Critical finite-size-scaling amplitudes of a fully anisotropic three-dimensional Ising model

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A fully anisotropic simple-cubic Ising lattice in the geometry of periodic cylinders $n\times n\times\infty$ is investigated by the transfer-matrix finite-size-scaling method. In addition to the previously obtained critical amplitudes of the inverse correlation lengths and singular part of the free energy [M. A. Yurishchev, Phys. Rev. B **50**, 13 533 (1994)], the amplitudes of the usual (''linear'') and nonlinear susceptibilities and the amplitude of the second derivative of the spin-spin inverse correlation length with respect to the external field are calculated. The behavior of critical amplitude combinations (which, in accordance with the Privman-Fisher equations, do not contain in their composition the nonuniversal metric coefficients and geometry prefactor) are studied as a function of the interaction anisotropy parameters. A universality domain for the amplitude ratios is found in the quasi-one-dimensional regime of interactions in the system. In the case of a fully *isotropic* three-dimensional Ising model for which the high precision values of the critical coupling and critical-point free energy are available, improved estimates are obtained for the following four universal quantities: (1) the amplitude of spin-spin inverse correlation length, (2) the amplitude of singular part of the free energy, (3) the ratio of the amplitude of a second derivative of the spin-spin inverse correlation length with respect to the external field to the usual susceptibility amplitude, and (4) the ratio of the nonlinear susceptibility amplitude to the square of the linear susceptibility amplitude (i.e., for the finite-size counterpart of the four-point renormalized coupling constant). [S1063-651X(97)07303-0]

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I. INTRODUCTION

In Ref. [1] (hereafter referred to as I), the critical finite-size amplitudes of the inverse correlation lengths and the ''singular'' part of the free energy per spin have been calculated for the three-dimensional ferromagnetic Ising model on a simple-cubic lattice with fully anisotropic interactions. The amplitudes have been obtained by a finite-size-scaling (FSS) analysis of the transfer-matrix (TM) data for subsystems having a shape of $n\times n\times\infty$ cylinders with periodic boundary conditions in both transverse directions.

The results showed that the ratios of the above critical amplitudes practically do not depend on the anisotropy parameter J_x/J_z if the second parameter J_y/J_x is fixed (the parallelepipeds $n\times n\times\infty$ are assumed to be stretched along the z axis; J_x and J_y are the interaction constants in the transverse directions of a cylinder, and J_z is the interaction constant in the longitudinal direction). Furthermore, it has been found that the amplitude ratios are independent of the second anisotropy parameter, J_y/J_x, in the vicinity of $J_y/J_x=1$. Unfortunately, a wrong conclusion concerning the amplitude ratio constancy in the full range of the J_y/J_x values has been made in I.

In addition to the amplitude of the spin-spin inverse correlation length (A_s) and the free-energy amplitude (A_f), in the present paper we calculate the amplitudes of linear and nonlinear susceptibilities (A_χ and $A_{\chi^{(4)}}$, respectively), as well as the amplitude of the second derivative of the spin-spin inverse correlation length with respect to the external field ($A_{\kappa''_{hh}}$). The calculations are performed again for the cyclic clusters $n\times n\times\infty$ with the maximum number of lattice layers in each transverse direction $n=4$ (i.e., for the sizes of TMs up to $65\,536\times65\,536$). Guiding ourselves by the functional equations of Privman and Fisher [2–4], we construct from critical amplitudes the combinations $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}}A_s/A_\chi^2$, which, as A_s/A_f, do not contain the certain nonuniversal coefficients. The analysis shows that those amplitude ratios are universal with respect to the anisotropy parameter $J_x/J_z\rightarrow0$ but depend on the parameter J_y/J_x. However, the J_y/J_x dependencies exhibit smooth extrema near $J_y/J_x=1$, and therefore the amplitude ratios have a local universality in their vicinity upon the second anisotropy parameter of the model.

In the present paper we find also the values of A_s, A_f, $A_{\kappa''_{hh}}/A_\chi$, and $A_{\chi^{(4)}}/A_\chi^2$ for $n=2$, 3, and 4 in the case of the fully isotropic simple-cubic Ising lattice by using the available high accurate estimates for the critical point and critical free energy and give three-point extrapolations for these quantities.

II. SPATIAL ANISOTROPY AND THE PRIVMAN-FISHER EQUATIONS

In the case of d-dimensional cylinders with sizes of $L_1\times L_2\times\cdots\times L_{d-1}\times\infty$, the Privman-Fisher equations, which allow one to identify for the hyperscaling systems the universal combinations of critical finite-size amplitudes, have the form [2]

$$\widetilde{\kappa}(t,h)=L_0^{-1}X(C_1tL_0^{y_T},C_2hL_0^{y_h};L_1/L_0,\ldots,L_{d-1}/L_0) \tag{1}$$

and

$$\widetilde{f}^{(s)}(t,h)=L_0^{-d}Y(C_1tL_0^{y_T},C_2hL_0^{y_h};L_1/L_0,\ldots,L_{d-1}/L_0). \tag{2}$$

In these equations, $\widetilde{\kappa}$ is the inverse correlation length in the longitudinal direction of the cylinder, $\widetilde{f}^{(s)}$ is the singular part of the free-energy density measured in units of $-k_BT$, $t=(T-T_c)/T_c$ is the reduced temperature, h is the normalized external field, y_T and y_h are critical exponents, C_1 and C_2 are system-dependent metric factors, and L_0 is a scale length. The FSS functions $X(x_1,x_2;l_1,l_2,\ldots)$ and $Y(x_1,x_2;l_1,l_2,\ldots)$ are universal (within the limits of a given universality class) but may depend on the type of boundary conditions and, as we see, on the aspect ratios $l_i=L_i/L_0$. For the scaling length L_0, one can take $L_0=(L_1L_2\cdots L_{d-1})^{1/(d-1)}$ or put $L_0=\min(L_1,L_2,\ldots,L_{d-1})$, etc.

Let us turn in Eqs. (1) and (2) to the dimensionless quantities, which are immediately defined by the parameters of a subsystem Hamiltonian. Let the elementary cell of a simple-cubic lattice have the sizes of $a_1\times a_2\times\cdots\times a_d$ and let the subsystem ''frame'' be a cylinder $n_1\times n_2\times\cdots\times n_{d-1}\times\infty$, where n_i is a number of spins in the ith transverse direction. We will, however, restrict ourselves to the case of cylinders with *square* cross section, i.e., $n_1=n_2=\cdots=n_{d-1}=n$. Then $L_i=na_i$, $\widetilde{\kappa}=a_d^{-1}\kappa_n$, and $\widetilde{f}^{(s)}=(a_1a_2\cdots a_d)^{-1}f_n^{(s)}$, where κ_n and $f_n^{(s)}$ are, respectively, the dimensionless inverse correlation length and singular part of the free energy per site. (Below, however, we will often omit, for brevity, the word ''dimensionless.'') In the new variables the Privman-Fisher equations can be written as

$$\kappa_n(t,h)=n^{-1}GX(C_1tn^{y_T},C_2hn^{y_h};a_2/a_1,\ldots,a_{d-1}/a_1) \tag{3}$$

and

$$f_n^{(s)}(t,h)=n^{-d}GY(C_1tn^{y_T},C_2hn^{y_h};a_2/a_1,\ldots,a_{d-1}/a_1), \tag{4}$$

where $G=G(a_2/a_1,\ldots,a_{d-1}/a_1,a_d/a_1)$ is the geometry prefactor. We assume that at least two lattice spacings in the system are finite and nonzero; without loss of generality, we take them as a_1 and a_d.

