Algorithm of the finite-lattice method for high-temperature expansion of the Ising model in three dimensions

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We propose an algorithm of the finite-lattice method to generate the high-temperature series for the Ising model in three dimensions. It enables us to extend the series for the free energy of the simple-cubic lattice from the previous series of 26th order to 46th order in the inverse temperature. The obtained series give the estimate of the critical exponent for the specific heat in high precision.

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I. INTRODUCTION

The finite-lattice method [1–3] is a powerful tool to generate the high- and low-temperature series for the spin models in the infinite volume limit. It avoids the tedious work of counting all the diagrams in the graphical method, and reduces the problem to the calculation of the partition function. In two dimensions, the total amount of the calculations for the finite-lattice method increases exponentially with the maximum order N of the series. On the other hand, in three dimensions, the total amount of the calculations increases exponentially with N^2 [4] and, except for some cases [5–13], many of the expansion series have been calculated by the graphical method. Here we present an algorithm of the finite-lattice method for the high-temperature expansion in three dimensions, in which the total amount of the calculation increases exponentially with $N \ln N$, and this enables us to generate the series to much higher orders than not only the standard algorithm of the finite-lattice method but also the graphical method. In fact applying the algorithm, we will extend the high-temperature series for the free energy density of the simple-cubic Ising model to 46th order in the inverse temperature from 26th order obtained by the standard algorithm of the finite-lattice method.

In Sec. II, we briefly review the standard finite-lattice method to generate the high-temperature series of the Ising model in three dimensions. In Sec. III, we present our algorithm of the finite-lattice method. In Sec. IV, we apply our algorithm to obtain the high-temperature series for the free energy density of the simple-cubic Ising model. The series are analyzed to estimate the critical exponent of the specific heat. Section V is devoted to summary and discussion.

II. FINITE-LATTICE METHOD

We consider the Ising model with spins $s_k = \pm 1$ on the sites k of the simple-cubic lattice with the Hamiltonian

$$H = -J \sum_{\langle k,k' \rangle} s_k s_{k'}. \tag{1}$$

Here the summation is taken for all the bonds connecting the nearest neighbor sites k and k'. The partition function is given by

$$Z = \sum_{\{s_k\}} \exp(-H/kT), \tag{2}$$

where the summation is the average over all of the spin variables,

$$\sum_{\{s_k\}} = \frac{1}{2} \sum_{s_1 = \pm 1} \frac{1}{2} \sum_{s_2 = \pm 1} \cdots. \tag{3}$$

In the finite-lattice method, to generate the high-temperature series for the free energy density to order N in the inverse temperature, we first calculate the partition function $Z(l_x \times l_y \times l_z)$ for the finite size lattices with $2(l_x + l_y + l_z) \leqslant N$. Here we use the notation for the lattice size such that the $1 \times 1 \times 1$ lattice means the unit cube composed of $2 \times 2 \times 2$ sites. The Boltzmann factor for each bond is expressed as

$$\exp(\beta s_k s_{k'}) = \cosh(\beta)(1 + t s_k s_{k'}), \tag{4}$$

with $\beta = J/kT$ and $t = \tanh(\beta)$. We define the bond configuration as the set of bonds to which factor $t s_k s_{k'}$ in Eq. (4) is assigned, while factor 1 is assigned to the other bonds of the finite size lattice. Nonvanishing contribution to the partition function comes only from the bond configuration C in which the bonds form one or more closed loops:

$$Z(l_x \times l_y \times l_z) = 1 + \sum_C \xi(C). \tag{5}$$

Here $\xi(C)$ is the contribution from the bond configuration C, and we are neglecting the trivial factor coming from the factor $\cosh(\beta)$ in the expansion of the Boltzmann factor in Eq. (4). In order to obtain the series to order t^N, the summation is taken for all possible bond configurations that have $N_b \leqslant N$

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except for the trivial configuration with $N_b=0$, where N_b is the number of the bonds in each bond configuration.

