Hyperuniversality of a fully anisotropic three-dimensional Ising model

M. A. Yurishchev
Radiophysical Research Institute, 603600 Nizhny Novgorod, Russia
(Received 3 May 1994; revised manuscript received 25 July 1994)

For the fully anisotropic simple-cubic Ising lattice, the critical finite-size scaling amplitudes of both the spin-spin and energy-energy inverse correlation lengths and the singular part of the reduced free-energy density are calculated by the transfer-matrix method and a finite-size scaling for cyclic $L \times L \times \infty$ clusters with $L = 3$ and 4. Analysis of the data obtained shows that the ratios and the directional geometric means of the above amplitudes are universal.

I. INTRODUCTION

Conforming with the Privman-Fisher hyperuniversality hypothesis, the finite-size scaling (FSS) equations for the inverse correlation lengths and the singular part of the reduced free-energy density near the bulk phase transition of a system have, respectively, the form (for reviews see Refs. 1 and 2)

$$\kappa_{i,L}(t,h) = L^{-1} X_i(C_1 t L^{y_T}, C_2 h L^{y_h}) \tag{1}$$

and

$$f_L^{(s)}(t,h) = L^{-d} Y(C_1 t L^{y_T}, C_2 h L^{y_h}) \, . \tag{2}$$

Here L is a characteristic size of finite or partly finite subsystem, the index i labels the types of correlation lengths [spin-spin ($i = 1$), energy-energy ($i = 2$), etc.], d is the space dimensionality, $t = (T - T_c)/T_c$, h is an external field, y_T and y_h are the critical exponents, $X_i(x,y)$ and $Y(x,y)$ are the scaling functions which, within the limits of universality classes, can otherwise depend on the type of boundary conditions and the subsystem shape; all nonuniversality of a model is absorbed in the metric factors C_1 and C_2. Equations (1) and (2) allow one to find the universal combinations for the FSS amplitudes at the phase-transition point $t = h = 0$. In particular, the amplitudes for the inverse correlation lengths $A_s = X_1(0,0)$ and $A_e = X_2(0,0)$ and for the free energy $A_f = Y(0,0)$ must be universal themselves. In the case of strips with periodic boundary conditions, they are (see, e.g., Ref. 2)

$$A_s = \pi\eta \, , \quad A_e = \pi\eta_e \, , \quad A_f = \frac{\pi c}{6}, \tag{3}$$

where η and η_e are the exponents of the decay law correspondingly of the spin-spin and energy-energy correlation functions ($\eta = 1/4$ and $\eta_e = 2$ for the flat Ising model) and c is the central charge of Virasoro algebra ($c = 1/2$ for the two-dimensional Ising lattice).

All foregoing statements are applied to the *spatially isotropic* systems. Lattice anisotropy is a marginal effect and hence the amplitudes and their combinations, strictly speaking, must depend on anisotropy parameters.[2] However in the case of the anisotropic two-dimensional Ising model, it has been established[3,4] that although the inverse correlation-length and free-energy amplitudes get a nonuniversal factor, R_α (α labels the directions along which an $L \times \infty$ strip is infinite; here, $\alpha = x, z$), it is common and the directional geometric mean $\bar{R} = (R_x R_z)^{1/2}$ is a constant (equaling the unity). Therefore, the universality is preserved for the ratios and the directional geometric means of these amplitudes.

In the light of above, it would be interesting to clear the matter up in three dimensions. Such an attempt is undertaken in the present paper. We consider the three-dimensional Ising model on a simple-cubic lattice with different interaction constants J_x, J_y, and J_z along all three spatial directions. The lattice is approximated by the $L \times L \times \infty$ bars with periodic boundary conditions in both transverse directions. Such boundaries eliminate undesirable surface effects and hence improve the quality of approximation. By the transfer matrix (TM) method combined with FSS analysis for the subsystems with sizes $L = 3$ and 4, we determine at first the critical temperatures depending upon anisotropy parameters J_x/J_z and J_y/J_x. (We consider a system at least with two nonzero couplings; unless otherwise stated, the $L \times L \times \infty$ parallelepipeds are taken infinitely long in the z direction.) After this, the FSS amplitudes of the inverse correlation lengths and the free energy are calculated at the critical points found. The obtained results demonstrate the independence of the amplitude ratios on the parameter J_x/J_z when J_y/J_x is fixed. Moreover, the analysis shows that the ratios are also independent on the second anisotropy parameter J_y/J_x at any rate in the region $J_y/J_x \simeq 1$. Finally, our calculations give evidence in the constancy of the directional geometric mean of the spin-spin inverse correlation length amplitude in three dimensions. Together with an invariance of the ratios, this implies that the directional geometric means of other amplitudes must be universal also.

II. MODEL AND SOLUTION OF THE EIGENPROBLEMS

The Hamiltonian of Ising model on a simple-cubic lattice with nearest-neighbor interactions reads

$$\mathcal{H} = -\sum_{ijk} S_{ijk}(J_x S_{i+1jk} + J_y S_{ij+1k} + J_z S_{ijk+1}) \ . \quad (4)$$

The spin-field variables S_{ijk} are located in the lattice sites and take the values ± 1.

The transfer matrix V of an $L \times L \times \infty$ subsystem is introduced by elements

$$\langle S_{11}, S_{12}, \ldots, S_{LL}|V|S'_{11}, S'_{12}, \ldots, S'_{LL}\rangle = \prod_{i,j=1}^{L} \exp[\tfrac{1}{2}K_x(S_{ij}S_{i+1j} + S'_{ij}S'_{i+1j}) + \tfrac{1}{2}K_y(S_{ij}S_{ij+1} + S'_{ij}S'_{ij+1}) + K_z S_{ij}S'_{ij}] \ , \quad (5)$$

where $K_\alpha = J_\alpha/k_BT$ (now $\alpha = x, y, z$); $S_{iL+1} = S_{i1}$ and $S_{L+1j} = S_{1j}$ by all $i, j = 1, 2, \ldots, L$. The matrix V is real, symmetric, and has an order of 2^N where $N = L^2$ equals the number of chains in a system; that is dense and all its elements are positive.

