Eliminated corrections to scaling around a renormalization-group fixed point: Transfer-matrix simulation of an extended $d=3$ Ising model

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Extending the parameter space of the three-dimensional ($d=3$) Ising model, we search for a regime of eliminated corrections to finite-size scaling. For that purpose, we consider a real-space renormalization group (RSRG) with respect to a couple of clusters simulated with the transfer-matrix (TM) method. Imposing a criterion of "scale invariance," we determine a location of the nontrivial RSRG fixed point. Subsequent large-scale TM simulation around the fixed point reveals eliminated corrections to finite-size scaling. As anticipated, such an elimination of corrections admits systematic finite-size-scaling analysis. We obtained the estimates for the critical indices as $\nu=0.6245(28)$ and $y_h=2.4709(73)$. As demonstrated, with the aid of the preliminary RSRG survey, the transfer-matrix simulation provides rather reliable information on criticality even for $d=3$, where the tractable system size is restricted severely.

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I. INTRODUCTION

The transfer-matrix method has an advantage over the Monte Carlo method in that it provides information free from the statistical (sampling) error and the problem of slow relaxation to thermal equilibrium. On one hand, the tractable system size with the transfer-matrix method is severely limited, because the transfer-matrix size increases exponentially as the system size N enlarges; here, N denotes the number of spins constituting a unit of the transfer-matrix slice. Such a limitation becomes even more serious in large dimensions ($d \geqslant 3$). Actually, for large d, the system size N ($=L^{d-1}$) increases rapidly as the linear dimension L enlarges, and it soon exceeds the limit of available computer resources. Because of this difficulty, the usage of the transfer-matrix method has been restricted mainly within $d=2$.

In this paper, we report an attempt to eliminate the finite-size corrections of the $d=3$ Ising model by tuning the interaction parameters. As anticipated, such an elimination of corrections admits systematic finite-size-scaling analysis of the numerical data with restricted system sizes. To be specific, we consider the $d=3$ Ising ferromagnet with extended interactions,

$$H=-J_{NN}\sum_{\langle i,j\rangle} S_iS_j - J_{NNN}\sum_{\langle\langle i,j\rangle\rangle} S_iS_j - J_{\Box}\sum_{[i,j,k,l]} S_iS_jS_kS_l, \quad (1)$$

where the Ising spins $S_i=\pm 1$ are placed at the cubic-lattice points specified by the index i. The summations $\Sigma_{\langle i,j\rangle}$, $\Sigma_{\langle\langle i,j\rangle\rangle}$, and $\Sigma_{[i,j,k,l]}$ run over all nearest-neighbor pairs, next-nearest-neighbor (plaquette diagonal) spins, and round-a-plaquette spins, respectively. Within the extended parameter space ($J_{NN},J_{NNN},J_{\Box}$), we search for a regime of eliminated corrections to scaling. For that purpose, we consider a real-space renormalization group for a couple of clusters, whose thermodynamics is simulated with the transfer-matrix method; see Fig. 1. We then determine a location of the renormalization-group fixed point. Following this preliminary renormalization-group survey, we perform extensive transfer-matrix simulation around this fixed point. Thereby, we show that the corrections-to-scaling behavior is improved around the fixed point. Here, we utilized an improved version of the transfer-matrix method [1–7], and succeeded in treating a variety of system sizes $N=5,6,\ldots,15$; note that conventionally, the tractable system sizes are restricted to $N=4,9,16,\ldots$. Apparently, such an extension of available system sizes provides valuable information on criticality.

In fairness, it has to be mentioned that our research owes its basic idea to the following pioneering studies. First, an attempt to eliminate the finite-size corrections was reported in Ref. [8], where the authors investigate the $d=3$ Ising model with the (finely tuned) second- and third-neighbor interactions; see also the studies [9–11] in the lattice-field-theory context. Their consideration could be viewed as an interesting application of the Monte Carlo renormalization group [12] to exploit the virtue of the fixed point. (The Monte Carlo renormalization group provides an explicit realization of the renormalization-group idea in the real space.) The aim of this paper is to develop an alternative approach to the elimination of corrections via the transfer-matrix method,

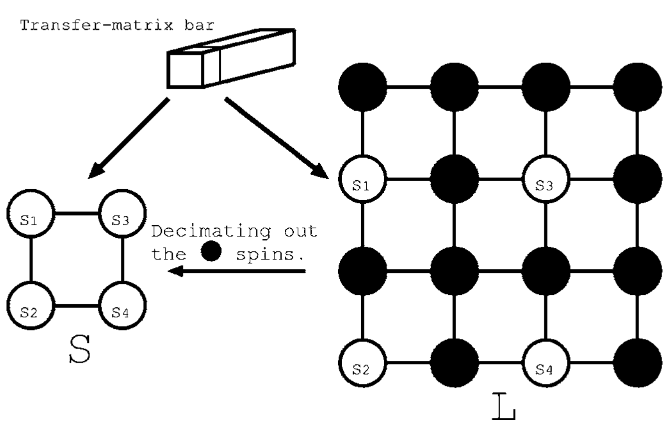

FIG. 1. A schematic drawing of our real-space renormalization group (decimation) for the $d=3$ Ising model with the extended interactions Eq. (1). As indicated, the thermodynamics is simulated with the transfer-matrix method. Imposing a criterion of scale invariance, Eq. (4), we determined the renormalization-group fixed point Eq. (7) numerically; see text for details.

