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UNIVERSALITY IN THE PARTIALLY ANISOTROPIC THREE-DIMENSIONAL ISING LATTICE

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Using transfer-matrix extended phenomenological renormalization-group methods, we study the critical properties of the spin-1/2 Ising model on a simple-cubic lattice with partly anisotropic coupling strengths $\vec{J} = (J', J', J)$. The universality of both fundamental critical exponents y_t and y_h is confirmed. It is shown that the critical finite-size scaling amplitude ratios $U = A_{\chi^{(4)}} A_\kappa / A_\chi^2$, $Y_1 = A_{\kappa''}/A_\chi$, and $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}}$ are independent of the lattice anisotropy parameter $\Delta = J'/J$. For the Y_2 invariant of the three-dimensional Ising universality class, we give the first quantitative estimate $Y_2 \approx 2.013$ (shape $L \times L \times \infty$, periodic boundary conditions in both transverse directions).

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1. INTRODUCTION

The phenomenological renormalization-group (RG) method in which the transfer-matrix technique and finite-size scaling (FSS) ideas are combined is a powerful tool for investigation of critical properties in different two-dimensional systems [1, 2]. Unfortunately, its application in three and more dimensions is sharply retarded due to huge sizes of the transfer matrices arising in approximations of d-dimensional lattices by $L^{d-1} \times \infty$ subsystems.

Indeed, even in the simplest case of systems with only two states of a site (the spin-1/2 Ising model), the size of the transfer matrix in three dimensions ($d = 3$) increases as 2^{L^2} (instead of the essentially more sparing law 2^L in two dimensions). Hence, for the $3 \times 3 \times \infty$ cluster, the eigenproblem of the 512×512 transfer matrix must be solved; for the $4 \times 4 \times \infty$ subsystem, the problem is for the $65\,536 \times 65\,536$ matrix; and for the $5 \times 5 \times \infty$ cluster, it is required to find the eigenvalues and eigenvectors of dense matrices with huge sizes of $33\,554\,432$ by $33\,554\,432$.

One can solve the full eigenproblem for the transfer matrices of Ising parallelepipeds $L \times L \times \infty$ with the side length $L \leq 4$. Our aim in this paper is to use such solutions with the maximum effect and extract as much accurate information about physical properties of the bulk system as possible.

The ordinary phenomenological RG is based on the FSS equations for correlation lengths [1, 2]. However, it is known [3–5] that the phenomenological RG can be built up using other quantities with a power divergence at the phase transition point. It is remarkable that such modified renormalizations can provide more precise results with the same sizes of subsystems [6].

In this paper, we calculate the values of different invariants of the 3D Ising universality class and discuss their universal and extrauniversal properties.

2. BASIC EQUATIONS

We start from the ordinary FSS equations [1, 2] for the inverse correlation length $\kappa_L(t, h)$ and the singular part of the dimensionless free-energy density $f_L^s(t, h)$, but we write them for the derivatives with respect to the reduced temperature $t = (T - T_c)/T_c$ and the external field h,

$$\kappa_L^{(m,n)}(t, h) = b^{my_t + ny_h - 1} \kappa_{L/b}^{(m,n)}(t', h') \qquad (1)$$

and

$$f_L^{s\,(m,n)}(t, h) = b^{my_t + ny_h - d} f_{L/b}^{s\,(m,n)}(t', h'). \qquad (2)$$

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Here,

$$\kappa_L^{(m,n)}(t,h) = \frac{\partial^{m+n}\kappa_L}{\partial t^m \partial h^n}$$

and similarly for $f_L^{s\,(m,n)}$; y_t and y_h are the thermal and magnetic critical exponents of the system, respectively; and $b = L/L'$ is the rescaling factor. In deriving Eqs. (1) and (2), we used a linearized form of the RG equations $t' \approx b^{y_t} t$ and $h' \approx b^{y_h} h$.