The principal task is to find the eigenvalues of V because, for example, the density of a free energy measured in units of $-k_BT$ is given by

$$f_L = N^{-1} \ln \Lambda_0 \ , \quad (6)$$

where Λ_0 is the largest eigenvalue of a TM. The inverse longitudinal correlation lengths (mass gaps) equal

$$\kappa_{i,L} = \ln(\Lambda_0/\Lambda_i) \ , \quad (7)$$

where $\Lambda_1, \Lambda_2 \ldots$ are the next (after Λ_0) dominant eigenvalues of TM for the subsystem.

In order to solve the TM eigenproblem for L as large as possible, we reduce the TM's to the block-diagonal forms using a symmetry under the transformations of the group $Z_2 \times T \wedge C_{2v}$. Here Z_2 is a group of global spin inversions $S \to -S$, T is a group of translations in the transverse directions of a bar, and C_{2v} is the point group consisting of rotations around the axis of a subsystem at angles multiple to π and the reflections in planes going through this axis and the middles of opposite sides of an $L \times L \times \infty$ parallelepiped.

There is no necessity to perform the full quasidiagonalization of TM's because the leading eigenvalues are distributed only among two subblocks. Owing to the Perron theorem,[5] Λ_0 lies in the subblock of an identity irreducible representation. Λ_1 is located in the other subblock — it is built on the basis functions which are symmetrical under all transformations of the space subgroup $T \wedge C_{2v}$ and antisymmetrical under the transformations including a spin inversion. Λ_2 is situated again in the subblock of an identity irreducible representation. (In connection with this see, for example, Ref. 3.)

As a group-theoretical analysis shows (see Appendix A), both subblocks containing the largest eigenvalues have sizes of 18×18 in the case of $3 \times 3 \times \infty$ cluster. For a cylinder $4 \times 4 \times \infty$, the TM 65 536 by 65 536 is reduced to a block-diagonal form in which the required subblocks have the orders 787 and 672. The final extraction of needed eigenvalues of TM's was carried out by a numerical solution of eigenproblems for the corresponding subblocks. By this, we applied the conjugate gradient method[6] and, if necessary, used also the library functions *tred2* and *tqli*.[7] Calculations were run on IBM PC-486 computer in the operating system LINUX.

III. CALCULATION OF THE CRITICAL AMPLITUDES

So, the FSS amplitudes for the inverse correlation lengths of the spin-spin and energy-energy correlation functions are equal to

$$A_s = L\kappa_{1,L} \quad (8)$$

and

$$A_e = L\kappa_{2,L} \ , \quad (9)$$

where $\kappa_{1,L}$ and $\kappa_{2,L}$ have been taken at the phase-transition point T_c (by $h = 0$). This point itself was determined from the renormalization-group equation

$$L\kappa_{1,L}(T_c) = (L-1)\kappa_{1,L-1}(T_c) \quad (10)$$

with $L = 4$. The amplitude for the singular part of a free-energy density, A_f, is found from a system of equations

$$f_L = f_0 + L^{-d}A_f \quad (11)$$

with $L = 3$ and 4. Here f_0 denotes the regular (background) part of a free-energy density; f_3 and f_4 are taken again at the critical points.

The critical temperatures, amplitudes, and background f_0 calculated at different values of the anisotropy parameters J_x/J_z and J_y/J_x are collected in Table I. In Eq. (11), the spatial dimensionality has been put $d = 2$ for $J_y = 0$ and $d = 3$ for $J_y \neq 0$. It should also be noted that, for finite L, Eq. (7) leads to the wrong values for $\kappa_{2,L}$ in the limit of noninteracting strips ($J_y = 0$). Due to $\lambda_1^2 > \lambda_0\lambda_2$ ($\lambda_0 > \lambda_1 > \lambda_2$ are the largest eigenvalues of a transfer matrix for the strip), $\Lambda_2 = (\lambda_0\lambda_1)^2$ by $L = 4$ and therefore $\kappa_{2,L} = \ln[\lambda_0^4/(\lambda_0\lambda_1)^2] = 2\kappa_{1,L}$. However, the correct values are given by formula $\kappa_{2,L} = \ln(\lambda_0/\lambda_2)$ which has been used to build up the Table I.

In Table II, we present the data for the directional geometric mean of the spin-spin inverse correlation length amplitude $\bar{A}_s$. Calculations were performed by the equation

$$\bar{A}_s = \begin{cases} (A_s^{(x)}A_s^{(z)})^{1/2} & \text{if } J_y = 0 \ , \\ (A_s^{(x)}A_s^{(y)}A_s^{(z)})^{1/3} & \text{if } J_y \neq 0 \ , \end{cases} \quad (12)$$

where $A_s^{(\alpha)}$ is the amplitude of the spin-spin inverse correlation length when the bar $L \times L \times \infty$ was stretched (for given J_x, J_y, and J_z) along the α direction.

IV. DISCUSSION

Consider first the behavior of absolute amplitudes. For the three-dimensional systems, available information about them is very scanty. In the periodic cylinder ge-

TABLE I. Critical temperatures, background, critical FSS amplitudes, and their ratios for different values of the anisotropy parameters J_x/J_z and J_y/J_x.

