pure Heisenberg model.

According to the modern theory of PT and CP, the universality class of the critical behavior depends primarily on[1,2] (i) the space dimension D, (ii) the number of components of the order parameter n, (iii) Hamiltonian symmetry, and (iv) the length of the characteristic interaction.

However, a number of available data suggest that the universality class of frustrated systems can depend not only on above mentioned factors. This is confirmed by the MC results obtained for lattices with different geometries.[6–13] Asymptotic values of the critical parameters for such systems are also of insufficient accuracy. In this respect, the purpose of this work is to determine the critical parameters of the 3D frustrated antiferromagnetic Heisenberg model on a layered-triangular lattice using the reliable well-tried schemes within a unified approach and with high accuracy.

Frustrated spin systems are rather complex objects for investigation even by means of the MC method. As it is known, the MC method meets with the so-called critical slowing down in the vicinity of the critical point, which in FS becomes an even more serious problem. Moreover, for frustrated systems, a huge number of local-minimum-energy states are a characteristic. The usual MC methods meet with failure in it. Therefore, many new algorithms of the MC method have been developed in recent years. The replica algorithms of the MC method turned out to be the most powerful and efficient for investigation of CP in different spin systems and models.[14–16] For this reason, the 3D frustrated antiferromagnetic Heisenberg model in our work is investigated using the classical Metropolis algorithm[17] and the highly effective replica-exchange method (REM).[14–16] The simulation of the REM is realized by two steps: (i) two replicas of different temperatures are simulated simultaneously, and (ii) after 100 Monte Carlo steps spin, the replicas exchange by data in accordance with the Metropolis scheme with probability of

$$w(X \to X') = \begin{cases} 1 & \text{for } \Delta \leqslant 0 \\ \exp(-\Delta) & \text{for } \Delta > 0, \end{cases}$$

where $\Delta = (T - T')(U - U')$, T and T' are the temperatures, and U and U' are the energies of adjacent replicas, correspondingly.

The main advantage of REM is that an exchange probability is known *a priori*, when for other methods, determination of probability is very tiring and takes much time. In the replica exchange algorithm, a random walk in "temperature space" for each replica is realized, which induces a random walk in the potential energy field. This solves the problem of getting trapped in the system of states with the local minimum energy. However, to improve this method, an increase of replicas is needed, which requires a more powerful computer to simulate the complex systems.

The calculations are carried out for the systems with periodic boundary conditions and linear sizes $L \times L \times L = N$, $L = 9 - 30$. A correlation of interplane and intraplane exchange alters in a range $R = |J'/J| = 0.01 - 1.0$. To average the thermodynamic parameters at each certain value of L, ten Markovian chains starting from different random initial configurations are used. The length of equilibrium section is 100 times larger than the length of nonequilibrium section in each chain. The thermodynamic parameter values obtained in such a way are averaged over ten configurations. These data are used in the diagrams.

III. RESULTS OF SIMULATION

To research the temperature dependences of the heat capacity and the susceptibility, the following equations are used:[9,18–20]

$$C = (NK^2)(\langle U^2 \rangle - \langle U \rangle^2), \tag{2}$$

$$\chi = \begin{cases} (NK)(\langle m^2 \rangle - \langle |m|^2 \rangle), & T < T_N \\ (NK)\langle m^2 \rangle, & T \geqslant T_N, \end{cases} \tag{3}$$

$$\chi_k = \begin{cases} (NK)(\langle {m_k}^2 \rangle - \langle |m_k|^2 \rangle), & T < T_k \\ (NK)\langle {m_k}^2 \rangle, & T \geqslant T_k, \end{cases} \tag{4}$$

where $K = |J|/k_B T$, N is the number of particles, U is the internal energy, m is the magnetic order parameter, m_k is the chiral order parameter, and χ_k is the chiral susceptibility.