In the traditional phenomenological RG theory [1, 2], Eq. (1) with $m = n = 0$ is considered as an RG mapping $(t,h) \to (t',h')$ for a cluster pair (L, L'). The critical temperature T_c is then estimated from the equation

$$L\kappa_L(T_c) = L'\kappa_{L'}(T_c). \tag{3}$$

The phenomenological renormalization $(t,h) \to (t',h')$ can also be realized by using any of relations (1) and (2) or their combination. It has been shown by the author [6] that some of such extended renormalizations lead to more rapid convergence in L than the standard phenomenological RG transformation. In particular, test examples on the fully isotropic systems [6] have shown that the relations

$$\left.\frac{\kappa_L''}{L^{d-1}\chi_L}\right|_{T_c} = \left.\frac{\kappa_{L'}''}{(L')^{d-1}\chi_{L'}}\right|_{T_c}, \tag{4}$$

$$\left.\frac{\chi_L^{(4)}}{L^d \chi_L^2}\right|_{T_c} = \left.\frac{\chi_{L'}^{(4)}}{(L')^d \chi_{L'}^2}\right|_{T_c} \tag{5}$$

locate T_c more accurately in comparison with the ordinary RG equation (3). In relations (4) and (5), the derivative $\kappa_L'' = \partial^2\kappa_L/\partial h^2$, the zero-field susceptibility $\chi_L = f_L^{s\,(0,2)}$, and the nonlinear susceptibility $\chi_L^{(4)} = f_L^{s\,(0,4)}$ can be evaluated by standard formulas via the eigenvalues and eigenvectors of transfer matrices (see, e.g., [7–9]).

To find the thermal critical exponent y_t, we applied two approaches. First, we again used the standard finite-size expression

$$y_t = \frac{\ln[L\dot{\kappa}_L/(L'\dot{\kappa}_{L'})]}{\ln(L/L')}, \tag{6}$$

which follows from Eq. (1) with $m = 1$, $n = 0$; $\dot{\kappa}_L = \partial\kappa_L/\partial t$. Second, we took the formula

$$y_t = \frac{\kappa_{L'}\dot{\kappa}_L - \kappa_L\dot{\kappa}_{L'}}{(\kappa_L\kappa_{L'}\dot{\kappa}_L\dot{\kappa}_{L'})^{1/2}\ln(L/L')}. \tag{7}$$

This expression is a direct consequence of the well-known Roomany–Wyld approximant to the Callan–Symanzik β-function [2].

To calculate the magnetic critical exponent y_h, we also used two ways,

$$y_h = \frac{d}{2} + \frac{\ln(\chi_L/\chi_{L'})}{2\ln(L/L')} \tag{8}$$

and

$$y_h = \frac{1}{2} + \frac{\ln(\kappa_L''/\kappa_{L'}'')}{2\ln(L/L')} \tag{9}$$

(these finite-size relations follow from Eqs. (1) and (2)).

In addition, we calculated the universal ratios of the critical FSS amplitudes. Ratios of this type can be identified from the Privman–Fisher functional expressions [10]. For the discussed anisotropic systems, they are given by [8]

$$\kappa_L(t,h) = L^{-1}G_0\mathcal{K}(C_1 t L^{y_t}, C_2 h L^{y_h}), \tag{10}$$

$$f_L^s(t,h) = L^{-d}G_0\mathcal{F}(C_1 t L^{y_t}, C_2 h L^{y_h}). \tag{11}$$

The scaling functions $\mathcal{K}(x_1,x_2)$ and $\mathcal{F}(x_1,x_2)$ are the same within the limits of a given universality class, but they may depend on the boundary conditions and the subsystem shape (a cube, infinitely long parallelepipeds, etc.). Thus, all nonuniversality, including the lattice anisotropy parameter Δ, is absorbed in the geometry prefactor G_0 and metric coefficients C_1 and C_2. The critical amplitude ratios from which the parameters G_0, C_1, and C_2 drop out should be extrauniversal. In particular, the amplitude combinations

$$U = \frac{A_{\chi^{(4)}}A_\kappa}{A_\chi^2} = \frac{\kappa_L \chi_L^{(4)}}{L^{d-1}\chi_L^2} \tag{12}$$

(a Binder-like ratio for the spatially anisotropic systems),

$$Y_1 = \frac{A_{\kappa''}}{A_\chi} = \frac{\kappa_L''}{L^{d-1}\chi_L}, \tag{13}$$

$$Y_2 = \frac{A_{\kappa^{(4)}}}{A_{\chi^{(4)}}} = \frac{\kappa_L^{(4)}}{L^{d-1}\chi_L^{(4)}} \tag{14}$$

are expected to be independent of the lattice anisotropy parameter $\Delta = J'/J$.