and make the best use of its merits and characteristics. In fact, the four-spin interaction, appearing in our Hamiltonian (1), is readily tractable with the transfer-matrix method, whereas it can make a conflict with the Monte Carlo simulation; in fact, the four-spin interaction disables the use of cluster update. (Probably, as for the Monte Carlo simulation, it might be more rewarding to enlarge the system size rather than incorporate extra interactions.) Second, the extended interactions appearing in our Hamiltonian (1) are taken from the proposal by Ma [13], who investigated the $d=2$ Ising model and its renormalization-group flow. We consider that his renormalization-group scheme for $d=2$ is still of use to our $d=3$ case as well. Actually, in our transfer-matrix treatment, the system size along the transfer-matrix direction is infinite, and the remaining $d=2$ fluctuations are responsible for the finite-size corrections. We demonstrate that Ma's scheme leads to satisfactory elimination of finite-size corrections in $d=3$.

The rest of this paper is organized as follows. In Sec. II, we explain the real-space decimation (renormalization group) for the $d=3$ Ising model (1), and search for its fixed point. In Sec. III, we perform extensive transfer-matrix simulation around this fixed point. Here, we utilized an improved transfer-matrix method, which is explicated in the Appendix. The last section is devoted to summary and discussions.

II. SEARCH FOR A SCALE-INVARIANT POINT: A REGIME OF ELIMINATED IRRELEVANT INTERACTIONS

In this section, we search for a point of eliminated finite-size corrections of the extended Ising model, Eq. (1). For that purpose, we set up a real-space renormalization group, and look for the scale-invariant (fixed) point; the result is given by Eq. (7).

To begin with, we set up the real-space renormalization group. We consider a couple of rectangular clusters with the sizes 2×2 and 4×4; see Fig. 1. These clusters are labeled by the symbols S and L, respectively. (Because we utilize the transfer-matrix method, the system sizes perpendicular to these rectangles are both infinite.) Decimating out the spin variables indicated by the symbol ● of the L cluster, we obtain a reduced lattice structure identical to that of the S cluster. Our concern is to find a "scale invariance" condition with respect to this real-space renormalization group.

Before going into the explicit formulation of the renormalization group (fixed-point analysis), we explain briefly how we simulated the thermodynamics of these clusters. As mentioned above, we employ the transfer-matrix method. The transfer-matrix elements for the S cluster are given by the formula

$$T_{\{T_i\},\{S_i\}} = (W^{S_3S_4}_{S_1S_2})^{1+3b}(W^{T_1T_2}_{S_1S_2}W^{T_2T_4}_{S_2S_4}W^{T_4T_3}_{S_4S_3}W^{t_3T_1}_{S_3S_1})^{1+b}, \qquad (2)$$

where the component $W^{S_3S_4}_{S_1S_2}$ denotes the local Boltzmann weight for a plaquette, Eq. (A3), and the spin variables $\{S_i\}$ and $\{T_i\}$ $(i=1-4)$ denote the spin configurations for both sides of the transfer-matrix slice. The component $(\cdots)^{1+3b}$ originates in the plaquette interactions perpendicular to the transfer-matrix direction, whereas the remaining part $(\cdots)^{1+b}$ comes from the longitudinal ones. The parameter b controls the boundary interaction strength. Note that irrespective of b, the periodic boundary condition is maintained; namely, all 2×2 spins remain equivalent as b varies. Such a redundancy is intrinsic to the $L=2$ system. Here, we consider this redundant parameter as a freely tunable one. [For example, a naive implementation of the periodic boundary condition for a pair of spins may result in such an interaction as $H=-JS_1S_2-JS_2S_1=-2JS_1S_2$. Clearly, such a duplicated interaction is problematic. Possibly, the interaction $-(1+b)JS_1S_2$ with a certain moderate parameter b should be a favorable one. The significant point is that the periodic boundary condition is maintained with b varied.] We found that the choice $b=0.4$ is reasonable for the reasons mentioned afterward.

