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The critical two-dimensional Ising model is studied with four types boundary conditions: free, fixed ferromagnetic, fixed antiferromagnetic, and fixed double antiferromagnetic. Using bond propagation algorithms with surface fields, we obtain the free energy, internal energy, and specific heat numerically on square lattices with a square shape and various combinations of the four types of boundary conditions. The calculations are carried out on the square lattices with size $N \times N$ and $30 < N < 1000$. The numerical data are analyzed with finite-size scaling. The bulk, edge, and corner terms are extracted very accurately. The exact results are conjectured for the corner logarithmic term in the free energy, the edge logarithmic term in the internal energy, and the corner logarithmic term in the specific heat. The corner logarithmic terms in the free energy agree with the conformal field theory very well.

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I. INTRODUCTION

The two-dimensional Ising model is the best understood statistical model with a phase transition. It has been studied intensively since the work by Onsager [1–3]. Exact results of the model on finite sizes with various boundary conditions (BCs) have been studied [4–11]. Detailed knowledge has been obtained for the torus case [6,7], helical BCs [8], Brascamp-Kunz BCs [9–11], and an infinitely long cylinder [12]. The Ising model on the finite lattice plays an important role in the finite-size scaling [13,14], which finds extensive applications in the analysis of experimental, Monte Carlo, and transfer-matrix data, as well as in recent theoretical developments related to conformal invariance [15–17]. However, for the complete open BCs, i.e., with open edges and sharp corners, some interesting results have begun to appear in recent years [18–20]. In these works, the free BCs were studied. In this paper we consider the fixed BCs.

One of the methods to solve the two-dimensional Ising model with a free boundary is the bond propagation (BP) algorithm. It was developed to compute the partition function of the Ising model in two dimensions [21,22]. Subsequently, the BP algorithm for the internal energy and specific heat was developed [23]. It is so powerful that very large system sizes and very accurate numerical results can be reached. With this algorithm, the calculations have been carried out on square and triangular lattices with free boundaries [19,20,23]. The results of free energy, internal energy, and specific heat are surprisingly accurate to 10^{-26}. The exact edge and corner terms on the square lattice and triangular lattice with various shapes are conjectured.

Recently, one of the present authors developed the BP algorithm with a surface field [24], which is called the SFBP algorithm. We use the SFBP algorithm to study the two-dimensional Ising model with a fixed boundary. We have studied three types of fixed BCs: $\pm$ (ferromagnetic), a (antioferromagnetic), and b (double ferromagnetic), which are defined in Sec. II. The free BC is denoted by 0. We have carried out numerical calculations of the free energy, internal energy, and specific heat on the square lattice with a square shape. For each edge, we assign a type of BC. We present the results of ten BCs including $(++++)$ (where the four edges are assigned the $+$ type BC), $(aaaa)$, $(bbbb)$, $(+-+-)$, $(+0+0)$, $(+a+a)$, $(+b+b)$, $(a0a0)$, $(b0b0)$, and $(abab)$. The numerical calculations are carried out on the square lattices with size $N \times N$ and $30 < N < 1000$. The data points are more than 80. Through fitting the data, we get very accurate expansions of the free energy, internal energy, and specific heat. The corner logarithmic corrections in the free energy verify the conformal field theory (CFT) predictions [25–27]. The exact edge and corner logarithmic terms in the internal energy and specific heat are conjectured.

The accurate finite-size expansions at the critical point are helpful to the CFT and renormalization-group (RG) study of the boundary effects [28]. An interesting way to see the effect of the irrelevant operators is to compute the asymptotic expansion (in powers of L^{-1}) of the free energy and its derivatives with respect to the temperature at the critical point. In the corner terms of the free energy and in the edge and corner terms of the internal energy and specific heat, there are logarithmic corrections. The logarithmic terms are usually related to the singular part of the free energy [13]. Therefore, studying these logarithmic corrections is especially important.

Our paper is organized as follows. Since this paper is long, we first summarize our results in Sec. II. In Secs. III, IV, and V we present the fittings of the free-energy density, the internal energy, and the specific heat, respectively. Section VI summarizes our work.

II. CRITICAL TWO-DIMENSIONAL ISING MODEL WITH MIXED BOUNDARY CONDITIONS

Figure 1 shows some lattices with typical BCs. We have studied three types of fixed BCs. The first one is $+$ $(-)$

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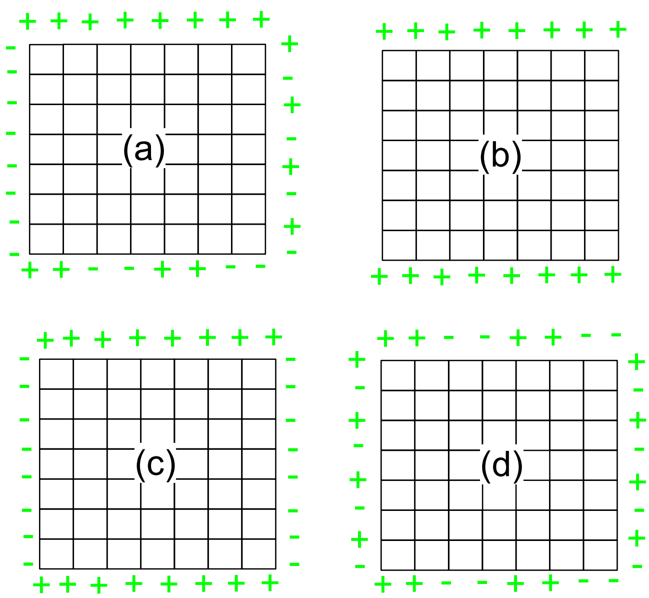

FIG. 1. (Color online) (a) The 8×8 lattice with BCs $(+ab-)$. (b) The 8×8 lattice with BCs $(+0+0)$. (c) The 8×8 lattice with BCs $(+-+-)$. (d) The 8×8 lattice with BCs $(baba)$.

type, where all the spins at the boundary are fixed to be positive (negative). We call it the ferromagnetic type. The second one is antiferromagnetic a type, where the spins at the boundary are fixed to be alternatively positive and negative. The third one is double antiferromagnetic b, where the spins at the boundary are fixed to be positive, positive, negative, and negative successively. Together with the free boundary (denoted by 0), we have four types of BCs. For a square, there are four edges; we denote the boundaries by $(\alpha_1,\alpha_2,\alpha_3,\alpha_4)$, where $\alpha_i = 0,+,-,a,b$. For example, as shown in Fig. 1(a), the BCs on the four edges are fixed to be $+$, a, b, and $-$ in proper order, respectively; then we denote the BCs by $(+ab-)$.