The order parameter of the system m is calculated by the equation[7]

$$m = \frac{3}{N}\sqrt{\langle M_A^2 + M_B^2 + M_C^2 \rangle / 3}, \tag{5}$$

where M_A, M_B, and M_C are magnetizations of three sublattices, respectively. The magnetization of sublattice is calculated in the following way[6]:

$$\langle |\vec{M}_r| \rangle = \langle \sqrt{S_x^2 + S_y^2 + S_z^2} \rangle, \quad r = A, B, C. \tag{6}$$

Antiferromagnetics of triangular lattice differ from usual ferromagnetics and antiferromagnetics, where a given direction in one of the sites determines a structure in whole. In case of antiferromagnetics with triangular lattice, there can be two different structures at a given direction of the spin in a site. A difference between these structures is described by a chirality vector.[10] The spin chirality is a critical value together with the vector antiferromagnetism. The fluctuations of the spin chirality are determined by new CEs β_k, γ_k, and ν_k.[8–13]

Recent theoretical, experimental, and numerical results predict a new chiral universality class of the critical behavior for frustrated systems.[11–13,21–23] A chiral order parameter for the system m_k is calculated by the expressions[8,9]

$$m_{kp} = \frac{2}{3\sqrt{3}} \sum_{\langle ij \rangle} [S_i \times S_j]_p, \tag{7}$$

$$m_k = \frac{1}{N} \sum_p m_{kp}, \tag{8}$$

where $p = (x, y, z)$ are the vector components.

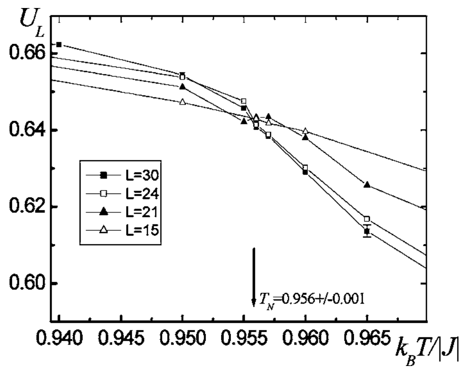

FIG. 1. Dependence of the Binder cumulant U_L on temperature $k_BT/|J|$ at $R=1$.

In order to determine the critical temperature T_N more precisely, we used the method of fourth-order Binder cumulants U_L (Ref. 24):

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2}. \tag{9}$$

According to the finite-size scaling theory, the point of intersection of the U_L cumulants in their temperature dependences is the critical point.[20]

The characteristic temperature dependences of the Binder cumulants U_L for magnetic order parameter at $R=1$ are plotted in Fig. 1 (here and in all subsequent figures, the statistical error does not exceed the size of the symbols of the dependences used for construction). By our estimations, an intersection of curves and least data spread are observed in a point $T=0.956\pm0.001$. This value is taken as the critical temperature $T_N=0.956(1)$. This approach turned out to be of low accuracy for the determination of the chiral critical temperature T_k. Therefore, the chiral critical temperature T_k is determined by means of a "cumulant crossing" method. Other authors recognize this method as accurate and precise for the determination of the chiral critical temperature T_k.[9,25,26] According to this method, the dependences $U_L(T)$ for the systems with different sizes are plotted in given scales $\ln^{-1}(L'/L)$, where L' and L are the sizes of two lattices and $L'>L$. The temperature extrapolation at $\ln^{-1}(L'/L)\to 0$ corresponds to the critical temperature for an infinite system $T_k(L\to\infty)$. Figure 2 represents a characteristic dependence of temperature T_k on the value $\ln^{-1}(L'/L)$ for different L at $R=1$. The lines in Fig. 2 are plotted by the least squares method. For $L\to\infty$, all lines crossed in a point $T=0.955\pm0.002$. This point corresponds to a value of the chiral critical temperature $T_k=0.955(2)$, which coincides with the value of the magnetic critical temperature $T_N=0.956(1)$. It is confirmed by the results in Refs. 8 and 9.

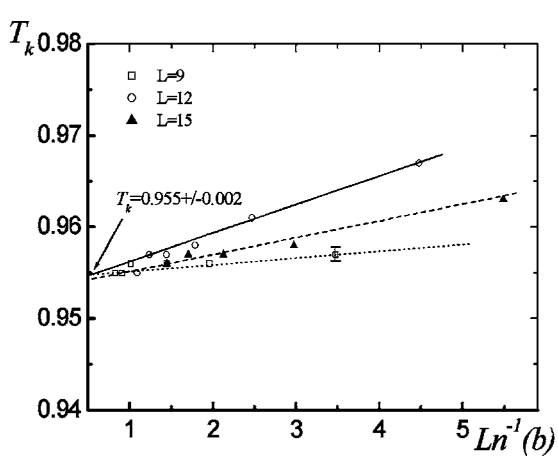

FIG. 2. Dependence of temperature T_k on $\ln^{-1}(L'/L)$ for different L at $R=1$.