J_y/J_x	J_x/J_z	k_BT_c/J_z	A_s	A_e	A_e/A_s	A_f	f_0	A_f/A_s
1.0	1.0	4.58104	1.4401	4.9627	3.44	0.4189	0.773	0.290
	0.1	1.35037	0.3613	1.2847	3.55	0.1044	0.959	0.288
	0.01	0.65458	0.0723	0.2576	3.56	0.0208	1.576	0.287
	0.001	0.40917	0.0115	0.0411	3.57	0.0033	2.451	0.286
0.75	1.0	4.18009	1.3345	4.5795	3.43	0.3953	0.775	0.296
	0.1	1.27931	0.3317	1.1712	3.53	0.0973	0.985	0.293
	0.01	0.63312	0.0653	0.2310	3.53	0.0191	1.623	0.292
	0.001	0.39985	0.0103	0.0365	3.54	0.0030	2.508	0.291
0.5	1.0	3.73973	1.2288	4.0812	3.32	0.3924	0.782	0.319
	0.1	1.19903	0.3005	1.0251	3.41	0.0943	1.019	0.313
	0.01	0.60815	0.0580	0.1981	3.41	0.0181	1.683	0.312
	0.001	0.38882	0.0090	0.0309	3.43	0.0028	2.578	0.311
0.25	1.0	3.22427	1.1256	3.3542	2.97	0.4407	0.803	0.391
	0.1	1.10117	0.2665	0.8151	3.05	0.1016	1.073	0.381
	0.01	0.57655	0.0500	0.1533	3.06	0.0190	1.767	0.380
	0.001	0.37453	0.0076	0.0235	3.09	0.0029	2.675	0.381
0.0	1.0	2.32081	0.8917	5.9901	6.71	0.2952	0.914	0.331
	0.1	0.91079	0.1856	1.3661	7.36	0.0616	1.232	0.331
	0.01	0.51058	0.0327	0.2418	7.39	0.0108	1.983	0.330
	0.001	0.34346	0.0048	0.0349	7.27	0.0016	2.915	0.333

ometry, it seems to be known only the estimates for the correlation-length amplitudes found by Monte Carlo simulations on the fully isotropic ($J_x = J_y = J_z$) lattices $L \times L \times 128$ with $L = 4, 6, 8$, and 10 (Ref. 8). For the inverse correlation-length amplitudes, these estimates ($L = 10$) yield $A_s = 1.342$ and $A_e = 4.78$. Appealing to Table I, one can convince oneself that our calculations conform with these values. Note also that the available high-temperature series for the free energy of a fully isotropic simple-cubic Ising lattice yields[9] $f_0 = 0.777\,11$ at criticality. Our estimate for the background, 0.773, is in good agreement with this magnitude.

In the two-dimensional case ($J_y = 0$), there exists, vice versa, complete information concerning the FSS amplitudes for the inverse correlation lengths and the free energy in the rectangular lattice with arbitrary anisotropy:[3,4]

$$A_s = \frac{\pi}{4}\left[\frac{\sinh(2J_x/k_BT_c)}{\sinh(2J_z/k_BT_c)}\right]^{1/2}, \tag{13}$$

TABLE II. Directional geometric mean of the spin-spin inverse correlation length amplitude $\bar{A}_s$ by different values of J_x/J_z and J_y/J_x.

J_x/J_z	J_y/J_x				
	0	0.25	0.5	0.75	1.0
1.0	0.891	1.57	1.46	1.43	1.44
0.1	0.833	2.00	1.87	1.80	1.76
0.01	0.577	2.02	2.01	2.01	2.02
0.001	0.294	1.48	1.51	1.54	1.57

$$A_e = 2\pi\left[\frac{\sinh(2J_x/k_BT_c)}{\sinh(2J_z/k_BT_c)}\right]^{1/2}, \tag{14}$$

and

$$A_f = \frac{\pi}{12}\left[\frac{\sinh(2J_x/k_BT_c)}{\sinh(2J_z/k_BT_c)}\right]^{1/2}, \tag{15}$$

where the critical temperature T_c satisfies to the equation

$$\sinh\left(\frac{2J_x}{k_BT_c}\right)\sinh\left(\frac{2J_z}{k_BT_c}\right) = 1\,. \tag{16}$$

Our numerical results reproduce these rigorous dependencies with acceptable accuracy. For the isotropic square Ising lattice, the critical free energy is (see Ref. 10)

$$f_0 = 2G/\pi + \tfrac{1}{2}\ln 2 = 0.929\,695\ldots \tag{17}$$

($G = 1^{-2} - 3^{-2} + 5^{-2} - \cdots$ is Catalan's constant). Appropriate value from Table I (f_0 at $J_x = J_z$ and $J_y = 0$) agrees to within 1.7% with the given exact quantity.

Inspecting Table I, we see the amplitudes vary in wide limits reaching several orders. The behavior is changed into a contrary one for their ratios. First what draws attention is that the ratios A_e/A_s and A_f/A_s stay practically unchanged with variation of J_x/J_z on three orders ($1 - 10^{-3}$) by given J_y/J_x. In the two-dimensional space ($J_y = 0$), the mean (here and below, over J_x/J_z) value of A_f/A_s equaling 0.331 conforms with the true value 1/3; the mean of A_e/A_s equals to 7.2 that agrees, in order of magnitude, with the exact value, 8, for the

A_e/A_s [see Eqs. (13)–(15)]. For the three-dimensional lattice with $J_x = J_y$, the mean value of A_f/A_s is 0.288. This quantity agrees with the estimate $A_f/A_s = 0.272$ which follows from the calculations of relative amplitudes for the inverse correlation lengths and the free energy in the Hamiltonian limit of a three-dimensional Ising model (square lattices $L \times L$ with sizes L up to 5).[11] According to Table I, the ratio for the inverse correlation-length amplitudes is $A_e/A_s = 3.53(6)$ in the discussed case. This estimate is in agreement with the mean values $A_e/A_s = 3.62(7)$, Ref. 12, and $A_e/A_s = 3.7(1)$, Ref. 8. Thus, the amplitude ratios A_e/A_s and A_f/A_s are not only universal with respect to the J_x/J_z but also their values agree quantitatively with available estimates in two limited cases: $J_y/J_x = 0$ and 1.