Then we make the Taylor expansion with respect to t of the logarithm of the partition function for each size of the lattice. The logarithm of the partition function can be written as

$$\ln Z(l_x\times l_y\times l_z)=\sum_{C_1}\xi(C_1)-\frac{1}{2}\sum_{C_1}\sum_{C_2}\xi(C_1)\xi(C_2)+\frac{1}{3}\sum_{C_1}\sum_{C_2}\sum_{C_3}\xi(C_1)\xi(C_2)\xi(C_3)+\cdots=\sum_{n}\frac{(-1)^n}{n}\sum_{C_1}\sum_{C_2}\cdots\sum_{C_n}\xi(C_1)\xi(C_2)\cdots\xi(C_n). \tag{6}$$

We define the superposed bond configuration $\tilde{C}=C_1+C_2+\cdots+C_n$ for each term in the right hand side of Eq. (6). We call two loops of the bonds connected if the two loops share at least one bond with each other, otherwise disconnected, and a set of loops are called connected if the set cannot be divided into two subsets such that any loop in one subset is disconnected with any loop in the other subset.

It is well known [14] that only the superposed configurations $\tilde{C}$ composed of the connected loops contribute to $\ln Z(l_x\times l_y\times l_z)$, i.e., all the terms in the right hand side of Eq. (6), which have the same superposed configuration composed of disconnected loops, cancel with each other with vanishing net contribution to $\ln Z$. We call this Theorem I.

Next we define recursively [2]

$$\phi(l_x\times l_y\times l_z)=\ln[Z(l_x\times l_y\times l_z)]-\sum_{\substack{l_x'\le l_x,l_y'\le l_y,l_z'\le l_z,\\ l_x'+l_y'+l_z'\ne l_x+l_y+l_z}}(l_x-l_x'+1)(l_y-l_y'+1)\times(l_z-l_z'+1)\phi(l_x'\times l_y'\times l_z'). \tag{7}$$

The terms $\phi(l_x'\times l_y'\times l_z')$ are subtracted in this equation corresponding to each $l_x'\times l_y'\times l_z'$ sublattice of the $l_x\times l_y\times l_z$ lattice and, by the translational invariance of the model, the same size of the sublattice has the same value of ϕ, giving the factor $(l_x-l_x'+1)(l_y-l_y'+1)(l_z-l_z'+1)$. It is straightforward [2] to prove using Theorem I that the Taylor expansion of $\phi(l_x\times l_y\times l_z)$ with respect to t includes the contribution from every connected superposed bond configuration that can be embedded into the $l_x\times l_y\times l_z$ lattice but cannot be embedded into any of its rectangular sublattices. We call this Theorem II.

The expansion series of the free energy density in the infinite volume limit is given by

$$f=\sum_{2(l_x+l_y+l_z)\le N}\phi(l_x\times l_y\times l_z). \tag{8}$$

The expansion series of $\phi(l_x\times l_y\times l_z)$ starts from the term of order t^n with $n=2(l_x+l_y+l_z)$, which comes from one closed loop of bonds which has two intersections with any plane perpendicular to the lattice bonds. Thus it is enough to restrict the lattice sizes for the summation in Eq. (8) to those that satisfy $2(l_x+l_y+l_z)\le N$ in order to obtain the series for f to order t^N.

In calculating the partition function of the finite size lattice, the transfer matrix formalism with the site-by-site construction [15,16] is used. The total amount of the calculation and the necessary computer memory is proportional to the number of the bond configurations in the smallest two-dimensional cross section of the finite size lattice, which is roughly $2^{l_xl_y}$ for $l_x\le l_y\le l_z$. To generate the expansion series to order β^N, the maximum size of the lattice to be taken into account is $l_x\sim l_y\sim l_z\sim N/6$, so the central processing unit (CPU) time and the memory increase exponentially with N^2 in this standard algorithm of the finite-lattice method.