One obtains from Eqs. (3) and (4) that

$$A_s=n\kappa_n(0,0)=GX(0,0;a_2/a_1,\ldots,a_{d-1}/a_1), \tag{5}$$

$$A_f=n^df_n^{(s)}(0,0)=GY(0,0;a_2/a_1,\ldots,a_{d-1}/a_1), \tag{6}$$

and analogously for the dimensionless critical finite-size-scaling amplitudes of the derivatives of $\kappa_n(t,h)$ or $f_n^{(s)}(t,h)$.

The geometry-prefactor form depends on the choice of L_0. The prefactor is defined with exactness up to some multiplicative function of $a_2/a_1,\ldots,a_{d-1}/a_1$, inasmuchas such a function can be introduced into the scaling functions X and Y or, vice versa, taken out from them. We will, however, set $G=1$ for the fully isotropic model.

In order to be able to employ the FSS theory, the ''lattice spacings'' a_i must be chosen so that in the vicinity of the phase transition point the bulk correlation lengths $\widetilde{\xi}_1,\ldots,\widetilde{\xi}_d$ along all the different spatial directions become equal among themselves: $\widetilde{\xi}_1=\widetilde{\xi}_2=\cdots=\widetilde{\xi}_d$. Such a rescaling of lattice spacings can be made for systems with the isotropic critical exponent ν of the bulk correlation lengths, i.e., when $\xi_i=\xi_0^{(i)}t^{-\nu}$ (Refs. [5–7]). The choice of a_i completes, in principle, the process of expressing the quantities entering into the Privman-Fisher equations via ''microscopic'' parameters—the interaction constants of the Hamiltonian. Note that the situation is paradoxical to a certain extent: in order to use the FSS theory for extracting information about a bulk system from properties of its finite subsystems, one must know before the correlation-length amplitudes of the bulk system.

In the two-dimensional anisotropic Ising lattice, which is a limited case $(J_y=0)$ of the three-dimensional Ising model under question, the dimensionless bulk correlation lengths for $T>T_c$ are [8] (see also, e.g., Ref. [9])

$$\begin{aligned}\xi_x(J_x/k_BT,J_z/k_BT)&=\xi_z(J_z/k_BT,J_x/k_BT)\\&=1/\ln[\coth(J_x/k_BT)\exp(-2J_z/k_BT)].\end{aligned} \tag{7}$$

[When $T<T_c$, the correlation length expressions differ from Eq. (7) by the factor $-1/2$, which is, however, unessential for the present considerations.] According to the isotropy requirement, $a_x\xi_x=a_z\xi_z$ and therefore for the square Ising lattice [5] (see also [6,10,11])

$$G=\frac{a_z}{a_x}=\lim_{T\to T_c}\frac{\xi_x}{\xi_z}=\left[\sinh\left(\frac{2J_z}{k_BT_c}\right)\right]^{-1}, \tag{8}$$

where the critical temperature T_c is determined by the equation

$$\sinh\left(\frac{2J_x}{k_BT_c}\right)\sinh\left(\frac{2J_z}{k_BT_c}\right)=1\,. \tag{9}$$

Equations (8) and (9) in parametric form yield the geometry factor $G(J_x/J_z)$. Note that up to date the anisotropy factors have been found for many exactly solved two-dimensional models of statistical physics [12–14].

In the three-dimensional space, Eqs. (3) and (4) are written as

$$\kappa_n(t,h)=n^{-1}GX(C_1tn^{y_T},C_2hn^{y_h};a_y/a_x) \tag{10}$$

and

$$f_n^{(s)}(t,h)=n^{-3}GY(C_1tn^{y_T},C_2hn^{y_h};a_y/a_x). \tag{11}$$

Due to the shape parameter a_y/a_x, the scaling functions depend on the coupling ratios, and therefore Eqs. (10) and (11) do not allow the existence of any universal amplitude combinations. An obvious exception, however, is given by the case when the interactions in the transverse directions of the parallelepiped $n\times n\times\infty$ are equal among themselves. On physical grounds, it is clear that $a_x=a_y$ by this, and consequently the critical amplitude combinations that do not contain C_1, C_2, and G will not depend upon the interaction constants in the system.

III. FORMULAS FOR THE SUSCEPTIBILITIES AND FOR THE INVERSE CORRELATION-LENGTH DERIVATIVE

For the amplitude ratio $A_{\kappa''_{hh}}/A_\chi$, it follows from Eqs. (3) and (4) that

$$\frac{A_{\kappa''_{hh}}}{A_\chi}=\frac{\kappa''_{hh}}{n^{d-1}\chi_n}, \tag{12}$$

where $\kappa''_{hh}=\partial^2\kappa_n/\partial h^2$, while $\chi_n=\partial^2 f_n/\partial h^2=\partial^2 f_n^{(s)}/\partial h^2$ is the susceptibility of the system (f_n denotes the dimensionless free energy per lattice site). Taking into account that $A_s=n\kappa_n$, one finds for the second amplitude combination

$$\frac{A_{\chi^{(4)}}A_s}{A_\chi^2}=\frac{\chi_n^{(4)}\kappa_n}{n^{d-1}\chi_n^2}, \tag{13}$$

where $\chi_n^{(4)}=-\partial^4 f_n/\partial h^4$ is a nonlinear susceptibility. Thus, the problem is to carry out the calculation of κ''_{hh} and $\chi_n^{(4)}$ for periodic cylinders $n\times n\times\infty$ at $h=0$ since the method of calculating κ_n and χ_n was already done in I.

To solve these problems, we use, as in I, the TM technique. The matrix elements of TM, $\mathcal{V}$, are given by

$$\langle S_{11},S_{12},\dots,S_{nn}|\mathcal{V}|S'_{11},S'_{12},\dots,S'_{nn}\rangle$$

$$=\prod_{i,j=1}^{n}\exp[\tfrac{1}{2}K_x(S_{ij}S_{i+1j}+S'_{ij}S'_{i+1j})+\tfrac{1}{2}K_y(S_{ij}S_{ij+1}+S'_{ij}S'_{ij+1})+K_zS_{ij}S'_{ij}+\tfrac{1}{2}h(S_{ij}+S'_{ij})]. \tag{14}$$

Here the spin variables S_{ij} take the values ±1; $S_{in+1}=S_{i1}$ and $S_{n+1j}=S_{1j}$ for all $i,j=1,2,\dots,n$; $K_\alpha=J_\alpha/k_BT$ $(\alpha=x,y,z)$. The matrix $\mathcal{V}$ is real, symmetric, and dense, having all its elements positive. The dimensionless free energy per spin equals

$$f_n=\frac{1}{n^2}\ln\Lambda_1, \tag{15}$$

where Λ_1 is the largest eigenvalue of $\mathcal{V}$. Further, the dimensionless spin-spin inverse correlation length in the longitudinal direction of a parallelepiped $n\times n\times\infty$ is

$$\kappa_n=\ln(\Lambda_1/\Lambda_2), \tag{16}$$

where Λ_2 denotes the second largest eigenvalue of the matrix $\mathcal{V}$.