We study the Ising model with these BCs using SFBP algorithms [24]. The fixed BCs are realized in the SFBP algorithm in the following way. Consider an $(N+2)\times(N+2)$ lattice with coupling constant J between spins. If the bottom (the zeroth row of spins) is assigned to be a $+$ type boundary, it is equivalent to applying a field with an intensity of J to the first row of spins without the zeroth row of spins. If the boundary is type 0, the surface field on the first row is zero. If the boundary is type a, the surface fields on the first row of spins are $+J$ and $-J$ alternatively. If the boundary is type b, the surface field on the first row of spins is $+J$, $+J$ $-J$, and $-J$ successively. The other edges can be dealt with similarly. Then the $(N+2)\times(N+2)$ lattice with fixed BCs becomes an $N \times N$ lattice with a surface field. In other words, we can solve the Ising model with a surface field to study the fixed boundary. Consider the Ising model with a surface field

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - \sum_{i\in\Gamma} H_i\sigma_i, \tag{1}$$

where Γ is the boundary and the surface field is assigned according to the BCs, which is discussed above. We calculate the partition function

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}} \tag{2}$$

and then get the free-energy density

$$f = -\frac{\ln Z}{S}, \tag{3}$$

where $S = N^2$ is the number of spins. The internal energy density is defined by

$$u = -\frac{1}{S}\frac{\partial \ln Z}{\partial \beta} \tag{4}$$

and the specific heat per spin by

$$c = \frac{1}{S}\frac{\partial^2 \ln Z}{\partial \beta^2}. \tag{5}$$

We have calculated the free energy, internal energy, and specific heat at the critical point $\beta J = \beta_c J = \frac{1}{2}\ln(1+\sqrt{2})$ with various BCs. We only present the results with ten BCs including $(++++)$, $(aaaa)$, $(bbbb)$, $(+a+a)$, $(+-+-)$, $(+b+b)$, $(+0+0)$, $(abab)$, $(0a0a)$, and $(0b0b)$. In the first three cases the BCs of the four edges are the same, so we can get the edge term easily. In all these cases, the BCs for the four corners are the same, so we can get the corner term easily.

We find that the critical free-energy density can be expanded into

$$f = f_0 + \frac{f_s}{N} + \frac{f_c \ln N}{N^2} + \sum_{k=2}^{k_{\max}} \frac{f_k}{N^k}, \tag{6}$$

where the surface term $f_s = \sum_{i=1}^{4} f_{\rm surf}(\alpha_i)$ is the sum of the four edges' contribution and $\alpha_i = +,-,0,a,b$ denote the BCs of the ith edge; the corner term $f_c = \sum_{i=1}^{4} f_{\rm corn}(\alpha_i\beta_i)$ is the sum of the four corners' contribution and $\alpha_i\beta_i = +-,+0,+a,+b,\ldots$ denotes the BCs of the ith corner. For example, the contribution from a corner with two edges under BCs $+$ and 0 is denoted by $f_{\rm corn}(+0)$. We expand the free energy (the internal energy and specific heat in the next two sections) to as high an order as possible to make the deviation as small as possible. In all fittings of the free energy, we take $k_{\max} = 15$.

In our fittings we confirm the exact result given by Onsager [1], i.e.,

$$f_0 = -\ln\sqrt{2} - \frac{2}{\pi}G, \tag{7}$$

where $G = 1 - \frac{1}{3^2} + \frac{1}{5^2} - \frac{1}{7^2} + \cdots$. For the free BCs, the edge term $f_{\rm surf}(0)$ has been obtained in our previous work [19]. It is conjectured that

$$f_{\rm surf}(0) = \tfrac{1}{2}\left[\tfrac{1}{2}\ln(1+\sqrt{2}) - D_1\right], \tag{8}$$

where $D_1 = \int_0^{\pi} \ln[1+\sqrt{2}(1-\cos\theta)^{1/2}(3-\cos\theta)^{-1/2}]$. This is obtained by comparing our numerical result on the rectangle with the exact result on the cylinder by Au-Yang and Fisher [5].

In the fittings for the free-energy data, the other surface terms are given by

$$\begin{array}{cc} \alpha & f_{\rm surf}(\alpha) \\ \pm & -0.200\,695\,195\,538\,609\,403\,401\,008(3) \\ a & 0.058\,260\,180\,986\,743\,355\,740\,6(6) \\ b & 0.035\,973\,497\,122\,255\,346\,54(7). \end{array} \quad (9)$$

For $f_{\rm surf}(\pm)$ and $f_{\rm surf}(a)$, the following is satisfied:

$$f_{\rm surf}(\pm) + f_{\rm surf}(a) = \frac{1}{2}\ln(1+\sqrt{2}) - \frac{2}{\pi}G. \quad (10)$$

This is obtained by comparing the result on Brascamp-Kunz BCs [10], where the cylinder has an upper edge under + BCs and a bottom edge under a BCs.