Similarly to the above, we constructed the transfer matrix for the L cluster as

$$T_{\{T_{ij}\},\{S_{ij}\}} = \prod_{1\leq i,j\leq 4} (W^{S_{i,j+1}S_{i+1,j+1}}_{S_{ij}S_{i+1,j}}W^{T_{ij}T_{i+1,j}}_{S_{ij}S_{i+1,j}}W^{T_{ij}T_{i,j+1}}_{S_{ij}S_{i,j+1}}), \qquad (3)$$

with the 4×4 spin configurations $\{S_{ij}\}$ and $\{T_{ij}\}$ under the periodic boundary condition. In this case $(L=4)$, we have no ambiguity as to the boundary interaction.

Based on the above-mentioned simulation scheme, we calculate the location of the renormalization-group fixed point. We impose the following scale-invariance conditions:

$$\langle S_1S_2\rangle_S = \langle S_1S_2\rangle_L, \qquad (4)$$

$$\langle S_1S_4\rangle_S = \langle S_1S_4\rangle_L, \qquad (5)$$

$$\langle S_1S_2S_3S_4\rangle_S = \langle S_1S_2S_3S_4\rangle_L. \qquad (6)$$

Here, the symbol $\langle\cdots\rangle_{S(L)}$ denotes the thermal average for the S (L) cluster, and the arrangement of spin variables $\{S_i\}$ is shown in Fig. 1. We solved the above equations numerically, and found that a nontrivial solution does exist at

$$(\tilde{J}_{NN},\tilde{J}_{NNN},\tilde{J}_{\square}) = (0.108\,982\,866\,643\,5, 0.044\,577\,772\,795\,6, -0.006\,511\,795\,049\,2). \qquad (7)$$

The last digits may be uncertain due to the numerical round-off errors. The result is to be compared with that of the preceding Monte Carlo study $(\tilde{J}_{NN},\tilde{J}_{NNN},\tilde{J}_{3rd})=(0.1109, 0.033\,08, 0.014\,02)$ [8], where the authors incorporated the third-neighbor interaction $\tilde{J}_{3rd}$ and omitted $\tilde{J}_{\square}$ instead.

Let us make a few comments. First, in the next section, we confirm that the fixed point is indeed a good approximant to the phase-transition point. This fact indicates that the above renormalization-group analysis is sensible. Moreover, we calculated the fixed point $\tilde{J}_{NN}=0.224\,390\,442\,310\,6$ for the conventional Ising model $(J_{NNN},J_{\square})=(0,0)$. We again see that this transition point is in agreement with a critical point $J^*_{NN}=0.221\,654\,55(3)$ determined with the Monte Carlo method [14]. (Hence, the choice of the boundary interaction strength $b=0.4$ is justified.) Second, we stress that the above renormalization group is not intended to obtain a (quantitatively reliable) critical point nor the critical indices. The aim

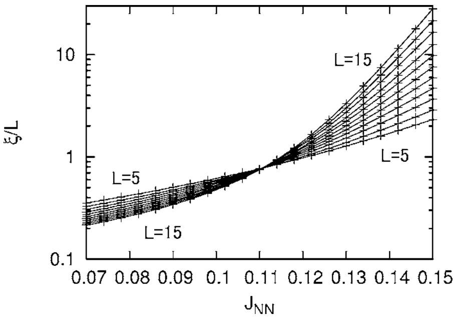

FIG. 2. Scaled correlation length ξ/L is plotted for the nearest-neighbor interaction J_{NN} and $N=5,6,\ldots,15$ ($N=L^2$); note that we survey the parameter space (8) including the renormalization-group fixed point (7). We observe a clear indication of criticality at $J_{NN}\sim 0.11$. Apparently, the finite-size-scaling behavior is improved as compared to that of Fig. 4 for the conventional Ising model.

of the above analysis is to truncate out the irrelevant interactions. The detailed analysis of criticality is made with the subsequent finite-size-scaling analysis. In other words, our numerical approach consists of two steps, and the remaining step is considered in the next section.

III. FINITE-SIZE-SCALING ANALYSIS OF THE CRITICAL EXPONENTS ν AND y_h

In Sec. II, we determined the position of the renormalization-group fixed point, Eq. (7). In this section, around the fixed point, we survey the criticality of the *temperature-driven* phase transition. That is, hereafter, we dwell on the one-parameter subspace

$$(J_{NN},J_{NNN},J_{\Box}) = J_{NN}\left(1,\frac{\tilde{J}_{NNN}}{\tilde{J}_{NN}},\frac{\tilde{J}_{\Box}}{\tilde{J}_{NN}}\right), \tag{8}$$

which contains the renormalization-group fixed point at $J_{NN}=\tilde{J}_{NN}$. We anticipate that corrections to scaling (influence of irrelevant operators) should be suppressed in this parameter space.