In order to derive the exact formulas for the zero-field derivatives of the free energy and inverse correlation length, we will use perturbation theory. For this one expands the TM in powers of h:

$$\mathcal{V}=V+hV_1+h^2V_2+h^3V_3+h^4V_4+O(h^5). \tag{17}$$

Let us use the symmetry of the model (in this context see I). $\mathcal{V}$ is invariant under the transformations of the group $T\wedge C_{2v}$ (T is a group of translations in the transverse directions of a cyclic bar $n\times n\times\infty$ and C_{2v} is the point group generated by two symmetry planes going through the middles of opposite faces of the system). Turn in Eq. (17) to the basis of the identity irreducible representation of the group $T\wedge C_{2v}$. Expansion (17) preserves the above form but now its terms are blocks corresponding to the indicated representation. Both eigenvalues Λ_1 and Λ_2 lie in the given block $\mathcal{V}$. Take now into consideration the symmetry Z_2 (a group of spin inversions). The matrices V, V_2, and V_4 are symmetrical and the matrices V_1 and V_3 are antisymmetrical (i.e., they change sign) under the spin inversion operation. Going by means of a similarity transformation into a new basis in which the original representation of the group is completely reducible, one obtains from Eq. (17)

$$\tilde{\mathcal{V}}=\begin{pmatrix}V^{(1)}&0\\0&V^{(2)}\end{pmatrix}+h\begin{pmatrix}0&V_1^{(12)}\\V_1^{(21)}&0\end{pmatrix}+h^2\begin{pmatrix}V_2^{(1)}&0\\0&V_2^{(2)}\end{pmatrix}+h^3\begin{pmatrix}0&V_3^{(12)}\\V_3^{(21)}&0\end{pmatrix}+h^4\begin{pmatrix}V_4^{(1)}&0\\0&V_4^{(2)}\end{pmatrix}+O(h^5). \tag{18}$$

For definiteness we suppose that the subblocks $V^{(1)}$, $V_2^{(1)}$, and $V_4^{(1)}$ correspond to the identity irreducible representation of the group Z_2. Denote the sizes of these subblocks by $N_1\times N_1$ and the sizes of the subblocks $V^{(2)}$, $V_2^{(2)}$, and $V_4^{(2)}$ by $N_2\times N_2$. Then, the matrices $V_1^{(12)}$ and $V_3^{(12)}$ have sizes $N_1\times N_2$; $V_1^{(21)}$ and $V_3^{(21)}$ are found by transposing $V_1^{(12)}$ and $V_3^{(12)}$, respectively. The numbers N_1 and N_2 can be obtained from a group-theoretical analysis. For the $2\times2\times\infty$ cluster, $N_1=5$ and $N_2=2$ (Ref. [15]); for the $3\times3\times\infty$ cluster, $N_1=N_2=18$ (Ref. [15]); and for $4\times4\times\infty$, $N_1=787$ and $N_2=672$ (Ref. [1]). Further, let $\lambda_i^{(1)}$ and ψ_i be the eigenvalues and corresponding eigenvectors of matrix $V^{(1)}$; let $\lambda_1^{(1)}=\lambda_1$ be the largest eigenvalue of the block $V^{(1)}$ and consequently of the ''nonperturbed'' transfer matrix V. Due to the Perron theorem, λ_1 is nondegenerate. Finally, let $\lambda_i^{(2)}$ and φ_i be the eigenpairs of $V^{(2)}$; $\lambda_1^{(2)}$ is the largest eigenvalue of block $V^{(2)}$. Note that $\lambda_1^{(2)}$ is also nondegenerate if we do not take the extreme cases, which can be examined separately.

Using the stationary perturbation theory for a nondegenerate level, we find the largest eigenvalue of $\mathcal{V}$ with accuracy up to the terms of second order in h:

$$\Lambda_1=\lambda_1+\left[\psi_1^+V_2^{(1)}\psi_1+\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{\lambda_1-\lambda_k^{(2)}}\right]h^2+O(h^4). \quad (19)$$

From here, the expression for the initial (zero-field) susceptibility follows as

$$\chi_n=\frac{2}{n^2\lambda_1}\left[\psi_1^+V_2^{(1)}\psi_1+\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{\lambda_1-\lambda_k^{(2)}}\right]. \quad (20)$$

The given formula, obtained by the perturbation-theory method, differs in a form from the one derived in I using the fluctuation-dissipation relation, but it is equivalent to it and yields the same values of the susceptibility.

In an analogous way, one obtains the following expression for the second largest eigenvalue of $\mathcal{V}$:

$$\Lambda_2=\lambda_1^{(2)}+\left[\varphi_1^+V_2^{(2)}\varphi_1+\sum_{k=1}^{N_1}\frac{(\psi_k^+V_1^{(12)}\varphi_1)^2}{\lambda_1^{(2)}-\lambda_k^{(1)}}\right]h^2+O(h^4). \quad (21)$$

From Eqs. (16), (19), and (21) we get the work formula for the second derivative of the spin-spin inverse correlation length at point $h=0$:

$$\kappa''_{hh}=2\left\{\frac{1}{\lambda_1}\left[\psi_1^+V_2^{(1)}\psi_1+\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{\lambda_1-\lambda_k^{(2)}}\right]-\frac{1}{\lambda_1^{(2)}}\left[\varphi_1^+V_2^{(2)}\varphi_1+\sum_{k=1}^{N_1}\frac{(\psi_k^+V_1^{(12)}\varphi_1)^2}{\lambda_1^{(2)}-\lambda_k^{(1)}}\right]\right\}. \quad (22)$$

Calculating the largest eigenvalue Λ_1 up to the terms of fourth order in h, we find the following result (suited for programming) for the initial nonlinear susceptibility:

$$\chi_n^{(4)}=\frac{12}{n^2\lambda_1}\left[\frac{1}{\lambda_1}Q^2-2(Q_1+Q_2+Q_3+Q_4+Q_5-Q_6+Q_7-Q_8)\right], \quad (23a)$$

with

$$Q=\psi_1^+V_2^{(1)}\psi_1+\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{\lambda_1-\lambda_k^{(2)}},$$

$$Q_1=\psi_1^+V_4^{(1)}\psi_1,\quad Q_2=\sum_{k=2}^{N_2}\frac{(\psi_1^+V_2^{(1)}\psi_k)^2}{\lambda_1-\lambda_k^{(1)}},\quad Q_3=2\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)(\psi_1^+V_3^{(12)}\varphi_k)}{\lambda_1-\lambda_k^{(2)}},$$

$$Q_4=2\sum_{k=1}^{N_2}\sum_{l=2}^{N_1}\frac{(\psi_1^+V_1^{(12)}\varphi_k)(\varphi_k^+V_1^{(21)}\psi_l)(\psi_l^+V_2^{(1)}\psi_1)}{(\lambda_1-\lambda_k^{(2)})(\lambda_1-\lambda_l^{(1)})},$$

$$Q_5=\sum_{k=1}^{N_2}\sum_{l=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)(\varphi_k^+V_2^{(2)}\varphi_l)(\varphi_l^+V_1^{(21)}\psi_1)}{(\lambda_1-\lambda_k^{(2)})(\lambda_1-\lambda_l^{(2)})}, \quad (23b)$$

$$Q_6=\psi_1^+V_2^{(1)}\psi_1\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{(\lambda_1-\lambda_k^{(2)})^2},$$

$$Q_7=\sum_{k=1}^{N_2}\sum_{l=2}^{N_1}\sum_{m=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)(\varphi_k^+V_1^{(21)}\psi_l)(\psi_l^+V_1^{(12)}\varphi_m)(\varphi_m^+V_1^{(21)}\psi_1)}{(\lambda_1-\lambda_k^{(2)})(\lambda_1-\lambda_l^{(1)})(\lambda_1-\lambda_m^{(2)})},$$

$$Q_8=\sum_{k=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_k)^2}{(\lambda_1-\lambda_k^{(2)})^2}\sum_{l=1}^{N_2}\frac{(\psi_1^+V_1^{(12)}\varphi_l)^2}{\lambda_1-\lambda_l^{(2)}}.$$