The corner terms $f_{\rm corn}$ are very interesting because they are universal and logarithmic. Cardy and Peschel studied the free energy within CFT [16]. They predicted that a corner with an angle $\pi/2$ and two edges under free BCs gives rise to the term $-\frac{c}{16}\frac{\ln N}{N^2}$ in the free-energy expansion, where $c = 1/2$ is the central charge. That is to say, $f_{\rm corn}(00) = -\frac{1}{32}$. This was verified in our previous work on the square lattice and triangular lattice with free BCs [19,20]. Later on, Imamura *et al.* study the corner terms with different BCs within CFT [25–27]. According to their results, the contribution to the free energy from a corner with two edges under α and β BCs $f_{\rm corn}(\alpha\beta)$ is given by

$$f_{\rm corn}(\alpha\beta) = 2\lambda_{\alpha\beta} - \frac{c}{16}, \quad (11)$$

where $\lambda_{\alpha\beta}$ is the conformal weight of the boundary operator inserted at the corner and $c = 1/2$ is the central charge for the Ising model. There are three different conformal weights in the Ising model, namely, $\lambda_{\alpha\beta} = 0$, 1/16, and 1/2. There are also three different conformally invariant boundary conditions, generally denoted by +, −, and f [29], where the first two describe fixed boundary conditions on the spin $s = +1$ or -1, respectively, and f corresponds to free boundary conditions. When boundary conditions on both sides of the corner are the same ($\alpha = \beta$), the boundary operator is just the identity operator with $\lambda = 0$. In the case when the boundary condition on one side of the corner is $\alpha = +$ and on the other side it is $\beta = -$, the boundary operator has conformal weight $\lambda = 1/2$; in the case when the boundary condition on one side of the corner is $\alpha = +$ or − and on the other side it is $\beta = 0$, a, or b, the boundary operator has conformal weight $\lambda = 1/16$. We also get the result that when boundary conditions on both sides of the corner are 0, a, or b, the boundary operator has conformal weight $\lambda = 0$. Thus we have obtained that the boundary conditions 0, a, and b are all free conformally invariant boundary conditions. Then we have the table for $f_{\rm corn}(\alpha\beta)$,

$$\begin{array}{cccccc} & + & - & 0 & a & b \\ + & -\frac{1}{32} & \frac{31}{32} & \frac{3}{32} & \frac{3}{32} & \frac{3}{32} \\ - & & -\frac{1}{32} & \frac{3}{32} & \frac{3}{32} & \frac{3}{32} \\ 0 & & & -\frac{1}{32} & -\frac{1}{32} & -\frac{1}{32} \\ a & & & & -\frac{1}{32} & -\frac{1}{32} \\ b & & & & & -\frac{1}{32}, \end{array} \quad (12)$$

where the first column is α and the first row is β. It is obvious that $f_{\rm corn}(\alpha\beta) = f_{\rm corn}(\beta\alpha)$.

Our numerical results verify these predictions with very high accuracy. The detailed fittings of the numerical data are presented in Sec. III. As one can see, the BCs 0, a, and b play the same role in the corner terms. In CFT, these BCs belong to the same type indeed. However, they play different roles in the internal energy and specific heat, which are shown in the following. This is the reason why we study these three types of BCs 0, a, and b.

We find that the critical internal energy can be expanded into

$$u = u_0 + \frac{u_s \ln N}{N} + \frac{u_c \ln N}{N^2} + \sum_{k=1}^{\infty} \frac{u_k}{N^k}, \quad (13)$$

where the surface term $u_s = \sum_{i=1}^4 u_{\rm surf}(\alpha_i)$ is the sum of the four edges' contribution and the corner term $u_c = \sum_{i=1}^4 u_{\rm corn}(\alpha_i\beta_i)$ is the sum of the four corners' contribution. In the expansions, we confirm the exact result of the bulk value [1]

$$u_0 = -\sqrt{2}. \quad (14)$$

From the results with various BCs, the surface terms are conjectured and are given by

$$\begin{array}{ccccc} \alpha & \pm & 0 & a & b \\ u_{\rm surf}(\alpha) & -\frac{1}{\pi} & \frac{1}{\pi} & \frac{1}{\pi} & \frac{1}{\pi}. \end{array} \quad (15)$$

The corner terms $u_{\rm corn}(\alpha\beta)$ conjectured from the numerics are summarized in the expression

$$\begin{array}{ccccc} & \pm & 0 & a & b \\ \pm & -\frac{2+\sqrt{2}}{2\pi} & \frac{1}{2\pi} & \frac{\sqrt{2}}{2\pi} & \frac{5\sqrt{2}}{8\pi} \\ 0 & & \frac{\sqrt{2}}{2\pi} & \frac{1}{2\pi} & \frac{4-\sqrt{2}}{8\pi} \\ a & & & \frac{2-\sqrt{2}}{2\pi} & \frac{8-5\sqrt{2}}{8\pi} \\ b & & & & \frac{4-3\sqrt{2}}{4\pi}, \end{array} \quad (16)$$

where α is shown in the left column and β is shown in the first row. The corner term $u_{\rm corn}(+-)$ is given by

$$u_{\rm corn}(+-) = -\frac{2+\sqrt{2}}{2\pi}. \quad (17)$$

It should be noted that $u_{\rm corn}(+-) = u_{\rm corn}(++)$ as compared with $f_{\rm corn}(+-) \neq f_{\rm corn}(++)$. The detailed fittings of the numerical data and the extraction of these coefficients are presented in Sec. IV.

The critical specific heat can be expanded into

$$c = A_0 \ln N + D_0 + \frac{c_s \ln N}{N} + \frac{c_c \ln N}{N^2} + \sum_{k=1}^{\infty} \frac{c_k}{N^k}, \quad (18)$$

where the surface term $c_s = \sum_{i=1}^4 c_{\rm surf}(\alpha_i)$ is the sum of the four edges' contribution and the corner term $c_c = \sum_{i=1}^4 c_{\rm corn}(\alpha_i\beta_i)$ is the sum of the four corners' contribution. In the fittings, we confirm the Onsager's exact result [1]

$$A_0 = \frac{8}{\pi}. \quad (19)$$

The surface terms conjectured from the numerics are given by

$$\begin{array}{ccccc} \alpha & \pm & 0 & a & b \\ c_{\rm surf}(\alpha) & \frac{4+\sqrt{2}}{\pi} & \frac{3\sqrt{2}}{\pi} & \frac{4-\sqrt{2}}{\pi} & \frac{4-2\sqrt{2}}{\pi}. \end{array} \tag{20}$$

The corner terms $c_{\rm corn}(\alpha\beta)$ conjectured from the numerics are summarized in the expression

$$\begin{array}{ccccc} & \pm & 0 & a & b \\ \pm & \frac{3+\sqrt{2}}{\pi} & \frac{3\sqrt{2}}{2\pi} & \frac{1}{\pi} & \frac{1-\sqrt{2}}{2\pi} \\ 0 & & \frac{3}{\pi} & \frac{3\sqrt{2}}{2\pi} & \frac{3\sqrt{2}-1}{2\pi} \\ a & & & \frac{3-\sqrt{2}}{\pi} & \frac{7-3\sqrt{2}}{2\pi} \\ b & & & & \frac{17-8\sqrt{2}}{4\pi}, \end{array} \tag{21}$$

where α is shown in the left column and β is shown in the first row. The corner term $c_{\rm corn}(+-)$ is given by

$$c_{\rm corn}(+-) = \frac{3+\sqrt{2}}{\pi}. \tag{22}$$

It should be noted that $c_{\rm corn}(+-) = c_{\rm corn}(++)$ as compared with $f_{\rm corn}(+-) \neq f_{\rm corn}(++)$. The detailed fittings of the numerical data and the extraction of these coefficients are presented in Sec. V.