III. ALGORITHM

In the standard algorithm of the finite-lattice method, the partition function for the finite size lattice is calculated with all the bond configurations taken into account. The point of our algorithm is that, in order to obtain the series to a given order, however, it is enough to consider only a restricted number of bond configurations.

Let us consider the anisotropic model of the simple-cubic Ising model with β_i and $t_i=\tanh(\beta_i)$ $(i=x,y,z)$ in the framework of the finite-lattice method described in Sec. II. The partition function $Z(l_x\times l_y\times l_z)$ can be written in exactly the same way as Eq. (5). In order to obtain the series to order $t_x^{N_x}t_y^{N_y}t_z^{N_z}$ in the standard algorithm, the summation is taken for all possible bond configurations $\{C\}$ that have $N_{bx}\le N_x$, $N_{by}\le N_y$, $N_{bz}\le N_z$ except for the trivial configuration with $N_{bx}=N_{by}=N_{bz}=0$, where N_{bx}, N_{by}, and N_{bz} are the number of the bonds in x, y, and z direction, respectively, for each bond configuration. Let us define n_{zi} as the number of the bonds in the z direction for the ith layer perpendicular to the z axis $(i=1,2,\ldots,l_z)$ for each bond configuration.

We find that the lowest order in t_z of the terms in $\phi(l_x\times l_y\times l_z)$ given by Eq. (7), which involve $\xi(C)$ for the bond configuration C with $\{n_{zi}\}$, is $\Sigma_{i=1}^{l_z}\max(n_{zi},2)$. We call this Theorem III.

The proof for this is the following. If $n_{zi}\ge 2$ for all $i=1,\cdots,l_z$ [see Figs. 1(a)–1(c)], $\Sigma_{i=1}^{l_z}\max(n_{zi},2)=\Sigma_{i=1}^{l_z}n_{zi}$ is equal to the order of $\xi(C)$ in t_z. Then it is obvious that Theorem III is true. If n_{zi} is zero for at least one of $i=1,\ldots,l_z$ [see Figs. 1(d) and 1(e)], the configuration C is either disconnected or can be embedded into some rectangular sublattice $l_x'\times l_y'\times l_z'$ with $l_z'<l_z$. Then, by Theorem II, the term $\xi(C)$ can contribute to $\phi(l_x\times l_y\times l_z)$ only when it is multiplied by one or more other $\xi(C')$'s in Eq. (6) so that their superposed configuration $\tilde{C}=C+C'(+\cdots)$ should be composed of connected loops that cannot be embedded into any rectangular sublattice of the $l_x\times l_y\times l_z$ lattice. In order to prevent embedding of the superposed configuration into any rectangular sublattice, $\tilde{n}_{zi}$ should satisfy $\tilde{n}_{zi}\ge 2$ for all i