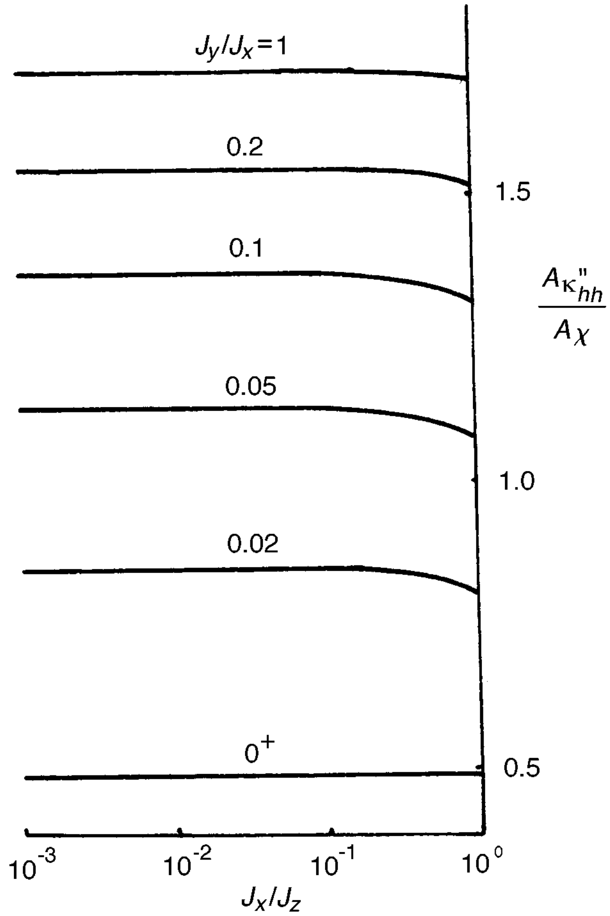

FIG. 1. Amplitude ratio $A_{\kappa''_{hh}}/A_\chi$ vs the anisotropy parameter J_x/J_z by different fixed values of J_y/J_x. Periodic cylinder $4\times4\times\infty$ at critical temperatures $T_c^{(3,4)}$.

Explicit expressions for the matrix elements of subblocks $V_1^{(12)}$, $V_2^{(1)}$, $V_2^{(2)}$, $V_3^{(12)}$, and $V_4^{(1)}$ are given in the Appendix. Notice that the full eigenproblems for the matrices $V^{(1)}$ and $V^{(2)}$ were solved by means of the *C* library function pair tred2 and tqli [16]. All calculations were carried out on a personal computer IBM PC-486 with the operating system FreeBSD.

IV. BEHAVIOR OF THE CRITICAL AMPLITUDE RATIOS

As already noted in Sec. II, the FSS amplitude combinations normally should depend on the interaction ratios, which change the shape of a subsystem. This is in agreement with basic ideas of the renormalization-group theory.

We will consider how the amplitude combinations behave versus the interaction anisotropy parameters in the three-dimensional Ising model. To eliminate as effectively as possible nonuniversal quantities from the critical FSS amplitude combinations, it is natural to consider the behavior of such combinations, which do not include in its composition the nonuniversal metric and geometry factors. In other words, it is reasonable to base again our choice of combinations on the Privman-Fisher equations.

For a cluster $n\times n\times\infty$, the values of linear and nonlinear susceptibilities and derivative κ''_{hh} are taken at critical temperatures, which were determined by the $(n-1,n)$ cluster pair, i.e., through the equation

$$(n-1)\kappa_{n-1}(T_c^{(n-1,n)})=n\kappa_n(T_c^{(n-1,n)}). \tag{24}$$

Since we are able to perform the calculations for subsystems with $n\leqslant4$, this allows us to have two independent iterations, with (2,3) and (3,4) pairs [a degenerate pair (1,2) was eliminated from the consideration due to its anomalies [17]]. Two steps of converging iterations give already a possibility to extract valuable information about tendencies in the change of quantities with increasing n.

The results for the critical temperatures and critical FSS amplitude ratios $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}}A_s/A_\chi^2$ depending on J_x/J_z and J_y/J_x in the cases of both cluster pairs (2,3) and (3,4) are collected in Table I.

Let us first discuss the behavior of amplitude ratios against J_x/J_z. Figure 1 [18] shows the dependencies of $A_{\kappa''_{hh}}/A_\chi$ on J_x/J_z at different fixed values of J_y/J_x. If $J_y/J_x=0$, the bar $n\times n\times\infty$ is reduced to statistically independent strips. In two-dimensional space, the dependence on an anisotropy parameter must be, as follows from Eqs. (3) and (4), absent. The $J_y/J_x=0$ plot given in Fig. 1 confirms this: in the case of the (3,4) approximation, the ratio $A_{\kappa''_{hh}}/A_\chi$ is unchanged within the relative root-mean-square error 0.08%. We expect the constancy of amplitude ratios also at $J_y/J_x=1$. The corresponding line shown in Fig. 1 can be considered as a straight one with an accuracy 0.31%. Importantly, the analogous error for the (2,3) pair is 0.45%. Thus, the deviations versus J_x/J_z fall as n increases.

For intermediate fixed values of J_y/J_x, the amplitude ratio has weak but still quite detectible dependence against J_x/J_z. As seen in Fig. 1, variances are most essential in the range $10^{-1}\lesssim J_y/J_x\leqslant1$. Now the amplitude ratio dependence does not tend to disappear with increasing n. For example, when $J_y/J_x=0.1$, the mean values and the root-mean-square uncertainties (the latter are shown in parentheses) for the quantity $A_{\kappa''_{hh}}/A_\chi$ in the range $10^{-3}\leqslant J_x/J_z\leqslant1$ equal 1.37(2) and 1.35(2) for the pairs (2,3) and (3,4), respectively.

A similar picture is observed for the $A_{\chi^{(4)}}A_s/A_\chi^2$ (see Table I) and for the A_s/A_f (Table I of Ref. [1]). As a whole one can conclude that the critical FSS amplitude combinations that do not contain the nonuniversal factors C_1, C_2, and G display a tendency to the universality under the anisotropy parameter J_x/J_z when this is small (i.e., by a quasi-one-dimensional nature of interactions in the system).

We discuss now the behavior of the amplitude ratios as a function of the second anisotropy parameter, namely, J_y/J_x. In I the amplitudes of the inverse correlation lengths and the free energy have been calculated for $J_y/J_x\in[0,1]$. The amplitude A_f was found from a set of two equations,

$$f_n=f_\infty+n^{-d}A_f, \tag{25}$$

with $n=3$ and 4 [‘‘background’’ f_∞ is a second unknown variable in Eq. (25)]. In this paper we prolong such calculations to $J_y/J_x=4$ and use not only the (3,4) pair but also the (2,3) one, to observe the evolution with increasing n. The results are shown in Fig. 2. It can be seen from the figure that when the parameter J_y/J_x increases from zero, the ratio A_s/A_f first increases monotonically from some finite value, which decreases with growth of cluster size. Then the A_s/A_f attains a smooth maximum near $J_y/J_x=1$. Lastly, the ratio A_s/A_f falls monotonically as J_y/J_x becomes large.