Throughout this section, we employ an improved version of the transfer-matrix method (Novotny's method) [1]. (To avoid confusion, we stress that in Sec. II, we used the conventional transfer-matrix method.) A benefit of Novotny's method is that we are able to treat an arbitrary (integral) number of spins $N=5,6,\ldots,15$, constituting a unit of the transfer-matrix slice; note that conventionally the number of spins is restricted to $N=4,9,16,\ldots$. We explicate this simulation algorithm in the Appendix.

A. Eliminated corrections to scaling

In Fig. 2, we plotted the scaled correlation length ξ/L for J_{NN} and a variety of system sizes $N=5,6,\ldots,15$. We evaluated the correlation length ξ with use of the formula $\xi=1/\ln(\lambda_1/\lambda_2)$ with the dominant (subdominant) eigenvalue λ_1 (λ_2) of the transfer matrix. As explained in the Appendix, the linear dimension L is simply given by

$$L=\sqrt{N}, \tag{9}$$

with the number of spins N; see Fig. 8.

From Fig. 2, we see a clear indication of criticality at $J_{NN}\approx 0.11$; note that the intersection point of the curves indicates a critical point. Afterward, we compare this result to that of the conventional Ising model $(J_{NNN},J_{\Box})=(0,0)$ to elucidate the improvement of the scaling behavior. Here, we want to draw the reader's attention to the point that we treated various system sizes $N=5,6,\ldots,15$ with the aid of the Novotny method. Actually, in Fig. 2, we notice that a variety of system sizes are available. Clearly, such an extension of available system sizes is significant in the subsequent detailed finite-size-scaling analyses.

In Fig. 3, we present the scaling plot $(J_{NN}-J^*_{NN})L^{1/\nu}$ $-\xi/L$ for $12\leqslant N\leqslant 15$. with the scaling parameters J^*_{NN} $=0.110\,59$ and $\nu=0.6245$ determined in Figs. 5 and 6, respectively. We see that the data collapse into a scaling function satisfactorily; actually, we can hardly observe corrections to the finite-size scaling.

In the above, we presented evidence that the corrections-to-scaling behavior is improved in the parameter space Eq. (8). Lastly, as a comparison, we provide the data for the conventional Ising model; namely, we set $(J_{NNN},J_{\Box})=(0,0)$

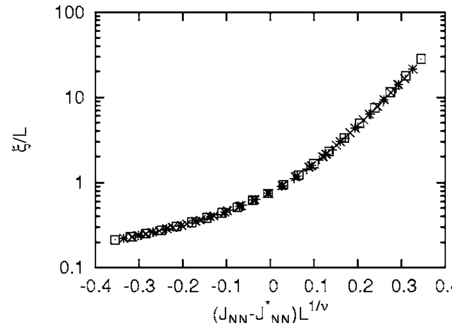

FIG. 3. The scaling plot for the correlation length, $(J_{NN}-J^*_{NN})L^{1/\nu}-\xi/L$, is shown for the system sizes $N=(+)$ 12, ($\times$) 13, (*) 14, and ($\Box$) 15; note the relation $N=L^2$. Here, we accepted the scaling parameters, $J^*_{NN}=0.110\,59$ and $\nu=0.6245$, determined in Figs. 5 and 6, respectively. We again confirm that corrections to scaling are suppressed significantly.

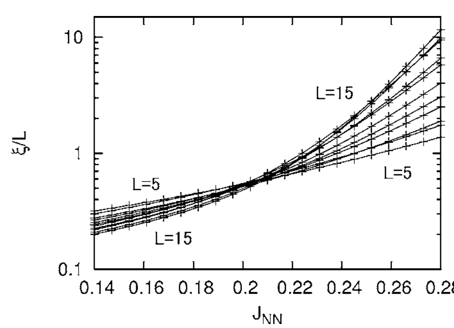

FIG. 4. Tentatively, we turned off the extended interactions ($J_{NNN}=0$ and $J_{\Box}=0$), and calculated the scaled correlation length ξ/L for various J_{NN} and $N=5,6,\ldots,15$. We notice that the data are scattered as compared to those in Fig. 2.

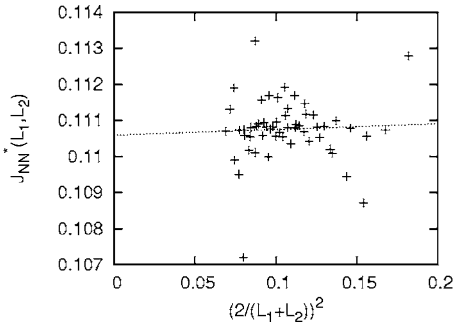

FIG. 5. The approximate critical interaction $J_{NN}^*(L_1,L_2)$ is plotted for $[2/(L_1+L_2)]^2$ with $5 \leqslant N_1 < N_2 \leqslant 15$ ($L_{1,2}=\sqrt{N_{1,2}}$). The least-squares fit to these data yields $J_{NN}^*=0.110\,59(52)$ in the thermodynamic limit $L \to \infty$.