We also studied the more complicated BCs such as $(+0-0)$, $(+-00)$, and $(+a-a)$. All the results satisfy the expansion form in Eqs. (6), (13), and (18). That is to say, the edge term is just the sum over those coming from each edge and the corner term is just the sum over those coming from each corner. However, these results are not presented in this paper.

Let us to summarize the results and make some remarks.

(i) The edge and corner logarithmic terms are additive, for example, for the surface free energy $f_c = \sum_{i=1}^4 f_{\rm corn}(\alpha_i\beta_i)$.

(ii) There is only one logarithmic correction, the corner term, in the free energy. There are only two logarithmic corrections, the edge and corner terms, in the internal energy. There are only three logarithmic corrections, the leading term, the edge, and corner terms, in the specific heat. The logarithmic terms are usually related to the singular part of the free energy [13]. Therefore, our results are helpful in determining the singular part of the free energy, which plays a key role in the RG and scaling theories.

(iii) As we can see, the role of BCs 0, a, and b is the same in the corner terms for the free energy, but different in the internal energy and specific heat. In Ref. [28], using CFT and RG theory, the authors classify the possible irrelevant operators for the Ising model with periodic BCs. Now we can ask a similar question: For the BCs $\pm$, 0, a, and b, what boundary states exist? What irrelevant operators cause the differences in the internal energy and specific heat for these BCs? These questions need to be answered by future work in CFT and RG theory.

III. CRITICAL FREE-ENERGY DENSITY

In the numerical calculation for all cases, the number of data points is more than 80 and the fitting interval of sizes is $30 < N < 1000$. For the BCs $(aaaa)$, $(+a+a)$, and $(a0a0)$, the lattice size is assigned to be $N = 2m$, where m is an integer considering the unit length is 2 for the a type boundary. For the BCs $(bbbb)$, $(+b+b)$, $(abab)$, and $(b0b0)$, the lattice size is assigned to be $N = 4m$ considering the unit length is 4 for the b type boundary. All the tables are given in Ref. [30].

To characterize the accuracy of our fittings, we define the maximal deviation

$$\delta_{\max} = \max\left|y_i - y_i^{\rm fit}\right|, \tag{23}$$

where y_i is the numerical data and $y_i^{\rm fit}$ is the value given by the fitting formula. We choose the maximum of the deviations from the data to the fitted ones to represent our fitting quality. We expand the the free energy, internal energy, and specific heat to as high an order as possible to make the $\delta_{\max}$ as small as possible. In every table of the fitting parameters, we give the maximum deviation. For example, in Table 1, $\delta_{\max} = 10^{-29}$. We list 30 digits for these results for the convenience of readers who may want to check other functional forms for the size dependence of the free energy.

The free-energy density is fitted with the formula

$$f = f_0 + \frac{f_s}{N} + \frac{f_c \ln N}{N^2} + \sum_{k=2}^{k_{\max}} \frac{f_k}{N^k}, \tag{24}$$

where $f_s = \sum_{i=1}^4 f_{\rm surf}(\alpha_i)$ is the sum of the four edges' contribution and $f_c = \sum_{i=1}^4 f_{\rm corn}(\alpha_i\beta_i)$ is the sum of the four corners' contribution. In all fittings of the free energy, we take $k_{\max} = 15$.

The bulk term is known from Onsager's exact result [1]

$$\begin{aligned} f_0 &= -\ln\sqrt{2} - \frac{2}{\pi}G \\ &= -0.929\,695\,398\,341\,610\,214\,985\,384\,973\,6\ldots, \end{aligned} \tag{25}$$

where $G = 1 - \frac{1}{3^2} + \frac{1}{5^2} - \frac{1}{7^2} + \cdots$. This bulk term can be the benchmark for our numerical results.

For the BCs $(++++)$ as shown in Table 1, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-27}. Assuming that the surface term is $f_s = 4f_{\rm surf}(+)$, we get

$$f_{\rm surf}(+) = -0.200\,695\,195\,538\,609\,403\,401\,008(3). \tag{26}$$

Similarly assuming that the corner term $f_c = 4f_{\rm corn}(++)$, we find that

$$f_{\rm corn}(++) = -\tfrac{1}{32} \tag{27}$$

is satisfied to an accuracy on the order of 10^{-20}. This agrees with the CFT discussion in Eq. (12).

The BCs (0000) have been studied in previous work [20,23]. The surface term is given by

$$\begin{aligned} f_{\rm surf}(0) &= \tfrac{1}{2}\left[\tfrac{1}{2}\ln(1+\sqrt{2}) - D_1\right] \\ &= 0.090\,865\,708\,492\,209\,378\,45\ldots. \end{aligned} \tag{28}$$

The corner term $f_{\rm corn}(00)$ has been studied in previous work [20] and is given by

$$f_{\rm corn}(00) = -\tfrac{1}{32}, \tag{29}$$

which is predicted by CFT [16].