It follows from the obtained data that the values of A_s/A_f are equal among themselves for J_y/J_x and $(J_y/J_x)^{-1}$ and this is better the smaller J_x/J_z. Clearly, the source of the $J_y/J_x \leftrightarrow (J_y/J_x)^{-1}$ symmetry is caused by the (approximate) J_x/J_z independence of amplitude ratios. The inversion symmetry leads in turn to an existence of extremum at $J_y/J_x=1$. Inasmuchas the extremum (maximum) is smooth, there is a local universality under the second anisotropy parameter J_y/J_x. We conclude that in the domain $0<J_x/J_z \ll 1$ and $|J_y/J_x-1| \ll 1$ there exists a complete universality of the amplitude ratio A_s/A_f. Note also that in the maximum region both curves go quite near one another; such a neighborhood characterizes the arrived convergence of (2,3) and (3,4) approximations.

We make the quantitative comparison of our data in the two-dimensional case. Space dimensionality d changes discontinuously from 3 to 2 in the limit $J_y/J_x \to 0$. This leads in turn to a finite jump in values of A_s/A_f at $J_y/J_x=0^+$ and $J_y/J_x=0$. Using Eq. (25) one finds for the $(n-1,n)$ pair that

$$(A_s/A_f)_0=\frac{n(n-1)(2n-1)}{3n(n-1)+1}(A_s/A_f)_{0^+}, \qquad (26)$$

where the subscripts 0 and 0^+ denote the values at $J_y/J_x=0$ and 0^+, respectively. Hence, recalculating the values at $J_y/J_x=0^+$ to the values at $J_y/J_x=0$, we obtain $(A_s/A_f)_0=3.0143$ for the (2,3) pair in the case $J_x/J_z=10^{-3}$. For the (3,4) pair at the same value of J_x/J_z, $(A_s/A_f)_0=3.0087$. In the two-dimensional Ising lattice, the exact value $A_s/A_f=3$ (in Fig. 2, it is shown by the

TABLE I. Critical-point amplitude ratios $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}}A_s/A_\chi^2$ as a function of anisotropy parameters J_x/J_z and J_y/J_x. Approximations by cluster pairs (2,3) and (3,4).

J_y/J_x	J_x/J_z		(2,3) pair			(3,4) pair	
		k_BT_c/J_z	$A_{\kappa''_{hh}}/A_\chi$	$A_{\chi^{(4)}}A_s/A_\chi^2$	k_BT_c/J_z	$A_{\kappa''_{hh}}/A_\chi$	$A_{\chi^{(4)}}A_s/A_\chi^2$
0^+	1.0	2.367640	0.65214	1.92695	2.320811	0.48946	1.44560
	0.5	1.699790	0.65173	1.92388	1.662411	0.48991	1.44730
	0.1	0.921068	0.65279	1.92832	0.910794	0.49034	1.44919
	0.01	0.513815	0.65309	1.92968	0.510586	0.49039	1.44940
	0.001	0.345015	0.65310	1.92972	0.343461	0.49039	1.44940
0.1	1.0	2.845802	1.34451	3.60933	2.817633	1.32110	3.48345
	0.5	1.979483	1.35368	3.62760	1.959011	1.34212	3.54079
	0.1	1.024601	1.38006	3.70054	1.019932	1.35995	3.59108
	0.01	0.550499	1.38661	3.71950	0.549216	1.36225	3.59760
	0.001	0.362466	1.38685	3.72021	0.361871	1.36233	3.59781
0.5	1.0	3.819394	1.65412	4.55222	3.739735	1.67447	4.59324
	0.5	2.533705	1.65621	4.54634	2.487136	1.68196	4.61381
	0.1	1.211125	1.67095	4.59073	1.199032	1.68882	4.63492
	0.01	0.611620	1.67545	4.60591	0.608159	1.68976	4.63782
	0.001	0.390357	1.67564	4.60656	0.388821	1.68979	4.63793
1.0	1.0	4.685960	1.68710	4.67454	4.581044	1.70507	4.70713
	0.5	3.024529	1.68407	4.64512	2.960469	1.71114	4.72047
	0.1	1.366300	1.69711	4.68102	1.350375	1.71743	4.73841
	0.01	0.658794	1.70231	4.69869	0.654587	1.71832	4.74101
	0.001	0.410971	1.70256	4.69953	0.409173	1.71835	4.74110
1.5	1.0	5.418190	1.68220	4.66797	5.310630	1.69188	4.66481
	0.5	3.442977	1.67334	4.61261	3.368233	1.69831	4.67598
	0.1	1.494583	1.68607	4.64298	1.475982	1.70726	4.70162
	0.01	0.695761	1.69307	4.66651	0.691216	1.70870	4.70596
	0.001	0.426622	1.69344	4.66777	0.424737	1.70875	4.70612
2.0	1.0	6.068336	1.66945	4.63471	5.975643	1.66826	4.58676
	0.5	3.819394	1.65412	4.55222	3.739735	1.67447	4.59324
	0.1	1.608392	1.66577	4.57383	1.587593	1.68729	4.63016
	0.01	0.727256	1.67510	4.60471	0.722535	1.68970	4.63763
	0.001	0.439633	1.67563	4.60652	0.437724	1.68979	4.63792

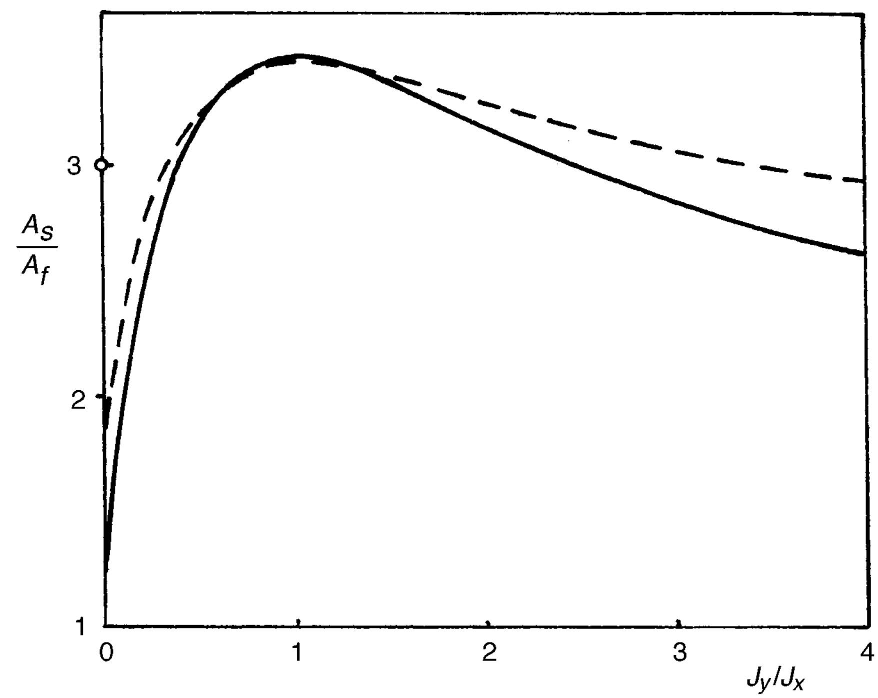

FIG. 2. Amplitude ratios A_s/A_f (averaged over $J_x/J_z = \{1, 10^{-1}, 10^{-2}, 10^{-3}\}$) as a function of J_y/J_x. Shown are the approximations by (2,3) and (3,4) cluster pairs—dashed and solid lines, respectively. Open circle on the ordinate axis is a value of A_s/A_f $(=3)$ for the two-dimensional Ising model.

open circle on the ordinate axis). Consequently, the error is reduced from 0.48% to 0.29% by going from (2,3) to (3,4) pair.

