Hyperuniversality of Fully Anisotropic Three-Dimensional Ising Model

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Abstract

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 above amplitudes are universal.

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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. [1,2])

\[ \kappa_i(L, t, h) = L^{-1} X_i(C_1 t L^{y_T}, C_2 h L^{y_h}) \]

and

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

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 else depend on the type of boundary conditions and the subsystem shape; all non-universality of a model is absorbed in the metric factors \( C_1 \) and \( C_2 \). Equations (1) and (2) allow 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])

\[ A_s = \pi \eta, \quad A_e = \pi \eta_e, \quad A_f = \frac{\pi c}{6}, \]

where \( \eta \) and \( \eta_e \) 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-lengths and free-energy amplitudes get a non-universal factor, \( R_\alpha \) (\( \alpha \) 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 (equalling 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 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 a 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 non-zero 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
\[
\mathcal{H} = -\sum_{ijk} S_{ijk} (J_x S_{i+1,jk} + J_y S_{ij+1,k} + J_z S_{ijk+1}).
\] (4)

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

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

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

where \( K_\alpha = J_\alpha / k_B T \) (now \( \alpha = x, y, z \)); \( S_{iL+1} = S_{i1} \) and \( S_{L+1,j} = S_{1j} \) 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 \( -k_B T \) is given by

\[
f_L = N^{-1} \ln \Lambda_0,
\] (6)

where \( \Lambda_0 \) is the largest eigenvalue of a TM. The inverse longitudinal correlation lengths (mass gaps) equal

\[
\kappa_{i,L} = \ln(\Lambda_0 / \Lambda_i),
\] (7)

where \( \Lambda_1, \Lambda_2 \ldots \) are the next (after \( \Lambda_0 \)) dominant eigenvalues of TM for the subsystem.

In order to solve the TM eigenproblem for \( L \) as large as possible, we reduce the TMs 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 \( \pi \) 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 TMs because the leading eigenvalues are distributed only among two subblocks. Owing to the Perron theorem \[3\], \( \Lambda_0 \) lies in the subblock of an identity irreducible representation. \( \Lambda_1 \) 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. $\Lambda_2$ 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 $18 \times 18$ 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 TMs 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

$$A_s = L\kappa_{1,L}$$

and

$$A_e = L\kappa_{2,L}.$$  \hspace{1cm} (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

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

with $L = 4$. The amplitude for the singular part of a free-energy density, $A_f$, is found from a system of equations
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 Eqs. (11), the spatial dimensionality has been put $d = 2$ for $J_y = 0$ and $d = 3$ for $J_y ≠ 0$. It should be noted also that, for finite $L$, Eq. (7) leads to the wrong values for $κ_{2,L}$ in the limit of non-interacting strips ($J_y = 0$). Due to $λ_1^2 > λ_0λ_2$ ($λ_0 > λ_1 > λ_2$ are the largest eigenvalues of a transfer matrix for the strip), $A_2 = (λ_0λ_1)^2$ by $L = 4$ and therefore $κ_{2,L} = ln[λ_0^4/(λ_0λ_1)^2] = 2κ_{1,L}$. However, the correct values are given by formula $κ_{2,L} = ln(λ_0/λ_2)$ 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 amplitudes $A_s$. Calculations were performed by the equation

\[
\bar{A}_s = \begin{cases} 
(A_s^{(x)}A_s^{(z)})^{1/2} & \text{if } J_y = 0 \\
(A_s^{(y)}A_s^{(z)})^{1/3} & \text{if } J_y ≠ 0 
\end{cases}
\]

where $A_s^{(α)}$ is the amplitude of the spin-spin inverse correlation length when the bar $L×L×∞$ 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 geometry, 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 $L×L×128$ 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 \[ f_0 = 0.77711 \] 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 \[3,4\]:

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

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

and

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

where the critical temperature \(T_c\) satisfies to the equation

\[
\sinh \left( \frac{2J_x}{k_BT_c} \right) \sinh \left( \frac{2J_z}{k_BT_c} \right) = 1. 
\]

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

\[
f_0 = 2G/\pi + \frac{1}{2} \ln 2 = 0.929695 \ldots
\]