From Table 2 for the BCs $(aaaa)$, assuming that $f_s = 4f_{\rm surf}(a)$, we get

$$f_{\rm surf}(a) = 0.058\,260\,180\,986\,743\,355\,740\,6(6). \tag{30}$$

In the exact result of an infinitely long strip with Brascamp-Kunz BCs, the edge term from the two edges in the expansion of the free-energy density is $f_1 = \frac{1}{2}\ln(1+\sqrt{2}) - \frac{2}{\pi}G$ [10]. The Brascamp-Kunz BCs are periodic in the x direction; in the y direction, the spins are up $(+1)$ along the upper border of the resulting cylinder and have alternative values along the lower border of the resulting cylinder. In our terminology, Brascamp-Kunz BCs are that the upper border has + BCs and the lower border has a BCs. Then it should have $f_1 = f_{\rm surf}(+) + f_{\rm surf}(a)$. From the above two equations, we find that it is satisfied indeed:

$$\begin{aligned} f_{\rm surf}(+) + f_{\rm surf}(a) &= -0.142\,435\,014\,551\,866\,047\,660\,4(6) \\ &\approx \frac{1}{2}\ln(1+\sqrt{2}) - \frac{2}{\pi}G \\ &= -0.142\,435\,014\,551\,866\,047\,660\,464\,2\ldots. \end{aligned} \quad (31)$$

In Ref. [10] the two borders are dealt with together. From our results, one can see that they can be dealt with separately.

For the BCs shown in Table 2, from the corner term f_c we get

$$f_{\rm corn}(aa) = -\tfrac{1}{32}, \quad (32)$$

where we assume $f_c = 4f_{\rm corn}(aa)$. The corner term f_c in Table 2 satisfies this equation to an accuracy on the order of 10^{-19}. This also agrees with the CFT discussion in Eq. (12).

From Table 3 for the BCs $(bbbb)$, assuming that $f_s = 4f_{\rm surf}(b)$, we get

$$f_{\rm surf}(b) = 0.035\,973\,497\,122\,255\,346\,54(7). \quad (33)$$

Assuming $f_c = 4f_{\rm corn}(bb)$, f_c satisfies

$$f_{\rm corn}(+-) = \tfrac{31}{32} \quad (34)$$

to an accuracy on the order of 10^{-16}. This agrees with the CFT result in Eq. (12).

In order to investigate the corner terms for two edges under different BCs, we also studied the BCs $(+-+-)$, $(+0+0)$, $(+a+a)$, $(+b+b)$, $(a0a0)$, $(b0b0)$, and $(abab)$. The parameters of the fitting of the free-energy density for these BCs are shown in Tables 4–10, respectively.

For the BCs $(+-+-)$ as shown in Table 4, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-23}. For the surface term, due the symmetry, it should have

$$f_{\rm surf}(-) = f_{\rm surf}(+). \quad (35)$$

On the one hand, the surface term value in Table 4 satisfies $f_s \approx 4f_{\rm surf}(+)$ [see Eq. (26)]. On the other hand, it should have $f_s = 2f_{\rm surf}(+) + 2f_{\rm surf}(-)$ for the BCs $(+-+-)$. Therefore, we have verified that $f_{\rm surf}(+) = f_{\rm surf}(-)$ in this case. For the corner term, assuming $f_c = 4f_{\rm corn}(+-)$, we get

$$f_{\rm corn}(+-) = \tfrac{31}{32} \quad (36)$$

to an accuracy on the order of 10^{-16}. This agrees with the CFT result in Eq. (12).

For the BCs $(+0+0)$ as shown in Table 5, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-26}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(+) + f_{\rm surf}(0)]$ [see Eqs. (26) and (28)]. Assuming $f_c = 4f_{\rm corn}(+0)$, f_c satisfies

$$f_{\rm corn}(+0) = \tfrac{3}{32} \quad (37)$$

to an accuracy on the order of 10^{-19}. This agrees with the CFT discussion in Eq. (12).

For the BCs $(+a+a)$ as shown in Table 6, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-26}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(+) + f_{\rm surf}(a)]$ [see Eqs. (26) and (30)]. Assuming $f_c = 4f_{\rm corn}(+a)$, f_c satisfies

$$f_{\rm corn}(+a) = \tfrac{3}{32} \quad (38)$$

to an accuracy on the order of 10^{-19}. This agrees with the CFT result in Eq. (12).

For the BCs $(+b+b)$ as shown in Table 7, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-24}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(+) + f_{\rm surf}(b)]$ [see Eqs. (26) and (33)]. From the corner term f_c we get

$$f_{\rm corn}(+b) = \tfrac{3}{32}, \quad (39)$$

assuming $f_c = 4f_{\rm corn}(+b)$. This agrees with the CFT discussion in Eq. (12). The f_c in Table IV coincides this value to an accuracy on the order of 10^{-17}.

For the BCs $(a0a0)$ as shown in Table 8, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-26}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(a) + f_{\rm surf}(0)]$ [see Eqs. (30) and (28)]. Assuming $f_c = 4f_{\rm corn}(a0)$, f_c satisfies

$$f_{\rm corn}(a0) = -\tfrac{1}{32} \quad (40)$$

to an accuracy on the order of 10^{-16}. This agrees with the CFT discussion in Eq. (12).

For the BCs $(b0b0)$ as shown in Table 9, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-23}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(b) + f_{\rm surf}(0)]$ [see Eqs. (33) and (28)]. Assuming $f_c = 4f_{\rm corn}(b0)$, f_c satisfies

$$f_{\rm corn}(b0) = -\tfrac{1}{32} \quad (41)$$

to an accuracy on the order of 10^{-16}. This also agrees with the CFT result in Eq. (12).

For the BCs $(abab)$ as shown in Table 10, the f_0 agree with the exact result in Eq. (25) to an accuracy on the order of 10^{-23}. The surface term satisfies $f_s \approx 2[f_{\rm surf}(a) + f_{\rm surf}(b)]$ [see Eqs. (30) and (33)]. Assuming $f_c = 4f_{\rm corn}(ab)$, f_c satisfies

$$f_{\rm corn}(ab) = -\tfrac{1}{32} \quad (42)$$

to an accuracy on the order of 10^{-16}. This agrees with the CFT result in Eq. (12).

As we can see, for the corner terms that are universal, the BCs a and b behave just like 0 (the free boundary). These boundary conditions flow to free BCs under boundary renormalization flow.

IV. CRITICAL INTERNAL ENERGY DENSITY

We find that the critical internal energy can be expanded into

$$u = u_0 + u_{\rm surf}\frac{\ln N}{N} + u_{\rm corn}\frac{\ln N}{N^2} + \sum_{k=1}^{\infty}\frac{B_k}{N^k}, \quad (43)$$

where the surface term $u_s = \sum_{i=1}^{4} u_{\rm surf}(\alpha_i)$ is the sum of the four edges' contribution and the corner term $u_c = \sum_{i=1}^{4} u_{\rm corn}(\alpha_i\beta_i)$ is the sum of the four corners' contribution. All BCs should have the same bulk internal energy u_0, which is obtained in Onsager's exact solution [1]

$$u_0 = -\sqrt{2} = -1.414\,213\,562\,373\,095\,048\,801\,688\,72\ldots. \tag{44}$$

This is the benchmark for our fittings.