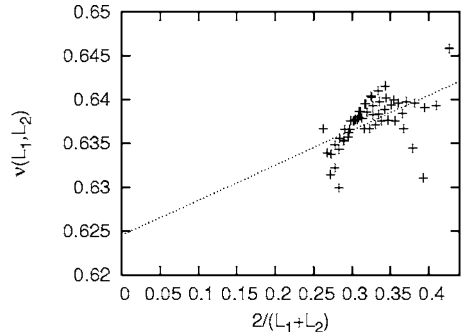

FIG. 6. The approximate correlation-length critical exponent $\nu(L_1,L_2)$ is plotted for $2/(L_1+L_2)$ with $5 \leqslant N_1 < N_2 \leqslant 15$ ($L_{1,2}=\sqrt{N_{1,2}}$). The least-squares fit to these data yields $\nu = 0.6245(28)$ in the thermodynamic limit $L \to \infty$.

tentatively. In Fig. 4, we plotted the scaled correlation length ξ/L for various J_{NN}. Apparently, the data suffer from ainsystematic finite-size corrections. The data scatter obscures the position of the critical point. (Nevertheless, we should mention that the data imply $J_{NN}^* \sim 0.2$, which does not contradict a recent Monte Carlo result $J_{NN}^*=0.221\,654\,55(3)$ [14].)

B. Phase-transition point J_{NN}^*

In the above, we obtain a rough estimate for the phase-transition point J_{NN}^*. In this section, we determine the transition point more precisely. In Fig. 5, we plotted the approximate transition point $J_{NN}^*(L_1,L_2)$ for $(2/(L_1+L_2))^2$. Here, the approximate transition point denotes the intersection point of the curves ξ/L (Fig. 2) for a pair of system sizes (L_1,L_2) $(5 \leqslant N_1 < N_2 \leqslant 15)$. That is, the following equation:

$$L_1\xi(L_1)|_{J_{NN}=J_{NN}^*(L_1,L_2)} = L_2\xi(L_2)|_{J_{NN}=J_{NN}^*(L_1,L_2)} \tag{10}$$

holds. In Fig. 5, we notice that the data exhibit suppressed systematic finite-size deviation, namely, the ansystematic data scatter is more conspicuous than the systematic deviation. The least-squares fit to these data yields the transition point

$$J_{NN}^* = 0.110\,59(52) \tag{11}$$

in the thermodynamic limit $L \to \infty$.

In order to check the reliability, we replaced the abscissa scale with $(2/(L_1+L_2))^{\omega+1/\nu}$ [15], where we used $1/\nu = 1.5868(3)$ and $\omega=0.821(5)$ reported in Ref. [14]. (In the next section, we present a consideration of the abscissa scale.) Thereby, we arrive at $J_{NN}^*=0.110\,62(43)$, which is consistent with the above result. (The error margin may be purely statistical.) We confirm that the choice of the abscissa scale is not very influential.

We notice that the transition point J_{NN}^* (11) and the renormalization-group fixed point $\tilde{J}_{NN}$ (7) are in good agreement with each other. This fact confirms that the renormalization-group analysis in Sec. II is indeed sensible. As mentioned in Sec. II we do not require fine accuracy as to the convergence of J_{NN}^* and $\tilde{J}_{NN}$. The aim of the renormalization-group analysis is to search for a regime of eliminated corrections rather than to obtain the precise location of the fixed point. The detailed analysis of criticality is performed in the subsequent finite-size-scaling analysis as demonstrated in the next section. [Actually, by tuning the boundary interaction parameter b (see Sec. II), we could attain better agreement between J_{NN}^* and $\tilde{J}_{NN}$. However, such a refinement does not affect the subsequent finite-size-scaling analysis very much.]

C. Critical exponents ν and y_h

In Sec. III A, we presented evidence of eliminated finite-size corrections. Encouraged by this result, in this section, we evaluate the critical exponents ν and y_h with use of the finite-size-scaling method (phenomenological renormalization group) [16].

In Fig. 6, we plotted the approximate correlation-length critical exponent

$$\nu(L_1,L_2) = \ln(L_1/L_2)/\ln\left(\frac{\partial[\xi(L_1)/L_1]}{\partial J_{NN}} \bigg/ \frac{\partial[\xi(L_2)/L_2]}{\partial J_{NN}}\right)\bigg|_{J_{NN}=J_{NN}^*(L_1,L_2)} \tag{12}$$

for $2/(L_1+L_2)$ with $5 \leqslant N_1 < N_2 \leqslant 15$. With use of the least-squares fit to these data, we obtain the estimate

$$\nu = 0.6245(28) \tag{13}$$

in the thermodynamic limit. The data in Fig. 6 exhibit appreciable systematic finite-size corrections. More specifically, the systematic deviation ($\sim 2\%$) is almost comparable to the insystematic data scatter. [This fact indicates that we cannot fully truncate out the irrelevant interactions within the parameter space $(J_{NN}, J_{NNN}, J_{\square})$.] In this sense, the above (extrapolated) value, Eq. (12), may contain a systematic (biased) error. Afterward, we present a few considerations on the extrapolation scheme. (Because our work is methodology oriented, we supply the least-squares-fit result as it is.)