A qualitatively similar picture takes place for the ratios $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}} A_s/A_\chi^2$ (Figs. 3 and 4). Here again the amplitude ratios have finite values at $J_y/J_x = 0^+$ that vanish with increasing n according to the $1/n$ law. There is again a monotonic increase for small values of J_y/J_x, a broad maximum near $J_y/J_x = 1$, and then a monotonic decrease by large J_y/J_x. The inversion symmetry $J_y/J_x \leftrightarrow (J_y/J_x)^{-1}$ applies again.

Let us compare the results for the discussed amplitude ratios in the two-dimensional limit. Since

$$(A_{\kappa''_{hh}}/A_\chi)_0 = n(A_{\kappa''_{hh}}/A_\chi)_{0^+}, \tag{27}$$

taking from Table I the values at $J_y/J_x = 0^+$, one finds that $(A_{\kappa''_{hh}}/A_\chi)_0$ equals 1.959 and 1.962 for the (2,3) and (3,4) approximations, respectively (the point $J_x/J_z = 10^{-3}$ has been used). These values are in good agreement with available estimates of the amplitude ratio for the two-dimensional isotropic Ising models, $A_{\kappa''_{hh}}/A_\chi = 1.95 - 1.96$ (Ref. [19]).

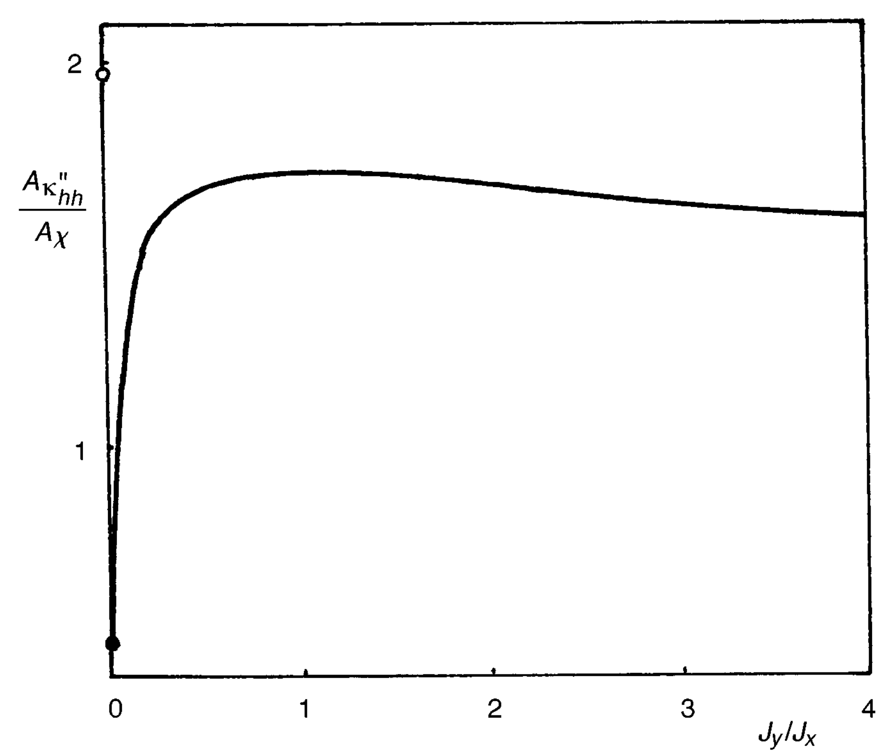

FIG. 3. Average amplitude ratio $A_{\kappa''_{hh}}/A_\chi$ vs J_y/J_x; periodic cylinder $4 \times 4 \times \infty$ at critical temperatures $T_c^{(3,4)}$. Full circle on the ordinate axis corresponds to the $A_{\kappa''_{hh}}/A_\chi$ at $J_y/J_x = 0^+$, while open one is a value of that ratio in the two-dimensional Ising lattice.

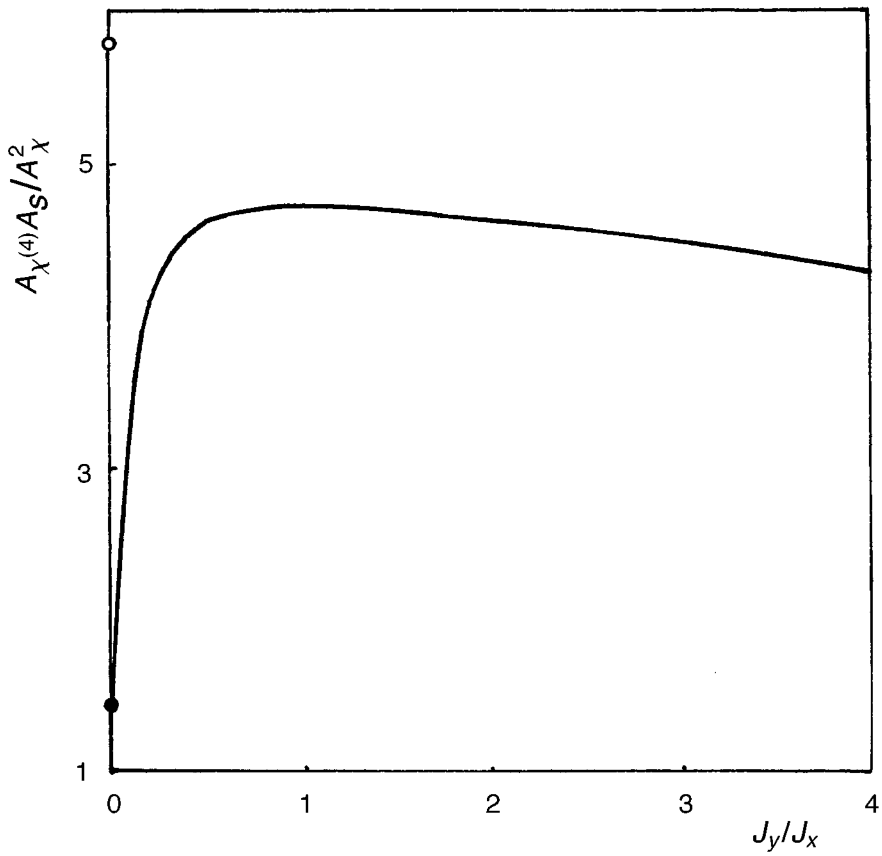

FIG. 4. The same as in Fig. 3 but for the amplitude ratio $A_{\chi^{(4)}}A_s/A_\chi^2$.

One can argue analogously for the combination $A_{\chi^{(4)}}A_s/A_\chi^2$, calculation being carried out by the formula

$$(A_{\chi^{(4)}}A_s/A_\chi^2)_0 = n(A_{\chi^{(4)}}A_s/A_\chi^2)_{0^+}. \tag{28}$$

Taking from Table I the necessary data, we find that at $J_x/J_z=10^{-3}$ the ratio $(A_{\chi^{(4)}}A_s/A_\chi^2)_0=5.7892$ and 5.7976 for the pairs (2,3) and (3,4), respectively. These results are in excellent agreement with the value $A_{\chi^{(4)}}A_s/A_\chi^2=5.797\,28(5)$ following from the calculations [20].