For the free BCs (0000), the edge terms $u_{\rm surf}(0)$ and $U_{\rm corn}(0)$ have been obtained in previous work [19]. According to the definition of this paper, they are given by

$$u_{\rm surf}(0) = \frac{1}{\pi} \tag{45}$$

and

$$u_{\rm corn}(00) = \frac{\sqrt{2}}{2\pi}. \tag{46}$$

For the BCs (++++), the fitting parameters are shown in Table 11. We confirm the exact result for the bulk internal energy density to an accuracy on the order of 10^{-25}. Assuming $u_s = 4u_{\rm surf}(+)$, we conjecture that

$$u_{\rm surf}(+) = -\frac{1}{\pi}. \tag{47}$$

The corner term u_s in Table 11 agrees with this conjecture to an accuracy on the order of 10^{-21}. For the corner term, assuming $u_c = 4u_{\rm corn}(++)$, we conjecture that

$$u_{\rm corn}(++) = -\frac{2+\sqrt{2}}{2\pi}. \tag{48}$$

This is valid to an accuracy on the order of 10^{-18}.

Table 12 is for the BCs ($aaaa$). The fitted bulk term u_0 confirms the exact result to an accuracy on the order of 10^{-25}. Assuming $u_s = 4u_{\rm surf}(a)$, we conjecture that

$$u_{\rm surf}(a) = \frac{1}{\pi}. \tag{49}$$

The corner term u_s in Table 12 agrees with this conjecture to an accuracy on the order of 10^{-21}. For the corner term, assuming $u_c = 4u_{\rm corn}(aa)$, we conjecture that

$$u_{\rm corn}(aa) = \frac{2-\sqrt{2}}{2\pi}. \tag{50}$$

This is valid to an accuracy on the order of 10^{-18} (see Table 12).

Table 13 is for the BCs ($bbbb$). The fitted bulk term u_0 confirms the exact result for the bulk internal energy density to an accuracy on the order of 10^{-22}. Assuming $u_s = 4u_{\rm surf}(b)$, we conjecture that

$$u_{\rm surf}(b) = \frac{1}{\pi}. \tag{51}$$

The corner term u_s in Table 13 agrees with this conjecture to an accuracy on the order of 10^{-18}. For the corner term, assuming $u_c = 4u_{\rm corn}(bb)$, we conjecture that

$$u_{\rm corn}(bb) = \frac{4-3\sqrt{2}}{4\pi}. \tag{52}$$

This is valid to an accuracy on the order of 10^{-15} (see Table 13).

As shown in Table 14 for BCs (+−+−), we confirm the exact result for the bulk internal energy density to an accuracy on the order of 10^{-21}. Assuming $u_s = 2u_{\rm surf}(+) + 2u_{\rm surf}(-)$ and using Eq. (47), we get

$$u_{\rm surf}(-) = -\frac{1}{\pi} \tag{53}$$

to an accuracy on the order of 10^{-17}. The symmetry requires that $u_{\rm surf}(-) = u_{\rm surf}(+)$. The edge term u_s in Table 14 agrees with this conjecture to an accuracy on the order of 10^{-17}.

For the corner term, assuming $u_c = 4u_{\rm corn}(+-)$, we conjecture that

$$u_{\rm corn}(+-) = -\frac{2+\sqrt{2}}{2\pi} = u_{\rm corn}(++). \tag{54}$$

This is valid to an accuracy on the order of 10^{-14}.

Table 15 is for the BCs (+0+0). The fitted bulk term u_0 agrees with the exact result to an accuracy on the order of 10^{-25}. Assuming $u_s = 2u_{\rm surf}(+) + 2u_{\rm surf}(0)$, we should have $u_s = 0$ following Eqs. (47) and (45). The surface term in Table 15 $|u_s| < 10^{-20}$ is nearly zero. For the corner term, assuming $u_c = 4u_{\rm corn}(+0)$, we conjecture that

$$u_{\rm corn}(+0) = \frac{1}{2\pi}. \tag{55}$$

This is valid to an accuracy on the order of 10^{-18} (see Table 15).

Table 16 is for the BCs ($+a+a$). The fitted bulk term u_0 agrees with the exact result $u_0 = \sqrt{2}$ to an accuracy on the order of 10^{-25}. Assuming $u_s = 2u_{\rm surf}(+) + 2u_{\rm surf}(a)$, we should have $u_s = 0$ following Eqs. (47) and (51). The surface term in Table 16 $|u_s| < 10^{-20}$ is nearly zero indeed. For the corner term, assuming $u_c = 4u_{\rm corn}(+a)$, we conjecture that

$$u_{\rm corn}(+a) = \frac{\sqrt{2}}{2\pi}. \tag{56}$$

This is valid to an accuracy on the order of 10^{-15} (see Table 16).

Table 17 is for the BCs ($+b+b$). The fitted bulk term u_0 agrees with the exact result $u_0 = \sqrt{2}$ to an accuracy on the order of 10^{-22}. Assuming $u_s = 2u_{\rm surf}(+) + 2u_{\rm surf}(b)$, we should have $u_s = 0$ following Eqs. (47) and (51). The surface term in Table 17 $|u_s| < 10^{-17}$ is nearly zero. For the corner term, assuming $u_c = 4u_{\rm corn}(+a)$, we conjecture that

$$u_{\rm corn}(+b) = \frac{5\sqrt{2}}{8\pi}. \tag{57}$$

This is valid to an accuracy on the order of 10^{-15} (see Table 17).

Table 18 is for the BCs ($a0a0$). The fitted bulk term u_0 agrees with the exact result $u_0 = \sqrt{2}$ to an accuracy on the order of 10^{-25}. Assuming $u_s = 2u_{\rm surf}(0) + 2u_{\rm surf}(a)$, we should have $u_s = 4/\pi$ following Eqs. (49) and (45). For the corner term, assuming $u_c = 4u_{\rm corn}(a0)$, we conjecture that

$$u_{\rm corn}(a0) = \frac{1}{2\pi}. \tag{58}$$

This is valid to an accuracy on the order of 10^{-18} (see Table 18).