\((G = 1^{-2} - 3^{-2} + 5^{-2} - \ldots \text{ is Catalan’s constant})\). Appropriate value from table I \((f_0 \text{ at } J_x = J_z \text{ and } J_y = 0)\) 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 \(A_f/A_s\) equalling to 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 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 TMs 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 $\nu$ and $\gamma/\nu$. The calculation was performed via the ordinary FSS formulae (see, e. g., Ref. \[13\]):

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

and

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

in which we put $L = 4$. Here $\kappa'_{1,L}$ is the derivative of $\kappa_{1,L}$ with respect to the temperature and $\chi_{L-1}$ and $\chi_{L}$ are the magnetic susceptibilities of subsystems at the phase-transition point. (Formule for the susceptibilities are derived in Appendix B.) How the calculation gives the critical exponents $\nu$ and, especially, $\gamma/\nu$ are practically constants with respect to $J_x/J_z \sim 10^{-3}$). 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 $\nu$ and $\gamma/\nu$ preserve the unchanged values equalling, respectively, to 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, it is clear-cut displayed the region $0 \leq J_y/J_x < 0.1 - 0.2$ 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 Eqs. (11) with $L = 2, 3, \text{and } 4$ 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 $d^*$ does not 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 Eqs. (11) with $L = 3$ and $4$ suffers from a similar defect. By finding of $A_e$ and $A_f$, it is not allowed to change 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 $A_e A_f/A_s^2$. 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 to the incorrect limits.

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

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

(20)
and

\[ f_{L, \alpha}^{(s)}(0, 0) = L^{-d} R_\alpha Y(0, 0), \quad (21) \]

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 \( J_y/J_x \rightarrow 1 \). 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 Eqs. (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. 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 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.

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**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 $\sigma_v$ and $\sigma'_v$. In the transfer matrix space $|S_{11}, S_{12}, \ldots, S_{LL}\rangle$, they are defined as

\[ I|S_{11}, S_{12}, \ldots, S_{LL}\rangle = | -S_{11}, -S_{12}, \ldots, -S_{LL}\rangle , \quad (A1) \]

\[ t_x|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle = |S_{1L}, S_{11}, \ldots, S_{1L-1}; S_{2L}, S_{21}, \ldots, S_{2L-1}; S_{LL}, S_{L1}, \ldots, S_{LL-1}\rangle \quad (A2) \]

\[ t_y|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle = |S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}; S_{11}, S_{12}, \ldots, S_{1L}\rangle \quad (A3) \]

\[ \sigma_v|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle = |S_{L1}, S_{L2}, \ldots, S_{LL}; \ldots; S_{21}, S_{22}, \ldots, S_{2L}; S_{11}, S_{12}, \ldots, S_{1L}\rangle \quad (A4) \]

\[ \sigma'_v|S_{11}, S_{12}, \ldots, S_{1L}; S_{21}, S_{22}, \ldots, S_{2L}; \ldots; S_{L1}, S_{L2}, \ldots, S_{LL}\rangle = |S_{1L}, \ldots, S_{12}, S_{11}; S_{2L}, \ldots, S_{22}, S_{21}; S_{LL}, \ldots, S_{L2}, S_{L1}\rangle . \quad (A5) \]

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

\[ \langle S_{11}, S_{12}, \ldots, S_{LL}|S'_{11}, S'_{12}, \ldots, S'_{LL}\rangle = \delta_{S_{11}S'_{11}} \delta_{S_{12}S'_{12}} \ldots \delta_{S_{LL}S'_{LL}} \quad (A6) \]
\(\delta_{SS'} = \frac{1}{2}|S + S'|\) is a Kronecker symbol, we find the original representation \(\Gamma\) of the group.