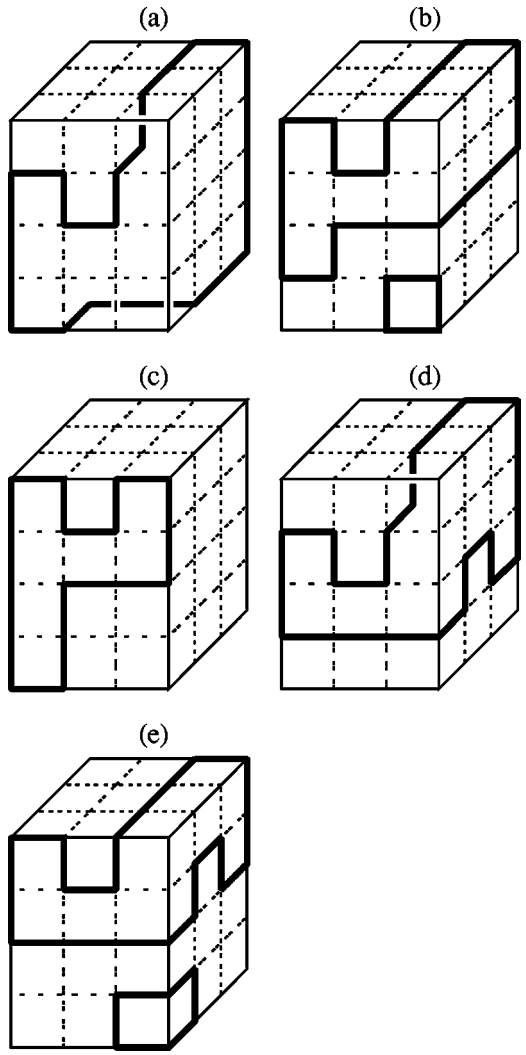

FIG. 1. Examples of the bond configuration for $Z(l_x \times l_y \times l_z)$ with $l_x=3$, $l_y=3$, $l_z=4$.

$=1,2,\ldots,l_z$, where $\tilde{n}_{zi}$ is the number of the bonds in the z direction for the superposed bond configuration $\tilde{C}$. Therefore the lowest order of the term in $\phi(l_x \times l_y \times l_z)$ to which the configuration C can contribute is again $\Sigma_{i=1}^{l_z} \max(n_{zi},2)$.

Thus to obtain the series for $\phi(l_x \times l_y \times l_z)$ to order N_x, N_y, and $N_z=2l_z+\Delta N_z$ in t_x, t_y, and t_z, respectively, we introduce in our algorithm $\phi(l_x \times l_y \times l_z, \Delta N_z)$ defined recursively by

$$\begin{aligned}\phi(l_x \times l_y \times l_z, \Delta N_z) &= \ln[Z(l_x \times l_y \times l_z, \Delta N_z)] \\ &- \sum_{\substack{l_x' \le l_x, l_y' \le l_y, l_z' \le l_z, \\ l_x'+l_y'+l_z' \ne l_x+l_y+l_z}} (l_x - l_x' + 1) \\ &\times (l_y - l_y' + 1)(l_z - l_z' + 1)\phi(l_x' \times l_y' \times l_z', \Delta N_z). \end{aligned} \tag{9}$$

Here the partition function $Z(l_x \times l_y \times l_z, \Delta N_z)$ is calculated only with the bond configurations taken into account which have $N_{bx} \le N_x$, $N_{by} \le N_y$ and n_{zi} with

$$\sum_{i=1}^{l_z} \max(n_{zi},2) \le 2l_z + \Delta N_z. \tag{10}$$

By Theorem III, any configuration that has $\Sigma_{i=1}^{l_z} \max(n_{zi},2) > 2l_z + \Delta N_z$ contributes to $\phi(l_x \times l_y \times l_z, \Delta N_z)$ in the order greater than $2l_z + \Delta N_z$. As an example, if we take $\Delta N_z = 2$ for the $3 \times 3 \times 4$ lattice, we should take account of Figs. 1(a)–1(c), each of which has $\Sigma_{i=1}^{l_z} \max(n_{zi},2) \le 10$, and we should neglect Figs. 1(d) and 1(e), each of which has $\Sigma_{i=1}^{l_z} \max(n_{zi},2) > 10$, among the configurations given in Fig. 1 according to the condition of Eq. (10). In spite of the fact that the configuration Figs. 1(a)–1(e) all have the same $\Sigma_{i=1}^{l_z} n_{zi} = 10$, the first three contribute to $\phi(3 \times 3 \times 4)$ to order t_z^{10} while the other two do not.