Table 19 is for the BCs ($b0b0$). The fitted bulk term u_0 agrees with the exact result $u_0 = \sqrt{2}$ to an accuracy on the order of 10^{-21}. Assuming $u_s = 2u_{\text{surf}}(0) + 2u_{\text{surf}}(b)$, we should have $u_s = 4/\pi$ following Eq. (51) and (45). For the corner term, assuming $u_c = 4u_{\text{corn}}(b0)$, we conjecture that

$$u_{\text{corn}}(b0) = \frac{4-\sqrt{2}}{8\pi}. \tag{59}$$

This is valid to an accuracy on the order of 10^{-14} (see Table 19).

Table 20 is for the BCs $(abab)$. The fitted bulk term u_0 agrees with the exact result $u_0 = \sqrt{2}$ to an accuracy on the order of 10^{-22}. Assuming $u_s = 2u_{\text{surf}}(a) + 2u_{\text{surf}}(b)$, we should have $u_s = 4/\pi$ following Eqs. (51) and (49). For the corner term, assuming $u_c = 4u_{\text{corn}}(ab)$, we conjecture that

$$u_{\text{corn}}(ab) = \frac{8-5\sqrt{2}}{8\pi}. \tag{60}$$

This is valid to an accuracy on the order of 10^{-15} (see Table 20).

It is worth mentioning an interesting case in which the BCs are $(++00)$. There is no finite-size correction in the internal energy. The internal energy density is equal to $-\sqrt{2}$ to an accuracy on the order of 10^{-28} for $30 < N < 1000$ in the numerical results. According to the discussion above, the edge and corner terms are expected to cancel. It is surprising that the corrections at every order cancel. This is similar to the cylinder with Brascamp-Kunz BCs [10] in which the critical internal energy density is exactly $-\sqrt{2}$.

One can show that this is an exact result. At first one can show that a lattice with $(++00)$ BCs is self-dual. In Fig. 2 we use a 3×3 lattice to explain why such a lattice is self-dual. In the first step, one connects all sites on the boundaries with fixed spins to additional points. In the second step one constructs in the usual way a dual lattice. To the faces of the lattice one should assign the sites of the dual lattice (note that there is also one face outside the lattice) and two sites of the dual lattice that are separated by the bond of the original lattice should be connected by the bond of the dual lattice. The sites of the dual lattice are denoted by open cycles and the bonds by dashed lines. Finally, one arrives at the same lattice. Since this lattice is self-dual, then one can take the derivative over βJ from the duality relation [31] and obtain that $u = -\coth(2\beta_c J) = -\sqrt{2}$.

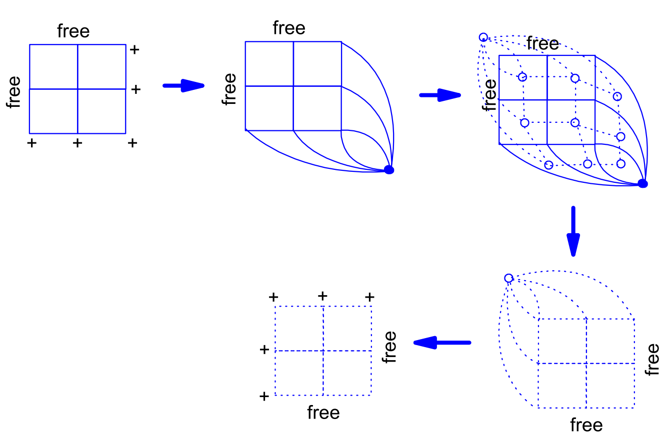

FIG. 2. (Color online) Self-duality of the 3×3 lattice with $(++00)$ BCs.

V. CRITICAL SPECIFIC HEAT

The critical specific heat can be expanded into

$$c = A_0 \ln N + D_0 + c_{\text{surf}}\frac{\ln N}{N} + c_{\text{corn}}\frac{\ln S}{S} + \sum_{k=1}^{\infty}\frac{c_k}{N^k}, \tag{61}$$

where the surface term $c_s = \sum_{i=1}^{4} c_{\text{surf}}(\alpha_i)$ is the sum of the four edges' contribution and the corner term $c_c = \sum_{i=1}^{4} c_{\text{corn}}(\alpha_i\beta_i)$ is the sum of the four corners' contribution. The exact value of A_0 is known from Onsager's solution [1]

$$A_0 = \frac{8}{\pi} = 2.546\,479\,089\,470\,325\,372\,302\,140\ldots. \tag{62}$$

This is the benchmark of our fittings.

Table 21 is for the BCs $(++++)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-23}. Assuming $c_s = 4c_{\text{surf}}(+)$, we conjecture that

$$c_{\text{surf}}(+) = \frac{4+\sqrt{2}}{\pi}. \tag{63}$$

The surface term in Table 21 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\text{corn}}(++)$, we conjecture that

$$c_{\text{corn}}(++) = \frac{3+\sqrt{2}}{\pi}. \tag{64}$$

This is valid to an accuracy on the order of 10^{-16} (see Table 21).

The specific heat for the boundary conditions (0000) has been studied in Ref. [23]. According to the definition of the present paper, the surface term is given by

$$c_{\text{surf}}(0) = \frac{3\sqrt{2}}{\pi} \tag{65}$$

and the corner term is given by

$$c_{\text{corn}}(00) = \frac{3}{\pi}. \tag{66}$$

Table 22 is for the BCs $(aaaa)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-22}. Assuming $c_s = 4c_{\text{surf}}(a)$, we conjecture that

$$c_{\text{surf}}(a) = \frac{4-\sqrt{2}}{\pi}. \tag{67}$$

The surface term in Table 22 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\text{corn}}(aa)$, we conjecture that

$$c_{\text{corn}}(aa) = \frac{3-\sqrt{2}}{\pi}. \tag{68}$$

This is valid to an accuracy on the order of 10^{-16} (see Table 22).

