

Exact finite-size corrections for the square-lattice Ising model with Brascamp-Kunz boundary conditions

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Finite-size scaling, finite-size corrections, and boundary effects for critical systems have attracted much attention in recent years. Here we derive exact finite-size corrections for the free energy F and the specific heat C of the critical ferromagnetic Ising model on the $\mathcal{M} \times 2\mathcal{N}$ square lattice with Brascamp-Kunz (BK) boundary conditions [J. Math. Phys. **15**, 66 (1974)] and compare such results with those under toroidal boundary conditions. When the ratio $\xi/2 = (\mathcal{M} + 1)/2\mathcal{N}$ is smaller than 1 the behaviors of finite-size corrections for C are quite different for BK and toroidal boundary conditions; when $\ln(\xi/2)$ is larger than 3, finite-size corrections for C in two boundary conditions approach the same values. In the limit $\mathcal{N} \rightarrow \infty$ we obtain the expansion of the free energy for infinitely long strip with BK boundary conditions. Our results are consistent with the conformal field theory prediction for the mixed boundary conditions by Cardy [Nucl. Phys. **B 275**, 200 (1986)] although the definitions of boundary conditions in two cases are different in one side of the long strip.

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I. INTRODUCTION

In the study of phase transitions and critical phenomena, it is extremely important to understand finite-size corrections to thermodynamical quantities. In experiments and in numerical studies of model systems, it is essential to take into account finite-size effects in order to extract correct infinite-volume predictions from the data. Finite-size scaling [1–3] concerns the critical behavior of systems in which one or more directions are finite, even though microscopically large, it is valuable in the analysis of experimental and numerical data in many situations, for example, for films of finite thickness. As soon as one has a finite system one must consider the question of boundary conditions on the outer surfaces or “walls” of the system. The systems under various boundary conditions have the same per-site free energy, internal energy, specific heat, etc., in the bulk limit, whereas the finite-size corrections are different. To understand the effects of boundary conditions on finite-size scaling and finite-size corrections, it is valuable to study model systems, such as percolation model [4] and the Ising model [5–9]. Therefore, in recent decades there have been many investigations on finite-size scaling, finite-size corrections, and boundary effects for critical model systems [10–21]. Of particular importance in such studies are exact results where the analysis can be carried out without numerical errors.

The Ising model has exact solutions on finite lattices with many kinds of boundary conditions, including cylindrical [5], toroidal [6–8], and Mobius strip and Klein bottle [16]. This class also includes the special boundary conditions introduced by Brascamp and Kunz [9]. The calculation of the exact partition function of the two-dimensional Ising model in the zero field wrapped on the cylinder was performed by Onsager in 1944 [5]. Exploiting the exactly known partition function of the two-dimensional Ising model on finite

$M \times N$ square lattice with toroidal boundary conditions [6], Ferdinand and Fisher [7] computed the finite-size corrections to the free energy, the internal energy, and the specific heat up to order N^{-1} . Recently, there has been much effort in understanding the behavior of finite-size corrections of the free energy, internal energy, and specific heat. Izmailian and Hu [15] and Salas [17] extended the results of [7] for the free energy and the internal energy up to order N^{-5} and for the specific heat up to order N^{-3} . Lu and Wu [16] obtained expressions for the partition function of the Ising model on a quadratic lattice embedded on a Mobius strip and a Klein bottle. They find finite-size corrections for free energy to order N^{-1} . Brascamp and Kunz [9] calculated the partition function of the Ising model on the $M \times 2N$ square lattice for special boundary conditions shown in Fig. 1. Recently Janke and Kenna [19] have calculated the finite-size corrections of the specific heat for this boundary condition up to M^{-3} order. Very recently, Ivashkevich, Izmailian, and Hu [20] provided a systematic method to compute finite-size corrections to the partition function and their derivatives of the Ising model on torus. Their approach is based on an intimate rela-