3. RESULTS AND DISCUSSION

We have carried out calculations for the subsystems $L \times L \times \infty$ with $L = 3$, 4. To avoid undesirable surface effects, the periodic boundary conditions were imposed in both transverse directions of parallelepipeds $L \times L \times \infty$. Thus, the transfer matrices for which the eigenproblem was solved were dense matrices of sizes up to $65\,536 \times 65\,536$. To solve the eigenproblem, we took the internal and lattice symmetries of subsystems into account and used the block-diagonalization method (see, e.g., [7, 9]). Calculations were performed on an 800 MHz Pentium III PC running the FreeBSD operating system.

3.1. Critical temperature

The critical temperature estimates coming from solutions of transcendental equations (4) and (5) are collected in Table 1.

In the purely isotropic case ($J' = J$), there are high-precision numerical estimates for the critical point of the three-dimensional Ising model. The most precise values for it have been obtained by Monte Carlo simulations [11, 12]: $K_c = 0.221\,654\,59(10)$, i.e., $k_B T_c/J = 1/K_c = 4.511\,5240(21)$.

Inspecting Table 1, one can see that the estimates for $J' = J$ that follow from Eq. (4) and (5) are the lower and upper bounds respectively. Therefore, their mean value has the accuracy of 0.01 %. We also note that our mean estimate is better than the value $k_B T_c/J = 4.533\,71$ obtained in Ref. [13] (see also [14]) for the fully isotropic lattice using the ordinary phenomenological renormalization of the bars with $L = 4, 5$.

We now discuss the anisotropic case. Here, there is the well-known exact asymptotic formula for the critical temperature [15],

$$\left(\frac{k_B T_c}{J}\right)_{asym} = \frac{2}{\ln(J/2J') - \ln\ln(J/2J') + O(1)} \tag{15}$$

Table 1. Lower and upper bounds on the critical temperature and their mean values (improved estimates of $k_B T_c/J$) in the three-dimensional simple-cubic spin-1/2 Ising lattice vs $\Delta = J'/J$. Calculations with a cluster pair $(3, 4)$

Δ	Eq. (4)	Eq. (5)	mean
1.0	4.47965814	4.54424309	4.51195062
0.5	2.91008665	2.94295713	2.92652189
0.1	1.33649605	1.34570054	1.34109829
0.05	1.03544938	1.04144927	1.03844933
0.01	0.65054054	0.65323146	0.65188600
0.005	0.55440490	0.55643112	0.55541801
0.001	0.40743000	0.40859011	0.40801006

as $J'/J \to 0$. It is a direct consequence of the molecular-field approximation in which the linear Ising chain is taken as a cluster.

Unfortunately, simple formula (15) yields considerable errors in the region $10^{-3} \le J'/J \le 1$. Its modifications in the spirit of Ref. [16],

$$\frac{k_B T_c}{J} \approx \frac{2}{\ln(J/J') - \ln\ln(J/J')},$$

lead to a loss of monotonic convergence as J'/J varies from unity to zero.

We choose infinitely long clusters $L \times L \times \infty$ stretched in a lattice direction with the dominant interaction J. Such a cluster geometry reflects the physical situation in the system. We may therefore expect more precise results for the critical temperature as the anisotropy of the quasi-one-dimensional lattice increases. We may also expect a monotonic convergence for the estimates in Eq. (4) and (5) because there must be physical reasons (finite length of clusters in the longitudinal direction, etc.) for a nonmonotonic or oscillatory character of behavior; they are absent in our approximations. That is, if Eq. (4) yields the lower bound in the most unfavorable case $J' = J$, then it should preserve such behavior for all $J' < J$. Similar arguments are valid for the estimates following from Eq. (5); these estimates are upper.

We note that the mean values in Table 1 are not only better than the estimates of $k_B T_c/J$ calculated with the $(3, 4)$ cluster pair by the standard phenomenological RG method, but also better than their improvements found by means of three-point extrapolations from the sizes $L = 2$, 3, 4 to the bulk limit [17].