We now discuss the dependence on J_y/J_x in the intermediate region. In the limit $J_y/J_x \to 0$, the $L \times L \times \infty$ bar decomposes into L of independent strips $L \times \infty$ and consequently the TM of the bar is factorized into the direct product of TM's for the strips. Since the TM of the bar is finite by finite L, its eigenvalues are *continuous* functions of model parameters. Hence there must exist the $d = 3 \to d = 2$ transition region when $J_y/J_x \to 0$. To estimate its sizes by using L, we have calculated the critical exponents ν and γ/ν. The calculation was performed via the ordinary FSS formulas (see, e.g., Ref. 13):

$$\nu = \frac{\ln[L/(L-1)]}{\ln[L\kappa'_{1,L}/(L-1)\kappa'_{1,L-1}]} \tag{18}$$

and

$$\gamma/\nu = \frac{\ln(\chi_L/\chi_{L-1})}{\ln[L/(L-1)]}\,, \tag{19}$$

in which we put $L = 4$. Here $\kappa'_{1,L}$ is the derivative of $\kappa_{1,L}$ with respect to the temperature and χ_{L-1} and χ_L are the magnetic susceptibilities of subsystems at the phase-transition point. (Formulas for the susceptibilities are derived in Appendix B.) How the calculation gives the critical exponents ν and, especially, γ/ν are practically constants with respect to J_x/J_z $(= 1 - 10^{-3})$. Their dependences on J_y/J_x are shown in Fig. 1. Within the section $0.2 < J_y/J_x \leq 1$, the exponents ν and γ/ν preserve the unchanged values equaling, respectively, 0.67 and 1.97 that agrees with available estimates for these exponents in the case of the fully isotropic three-dimensional Ising model (Ref. 14 and references therein). By $J_y = 0$, our calculation yields $\nu = 1.06$ and $\gamma/\nu = 1.74$. These magnitudes conform closely with the exact values of discussed exponents in two dimensions: $\nu = 1$ and $\gamma/\nu = 7/4$. In Fig. 1, the region $0 \leq J_y/J_x < 0.1 - 0.2$ is clearly displayed where a smooth transition occurs from the $d = 3$ exponent values to the $d = 2$ ones. Consequently, one does not consider the $L \times L \times \infty$ lattice with $L \leq 4$ as a three-dimensional one when $J_y/J_x < 0.2$. In order to support this conclusion, we have calculated the "effective" lattice dimensionality solving the system of Eq. (11) with $L = 2$, 3, and 4 and treating d in it as an unknown continuous variable d^*. (For the fully anisotropic $2 \times 2 \times \infty$ Ising lattice, there is an exact analytical solution.[15]) The conclusion is that d^* does not

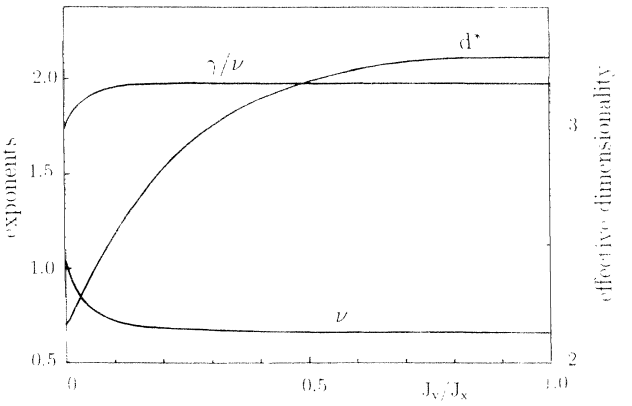

FIG. 1. Critical exponents ν and γ/ν (left scale) and the effective lattice dimensionality d^* (right scale) vs anisotropy parameter J_y/J_x.

depend on J_x/J_z and its plot on J_y/J_x is also presented in Fig. 1. This plot has a more qualitative character because in the calculation a cluster with an extremely small size $L = 2$ has been used. Nevertheless, the presented dependence indicates that the lattice dimensionality d^* is less than three by $J_y/J_x < 0.3$.

As mentioned in Sec. III, the energy-energy inverse correlation length $\kappa_{2,L}$ (and hence the amplitude A_e) has a false behavior in the limit $J_y/J_x \to 0$ due to finite sizes L. The scaling amplitude A_f obtained from Eq. (11) with $L = 3$ and 4 suffers from a similar defect. By finding of A_e and A_f, it is not allowed to interchange the order of the limits $L \to \infty$ and $J_y/J_x \to 0$. (Note in passing that the calculation of $\kappa_{1,L}$ and A_s is free upon such requirement.) Taking into account these circumstances, let us consider in Fig. 2 the obtained dependencies of ratios A_e/A_s and A_eA_f/A_s^2. The plots of both dependencies have the horizontal sections by small deviations of J_y/J_x from unity. Thus, the amplitude ratios do not depend on the second anisotropy parameter J_y/J_x in this region of its values. As J_y/J_x is decreased, both quantities tend