One important point in our algorithm of the finite-lattice method is that in the recursive definition of $\phi(l_x' \times l_y' \times l_z', \Delta N_z)$ with $l_x' \le l_x, l_y' \le l_y, l_z' \le l_z$, the common value of ΔN_z should be taken for all these lattices. It guarantees that the cancellation between the term in $\ln[Z(l_x \times l_y \times l_z)]$, which comes from the superposed bond configuration that can be embedded into the $l_x' \times l_y' \times l_z'$ sublattice, and the corresponding term in $\phi(l_x' \times l_y' \times l_z')$ in the right hand side of Eq. (7) will be kept in the right hand side of Eq. (9) by keeping or neglecting simultaneously the bond configuration for the partition function $Z(l_x \times l_y \times l_z)$, which can be embedded just into the $l_x' \times l_y' \times l_z'$ sublattice, and the same bond configuration for the partition function $Z(l_x' \times l_y' \times l_z')$.

The contribution of the bond configuration with $\{n_{zi}\}$ to the partition function of the finite size lattice can be calculated by the transfer matrix formalism as

$$Z(\{n_{zi}\}) = V_{0,j_1} t_z^{n_{z1}} V_{j_1,j_2} t_z^{n_{z2}} \cdots t_z^{n_{zl_z}} V_{j_{l_z},0}. \tag{11}$$

Here $V_{j_i,j_{i+1}}$ is the transfer matrix element with incoming n_{zi} spins and outgoing n_{zi+1} spins and the summations over the spin locations $j_1, j_2, \ldots$ of the $n_{z1}, n_{z2}, \ldots$ spins, respectively, are assumed in the right-hand side of Eq. (11). This transfer matrix element itself is the partition function in two dimensions with $n_{zi}+n_{zi+1}$ spins attached, which can be calculated to any order in t_x and t_y efficiently by the site-by-site construction [15,16]. The amount of the calculation for each transfer matrix element is proportional to the combinatorial factor $C((l_x+1)(l_y+1), n_{zi}+n_{zi+1})$, 2^{l_x}, and $l_x l_y$, which are the number of the cases for attaching the $n_{zi}+n_{zi+1}$ spins to the $(l_x+1)(l_y+1)$ sites, the number of states in site-by-site construction for the partition function of the Ising model in two dimensions, and the number of relevant bonds, respectively.

To obtain the series to order N in the isotropic model, we calculate the expansion series for each of the $\phi(l_x \times l_y \times l_z)$'s defined by Eq. (7) in the anisotropic model to order $t_x^{N_x} t_y^{N_y} t_z^{N_z}$ with $N_x+N_y+N_z=N$, using our algorithm described above, and set $t_x=t_y=t_z=t$ finally. When we use our algorithm for

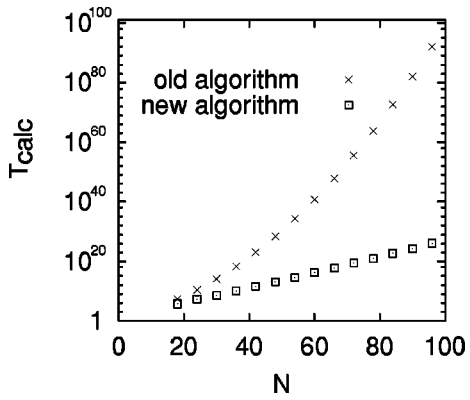

FIG. 2. Total amount of the calculation to generate the series to order N by the old algorithm and the new algorithm of the finite-lattice method.

each lattice size $l_x \times l_y \times l_z$ and each of the orders N_x, N_y, N_z, we can make the simultaneous exchange of the lattice axes and the corresponding orders as $(l_x \times l_y \times l_z; N_x, N_y, N_z) \rightarrow (l_x \times l_z \times l_y; N_x, N_z, N_y)$ or $(l_x \times l_y \times l_z; N_x, N_y, N_z) \rightarrow (l_y \times l_z \times l_x; N_y, N_z, N_x)$, which have the chance to reduce the amount of the calculation for the transfer matrix elements.