In Fig. 7, we plotted the approximate exponent y_h,

$$y_h(L_1,L_2) = \ln\left(\frac{\partial^2[\xi(L_1)/L_1]}{\partial H^2} \Bigg/ \frac{\partial^2[\xi(L_2)/L_2]}{\partial H^2}\right)\Bigg|_{J_{NN}=J^*_{NN}(L_1,L_2)} \Bigg/ [2\ln(L_1/L_2)], \tag{14}$$

for $2/(L_1+L_2)$ with $5 \leq N_1 < N_2 \leq 15$. In order to incorporate the magnetic field H, we added the Zeeman term, $-H\Sigma_i S_i$, to the Hamiltonian (1). Rather satisfactorily, the data $y_h(L_1,L_2)$ exhibit suppressed systematic corrections; the systematic deviation is almost negligible compared to the insystematic one. The least-squares fit to these data yields the estimate

$$y_h = 2.4709(73) \tag{15}$$

in the thermodynamic limit.

Provided by the above estimates ν and y_h, we obtain the following critical indices through the scaling relations:

$$\alpha = 0.1265(84), \tag{16}$$

$$\beta = 0.3304(48), \tag{17}$$

$$\gamma = 1.213(11). \tag{18}$$

Let us provide comparative results with an alternative extrapolation scheme. We replaced the scale of abscissa in Figs. 6 and 7 with $[2/(L_1+L_2)]^{\omega}$; here, we set the exponent ω=0.821(5) reported in Ref. [14]. (As mentioned below, this scheme may overestimate the amount of systematic finite-size corrections.) Accepting this abscissa scale, we arrive at ν=0.6216(34) and y_h=2.4694(90). These values appear to be consistent with the above ones within the error margins, confirming that the extrapolation scheme is not very influential.

We argue the underlying physics of the abscissa scale (extrapolation scheme) in detail. In principle, the exponent ω governs the dominant (systematic) finite-size corrections. On the other hand, in the present simulation, we are trying to truncate out such systematic corrections. Hence, in our data analysis, the usage of the exponent ω would be problematic. We consider that the systematic corrections should obey the scaling law like $L^{-\omega_{eff}}$ with a certain effective exponent $\omega_{eff} > \omega$, at least in the regime of $5 \leq N \leq 15$; namely, we suspect that the abscissa scale with the exponent ω leads to an overestimation of systematic corrections. Actually, a recent Monte Carlo simulation reports the estimates ν =0.630 20(12) and y_h=2.4816(1) [14]. Here, we notice that their ν indicates a non-negligible deviation, whereas the value of y_h is in good agreement with ours. This fact confirms the above observation that $\nu(L_1,L_2)$ exhibits appreciable systematic corrections, and the extrapolated value may contain a biased error. Possibly, an adequate exponent ω_{eff} would be even larger than the value ω_{eff}=1 utilized in Fig. 6. Nevertheless, for the sake of simplicity, we do not pursue this issue further, and supply the least-squares-fit result as it is.

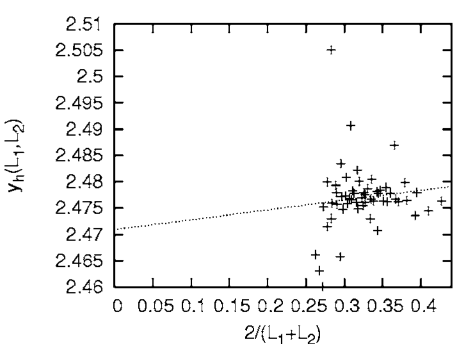

FIG. 7. The approximate critical exponent $y_h(L_1,L_2)$ is plotted for $2/(L_1+L_2)$ with $5 \leq N_1 < N_2 \leq 15$ $(L_{1,2}=\sqrt{N_{1,2}})$. The least-squares fit to these data yields y_h=2.4709(73) in the thermodynamic limit $L \to \infty$.

Lastly, we mention a recent extensive exact-diagonalization result by Hamer [17], who obtained ν =0.628 54(79) and y_h=2.482(10). He investigated the quantum d=2 transverse-field Ising model, relying on the belief that the quantum d=2 Ising model should belong to the same universality class as the d=3 Ising ferromagnet. The quantum version has an advantage in that the Hamiltonian elements are sparse (few nonzero elements), and one is able to treat a large cluster size 6×6. Comparing our data with his results, we notice that they are almost comparable with each other. Actually, the error margin of our y_h is even smaller than his result, although we treated the d=3 ferromagnet directly.