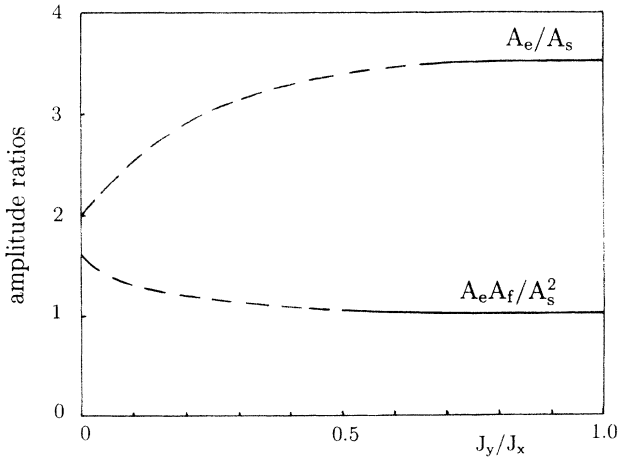

FIG. 2. The amplitude ratios A_e/A_s and A_eA_f/A_s^2 against the anisotropy parameter J_y/J_x. The curve parts which are considered as nonphysical ones are shown by a dashed line.

to the incorrect limits.

The recognized properties of the critical FSS amplitudes by a given orientation (α) of an $L \times L \times \infty$ bar in the anisotropic Ising lattice can be described by equations

$$\kappa_{i,L,\alpha}(0,0) = L^{-1} R_\alpha X_i(0,0) \tag{20}$$

and

$$f^{(s)}_{L,\alpha}(0,0) = L^{-d} R_\alpha Y(0,0) \, , \tag{21}$$

where $X_i(0,0)$ and $Y(0,0)$ are amplitudes of the isotropic model and $R_\alpha = R_\alpha(J_x/J_z, J_y/J_x)$. The given equations are true at $J_y/J_x = 0$ and, according to the presented data, when $J_y/J_x \to 1$. Equations (20) and (21) are likely to be valid also over the wider range of J_y/J_x. This is confirmed qualitatively by the calculation of A_f from Eq. (11) with $L = 2$, 3, and 4 (without supposition that $d = 3$ for all $J_y \neq 0$).

Discuss now the behavior of the directional geometric mean of the spin-spin inverse correlation length amplitude (Table II). In the two-dimensional case (column with $J_y/J_x = 0$), $\bar{A}_s$ loses a stability when $J_x/J_z \leq 10^{-2}$. This is obviously connected with small widths of strips by which we approximate the system. The situation is perceptibly better in three dimensions. Here $\bar{A}_s = 1.7(3)$, i.e. the percentage error equals 18%. With such accuracy, we may consider $\bar{A}_s$ as a constant.

V. CONCLUSIONS

In this paper, the TM-FSS calculations of critical temperatures, exponents, amplitudes, and free-energy background for the fully anisotropic three-dimensional Ising model have been carried out. The data obtained allow one to make the following inference concerning the structure of critical FSS amplitudes of the inverse correlation lengths and the free energy: Similarly to the two-dimensional case, all lattice-anisotropy parameters are absorbed in a separate prefactor which is common for named amplitudes and the directional geometric mean of which is the unity.

ACKNOWLEDGMENTS

The author would like to thank V. Privman, J. L. Cardy, M. Henkel, and H. L. Richards for helpful correspondence via e-mail. I am also grateful to A. M. Sterlin, A. P. Protogenov, and M. G. Teitelman for useful discussions. Finally, special thanks go to A. M. Babichenko and A. N. Karashtin for valuable consultations in programming.

APPENDIX A: QUASIDIAGONALIZATION OF THE TRANSFER MATRICES

The group $Z_2 \times T \wedge C_{2v}$ has an order $g = 8L^2$. Its generating elements are a spin inversion I, translations on one step t_x and t_y, and reflections in the symmetry planes σ_v and σ'_v. In the transfer matrix space $|S_{11}, S_{12}, \ldots, S_{LL}\rangle$, they are defined as

$$I|S_{11}, S_{12}, \ldots, S_{LL}\rangle = |-S_{11}, -S_{12}, \ldots, -S_{LL}\rangle \, , \tag{A1}$$

$$t_x|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle$$

$$= |S_{1L}, S_{11}, \ldots, S_{1L-1}; S_{2L}, S_{21}, \ldots, S_{2L-1}; S_{LL}, S_{L1}, \ldots, S_{LL-1}\rangle \, , \tag{A2}$$

$$t_y|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle$$

$$= |S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}; S_{11}, S_{12}, \ldots, S_{1L}\rangle \, , \tag{A3}$$

$$\sigma_v|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle$$

$$= |S_{L1}, S_{L2}, \ldots, S_{LL}; \ldots; S_{21}, S_{22}, \ldots, S_{2L}; S_{11}, S_{12}, \ldots, S_{1L}\rangle \, , \tag{A4}$$

$$\sigma'_v|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle$$

$$= |S_{1L}, \ldots, S_{12}, S_{11}; S_{2L}, \ldots, S_{22}, S_{21}; S_{LL}, \ldots, S_{L2}, S_{L1}\rangle \, . \tag{A5}$$

Other transformations of the group are the corresponding combinations of above operations. Multiplying from the left the equations like (A1)–(A5) on conjugate vectors and taking into account the orthonormality condition

$$\langle S_{11}, S_{12}, \ldots, S_{LL} | S'_{11}, S'_{12}, \ldots, S'_{LL} \rangle = \delta_{S_{11}S'_{11}} \delta_{S_{12}S'_{12}} \ldots \delta_{S_{LL}S'_{LL}} \quad \text{(A6)}$$

($\delta_{SS'} = \frac{1}{2}|S + S'|$ is a Kronecker symbol), we find the original representation Γ of the group.