We discuss now a reason that could lead to a disappearance of the parameter J_x/J_z from scaling functions for the system with the dominant intrachain interaction $(J_z \gg J_x, J_y)$. The bulk correlation-length amplitude is a function of the interaction constants. Let $\xi_0^{(x)}=\phi(J_x/k_BT_c, J_y/k_BT_c, J_z/k_BT_c)$. In a lattice that is infinite in all three directions, the function $\phi(x,y,z)$ is symmetrical under the replacement of its second and third arguments: $\phi(x,y,z)=\phi(x,z,y)$. Moreover, $\phi(0,y,z)=0$ which means the absence of correlations in the direction along which there are no interactions. Let the expansion on the first argument begin from a term x in some power q. In accordance with physical reasoning, it is apparent that in the infinite lattice the amplitude $\xi_0^{(y)}$ has the same functional form as $\xi_0^{(x)}$ but, of course, with replaced arguments: $\xi_0^{(y)}=\phi(J_y/k_BT_c, J_x/k_BT_c, J_z/k_BT_c)$. Further, the critical temperature of a quasi-one-dimensional Ising model is given by [21]

$$k_BT_c/J_z = 2\left[\ln\left(\frac{J_z}{J_x+J_y}\right) - \ln\ln\left(\frac{J_z}{J_x+J_y}\right) + O(1)\right]^{-1}. \tag{29}$$

TABLE II. Estimates of the universal critical amplitude combinations for the fully isotropic three-dimensional simple-cubic Ising lattice in the geometry of infinitely long cyclic parallelepipeds with the square cross section. For all quantities, with the exception of A_f, the three-point extrapolations were performed by the Shanks' transform (Ref. [24]). In the case of A_f as a realistic estimate, the last term of finite sequence has been taken.

n	A_s	A_f	$A_{\kappa''_{hh}}/A_\chi$	$A_{\chi^{(4)}}/A_\chi^2$
2	1.458347	0.451886	1.784594	3.497834
3	1.353169	0.409959	1.763848	3.661609
4	1.302661	0.378507	1.755304	3.759097
∞	1.26(5)	0.37(3)	1.749(6)	3.9(2)

Due to the fact that a decrease of k_BT_c/J_z is logarithmically slow, the arguments of function ϕ, $J_x/k_BT_c=(J_x/J_z)J_z/k_BT_c$ and $J_y/k_BT_c=(J_y/J_x)(J_x/J_z)J_z/k_BT_c$, are small for small J_x/J_z. Expanding the bulk correlation-length amplitudes in Taylor series and keeping only the leading asymptotical term, we obtain that as $J_x/J_z\to 0$ the aspect ratio $a_y/a_x\simeq(J_y/J_x)^{-q}$. The anisotropy parameter J_x/J_z did drop out.

In light of the above statements the Privman-Fisher equations for the quasi-one-dimensional system $(J_x,J_y\ll J_z)$ can be written as

$$\kappa_n(t,h)=n^{-1}G(J_x/J_z,J_y/J_x)X(C_1tn^{y_T},C_2hn^{y_h};J_y/J_x) \tag{30}$$

and

$$f_n^{(s)}(t,h)=n^{-d}G(J_x/J_z,J_y/J_x)Y(C_1tn^{y_T},C_2hn^{y_h};J_y/J_x), \tag{31}$$

where $d=|\mathrm{sgn}(J_x)|+|\mathrm{sgn}(J_y)|+|\mathrm{sgn}(J_z)|$. The geometry prefactor is normalized so that $G(1,1)=1$ and the dependence $G(J_x/J_z,0)$ is given by Eqs. (8) and (9).

We know that the $J_y/J_x\leftrightarrow(J_y/J_x)^{-1}$ invariance and the analyticity of scaling functions leads to the existence of a smooth extremum for the critical amplitude ratios of the $n\times n\times\infty$ parallelepipeds at $J_y/J_x=1$. In this context note that in the case of parallelepipeds with a *rectangular* cross section, $n_x\times n_y\times\infty$, one should expect the extrema for the certain ratios of critical amplitudes at $J_y/J_x=(n_y/n_x)^{1/q}$.

V. COMPLETELY ISOTROPIC LATTICE

At present, the critical point of the fully isotropic simple-cubic Ising lattice is located to a high degree of accuracy: $K_c=0.221\,655(1)$ (Ref. [22] and references therein). It is known also with large accuracy the free energy at criticality: $f_\infty=0.777\,90(2)$, Ref. [23]. On the other hand, we can carry out the calculations for subsystems $n\times n\times\infty$ with three numbers of lattice layers $n=2$, 3, and 4. This allows one, generally speaking, to perform the three-point extrapolations for accelerating the convergence and to improve the estimates of the universal critical amplitudes A_s and A_f and also the universal critical amplitude ratios $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}}/A_\chi^2$. The results are summarized in Table II.

One can compare our results with the available estimates. According to a Monte Carlo simulation on periodic cylinders $n\times n\times 128$ with $n=4$, 6, 8, and 10 (Ref. [25]), the critical FSS amplitude of the spin-spin inverse correlation length equals $A_s=1.30(3)$. Our estimate $A_s=1.26(5)$ is consistent with the one above.

Information concerning the absolute amplitude of the free energy can be extracted from the published data by the indirect route. Indeed, in accordance with the calculations [26] carried out in the quantum limit of a three-dimensional Ising model, $A_s/A_f=3.671(6)$. Using the above estimate $A_s=1.30(3)$ one finds $A_f=0.354(9)$. The value $A_f=0.37(3)$ given in Table II agrees with this estimate. Note that the critical FSS free-energy amplitude of the three-dimensional Ising lattice with the shape of periodic cubes is equal to $A_f^{\mathrm{cube}}=0.625(5)$, Ref. [23]. For a comparison note also that in the two-dimensional space the free-energy amplitudes of periodic Ising strips and squares are equal correspondingly to $\pi/12=0.261\,799$ and $\ln(2^{1/4}+2^{-1/2})=0.639\,911$ (see, e.g., Ref. [3]).

We do not know from the literature any estimates for the universal ratio $A_{\kappa''_{hh}}/A_\chi$ in three dimensions. One can note that out of all the four quantities discussed in this section, the combination $A_{\kappa''_{hh}}/A_\chi$ has the best convergence in n.

Finally, for the universal combination $A_{\chi^{(4)}}/A_\chi^2$, which is the finite-size cumulant ratio $\overline{g_\infty}$, there exists an estimate only in the order of magnitude: $\overline{g_\infty}\sim 3$ (Ref. [27], see also the reviews [3]). We have succeeded in obtaining this quantity to an accuracy of 5%.

VI. CONCLUSIONS

In this paper I have presented large-scale transfer-matrix calculations for different finite-size amplitudes of a fully anisotropic simple-cubic Ising lattice in the shape of $n\times n\times\infty$ bars with periodic boundaries in both transverse directions. The behavior of amplitude combinations (ratios) that do not contain the nonuniversal metric factors and geometry prefactor was studied depending on the interaction anisotropy parameters J_x/J_z and J_y/J_x. It has been established that these amplitude ratios practically cease to depend on the anisotropy parameter $J_x/J_z\to 0$ and, what is more, this is true for a wide interval, $J_x/J_z\lesssim 10^{-1}$.