IV. SUMMARY AND DISCUSSIONS

So far, it has been considered that the transfer-matrix method would not be very useful for problems in $d \geq 3$ because of its severe limitation as to tractable system size. In this paper, we demonstrated that the corrections-to-scaling behavior of the d=3 Ising model (1) is improved by adjusting the coupling constants to the values of the renormalization-group fixed point, Eq. (7). Actually, corrections to scaling in Figs. 2 and 3 are eliminated significantly as compared to those in Fig. 4 for the conventional Ising model. Moreover, we succeeded in treating a variety of system sizes N=5,6,…,15 with the aid of the Novotny method (see the Appendix); note that with the conventional approach, the available system sizes are restricted to

N=4,9,16,…. Clearly, such an extension of available system sizes provides valuable information on criticality. Owing to these improvements, we analyzed the criticality of the d=3 Ising model with the transfer-matrix method, and obtained the critical indices ν=0.6245(28) and y_h=2.4709(73).

As mentioned in the Introduction, an attempt to eliminate finite-size corrections has been pursued [8] in the context of the Monte Carlo renormalization group [12]. We consider that an approach with the transfer-matrix method is also of use because of the following reasons. First, we accepted a simple renormalization-group scheme shown in Fig. 1. As mentioned in the Introduction, this scheme was introduced originally as for the d=2 Ising model [13]. The advantage of the transfer-matrix method is that the system size along the transfer-matrix direction is infinite, and the remaining d=2 fluctuations are responsible for the finite-size corrections. Hence, such a (d=2)-like renormalization group is still of use to achieve elimination of corrections satisfactorily. Second, the transfer-matrix method is capable of the four-spin interaction appearing in our Hamiltonian (1). On the other hand, the Monte Carlo sampling conflicts with such a multispin interaction, because the multispin interaction disables the use of a cluster-update algorithm. (Probably an effort toward enlarging the system size would be rewarding from a technical viewpoint.)

In addition to these merits, we would like to emphasize again the point that the transfer-matrix approach with the Novotny method allows us to treat a variety of system sizes N=5,6,…,15. We consider that Novotny's method combined with the elimination of finite-size corrections would be promising to resolve the (seemingly intrinsic) drawback of the transfer-matrix method in $d \geq 3$. As a matter of fact, the basic idea of the present scheme would be generic, and it might have a potential applicability to a wide class of systems. An effort toward this direction is in progress, and it will be addressed in future study.

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APPENDIX: NOVOTNY'S TRANSFER-MATRIX METHOD

We explain the details of the transfer-matrix method utilized in Sec. III. (To avoid confusion, we remind the reader that in Sec. II, we utilized the conventional transfer-matrix method.) Our method is based on Novotny's formalism [1–4], which enables us to consider an arbitrary (integral) number of spins $\forall N$, constituting a unit of the transfer-matrix slice even for $d \geq 3$; note that conventionally, the number of spins is restricted to N=4,9,16,…. We made a modification to the Novotny formalism in order to incorporate the plaquette-type interactions. We already reported this method in Ref. [5], where we studied the multicriticality of the extended d=3 Ising model [18]. In the present paper, we implemented yet further modifications such as Eqs. (A8)–(A10). Hence, for the sake of self-consistency, we explicate the full details of the simulation scheme.

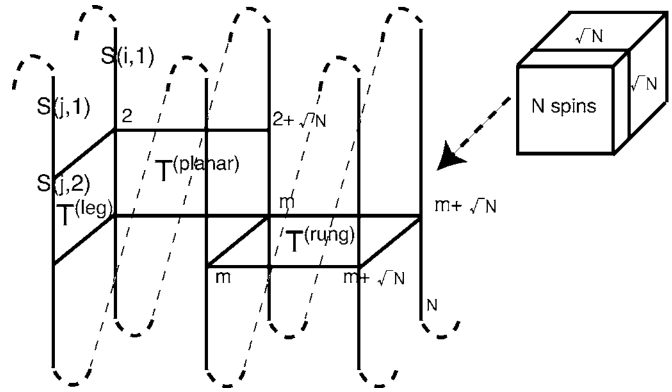

FIG. 8. A schematic drawing of a unit of the transfer-matrix slice for the d=3 Ising model with the extended interactions (1). The contributions from the "leg," "planar," and "rung" interactions are considered separately; see Eq. (A1). Within the transfer-matrix slice, the arrangement of the constituent spins is one dimensional (coiled structure). The dimensionality is raised up to d=2 by the bridges between the $\sqrt{N}$th-neighbor spins along the leg.