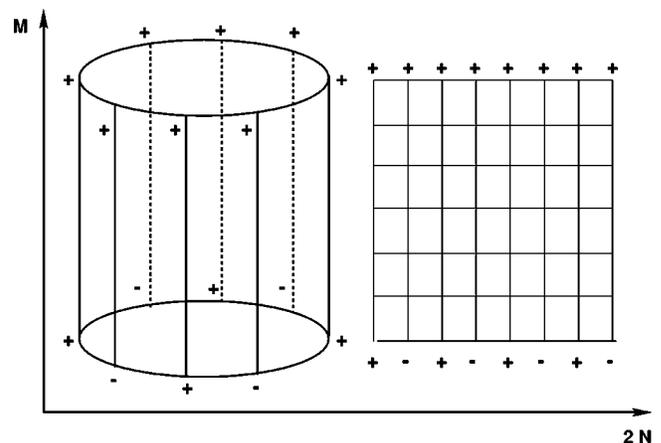


FIG. 1. The Brascamp-Kunz boundary conditions for the $M \times 2N$ lattice. Here $M = 7$ and $2N = 8$.

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tion between the terms of the asymptotic expansion and the so-called Kronecker's double series [20], which are directly related to elliptic θ functions. Expressing the final result in terms of θ functions avoids messy sums (as in some earlier works) and greatly simplifies the task of verifying the behavior of the different terms in the asymptotic expansion under duality transformation $M \leftrightarrow N$. Using this approach, Salas [21] computed the finite-size corrections to the free energy, internal energy, and specific heat of the critical Ising model on a triangular and honeycomb lattices wrapped on a torus.

Using the exact partition of Ref. [9] and the method of Ref. [20], in the present paper we derive exact finite-size corrections for the free energy F and the specific heat C of the critical ferromagnetic Ising model on the $\mathcal{M} \times 2\mathcal{N}$ square lattice with Brascamp-Kunz (BK) boundary conditions [9] and compare such results with those under toroidal boundary conditions [7,15]. We find that when the ratio $\xi/2 = (\mathcal{M}+1)/2\mathcal{N}$ is smaller than 1 the behaviors of finite-size corrections for C are quite different for BK and toroidal boundary conditions; when $\ln(\xi/2)$ is larger than 3, finite-size corrections for C in two boundary conditions approach the same values. In the limit $\mathcal{N} \rightarrow \infty$ we obtain the expansion of the free energy for infinitely long strip with BK boundary conditions. Our results are consistent with the conformal field theory prediction for the mixed boundary conditions by Cardy [11] although the definitions of boundary conditions in two cases are different on one side of the long strip.

This paper is organized as follows. In Sec. II we show how to lead the partition function of Ising model under the BK boundary conditions to the form of partition function with twisted boundary conditions. In Sec. III asymptotic expansion of the free energy is presented. In Sec. IV expansion of the specific heat is presented. Our results are summarized and discussed in Sec. V.

II. ISING MODEL UNDER BRASCAMP-KUNZ BOUNDARY CONDITIONS

For the Ising model on a lattice G of N sites, the i -th site of the lattice for $1 \leq i \leq N$ is assigned a classical spin variable s_i , which has values ± 1 . The spins interact according to the Hamiltonian

$$\beta H = -J \sum_{\langle ij \rangle} s_i s_j, \quad (1)$$

where J is the exchange energy, the sum runs over the nearest neighbor pairs of spins, and $\beta = 1/k_B T$ is the inverse temperature. The partition function of the Ising model is given by the sum over all spin configurations on the lattice

$$Z_{\text{Ising}}(J) = \sum_s e^{-\beta H(s)}. \quad (2)$$

As is mentioned in the Introduction there are a few boundary conditions for which the Ising model has been solved exactly. Among them is the special boundary conditions studied by BK [9]. They considered a lattice with $2\mathcal{N}$ sites in the x direction and \mathcal{M} sites in the y direction. The boundary conditions 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 the alternative values along the lower border of the resulting cylinder as is shown in Fig. 1. Recently Janke and Kenna [19] have analyzed the Ising model in two dimensions with these boundary conditions. They have derived exact expressions for the finite-size scaling of the specific heat up to the \mathcal{M}^{-3} order. In this paper we obtain all exact finite-size corrections for the free energy and the specific heat. Moreover, in our case, the terms of the asymptotic expansion are analytical functions. They are related to Kronecker's double series [22], which in turn can be expressed by elliptic θ functions [20].