All matrices of representation built commute with V. For instance, using Eqs. (5) and (A1), we have

$$\begin{aligned} &\langle S_{11}, S_{12}, \ldots, S_{LL} | I^{-1} V I | S'_{11}, S'_{12}, \ldots, S'_{LL} \rangle \\ &= \langle -S_{11}, -S_{12}, \ldots, -S_{LL} | V | -S'_{11}, -S'_{12}, \ldots, -S'_{LL} \rangle \\ &= \langle S_{11}, S_{12}, \ldots, S_{LL} | V | S'_{11}, S'_{12}, \ldots, S'_{LL} \rangle \end{aligned} \quad \text{(A7)}$$

so that $[V, I] = 0$. The same is valid for all other transformations of the group.

The traces of matrices built are characters of representation Γ. For the $3 \times 3 \times \infty$ case, the characters of original representation together with characters of irreducible representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$ to which correspond the subblocks containing the largest eigenvalues are given in Table III. Using this table and utilizing the formula for counting the multiplicities with which a given irreducible representation enters into an original representation (see, e.g., Ref. 16)

$$a_\mu = \frac{1}{g} \sum_i g_i \chi_i^{(\mu)^*} \chi_i \quad \text{(A8)}$$

TABLE III. Characters of the group $Z_2 \times T \wedge C_{2v}$ in the case $L = 3$; here $T \wedge C_{2v} \approx C_{3v} \times C_{3v}$.

	E	$3\sigma_v$ $3\sigma'_v$	$9\sigma_v\sigma'_v$	$2t_x$ $2t_y$ $4t_xt_y$	$6t_x\sigma_v$ $6t_y\sigma'_v$	$I, 3I\sigma_v, 3I\sigma'_v$ $9I\sigma_v\sigma'_v, 2It_x, 2It_y$ $4It_xt_y, 6It_x\sigma_v, 6It_y\sigma'_v$
$\Gamma^{(1)}$	1	1	1	1	1	1
$\Gamma^{(2)}$	1	1	1	1	1	-1
Γ	512	64	32	8	4	0

(g_i is a number of elements in ith class, $\chi_i^{(\mu)}$ is a character of element from the ith class in μth irreducible representation, and χ_i is a character of element from ith class in an original representation) we find the composition of representation Γ:

$$\Gamma = 18(\Gamma^{(1)} + \Gamma^{(2)}) + \cdots . \quad \text{(A9)}$$

It follows from here that in a basis where the representation Γ is completely reducible the transfer matrix of 512th order will take a quasidiagonal form in which both subblocks corresponding to the one-dimensional irreducible representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$ will have the sizes 18 by 18.

The basis vectors of irreducible representations on which the transfer matrix takes the discussed block-diagonal form are built with the help of projection operators.[16] In the case of an $L = 3$ subsystem, the basis vectors for the irreducible representations $\Gamma^{(1,2)}$ are

$$\begin{aligned}
\varphi_1^{(1,2)} &= (u_1 \pm u_{512})/\sqrt{2} , & \varphi_2^{(1,2)} &= \sum_i{}' G_i (u_8 \pm u_{505})/\sqrt{6} , \\
\varphi_3^{(1,2)} &= \sum_i{}' G_i (u_{74} \pm u_{439})/\sqrt{6} , & \varphi_4^{(1,2)} &= \sum_i{}' G_i (u_{85} \pm u_{428})/2\sqrt{3} , \\
\varphi_5^{(1,2)} &= \sum_i{}' G_i (u_2 \pm u_{511})/3\sqrt{2} , & \varphi_6^{(1,2)} &= \sum_i{}' G_i (u_4 \pm u_{509})/3\sqrt{2} , \\
\varphi_7^{(1,2)} &= \sum_i{}' G_i (u_{10} \pm u_{503})/3\sqrt{2} , & \varphi_8^{(1,2)} &= \sum_i{}' G_i (u_{28} \pm u_{485})/3\sqrt{2} , \\
\varphi_9^{(1,2)} &= \sum_i{}' G_i (u_{79} \pm u_{434})/3\sqrt{2} , & \varphi_{10}^{(1,2)} &= \sum_i{}' G_i (u_{11} \pm u_{502})/6 , \\
\varphi_{11}^{(1,2)} &= \sum_i{}' G_i (u_{15} \pm u_{498})/6 , & \varphi_{12}^{(1,2)} &= \sum_i{}' G_i (u_{75} \pm u_{438})/6 , \\
\varphi_{13}^{(1,2)} &= \sum_i{}' G_i (u_{16} \pm u_{497})/6 , & \varphi_{14}^{(1,2)} &= \sum_i{}' G_i (u_{76} \pm u_{437})/6 , \\
\varphi_{15}^{(1,2)} &= \sum_i{}' G_i (u_{30} \pm u_{483})/6 , & \varphi_{16}^{(1,2)} &= \sum_i{}' G_i (u_{84} \pm u_{429})/6 , \\
\varphi_{17}^{(1,2)} &= \sum_i{}' G_i (u_{12} \pm u_{501})/6\sqrt{2} , & \varphi_{18}^{(1,2)} &= \sum_i{}' G_i (u_{86} \pm u_{427})/6\sqrt{2} ,
\end{aligned} \quad \text{(A10)}$$

where

$$\begin{aligned} u_1 &= |1,1,1;1,1,1;1,1,1\rangle, \\ u_2 &= |1,1,1;1,1,1;1,1,-1\rangle, \ \ldots , \\ u_{512} &= |-1,-1,-1;-1,-1,-1;-1,-1,-1\rangle . \end{aligned} \quad \text{(A11)}$$

The plus and minus signs correspond to the basis vectors of irreducible representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$, respectively. For shortening of a listing, only the I-conjugated pairs of generating orths are shown in Eqs. (A10). The numbers of orths in a pair (n and n') are connected by a relation

$n' = 2^N + 1 - n$. Acting on such orths by operators $G_i \in T \wedge C_{2v}$ and taking on each step only the new u-orths (this peculiarity is marked by prime on the sum symbol), we obtain the expressions for the basis functions in explicit form.