It was shown that as a function of J_y/J_x the amplitude ratios have a smooth extremum (maximum) near $J_y/J_x=1$. As a result, the critical finite-size amplitude combinations are universal with respect to both anisotropy parameters in the domain $0<J_x/J_z\ll 1$ and $|J_y/J_x-1|\ll 1$.

A mechanism leading to the J_x/J_z independence of certain amplitude ratios was proposed. By this the $J_x\leftrightarrow J_y$ invariance together with the analyticity of the scaling functions explains the existence of a smooth extremum in the amplitude combinations at $J_y/J_x=1$.

In the case of fully isotropic interactions $(J_x=J_y=J_z)$ for which the high accuracy values of critical coupling and critical free energy are available, the better estimates have been found for the universal critical finite-size amplitudes of the spin-spin inverse correlation length and singular part of the free energy per site, as well as for the universal amplitude ratios $A_{\kappa''_{hh}}/A_\chi$ and $A_{\chi^{(4)}}/A_\chi^2$.

APPENDIX: MATRIX ELEMENTS OF V_1, V_2, V_3, AND V_4 IN THE QUASIDIAGONAL REPRESENTATION OF V

The sizes of upper and lower subblocks in the expansion (18) of TM for a cylinder $n\times n\times\infty$ are equal among themselves $(N_1=N_2)$ by odd n and unequal $(N_1\neq N_2)$ by even n. Consider the cases of even and odd n separately.

Matrix elements of subblocks $V^{(1)}$ and $V^{(2)}$ for the bars $3\times 3\times\infty$ and $4\times 4\times\infty$ have been done in [15] and I. For the $2\times 2\times\infty$ cluster, subblocks $V^{(1)}$ and $V^{(2)}$ have, respectively, the sizes 5×5 and 2×2 [15]. As for the $4\times 4\times\infty$ cluster, their matrix elements are given by

$$V_{ij}^{(1)}=A_{ij}G_{ij} \tag{A1a}$$

and

$$V_{ij}^{(2)}=A_{ij}\widetilde{G}_{ij}, \tag{A1b}$$

where

$$A_{ij}=\frac{\max(n_i,n_j)}{\sqrt{n_in_j}}\exp[\tfrac{1}{2}(m_i^a+m_j^a)K_x+\tfrac{1}{2}(m_i^b+m_j^b)K_y], \tag{A2}$$

$$G_{ij}=g_0^{(ij)}+2\sum_{s=1}^{(1/2)n^2}g_s^{(ij)}\cosh(2sK_z), \tag{A3a}$$

and

$$\widetilde{G}_{ij}=2\sum_{s=1}^{(1/2)n^2}\widetilde{g}_s^{(ij)}\sinh(2sK_z). \tag{A3b}$$

The coefficients n_i, m_i^a, m_i^b, and m_i for the periodic cylinder $2\times2\times\infty$ are

$$n_i=\{2,8,2,2,2\},\quad m_i^a=\{4,0,-4,-4,4\},$$

$$m_i^b=\{4,0,4,-4,-4\},\quad m_i=\{4,2,0,0,0\}. \tag{A4}$$

As in the case of $4\times4\times\infty$ cluster, the coefficients $g_s^{(ij)}$ satisfy again the condition

$$g_0^{(ij)}+2\sum_{s=1}^{(1/2)n^2}g_s^{(ij)}=\min(n_i,n_j). \tag{A5}$$

For $g_s^{(ij)}$ with $s\neq0$ one has

11) 01 21) 10 22) 01 31) 00 32) 10 33) 01 41) 00

42) 10 43) 00 44) 01 51) 00 52) 10

53) 00 54) 00 55) 01 . (A6)

Finally, the $\widetilde{g}_s^{(ij)}$ coefficients of a cluster $2\times2\times\infty$ equal

11) 01 21) 10 22) 01 . (A7)

Taking (from [15] and I) the basis functions of irreducible representations we find the matrix elements of subblocks $V_1^{(12)}$ for bars $n\times n\times\infty$ with even n (i.e., for cylinders $2\times2\times\infty$ and $4\times4\times\infty$):

$$(V_1^{(12)})_{ij}=\tfrac{1}{2}A_{ij}(m_jG_{ij}+m_i\widetilde{G}_{ij}), \tag{A8}$$

where $m_i=0$ by $i>N_2$; here and below we regard, for definiteness, $\widetilde{G}_{ij}=0$ when i or $j>N_2$. Analogously one evaluates for subblocks $V_2^{(1)}$ and $V_2^{(2)}$:

$$(V_2^{(1)})_{ij}=\frac{1}{2^2 2!}A_{ij}[(m_i^2+m_j^2)G_{ij}+2m_im_j\widetilde{G}_{ij}] \tag{A9a}$$

and

$$(V_2^{(2)})_{ij}=\frac{1}{2^2 2!}A_{ij}[(m_i^2+m_j^2)\widetilde{G}_{ij}+2m_im_jG_{ij}]. \tag{A9b}$$

The matrix elements of subblock $V_3^{(12)}$ are

$$(V_3^{(12)})_{ij}=\frac{1}{2^3 3!}A_{ij}[m_j(3m_i^2+m_j^2)G_{ij}+m_i(m_i^2+3m_j^2)\widetilde{G}_{ij}]. \tag{A10}$$

Lastly, for subblock $V_4^{(1)}$ we find

$$(V_4^{(1)})_{ij}=\frac{1}{2^4 4!}A_{ij}[(m_i^4+6m_i^2m_j^2+m_j^4)G_{ij} +4m_im_j(m_i^2+m_j^2)\widetilde{G}_{ij}]. \tag{A11}$$

In the case of a cluster $n\times n\times\infty$ with odd number of layers n, the formulas are more uniform because the same set of coefficients $g_s^{(ij)}$ enters into matrix elements for subblocks of both representations. Introducing the auxiliary quantities

$$H_{ij}^{(+)}=\sum_{s=1}^{(1/2)(n^2+1)}|g_s^{(ij)}|\exp[(2s-1)K_z\mathrm{sgn}(g_s^{(ij)})] \tag{A12a}$$

and

$$H_{ij}^{(-)}=\sum_{s=1}^{(1/2)(n^2+1)}|g_s^{(ij)}|\exp[-(2s-1)K_z\mathrm{sgn}(g_s^{(ij)})], \tag{A12b}$$

we obtain for even (k) terms of transfer-matrix expansion:

$$(V_k^{(1)})_{ij}=\frac{1}{2^k k!}A_{ij}[(m_i+m_j)^kH_{ij}^{(+)}+(m_i-m_j)^kH_{ij}^{(-)}] \tag{A13a}$$

and

$$(V_k^{(2)})_{ij}=\frac{1}{2^k k!}A_{ij}[(m_i+m_j)^kH_{ij}^{(+)}-(m_i-m_j)^kH_{ij}^{(-)}], \tag{A13b}$$

where A_{ij} equal (A2) but, of course, with their sets of coefficients. By odd k, i.e., for subblocks $V_k^{(12)}$, the expressions for the matrix elements have the form

$$(V_k^{(12)})_{ij}=\frac{1}{2^k k!}A_{ij}[(m_i+m_j)^kH_{ij}^{(+)}-(m_i-m_j)^kH_{ij}^{(-)}]. \tag{A14}$$

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