For the BK boundary conditions, the Ising partition function given in Ref. [9] can be rewritten as

$$Z_{\mathcal{M},2\mathcal{N}} = (\sqrt{2}e^\mu)^{2\mathcal{M}\mathcal{N}} \prod_{i=1}^{\mathcal{N}} \prod_{j=1}^{\mathcal{M}} F(i,j), \quad (3)$$

where $\mu = 1/2 \ln \sinh 2J$ and

$$F(i,j) = 4 \left[2 \sinh^2 \mu + \sin^2 \left(\frac{\pi(i-1/2)}{2\mathcal{N}} \right) + \sin^2 \left(\frac{\pi j}{2(\mathcal{M}+1)} \right) \right]. \quad (4)$$

Now we try to express the partition function $Z_{\mathcal{M},2\mathcal{N}}$ given by Eq. (3) to the form of partition function with twisted boundary conditions $Z_{\alpha,\beta}(\mu)$,

$$Z_{\alpha,\beta}^2(\mu) = \prod_{i=0}^{N-1} \prod_{j=0}^{M-1} 4 \left[\sin^2 \left(\frac{\pi(i+\alpha)}{N} \right) + \sin^2 \left(\frac{\pi(j+\beta)}{M} \right) + 2 \sinh^2 \mu \right], \quad (5)$$

for which a general theory about its asymptotic expansion has been given in Ref. [20]. For this purpose we can express the double products $\prod_{i=0}^{2\mathcal{N}-1} \prod_{j=0}^{2\mathcal{M}+1} F(i+1,j)$ through $\prod_{i=1}^{\mathcal{N}} \prod_{j=1}^{\mathcal{M}} F(i,j)$ as

$$\begin{aligned} \prod_{i=0}^{2\mathcal{N}-1} \prod_{j=0}^{2\mathcal{M}+1} F(i+1,j) &= \left(\prod_{i=1}^{\mathcal{N}} \prod_{j=1}^{\mathcal{M}} F(i,j) \right)^4 \\ &\times \prod_{i=0}^{2\mathcal{N}-1} F(i+1,0) F(i+1,\mathcal{M}+1). \end{aligned} \quad (6)$$

Here we use the properties of function $F(i,j)$

$$F(2\mathcal{N}+1-k,j) = F(k,j) \quad \text{and} \quad F(i,2\mathcal{M}+2-k) = F(i,k). \quad (7)$$

This transformation leads the rectangular lattice $\mathcal{M} \times 2\mathcal{N}$ under consideration to the lattice $2(\mathcal{M}+1) \times 2\mathcal{N}$. In what follows we will use, for convenience, the definition of the aspect ratio as $\xi = (\mathcal{M}+1)/\mathcal{N}$ instead of the conventional one ($\xi = \mathcal{M}/2\mathcal{N}$).

The left-hand side of Eq. (6) is nothing but the partition function with twisted boundary conditions $Z_{1/2,0}^2(\mu)$ given by Eq. (5) with $N = 2\mathcal{N}$ and $M = 2(\mathcal{M}+1)$. With the help of the identity [23]

$$\prod_{i=0}^{2\mathcal{N}-1} 4 \left[\sinh^2 \omega + \sin^2 \left(\frac{\pi(i+1/2)}{2\mathcal{N}} \right) \right] = 4 \cosh^2(2\mathcal{N}\omega)$$

the second product in the right-hand side of Eq. (6) can be transformed into the form

$$\prod_{i=0}^{2\mathcal{N}-1} F(i+1,0)F(i+1,\mathcal{M}+1) = [4 \cosh\{2\mathcal{N}\omega_\mu(0)\} \cosh\{2\mathcal{N}\omega_\mu(\pi/2)\}]^2, \quad (8)$$

where

$$\omega_\mu(k) = \operatorname{arcsinh} \sqrt{\sin^2 k + 2 \operatorname{sh}^2 \mu} \quad (9)$$

is a lattice dispersion relation.