Finally, having the basis vectors for the irreducible representations, one can find the matrix elements of subblocks with the transfer matrix eigenvalues under search. For the $3 \times 3 \times \infty$ task, the matrix elements of subblocks corresponding to the irreducible representations $\Gamma^{(1,2)}$ have been given with all necessary coefficients in Ref. 15.

In the case of $4 \times 4 \times \infty$ subsystem, the basis vectors of $\Gamma^{(1)}$ and $\Gamma^{(2)}$ can be taken in the form

$$\psi_1^{(1,2)} = (e_1 \pm e_{65\,536})/\sqrt{2}\,, \qquad \psi_2^{(1,2)} = \sum_i{}' G_i(e_2 \pm e_{65\,535})/4\sqrt{2}\,,$$
$$\cdots$$
$$\psi_{671}^{(1,2)} = \sum_i{}' G_i(e_{13\,670} \pm e_{51\,867})/4\sqrt{2}\,, \qquad \psi_{672}^{(1,2)} = \sum_i{}' G_i(e_{13\,674} \pm e_{51\,863})/8\sqrt{2}\,, \tag{A12}$$
$$\psi_{673}^{(1)} = \tfrac{1}{2}\sum_i{}' G_i e_{256}\,, \quad \cdots \qquad \psi_{787}^{(1)} = (e_{23\,131} + e_{42\,406})/\sqrt{2}\,,$$

where

$$e_1 = |1,1,\ \ldots\ ,1\rangle,\ ,\quad e_2 = |1,1,\ \ldots\ ,-1\rangle,\ \ldots\ ,$$
$$e_{65\,536} = |-1-,1,\ \ldots\ ,-1\rangle\,. \tag{A13}$$

The basis functions (A12) from 1 to 672 and then from 673 to 787 are ordered with the numbers of the first generating e-orths increasing. Using Eqs. (5), (A12), and (A13), we evaluate the matrix elements $V_{ij}^{(1,2)} = \psi_i^{(1,2)^+} V \psi_j^{(1,2)}$ for subblocks corresponding to the irreducible representations $\Gamma^{(1,2)}$. The matrix elements are

$$V_{ij}^{(1)} = \frac{\max(n_i,n_j)}{\sqrt{n_i n_j}}\left[g_0^{(i,j)} + 2\sum_{s=1}^{8} g_s^{(i,j)}\cosh(2sK_z)\right] \times \exp[\tfrac{1}{2}(m_i^a + m_j^a)K_x + \tfrac{1}{2}(m_i^b + m_j^b)K_y] \tag{A14}$$

and

$$V_{ij}^{(2)} = 2\frac{\max(n_i,n_j)}{\sqrt{n_i n_j}}\left[\sum_{s=1}^{8} \tilde{g}_s^{(i,j)}\sinh(2sK_z)\right] \times \exp[\tfrac{1}{2}(m_i^a + m_j^a)K_x + \tfrac{1}{2}(m_i^b + m_j^b)K_y]\,, \tag{A15}$$

where n_i are lengths of basis vectors, m_i^a and m_i^b are the reduced partial energies of spin configurations in orths of ith vector. All coefficients $g_s^{(i,j)}$ are non-negative and satisfy to the "sum rules"

$$g_0^{(i,j)} + 2\sum_{s=1}^{8} g_s^{(i,j)} = \min(n_i,n_j)\,. \tag{A16}$$

We did not keep the coefficients $g_0^{(i,j)}$ but restored them for each matrix element $V_{ij}^{(1)}$ from Eq. (A16). As the calculation shows, the coefficients $g_s^{(i,j)}$ with $s \neq 0$ are not greater than 60. Hence, it is enough to take one byte for every element of the g-array, i.e., to use the data type "char" in C code. Thus, 2 480 624 bytes of a memory are required to store the g-coefficients for a triangle part of symmetric matrix $V^{(1)}$. The values of coefficients $\tilde{g}_s^{(i,j)}$ lie in the range from -28 to $+40$ and we alloted in addition the 1 809 024 bytes of a memory for the $\tilde{g}$-coefficients of matrix $V^{(2)}$.

APPENDIX B: FORMULAS FOR THE CALCULATION OF SUSCEPTIBILITIES

In deriving of formulas for χ_L, we will point out from a fluctuation-dissipation relation connecting the susceptibility with a magnetic moment $\mathcal{M}$ (see, for example, Ref. 17):

$$\chi_L(T) = \frac{1}{k_B T}\lim_{M\to\infty}\frac{1}{L^2 M}\langle \mathcal{M}^2\rangle\,. \tag{B1}$$

Here $\mathcal{M} = \sum_{ijk} S_{ij}^k$ where $S_{ij}^k \equiv S_{ijk}$ is the total magnetic moment of $L\times L\times M$ periodic subsystem; the brackets refer to average on Gibbs distribution. Taking into account the translational invariance of a cluster in the longitudinal (z) direction, one can write Eq. (B1) in the form

$$\chi_L(T) = \frac{1}{L^2 k_B T}\lim_{M\to\infty}\sum_{r=0}^{M-1}\langle (S_{11}^k + S_{12}^k + \cdots + S_{LL}^k) \times (S_{11}^{k+r} + S_{12}^{k+r} + \cdots + S_{LL}^{k+r})\rangle\,. \tag{B2}$$