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

\[
\langle S_{11}, S_{12}, \ldots, S_{LL} | I^{-1} V I | S'_{11}, S'_{12}, \ldots, S'_{LL} \rangle \\
= \langle -S_{11}, -S_{12}, \ldots, -S_{LL} | V | -S'_{11}, -S'_{12}, \ldots, -S'_{LL} \rangle \\
= \langle S_{11}, S_{12}, \ldots, S_{LL} | V | S'_{11}, S'_{12}, \ldots, S'_{LL} \rangle 
\]

(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 \(\Gamma\). 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])

\[
a_\mu = \frac{1}{g} \sum_i g_i \chi_i^{(\mu)} \chi_i
\]

(A8)

\((g_i\) is a number of elements in \(i\)th class, \(\chi_i^{(\mu)}\) is a character of element from \(i\)th class in \(\mu\)th irreducible representation, and \(\chi_i\) is a character of element from \(i\)th class in an original representation) we find the composition of representation \(\Gamma\):

\[
\Gamma = 18(\Gamma^{(1)} + \Gamma^{(2)}) + \ldots
\]

(A9)

It follows from here that in a basis where the representation \(\Gamma\) is completely reducible the transfer matrix of 512-th 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 a 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{align}
\varphi_{1,2}^{(1,2)} &= (u_1 \pm u_{512})/\sqrt{2} & \varphi_{2}^{(1,2)} &= \sum' G_i (u_8 \pm u_{505})/\sqrt{6} \\
\varphi_{3}^{(1,2)} &= \sum' G_i (u_{74} \pm u_{439})/\sqrt{6} & \varphi_{4}^{(1,2)} &= \sum' G_i (u_{85} \pm u_{428})/2\sqrt{3} \\
\varphi_{5}^{(1,2)} &= \sum' G_i (u_2 \pm u_{511})/3\sqrt{2} & \varphi_{6}^{(1,2)} &= \sum' G_i (u_4 \pm u_{509})/3\sqrt{2} \\
\varphi_{7}^{(1,2)} &= \sum' G_i (u_{10} \pm u_{503})/3\sqrt{2} & \varphi_{8}^{(1,2)} &= \sum' G_i (u_{28} \pm u_{485})/3\sqrt{2} \\
\varphi_{9}^{(1,2)} &= \sum' G_i (u_{79} \pm u_{434})/3\sqrt{2} & \varphi_{10}^{(1,2)} &= \sum' G_i (u_{11} \pm u_{502})/6 \\
\varphi_{11}^{(1,2)} &= \sum' G_i (u_{15} \pm u_{498})/6 & \varphi_{12}^{(1,2)} &= \sum' G_i (u_{75} \pm u_{438})/6 \\
\varphi_{13}^{(1,2)} &= \sum' G_i (u_{16} \pm u_{497})/6 & \varphi_{14}^{(1,2)} &= \sum' G_i (u_{76} \pm u_{437})/6 \\
\varphi_{15}^{(1,2)} &= \sum' G_i (u_{30} \pm u_{483})/6 & \varphi_{16}^{(1,2)} &= \sum' G_i (u_{84} \pm u_{429})/6 \\
\varphi_{17}^{(1,2)} &= \sum' G_i (u_{12} \pm u_{501})/6\sqrt{2} & \varphi_{18}^{(1,2)} &= \sum' G_i (u_{86} \pm u_{427})/6\sqrt{2},
\end{align}

where

\begin{align}
&u_1 = \{1,1,1;1,1,1;1,1\}, u_2 = \{1,1,1;1,1,1;1,1,1\}, \ldots , \\
u_{512} = \{-1,-1,-1;3,-1,-1;1,-1,-1\}. \tag{A11}
\end{align}

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 \((n\text{ and }n')\) are connected by a relation \(n' = 2^N + 1 - n\). Acting on such orths by operators \(G_i \in \mathbb{T} \land C_{2v}\) 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. [13].

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
\[ \psi_{1,2}^{(1,2)} = (e_1 \pm e_{65,536}) / \sqrt{2} \]

\[ \psi_{2}^{(1,2)} = \sum_i G_i (e_2 \pm e_{65,535}) / 4 \sqrt{2} \]

\[ \psi_{671}^{(1,2)} = \sum_i G_i (e_{13,670} \pm e_{51,867}) / 4 \sqrt{2} \]

\[ \psi_{672}^{(1,2)} = \sum_i G_i (e_{13,674} \pm e_{51,863}) / 8 \sqrt{2} \]

\[ \psi_{673}^{(1)} = \frac{1}{2} \sum_i G_i e_{256} \]

\[ \psi_{787}^{(1)} = (e_{23,131} + e_{42,406}) / \sqrt{2}, \]

where

\[ e_1 = |1,1,\ldots,1>, \quad e_2 = |1,1,\ldots,-1>, \ldots, \quad e_{65,536} = |-1,-1,\ldots,-1> \]  