We estimate the total amount of the calculation time $T_{\mathrm{calc}}(N)$ to generate the free energy series to order N by listing up all the transfer matrices needed and summing up the estimated time to calculate each of the matrices, which is plotted in Fig. 2, together with the estimated total calculation time for the old algorithm of the finite-lattice method. The numerical estimation for the new algorithm agrees well with the actually used calculation time for $N \leqslant 46$. We see that the calculation time for the old algorithm grows exponentially with N^2, while that for the new algorithm can be fitted by $A \exp(BN \ln N + CN + D \ln N)$ with $B \sim 0.15$, $C \sim -0.24$, and $D \sim 3.6$. We can simply understand this $\exp(BN \ln N + \cdots)$ behavior as follows. The maximum size of the lattice to be taken into account is $l_x = l_y = l_z = N/6$, for which $\Delta N_z = 0$ and we have only to consider the bond configurations with $n_{zi} = 2$ for all $i = 1,2, \ldots, l_z$. The largest amount of the calculation is to be paid for the partition function of the lattice that has smaller size of $l_x \sim l_y \sim l_z \sim N/12$, for which the maximum of $n_{zi} + n_{zi+1}$ is about $N/6$ and the product of the above factors is $C((N/12)^2, N/6) 2^{N/12} (N/12)^2$, and it grows as $\exp(BN \ln N + CN + D \ln N)$ with $B = 1/6$ for large N.

IV. RESULT

Using our algorithm of the finite-lattice method, we have calculated the high-temperature series for the free energy density of the simple-cubic Ising model to order $N = 46$. The coefficients of the obtained series

$$f = 3 \cosh(\beta) + \sum_n a_n t^n; \quad t = \tanh(\beta) \tag{12}$$

are listed in Table I. They agree with those given by Bhanot *et al.* [5] to order $N = 24$ and by Guttmann and Enting [6] to order $N = 26$. We have added ten new terms to these previous series. To obtain the series of order $N = 26$ in our algorithm, we needed only the computer memory of 1 Mbytes and the CPU time of 5 min in a standard PC, and to order $N = 46$ we used the total memory of 2 Gbytes and the CPU time of 25 h in CP-PACS at Tsukuba University.

TABLE I. High-temperature expansion coefficients for the free energy density of the simple-cubic Ising model.

n	a_n
2	0
4	3
6	22
8	375/2
10	1980
12	240 44
14	319 170
16	180 590 31/4
18	201 010 408/3
20	516 228 363 3/5
22	163 970 407 50
24	266 958 797 382
26	443 759 665 054 8
28	525 549 581 866 326/7
30	644 828 436 349 120 2/5
32	179 577 198 475 709 847/8
34	395 251 648 062 268 272
36	210 936 621 888 205 205 21/3
38	126 225 408 651 399 082182
40	456 921 753 319 676 199 778 5/2
42	291 912 871 109 686 238 579 40/7
44	841 0722 262 379 235 048 686 604/11
46	141 203 142 047 137 197 668 882 10

Following is the result of the preliminary analysis of the series for the specific heat $C(t) = \Sigma_n c_n t^n$. We plot in Fig. 3, the critical exponent α versus the critical value β_c for the first-order inhomogeneous differential approximants [17] of the series of $N = 40$–46. From the linear dependence of α on β_c we find $\alpha = 0.1045(1)$ or $\alpha = 0.1077(2)$ at the value $\beta_c = 0.221\,654\,59(10)$ [18] or $\beta_c = 0.221\,659\,5(15)$ [19] ob-

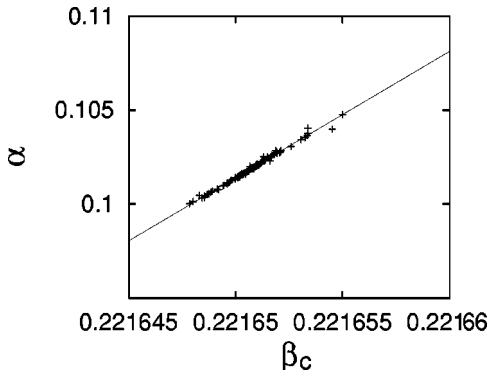

FIG. 3. Critical exponent α versus the critical value β_c for the inhomogeneous differential approximants of the first order.