To calculate the statistical means, we use the transfer matrix technique. Let us introduce in addition the spin matrices making by this the one-dimensional order of pair of indices $i,j \to l = L(i-1)+j$:

$$\hat{S}_l = \underbrace{1\times\cdots\times 1}_{l-1}\times\sigma_z\times\underbrace{1\times\cdots\times 1}_{N-l}\,, \tag{B3}$$

where 1 denotes the unit matrix of second order and σ_z is Pauli's z matrix; $N = L^2$. This allows one to rewrite Eq. (B2) as

$$\chi_L(T) = \frac{1}{L^2 k_B T} \lim_{M\to\infty} \frac{1}{\mathrm{Tr} V^M} \sum_{r=0}^{M-1} \mathrm{Tr}[(\hat{S}_1 + \cdots + \hat{S}_N) \times V^r (\hat{S}_1 + \cdots + \hat{S}_N) V^{M-r}] \,. \quad \text{(B4)}$$

From here, by passing under the trace symbol into diagonal representation of the transfer matrix and by taking into account the nondegeneracy of its largest eigenvalue, we obtain

$$\chi_L(T) = \frac{1}{L^2 k_B T} \sum_{i=1}^{2^N-1} \frac{\Lambda_0 + \Lambda_i}{\Lambda_0 - \Lambda_i} |F_i^+ (\hat{S}_1 + \cdots + \hat{S}_N) F_0|^2 \,, \quad \text{(B5)}$$

where $F_0, F_1, \ldots$ are eigenvectors of matrix V corresponding to its eigenvalues $\Lambda_0, \Lambda_1, \ldots$. Further, the operator $\hat{S} = \hat{S}_1 + \cdots + \hat{S}_N$ is invariant with respect to all purely spatial transformations and breaks the Z_2 symmetry. Therefore, the matrix elements entering into Eq. (B5) are not zero only for "transitions" from the identity irreducible representation $\Gamma^{(1)}$ just into the irreducible representation $\Gamma^{(2)}$.

Vector F_0 is a linear combination of basis functions only of the identity irreducible representation. In the case of $3 \times 3 \times \infty$,

$$F_0 = \sum_{i=1}^{18} f_i^{(0)} \varphi_i^{(1)} \,, \quad \text{(B6)}$$

where $f_i^{(0)}$ are components of eigenvector answering to the largest eigenvalue (Λ_0) of subblock of the identity irreducible representation. Using Eqs. (A10), we find that

$$\hat{S} \varphi_i^{(1)} = m_i \varphi_i^{(2)} \,, \quad \text{(B7)}$$

where

$$m_i = \{9, 3, 3, 3, 7, 5, 5, 1, 1, 5, 3, 3, 1, 1, 1, 1, 3, 1\} \,, \quad \text{(B8)}$$

m_i is the magnetic moment of spin configurations in the ith basis vector. As a result, we obtain from Eq. (B5) the following work formula for a calculation of the susceptibility:

$$\chi_3(T) = \frac{1}{9 k_B T} \sum_{i=1}^{18} \frac{\Lambda_0 + \Lambda_i^{(2)}}{\Lambda_0 - \Lambda_i^{(2)}} \left[\sum_{j=1}^{18} m_j f_j^{(0)} f_j^{(i)} \right]^2 \,. \quad \text{(B9)}$$

Here $f_j^{(i)}$ are components of ith eigenvector corresponding to eigenvalue $\Lambda_i^{(2)}$ for the subblock of irreducible representation $\Gamma^{(2)}$.

Analogous formula take place for the $L = 4$ subsystem:

$$\chi_4(T) = \frac{1}{16 k_B T} \sum_{i=1}^{672} \frac{\Lambda_0 + \Lambda_i^{(2)}}{\Lambda_0 - \Lambda_i^{(2)}} \left[\sum_{j=1}^{672} m_j f_j^{(0)} f_j^{(i)} \right]^2 \,. \quad \text{(B10)}$$

All quantities entering in this expression should be taken, of course, for the $4 \times 4 \times \infty$ model.

Therefore, the calculation of susceptibilities requires the solution of a part eigenproblem for the subblock of an identity irreducible representation and the solution of a full eigenproblem for a second subblock which corresponds to the irreducible representation $\Gamma^{(2)}$. The part eigenproblem was solved again by the conjugate gradient method and the full one — by using the library C pair *tred2 - tqli*.

[1] V. Privman, in *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).

[2] V. Privman, P. C. Hohenberg, and A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1991), Vol. 14.

[3] P. Nightingale and H. Blöte, J. Phys. A **16**, L657 (1983).

[4] J. O. Indekeu, M. P. Nightingale, and W. V. Wang, Phys. Rev. B **34**, 330 (1986).

[5] R. F. Gantmacher, *The Theory of Matrices* (Nauka, Moscow, 1988).

[6] W. W. Bradbury and R. Fletcher, Num. Math. **9**, 259 (1966); A. Ruhe, in *Numerische Behandlung von Eigenwertaufgaben*, edited by L. Collatz (Birkhäuser, Basel and Stuttgart, 1974); the used in the paper C code based on a conjugate gradient method has been written by A. M. Sterlin (unpublished).

[7] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing* (Cambridge University, Cambridge, 1992).

[8] R. A. Weston, Phys. Lett. B **248**, 340 (1990).

[9] A. J. Guttmann and I. G. Enting, J. Phys. A **26**, 807 (1993).

[10] A. E. Ferdinand and M. E. Fisher, Phys. Rev. **185**, 832 (1969).

[11] M. Henkel, J. Phys. A **19**, L247 (1986); **20**, 3969 (1987).

[12] M. Henkel, J. Phys. A **20**, L769 (1987).

[13] P. Nightingale, J. Appl. Phys. **53**, 7927 (1982).

[14] A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991).

[15] M. A. Yurishchev, J. Phys. Condens. Matter **5**, 8075 (1993).

[16] M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Addison-Wesley, London, 1964).

[17] H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Clarendon, Oxford, 1971).