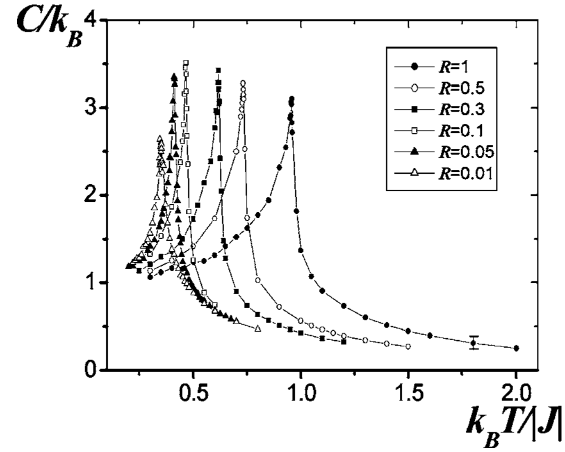

FIG. 3. Dependence of the heat capacity C/k_B on temperature $k_BT/|J|$ for system with $L=24$.

Temperature dependences of heat capacity C (Fig. 3) and susceptibility χ (Fig. 4) have sharply defined maxima in the critical region. A decrease of interplane and intraplane exchanges R leads to a decrease of a phase transition temperature and, respectively, to displacement of heat capacity and susceptibility maxima into the low temperature region. For the susceptibility, this displacement is accompanied by the increase of maxima. While the heat capacity maxima first increase, one observes a gradual decreasing at $R\leqslant 0.05$. As for the susceptibility, the maximum increases with decrease of R.

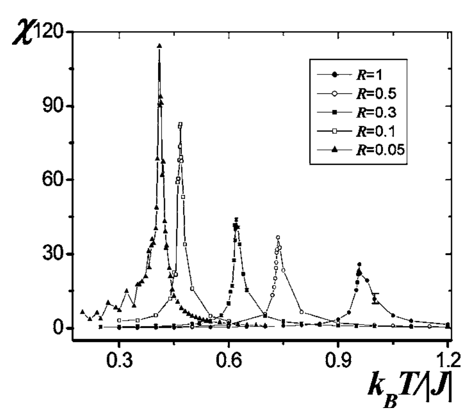

FIG. 4. Dependence of the susceptibility χ on temperature $k_BT/|J|$ for system with $L=24$.

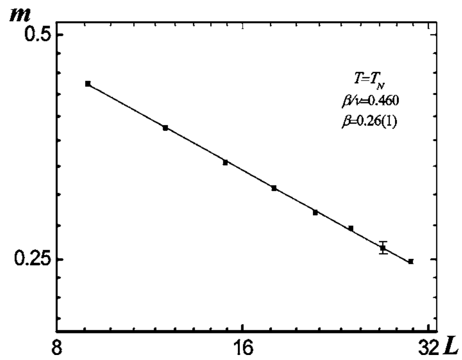

FIG. 5. Dependence of order parameter m on linear sizes of system L at $T=T_N$ at $R=1$.

The static chiral and magnetic CEs of the heat capacity α, the susceptibility γ, γ_k, the magnetization β, β_k, and the correlation length ν, ν_k are calculated by means of the finite-size scaling theory.[6,19,25–28]

The following expressions are obtained from the finite-size scaling theory in the system with $L\times L\times L$ size at $T=T_N$ and sufficiently large L (Refs. 5, 9, 19, and 27–30):

$$m \propto L^{-\beta/\nu}, \quad (10)$$

$$m_k \propto L^{-\beta_k/\nu_k}, \quad (11)$$

$$\chi \propto L^{\gamma/\nu}, \quad (12)$$

$$\chi_k \propto L^{\gamma_k/\nu_k}, \quad (13)$$

$$V_n = L^{1/\nu} g_{V_n}, \quad (14)$$

$$V_{nk} = L^{1/\nu_k} g_{V_n}, \quad (15)$$

where g_{V_n} is a constant, and V_n and V_{nk} can be calculated from the following equations:

$$V_i = \frac{\langle m^i E\rangle}{\langle m^i\rangle} - \langle E\rangle \quad (i=1,2,3,4), \quad (16)$$

$$V_{ki} = \frac{\langle m_k^i E\rangle}{\langle m_k^i\rangle} - \langle E\rangle \quad (i=1,2,3,4). \quad (17)$$

These expressions are used to determine β, β_k, γ, γ_k, ν, and ν_k.