Using Eqs. (4)–(6) and (8), the partition function $Z_{\mathcal{M},2\mathcal{N}}$ can be expressed as

$$Z_{\mathcal{M},2\mathcal{N}}^2 = \frac{(\sqrt{2}e^\mu)^{4\mathcal{M}\mathcal{N}}}{4 \cosh[2\mathcal{N}\omega_\mu(0)] \cosh[2\mathcal{N}\omega_\mu(\pi/2)]} Z_{1/2,0}(\mu). \quad (10)$$

For our further purposes we transform the partition function $Z_{1/2,0}$ into the simpler form

$$Z_{1/2,0}(\mu) = \prod_{n=0}^{N-1} 2 \sinh \left[M \omega_\mu \left(\frac{\pi(n+1/2)}{N} \right) \right], \quad (11)$$

where $N=2\mathcal{N}$ and $M=2(\mathcal{M}+1)$.

III. ASYMPTOTIC EXPANSION OF THE FREE ENERGY

In the preceding section it was shown that the partition function of the $\mathcal{M} \times 2\mathcal{N}$ Ising model with BK boundary conditions can be expressed in terms of the partition function with twisted boundary conditions $Z_{1/2,0}$, which has been well studied in Ref. [20]. Further we will use it and for simplicity we will remind some necessary parts from there. For reader's convenience, all the technical details of our calculations and definitions of the special functions are summarized in the appendices at the end of this paper. Considering the logarithm of the partition function with twisted boundary conditions, Eq. (11), we note that it can be transformed as

$$\ln Z_{1/2,0}(0) = M \sum_{n=0}^{N-1} \omega_0 \left(\frac{\pi(n+1/2)}{N} \right) + \sum_{n=0}^{N-1} \ln(1 - e^{-2M\omega_0(\pi(n+1/2)/N)}). \quad (12)$$

The second sum here vanishes in the limit $M \rightarrow \infty$ when our lattice turns into infinitely long cylinder of circumference N . Therefore, the first sum gives the logarithm of the partition function with twisted angle $1/2$ on that cylinder. Its asymptotic expansion can be found with the help of the Euler-Maclaurin summation formula [24]

$$M \sum_{n=0}^{N-1} \omega_0 \left(\frac{\pi(n+1/2)}{N} \right) = \frac{S}{\pi} \int_0^\pi \omega_0(x) dx - \pi \xi B_2^{1/2} - 2 \pi \xi \sum_{p=1}^{\infty} \left(\frac{\pi^2 \xi}{S} \right)^p \frac{\lambda_{2p}}{(2p)!} \frac{B_{2p+2}^{1/2}}{2p+2}. \quad (13)$$

Here $S = NM = 4\mathcal{N}(\mathcal{M}+1)$, $B_p^{1/2}$ are the Bernoulli polynomials B_p^α at $\alpha = 1/2$, which are related to the Bernoulli numbers $B_p^\alpha \equiv B_p^0$ as $B_p^{1/2} = (2^{1-p} - 1)B_p$ and $\xi = M/N = (\mathcal{M}+1)/\mathcal{N}$. We have also used the symmetry property $\omega_0(k) = \omega_0(\pi - k)$ of the lattice dispersion relation given by Eq. (9) and its Taylor expansion

$$\omega_0(k) = k \left(\lambda + \sum_{p=1}^{\infty} \frac{\lambda_{2p}}{(2p)!} k^{2p} \right), \quad (14)$$

where $\lambda = 1$, $\lambda_2 = -2/3$, $\lambda_4 = 4$, etc.

We may transform the second term in Eq. (12) as

$$\sum_{n=0}^{N-1} \ln(1 - e^{-2M\omega_0(\pi(n+1/2)/N)}) = \ln \frac{\theta_4}{\eta} + \pi \xi B_2^{1/2} - 2 \pi \xi \sum_{p=1}^{\infty} \left(\frac{\pi^2 \xi}{S} \right)^p \frac{\Lambda_{2p}}{(2p)!} \times \frac{\operatorname{Re} K_{2p+2}^{1/2,0}(i\lambda \xi) - B_{2p+2}^{1/2}}{2p+2}, \quad (15)$$