In the range $10^{-2} \le J'/J \le 1$, there are also the data for the critical temperature of a simple-cubic Ising lattice that were extracted from the Padé-approximant analysis of the high-temperature series [18]. For $J' = J$, according to these data, $k_B T_c/J = 4.5106$, which is lower by 0.014 % in comparison with the results in Ref. [12]. For $J'/J = 0.1$, the authors of Ref. [18] found the value $k_B T_c/J = 1.343$. This quantity somewhat overestimates the mean value in Table 1. Finally, for $J'/J = 0.01$, the series method [18] yields $k_B T_c/J = 0.65$, which goes out of our lower bound. This is not surprising because the calculations based on the high-temperature series rapidly deteriorate owing to the very limited number (≤ 11) of terms available in such series for the anisotropic lattices.

Therefore, we may treat the values found from Eqs. (4) and (5) as lower and upper bounds on the real critical temperature. Their mean value for each J'/J yields the best estimate that we achieve in this paper

Table 2. Estimates of the thermal and magnetic critical exponents for different values of $\Delta = J'/J$. Calculations with a cluster pair $(3,4)$

Δ	$k_B T_c/J$	y_t		y_h	
		Eq. (6)	Eq. (7)	Eq. (8)	Eq. (9)
1.0	4.51195062	1.5760695	1.7246286	2.5971647	2.5886128
0.5	2.92652189	1.5256373	1.6636718	2.5902006	2.5819462
0.1	1.34109829	1.4700811	1.5972576	2.5843305	2.5766511
0.05	1.03844933	1.4533899	1.5791439	2.5836720	2.5761101
0.01	0.65188600	1.4236178	1.5480583	2.5832982	2.5758028
0.005	0.55541801	1.4141719	1.5383503	2.5832029	2.5757888
0.001	0.40801006	1.3984754	1.5222765	2.5834573	2.5757953
		$1.47\{6\}$	$1.60\{7\}$	$2.586\{5\}$	$2.579\{5\}$

for the reduced critical temperature $k_B T_c/J$ (the last column in Table 1). Hence, its absolute error is not larger in any case than half the difference of the corresponding upper and lower bounds. Using the data in Table 1, we establish that the relative errors for $k_B T_c/J$ monotonically decrease from 0.72 % to 0.14 % as J'/J goes from 1 to 10^{-3}.

3.2. Invariants of the three-dimensional Ising universality class

With the improved estimates for the critical temperature of an anisotropic simple-cubic lattice, we now calculate some invariants of the three-dimensional Ising model universality class.

3.2.1. Critical exponents

According to the RG theory, critical exponents are determined entirely by a fixed point and do not depend on the lattice anisotropy. For a three-dimensional Ising model, the universality of critical exponents has been confirmed for $\Delta \in [0.2, 5]$ by the high-temperature series calculations [19].

At present, the most precise estimates of critical exponents are provided by the high-temperature expansions for ordinary models [20] and for models with improved potentials characterized by suppressed leading scaling corrections [21]. For the three-dimensional (fully isotropic) Ising lattice, these methods yield $\nu = 0.63012(16)$ and $\gamma = 1.2373(2)$. Hence, $y_t = 1/\nu = 1.5870(4)$ and $y_h = (d + \gamma/\nu)/2 = 2.48180(18)$.

In Table 2, we report our estimates for the critical exponents y_t and y_h. It follows from those data that as the lattice anisotropy parameter Δ varies by three orders (from unity to 10^{-3}), the estimates of critical exponents are changed only by a few per cent or less. In particular, calculations via Eqs. (6) and (7) with the cluster pair $(3,4)$ yield $y_t = 1.47\{6\}$ and $y_t = 1.60\{7\}$ respectively. (Here and below, the numbers in curly brackets are dispersions of averages over the lattice anisotropy parameter Δ.) Their variations are in the range 4–4.4 %. Similar calculations of the magnetic critical exponent performed with Eqs. (8) and (9), also with the pair $(3,4)$, lead to $y_h = 2.586\{5\}$ and $y_h = 2.579\{5\}$, correspondingly. Relative dispersions of these estimates are about 0.2 %.

Thus, our calculations confirm the universality of both critical exponents in an essentially wider range of Δ than in earlier investigations. Systematic errors of the achieved estimates arise due to small sizes L of the subsystems used.