In Ref. 29, it is shown that a similar equation for the heat capacity does not hold true, and for the approximation of the temperature dependence on L, the following equation is practically used[7–9]:

$$C_{\max}(L) = A_1 - A_2 L^{\alpha/\nu}, \quad (18)$$

where A_1 and A_2 are certain coefficients.

A characteristic dependence of the magnetic order parameter m on linear sizes of lattice L in the log-log scale is depicted in Fig. 5. All data are plotted on the line, and the curve inclination angle defines the value β/ν. We determine the values α/ν, β_k/ν_k, γ/ν, γ_k/ν_k, $1/\nu$, and $1/\nu_k$ for different R by this scheme. The obtained values ν and ν_k are used to calculate the exponents α, β, β_k, γ, and γ_k. All values obtained in such a way are listed in Tables I–III.

A procedure used for the derivation of the Fisher exponent η is worth special notice. Using the ratio between the susceptibility χ and the correlation length[31] ξ,

$$\chi \propto \xi^{\gamma/\nu}, \quad (19)$$

and the relation $\eta=2-\gamma/\nu$ connecting the exponents η and ν, we get

TABLE I. Values of the critical parameters for the Heisenberg model at $R=1$.

Critical parameter	Data of this work (Metropolis algorithm)	Data of this work (REM)	Method MC[a]	Method MC[b]	Method MC[c]	Expt.[d]	Unfrustrated Heisenberg model[e]
T_N	0.957(2)	0.956(1)	0.954(2)	0.955(2)	0.9577(2)	[f]	1.443
T_k	0.955(2)	0.955(2)	[f]	0.958(2)	0.9577(2)	[f]	[f]
ν	0.53(3)	0.59(2)	0.53(3)	0.59(2)	0.586(8)	0.54(3)	0.7112(5)
α	0.37(5)	0.26(3)	0.4(1)	0.24(8)	[f]	0.39(9)	−0.1336(15)
β	0.26(3)	0.26(1)	0.25(2)	0.30(2)	0.285(11)	0.25(1)	0.3689(3)
γ	1.11(6)	1.23(4)	1.1(1)	1.17(7)	1.185(3)	1.10(5)	1.3960(9)
ν_k	0.60(3)	0.59(2)	[f]	0.60(2)	0.60(2)	[f]	[f]
β_k	0.45(3)	0.43(2)	[f]	0.55(2)	0.50(2)	0.44(2)	[f]
γ_k	0.93(6)	0.87(5)	[f]	0.72(2)	0.82(2)	0.84(7)	[f]
η	−0.10(5)	−0.09(3)	[f]	[f]	[f]	[f]	0.0375(5)

[a]Reference 7.
[b]Reference 8.
[c]Reference 9.
[d]Reference 10.
[e]Reference 4.
[f]Not available.

TABLE II. Values of the magnetic critical parameters for the Heisenberg model for different R.

R	T_N	ν	α	β	γ	$\alpha+2\beta+\gamma=2$
1	0.956(1)	0.59(2)	0.26(3)	0.26(2)	1.23(4)	2.02
0.8	0.872	0.60	0.24	0.26	1.26	2.02
0.7	0.829	0.61	0.22	0.28	1.29	2.07
0.6	0.783	0.59	0.22	0.29	1.22	2.02
0.4	0.677	0.60	0.24	0.27	1.27	2.05
0.3	0.619	0.60	0.26	0.29	1.23	2.07
0.1	0.468	0.59	0.24	0.28	1.17	1.97
0.075	0.442	0.55	0.26	0.24	1.23	1.97
0.05	0.413	0.55	0.15	0.22	1.11	1.70
0.01	0.353	0.48	0.09	0.27	0.82	1.45

$$\ln(\chi/\xi^2) = c - \eta \ln \xi, \qquad (20)$$

where c is a constant. For systems with finite sizes, the equality $\xi = L$ is satisfied. Then, at $T = T_N$, we have

$$\ln(\chi/L^2) = c - \eta \ln L. \qquad (21)$$

On the basis of Eq. (21), the Fisher exponent η is defined. Data are also presented in the Table I. Here, also demonstrated are the numerical[7–9] and experimental[10] results at $R=1$ of other authors and values of critical parameters for nonfrustrated model.[4]

In Ref. 10, presented are the experimental results for the chirality of antiferromagnetic $CsMnBr_3$ with triangular lattice. This material has a hexagonal structure $P6_3/mmc_1$. The antiferromagnetism in the ab plane appears at $T_N = 8.3$ K. This phase transition is studied experimentally,[32–36] where the critical parameters are calculated from the data for scattering of nonpolar neutrons and are not of high accuracy.