where $\eta = (\theta_2 \theta_3 \theta_4/2)^{1/3}$ is the Dedekind- η function; θ_2 , θ_3 , θ_4 are elliptic θ functions and $K_{2p+2}^{1/2,0}(i\lambda \xi)$ are Kronecker's double series [20,22] (see also Appendix A). Taking into account the relation between moments and cumulants (Appendix B), the differential operators Λ_{2p} that have appeared here can be expressed via coefficients λ_{2p} of the expansion of the lattice dispersion relation as

$$\Lambda_2 = \lambda_2,$$

$$\Lambda_4 = \lambda_4 + 3 \lambda_2^2 \frac{\partial}{\partial \lambda},$$

$$\Lambda_6 = \lambda_6 + 15 \lambda_4 \lambda_2 \frac{\partial}{\partial \lambda} + 15 \lambda_2^3 \frac{\partial^2}{\partial \lambda^2},$$

⋮

$$\Lambda_p = \sum_{r=1}^p \sum \left(\frac{\lambda_{p_1}}{p_1!} \right)^{k_1} \cdots \left(\frac{\lambda_{p_r}}{p_r!} \right)^{k_r} \frac{p!}{k_1! \cdots k_r!} \frac{\partial^k}{\partial \lambda^k}.$$

Here the summation is over all positive numbers $\{k_1 \cdots k_r\}$ and different positive numbers $\{p_1, \dots, p_r\}$ such that $p_1 k_1 + \cdots + p_r k_r = p$ and $k = k_1 + \cdots + k_r - 1$.

Substituting Eqs. (13) and (15) into Eq. (12) we finally obtain exact asymptotic expansion of the logarithm of the partition function with twisted boundary conditions in terms of Kronecker's double series

$$\begin{aligned} \ln Z_{1/2,0}(0) &= \frac{S}{\pi} \int_0^\pi \omega_0(x) dx + \ln \frac{\theta_4}{\eta} \\ &\quad - 2 \pi \xi \sum_{p=1}^{\infty} \left(\frac{\pi^2 \xi}{S} \right)^p \frac{\Lambda_{2p}}{(2p)!} \frac{\text{Re} K_{2p+2}^{1/2,0}(i\lambda \xi)}{2p+2}, \end{aligned} \quad (16)$$

where $\int_0^\pi \omega_0(x) dx = 2G$ and $G = 0.915966$ is Catalan's constant.

After reaching this point, one can easily write down the exact asymptotic expansion of the free energy, $F = -\ln Z_{\mathcal{M},2\mathcal{N}}$, at the critical point. Plugging Eq. (16) back in Eq. (10) we finally obtain

$$\begin{aligned} F &= -2\mathcal{M}\mathcal{N} \left(\frac{1}{2} \ln 2 + \frac{2G}{\pi} \right) + 2\mathcal{N} \left[\frac{1}{2} \ln(1 + \sqrt{2}) - \frac{2G}{\pi} \right] \\ &\quad - \frac{1}{2} \ln \frac{\theta_4}{2\eta} + \pi \xi \sum_{p=1}^{\infty} \left(\frac{\pi}{2\mathcal{N}} \right)^{2p} \frac{\Lambda_{2p}}{(2p)!} \frac{\text{Re} K_{2p+2}^{1/2,0}(i\lambda \xi)}{2p+2}. \end{aligned} \quad (17)$$

Note that Kronecker's functions $K_p^{1/2,0}(i\lambda \xi)$ can be expressed in terms of the elliptic θ function only. Thus, Eq. (17) can be rewritten in the following form:

$$F = 2\mathcal{M}\mathcal{N}f_{\text{bulk}} + 2\mathcal{N}f_1 + f_0 + \sum_{p=1}^{\infty} \frac{f_{2p}}{(2\mathcal{N})^{2p}}, \quad (18)$$

where

$$f_{\text{bulk}} = -\frac{1}{2} \ln 2 - \frac{2G}{\pi} = -0.929695 \dots, \quad (19)$$

$$f_1 = \frac{1}{2} \ln(1 + \sqrt{2}) - \frac{2G}{\pi} = -0.142435 \dots, \quad (20)$$

$$f_0 = -\frac{1}{2} \ln \frac{\theta_4}{2\eta}, \quad (21)$$

$$f_2 = -\frac{\pi^3 \xi}{360} \left(\frac{7}{8} \theta_4^8 - \theta_2^4 \theta_3^4 \right), \quad (22)$$