Table 23 is for the BCs $(bbbb)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-19}. Assuming $c_s = 4c_{\text{surf}}(b)$, we conjecture that

$$c_{\text{surf}}(b) = \frac{4-2\sqrt{2}}{\pi}. \tag{69}$$

The surface term in Table 23 agrees with this conjecture to an accuracy on the order of 10^{-15}. For the corner term, assuming

$c_c = 4c_{\rm corn}(bb)$, we conjecture that

$$c_{\rm corn}(bb) = \frac{17 - 8\sqrt{2}}{4\pi}. \quad (70)$$

This is valid to an accuracy on the order of 10^{-12} (see Table 23).

Table 24 is for the BCs $(+-+-)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-23}. Assuming $c_s = 2c_{\rm surf}(+) + 2c_{\rm surf}(-)$ and $c_{\rm surf}(-) = c_{\rm surf}(+)$, we have $c_s = 4(4 + \sqrt{2})/\pi$ following Eq. (63). The surface term in Table 24 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\rm corn}(+-)$, we conjecture that

$$c_{\rm corn}(+-) = \frac{3 + \sqrt{2}}{\pi}. \quad (71)$$

This is valid to an accuracy on the order of 10^{-16} (see Table 24).

Table 25 is for the BCs $(+0+0)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-23}. Assuming $c_s = 2c_{\rm surf}(+) + 2c_{\rm surf}(0)$, we should have $c_s = 8(1 + \sqrt{2})/\pi$ following Eqs. (63) and (65). The surface term in Table 25 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\rm corn}(+0)$, we conjecture that

$$c_{\rm corn}(+0) = \frac{3\sqrt{2}}{2\pi}. \quad (72)$$

This is valid to an accuracy on the order of 10^{-16} (see Table 25).

Table 26 is for the BCs $(+a+a)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-23}. Assuming $c_s = 2c_{\rm surf}(+) + 2c_{\rm surf}(a)$, we should have $c_s = 16/\pi$ following Eqs. (63) and (67). The surface term in Table 26 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\rm corn}(+a)$, we conjecture that

$$c_{\rm corn}(+a) = \frac{1}{\pi}. \quad (73)$$

This is valid to an accuracy on the order of 10^{-16} (see Table 26).

Table 27 is for the BCs $(+b+b)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-20}. Assuming $c_s = 2c_{\rm surf}(+) + 2c_{\rm surf}(b)$, we should have $c_s = 2(8 - \sqrt{2})/\pi$ following Eqs. (63) and (69). The surface term in Table 27 agrees with this conjecture to an accuracy on the order of 10^{-16}. For the corner term, assuming $c_c = 4c_{\rm corn}(+b)$, we conjecture that

$$c_{\rm corn}(+b) = \frac{1 - \sqrt{2}}{2\pi}. \quad (74)$$

This is valid to an accuracy on the order of 10^{-13} (see Table 27).

Table 28 is for the BCs $(a0a0)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-23}. Assuming $c_s = 2c_{\rm surf}(a) + 2c_{\rm surf}(0)$, we should have $c_s = 2(4 + 2\sqrt{2})/\pi$ following Eqs. (65) and (67). The surface term in Table 28 agrees with this conjecture to an accuracy on the order of 10^{-19}. For the corner term, assuming $c_c = 4c_{\rm corn}(a0)$, we conjecture that

$$c_{\rm corn}(a0) = \frac{3\sqrt{2}}{2\pi}. \quad (75)$$

This is valid to an accuracy on the order of 10^{-16} (see Table 28).

Table 29 is for the BCs $(b0b0)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-19}. Assuming $c_s = 2c_{\rm surf}(b) + 2c_{\rm surf}(0)$, we should have $c_s = 2(4 + \sqrt{2})/\pi$ following Eqs. (65) and (69). The surface term in Table 29 agrees with this conjecture to an accuracy on the order of 10^{-15}. For the corner term, assuming $c_c = 4c_{\rm corn}(b0)$, we conjecture that

$$c_{\rm corn}(b0) = \frac{3\sqrt{2} - 1}{2\pi}. \quad (76)$$

This is valid to an accuracy on the order of 10^{-12} (see Table 29).

Table 30 is for the BCs $(abab)$. The fitted bulk term A_0 agrees with the exact result to an accuracy on the order of 10^{-19}. Assuming $c_s = 2c_{\rm surf}(b) + 2c_{\rm surf}(a)$, we should have $c_s = 2(8 - 3\sqrt{2})/\pi$ following Eqs. (67) and (69). The surface term in Table 30 agrees with this conjecture to an accuracy on the order of 10^{-15}. For the corner term, assuming $c_c = 4c_{\rm corn}(ab)$, we conjecture that

$$c_{\rm corn}(ab) = \frac{7 - 3\sqrt{2}}{2\pi}. \quad (77)$$

This is valid to an accuracy on the order of 10^{-12} (see Table 30).

For the constant term D_0, we have

$$D_0 \approx 2.939\,093\,476\,724\,904\,2 \quad (78)$$

for the BCs $(++++)$, $(aaaa)$, $(bbbb)$, $(a0a0)$, $(b0b0)$, and $(abab)$;

$$D_0 \approx 2.079\,572\,636\,155\,318\,549 \quad (79)$$

for $(+0+0)$, $(+a+a)$, and $(+b+b)$; and

$$D_0 \approx 4.927\,274\,829\,992\,747\,027\,120 \quad (80)$$

for $(+-+-)$. This indicates that the BCs 0, a, and b belong to the same type in this term.

We do not know of any conformal field predictions for the specific heat for the open boundaries. The discussion of the specific heat in terms of CFT and RG theory should be very interesting and is left for future work.

VI. CONCLUSION

We have studied the critical free energy, internal energy, and specific heat on square lattices with different fixed boundaries. Due to the extraordinarily high accuracy, we have conjectured all the exact edge and corner logarithmic corrections. These results indicate that the Ising model with fixed boundary conditions may have analytical solutions.

For convenience, we studied only the square shape because our emphasis is the edge and corner logarithmic corrections. To study the geometry's effect, one should study different aspect ratios (of the horizontal size and the vertical size). In previous work [19,20,23], the logarithmic corrections were geometry independent for the Ising model with free BCs. We did not studied the geometry's effects for the BCs in this paper.

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