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 \( V_{ij}^{(1,2)} = \psi_i^{(1,2)} \psi_j^{(1,2)} \) for subblocks corresponding to the irreducible representations \( \Gamma^{(1,2)} \). The matrix elements are

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

and

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

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 \( i \)th vector. All coefficients \( g_s^{(i,j)} \) are non-negative and satisfy to the “sum rules”

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

We did not keep the coefficients \( g_0^{(i,j)} \) but restored them for each matrix element \( V_{ij}^{(1)} \) from Eqs. (A16). As a 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, it is required 2 480 624 bytes of a memory to store the
The values of coefficients $\tilde{g}^{(i,j)}$ lie in the range from $-28$ to $+40$ and we allotted in addition the 1809024 bytes of a memory for the $\tilde{g}$-coefficients of matrix $V^{(2)}$.

APPENDIX B: FORMULAE FOR THE CALCULATION OF SUSCEPTIBILITIES

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

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

(B1)

Here $\mathcal{M} = \sum_{ijk} S^k_{ij}$ where $S^k_{ij} \equiv S_{ijk}$ 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

$$
\chi_L(T) = \frac{1}{L^2 k_B T} \lim_{M \to \infty} \sum_{r=0}^{M-1} \langle (S^k_{11} + S^k_{12} + \ldots + S^k_{LL})(S^k_{11} + S^k_{12} + \ldots + S^k_{LL}) \rangle.
$$

(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 indexes $i, j \to l = L(i - 1) + j$:

$$
\hat{S}_l = 1 \times \ldots \times 1 \times \sigma_z \times 1 \times \ldots \times 1,
$$

(B3)

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

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

(B4)

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

$$
\chi_L(T) = \frac{1}{L^2 k_B T} \sum_{i=1}^{2N-1} \frac{\Lambda_0 + \Lambda_i}{\Lambda_0 - \Lambda_i} |F^+_i(\hat{S}_1 + \ldots + \hat{S}_N)F_0|^2,
$$

(B5)
where \( F_0, F_1, \ldots \) are eigenvectors of matrix \( V \) corresponding to its eigenvalues \( \Lambda_0, \Lambda_1, \ldots \).

Further, the operator \( \hat{S} = \hat{S}_1 + \ldots + \hat{S}_N \) 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 \( 3 \times 3 \times \infty \),

\[
F_0 = \sum_{i=1}^{18} f_i^{(0)} \varphi_i^{(1)},
\]

where \( f_i^{(0)} \) are components of eigenvector answering to the largest eigenvalue \( \Lambda_0 \) of subblock of the identity irreducible representation. Using Eqs. (A10), we find that

\[
\hat{S} \varphi_i^{(1)} = m_i \varphi_i^{(2)},
\]

where

\[
m_i = \{9, 3, 3, 3, 7, 5, 5, 1, 1, 5, 3, 3, 1, 1, 1, 1, 1, 3, 1\};
\]

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

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

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

Analogous formula take place for the \( L = 4 \) subsystem:

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

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 \textit{tred2 - tqli}.
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**TABLE I.** Critical temperatures, background, critical FSS amplitudes and their ratios for different values of the anisotropy parameters $J_x/J_z$ and $J_y/J_x$.

| $J_y/J_x$ | $J_x/J_z$ | $k_B T_c/J_z$ | $A_s$ | $A_e$ | $A_e/A_s$ | $A_f$ | $f_0$ | $A_f/A_s$ |
|-----------|-----------|---------------|-------|-------|-----------|-------|-------|-----------|
| 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 |
TABLE II. Directional geometric mean of the spin-spin inverse correlation length amplitude $\tilde{\lambda}$ 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 |
TABLE III. Characters of the group $Z_2 \times T \wedge C_{2v}$ in the case $L = 3$; here $T \wedge C_{2v} \approx C_{3v} \times C_{3v}$.

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

FIG. 1. Critical exponents $\nu$ and $\gamma/\nu$ (left scale) and the effective lattice dimensionality $d^*$ (right scale) versus anisotropy parameter $J_y/J_x$.

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 non-physical ones are shown by dashed line.