3.2.2. Critical FSS amplitude ratios

Critical amplitudes are determined by scaling functions. As a result, their «universal ratios» like

$$\frac{A_{\kappa^{(4)}}}{A_{\chi^{(4)}}} = \frac{\mathcal{K}^{(0,4)}(0,0)}{\mathcal{F}^{(0,4)}(0,0)}$$

depend, generally speaking, on the lattice anisotropy because it can change the shape of subsystems. But in the case of parallelepipeds $L^{d-1} \times \infty$ with unchanged (between themselves) transverse coupling constants, the shape of a sample (all its aspect ratios) is independent of the interaction in the longitudinal direction. Such a kind of universality is studied here.

Table 3 contains results of our calculations for the critical FSS amplitude ratios $U = A_{\chi^{(4)}} A_\kappa / A_\chi^2$,

Table 3. Estimates of the universal critical FSS amplitude ratios $U = A_{\chi^{(4)}} A_\kappa / A_\chi^2$, $Y_1 = A_{\kappa^{(2)}}/A_\chi$, and $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}}$ for the Ising system with the cylindrical geometry $L \times L \times \infty$ and periodic boundary conditions. Data for $L = 4$

Δ	$k_B T_c/J$	U	Y_1	Y_2
1.0	4.51195062	4.8956599	1.7550004	2.0146443
0.5	2.92652189	4.8967625	1.7572512	2.0136519
0.1	1.34109829	4.9011909	1.7596003	2.0129829
0.05	1.03844933	4.9014406	1.7597697	2.0129285
0.01	0.65188600	4.9015375	1.7598563	2.0128977
0.005	0.55541801	4.9015529	1.7598646	2.0128953
0.001	0.40801006	4.9015782	1.7598732	2.0128938
		4.900{3}	1.759{2}	2.0133{6}

$Y_1 = A_{\kappa''}/A_\chi$, and $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}}$. Calculations have been performed for $\Delta \in [10^{-3}, 1]$ using a cyclic cluster $4 \times 4 \times \infty$.

In accordance with the data in Table 3, the average ratio $U = 4.900\{3\}$. Hence, as the anisotropy parameter Δ varies by three orders, this quantity changes only by 0.06 %. With such accuracy, we may consider the given ratio a constant. In the case of a fully isotropic lattice, $A_\kappa = 1.26(5)$ and $A_{\chi^{(4)}}/A_\chi^2 = 3.9(2)$ [8], and therefore $A_{\chi^{(4)}} A_\kappa / A_\chi^2 = 4.9(5)$. Our values of U in Table 3 are in good agreement with this estimate.

It follows from Table 3 that $Y_1 = A_{\kappa''}/A_\chi = 1.759(2)$. Hence, the constancy of this universal amplitude ratio is estimated at least as a few times 10^{-3}. Our average value for Y_1 agrees well with the estimate for the isotropic lattice, $A_{\kappa''}/A_\chi = 1.749(6)$ [8].

According to the data in Table 3, the amplitude ratio $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}} = 2.0133\{6\}$. This quantity is therefore most stable of all the invariants of the three-dimensional Ising universality class that were investigated in this paper. We note that we are not aware of any quantitative estimates for $A_{\kappa^{(4)}}/A_{\chi^{(4)}}$.

4. CONCLUSIONS

In this paper, the large-scale transfer-matrix computations have been performed. Application of the extended phenomenological RG schemes has allowed finding tight bounds on the critical temperature in the anisotropic simple-cubic Ising lattice and improving the available estimates for it.

We calculated the thermal and magnetic critical exponents. Our results confirm the universality of y_t within 4–4.4 % and of y_h within 0.2 % over a remarkably wider range of Δ ($10^{-3} \le \Delta \le 1$) than in Ref. [19].

Finally, the presented results give clear evidence that the critical FSS amplitude ratios $U = A_{\chi^{(4)}} A_\kappa / A_\chi^2$, $Y_1 = A_{\kappa''}/A_\chi$, and $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}}$ are independent of the lattice anisotropy parameter $\Delta = J'/J$ with accuracies at least 0.1 %. Probably for the first time in the literature, we give an estimate for the universal quantity Y_2.

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