Before going into details, we mention the basic idea of the Novotny method. In Fig. 8, we presented a schematic drawing of a unit of the transfer-matrix slice. Note that in general, a transfer-matrix unit for a d-dimensional system should have a ($d-1$)-dimensional structure, because it is a cross section of the d-dimensional manifold. However, as shown in Fig. 8, the constituent N spins form a d=1 (coiled) alignment rather than d=2. The dimensionality is raised *effectively* to d=2 by the $\sqrt{N}$ th-neighbor interactions among these N spins; this is the essential idea of the Novotny method to constitute a transfer-matrix unit with arbitrary number of spins even for d=3.

In the following, we present the explicit formulas for the transfer-matrix elements. We decompose the transfer matrix into the following three components:

$$T(v) = T^{(leg)} \odot T^{(planar)}(v) \odot T^{(rung)}(v), \tag{A1}$$

where the symbol $\odot$ denotes the Hadamard (element by element) matrix multiplication. Note that the product of local Boltzmann weights gives rise to the global one. The physical content of each component is shown in Fig. 8.

The explicit expression for the element of $T^{(leg)}$ is given by the formula,

$$T_{ij}^{(leg)} = \langle i|A|j\rangle = W_{S(i,1)S(i,2)}^{S(j,1)S(j,2)} W_{S(i,2)S(i,3)}^{S(j,2)S(j,3)} \cdots W_{S(i,N)S(i,1)}^{S(j,N)S(j,1)}, \tag{A2}$$

where the indices i and j specify the spin configurations of both sides of the transfer-matrix slice. More specifically, the spin configuration $\{S(i,1), S(i,2), \ldots, S(i,N)\}$ is arranged along the leg; see Fig. 8. The factor $W_{S_1 S_2}^{S_3 S_4}$ denotes the local Boltzmann weight for the plaquette spins $\{S_i\}$ (i=1–4);

$$W_{S_1S_2}^{S_3S_4} = \exp\left[-\left(-\frac{J_{NN}}{4}(S_1S_2+S_2S_4+S_4S_3+S_3S_1) - \frac{J_{NNN}}{2}(S_1S_4+S_2S_3) - \frac{J_\square}{2}S_1S_2S_3S_4\right)\right]. \quad (A3)$$

Notably enough, the component $T^{(leg)}$ is nothing but a transfer matrix for the $d=2$ Ising model. The remaining components $T^{(planar)}$ and $T^{(rung)}$ introduce the $\sqrt{N}$th-neighbor couplings, and raise the dimensionality effectively to $d=3$.

The component $T^{(planar)}$ is given by

$$T_{ij}^{(planar)}(v) = \langle i|AP^v|i\rangle, \quad (A4)$$

with

$$v = \sqrt{N}, \quad (A5)$$

where the matrix P denotes the translation operator; namely, the state $P|i\rangle$ represents a shifted configuration $\{S(i,m+1)\}$. Hence, the insertion of $P^{\sqrt{N}}$ introduces the $\sqrt{N}$th-neighbor interactions among the N spins [1]. Similarly, we propose the following expression for the component $T^{(rung)}$:

$$T_{ij}^{(rung)}(v) = (\langle i| \otimes \langle j|)B[(P^v|i\rangle) \otimes (P^v|j\rangle)], \quad (A6)$$

with,

$$(\langle i| \otimes \langle j|)B(|k\rangle \otimes |l\rangle) = \prod_{m=1}^{N} W_{S(i,m)S(j,m)}^{S(k,m)S(l,m)}. \quad (A7)$$

The meaning of the formula should be apparent from Fig. 8.

The above formulations were already reported in Ref. [5]. In the following, we propose a number of additional improvements. First, we symmetrize the transfer matrix with the replacement [2]

$$T(v) \to T(v) \odot T(-v). \quad (A8)$$

Correspondingly, we substitute the strength of the coupling constants $J_\alpha \to J_\alpha/2$ in order to compensate the above duplication. Clearly, with the symmetrization, the symmetry of descending $(m=N,N-1,\ldots)$ and ascending $(m=1,2,\ldots)$ directions is restored. Moreover, we implement the following symmetrizations:

$$\langle i|AP^v|i\rangle \to \langle i|AP^v|i\rangle\langle i|P^{-v}A|i\rangle \quad (A9)$$

and

$$(\langle i| \otimes \langle j|)B[(P^v|i\rangle) \otimes (P^v|j\rangle)] \to (\langle i| \otimes \langle j|)B[(P^v|i\rangle) \otimes (P^v|j\rangle)][(\langle i|P^{-v}) \otimes (\langle j|P^{-v})]B(|i\rangle \otimes |j\rangle) \quad (A10)$$

as to Eqs. (A4) and (A6), respectively. Again, we have to redefine the coupling constants to compensate the duplication.

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