The exponents ν and ν_k calculated by REM coincide with those described in Refs. 8 and 9 within the limits of error and are also close to values $\nu = 0.55(3)$ from Ref. 12 and $\nu = 0.589(7)$ from Ref. 13. Our results show $\nu = \nu_k$. The exponents α, β, and γ differ from the data in Ref. 7 but agree with the results in Refs. 8–10 within the limits of error. The exponents β_k and γ_k are close to the exponents in Ref. 10. The chiral and magnetic CEs evaluated in this work are out of agreement. As for the critical temperatures $T_N = 0.956(1)$ and $T_k = 0.955(2)$ determined in this work and in Refs. 7–9 and also $T_k = 0.958(2)$ from Ref. 13, they coincide with each other. Our results are in good agreement with experimental results and major numerical results of other authors and with some results $\gamma = 1.06(5)$ and $\beta_k = 0.38(10)$ obtained on the basis of field theory[12] but differ from the data for nonfrustrated Heisenberg model.[4] So the 3D frustrated antiferromagnetic Heisenberg model in a layered-triangular lattice creates another universality class of the critical behavior.

The dependence of CE on the ratio of interplane and intraplane exchanges R is of great interest. To study this question, we have investigated the 3D frustrated antiferromagnetic Heisenberg model on a layered-triangular lattice at different R in range $R = 0.01 - 1.0$. For every R, all important magnetic and chiral critical parameters are calculated by means of the finite-size scaling theory and described procedure. Values of magnetic and chiral parameters are shown in Tables II and III, correspondingly. It should be noted that the values of critical parameters for different values of R from $R = 1.0$ to $R = 0.075$ do not depend on R and coincide within the limits of error. For all that, the ratio of scaling between critical exponents α, β, and γ is carried out with high accuracy. However when R becomes less than 0.075, a sharp change of all exponent values is observed. This change is accompanied by disturbance of scaling ratio between α, β,

TABLE III. Values of the chiral critical parameters for the Heisenberg model for different R.

R	T_k	ν_k	α	β_k	γ_k	$\alpha+2\beta_k+\gamma_k=2$
1	0.956(2)	0.59(2)	0.26(3)	0.43(2)	0.87(5)	1.99
0.8	0.872	0.60	0.24	0.42	0.96	2.04
0.7	0.829	0.61	0.22	0.48	0.96	2.14
0.6	0.783	0.59	0.22	0.46	0.85	1.99
0.4	0.677	0.60	0.24	0.43	0.90	2
0.3	0.619	0.60	0.26	0.48	0.81	2.03
0.1	0.468	0.59	0.24	0.47	0.82	2
0.075	0.442	0.55	0.26	0.42	0.87	1.97
0.05	0.413	0.55	0.15	0.31	0.60	1.37
0.01	0.353	0.48	0.09	0.40	0.52	1.41

and γ. Obviously, a character of the critical behavior of the model does not change with change of R from 1.0 to 0.075. However, at $R<0.075$, the crossover probably occurs and changes the critical behavior from three dimensional to quasi-two-dimensional.

IV. CONCLUSIONS

Thus, the critical properties of 3D frustrated antiferromagnetic Heisenberg model on a layered-triangular lattice are investigated using the classical (Metropolis) algorithm and REM of the MC method. The obtained results allow us to calculate all static CEs. Exponents α (heat capacity), γ, γ_k (susceptibility), β, β_k (magnetization), and ν, ν_k (correlation length), as well as the Fisher exponent η, are calculated from the correlations of the finite-size scaling theory within a unified approach. The results of the calculations show that the 3D frustrated antiferromagnetic Heisenberg model on a layered-triangular lattice belongs to another universality class. The universality class for the critical behavior of the model is revealed to be kept up to the value of interplane exchange interaction, $R=0.075$, and with further decrease of R, a transition from three-dimensional critical behavior to quasi-two-dimensional one is observed.

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