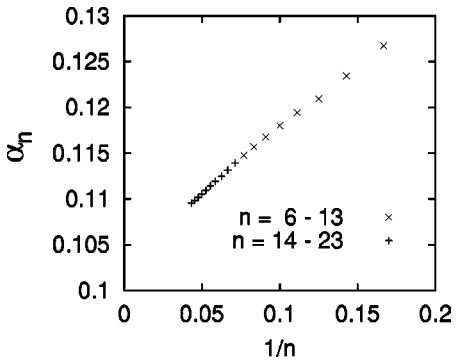

FIG. 4. Sequence α_n plotted versus $1/n$.

tained in the recent Monte Carlo simulations. The second-order inhomogeneous differential approximants give almost the same value. We also made the ratio analysis. The sequence $\alpha_n=(t_c^2 c_{2n}/c_{2n-2}-1)n+1$, which is expected to behave as $\alpha+b/n^{\Delta}+c/n+\cdots$ with the correction-to-scaling exponent $\Delta\sim 0.5$ [17], is plotted versus $1/n$ in Fig. 4 for $\beta_c=0.221\,654\,59$. The sequence for $n=14$–23 given by the new 10 coefficients has a bit different slope from the sequence for $n\leqslant 13$ given by the previously obtained series. The three-parameter fitting of the newly obtained sequence for $\beta_c=0.221\,654\,59$ gives $\alpha=0.1036(10)$, $b=-0.007(10)$, and $c=0.17(2)$ for $\Delta=0.5$. As for the case of $\beta_c=0.221\,659\,5$, it gives $\alpha=0.1082(14)$, $b=-0.033(10)$, and $c=0.21(2)$. These estimated values of α by the inhomogeneous differential approximation and by the ratio method are not inconsistent with each other. We see, on the other hand, that the estimated values of α depends crucially on the value of β_c, and in order to determine α precisely in these biased method we need more precise value of β_c. We also notice that the correction-to-scaling term is very small, which was already pointed out in the analysis of the shorter series [5,6].

From the hyperscaling relation $\alpha=2-d\nu$ the high-temperature series for the second moment correlation length gives $\alpha=0.1088(39)$ [20] and $\alpha=0.1096(5)$ [21], and the ϵ expansion gives $\alpha=0.1085(75)$ [22]. More direct estimation of $\alpha=0.110(2)$ was also given by the high-temperature series for the magnetic susceptibility of the antiferromagnetic critical point [21]. We note that our estimated value of α using $\beta_c=0.221\,654\,59$ is not consistent with these values (except for the value by the ϵ expansion), but the value using $\beta_c=0.221\,659\,5$ is rather closer to them.

V. SUMMARY

Our algorithm of the finite-lattice method has been given to generate long series of the high-temperature expansions for the Ising model in three dimensions. It drastically improves the computational efficiency of the finite-lattice method in three dimensions. The CPU time necessary to obtain the series to order β^N increases exponentially with $N\ln N$, while it increases exponentially with N^2 in the original version of the finite-lattice method. Our algorithm has been applied to the high-temperature expansion for the free energy of the simple-cubic Ising model, generating the series to order β^{46}, and it is much longer than those by the original version of the finite-lattice method and by the diagrammatic method.

The basic idea presented here in our algorithm of the finite-lattice method can be applied to the high-temperature expansion of other quantities such as the magnetic susceptibility and the correlation length for the Ising model in three dimensions, and it can also be applied to the models with continuous spin variables such as the XY model in three dimensions. Furthermore, the idea can be used in the low-temperature expansion for the spin models in three dimensions. We can expect that it will enable us to generate the expansion series in much higher orders compared with the presently available series.

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