$$\begin{aligned} f_4 &= -\frac{\pi^5 \xi}{48384} \left[\pi \xi \theta_3^4 \theta_4^4 \left(\theta_3^8 + \frac{5}{4} \theta_3^4 \theta_4^4 - \frac{5}{16} \theta_4^8 \right) + (\theta_2^4 + \theta_3^4) \right. \\ &\quad \left. \times \left(\frac{31}{16} \theta_4^8 + \theta_2^4 \theta_3^4 \right) \left(1 + 4 \xi \frac{\theta_2'}{\theta_2} \right) \right], \end{aligned} \quad (23)$$

$$\begin{aligned} f_6 &= \frac{\pi^7 \xi}{87091200} \left[70 \pi^2 \xi^2 \theta_3^4 \theta_4^4 \left(\theta_2^{16} + \frac{\theta_2^{12} \theta_4^4}{2} - \frac{81 \theta_2^8 \theta_4^8}{8} \right. \right. \\ &\quad \left. \left. - \frac{295 \theta_2^4 \theta_4^{12}}{16} - \frac{635 \theta_4^{16}}{64} \right) + 630 \pi \xi \theta_3^4 \theta_4^4 \left(\theta_2^{12} - \frac{3 \theta_2^8 \theta_4^4}{4} \right. \right. \\ &\quad \left. \left. - \frac{21 \theta_2^4 \theta_4^8}{8} - \frac{127 \theta_4^{12}}{64} \right) \left(1 + 4 \xi \frac{\theta_2'}{\theta_2} \right) + \left(\theta_2^{16} + 2 \theta_2^{12} \theta_4^4 \right. \right. \end{aligned}$$

$$\begin{aligned} &\quad \left. - \frac{3}{4} \theta_2^8 \theta_4^8 - \frac{7}{4} \theta_2^4 \theta_4^{12} - \frac{127}{128} \theta_4^{16} \right) \left(711 + 5040 \xi \frac{\theta_2'}{\theta_2} \right. \\ &\quad \left. + 8400 \xi^2 \frac{\theta_2'^2}{\theta_2^2} + 560 \xi^2 \frac{\theta_2''}{\theta_2} \right), \end{aligned} \quad (24)$$

$$\begin{aligned} f_8 &= -\pi^{12} \xi^4 \frac{\theta_4^4 \theta_3^4}{33634123776} (1280 \theta_2^{24} + 20224 \theta_2^{20} \theta_4^4 \\ &\quad + 83664 \theta_2^{16} \theta_4^8 + 210496 \theta_2^{12} \theta_4^{12} + 361115 \theta_2^8 \theta_4^{16} \\ &\quad + 323910 \theta_2^4 \theta_4^{20} + 107310 \theta_4^{24}) \\ &\quad - \pi^{11} \xi^3 \frac{\theta_4^4 \theta_3^4 \left(1 + 4 \xi \frac{\theta_2'}{\theta_2} \right)}{1868562432} (1280 \theta_2^{20} + 8832 \theta_2^{16} \theta_4^4 \\ &\quad + 19056 \theta_2^{12} \theta_4^8 + 33568 \theta_2^8 \theta_4^{12} + 38655 \theta_2^4 \theta_4^{16} \\ &\quad + 15330 \theta_4^{20}) - \frac{\pi^{10} \xi^2 \theta_4^4 \theta_3^4}{1177194332160} \left(3789 + 27720 \xi \frac{\theta_2'}{\theta_2} \right. \\ &\quad \left. + 48720 \xi^2 \frac{\theta_2'^2}{\theta_2^2} + 2240 \xi^2 \frac{\theta_2''}{\theta_2} \right) (1280 \theta_2^{16} + 3136 \theta_2^{12} \theta_4^4 \\ &\quad + 3216 \theta_2^8 \theta_4^8 + 5176 \theta_2^4 \theta_4^{12} + 2555 \theta_4^{16}) \\ &\quad - \frac{\pi^9 \xi (\theta_2^4 + \theta_3^4)}{235438866432} \left(1479 + 15156 \xi \frac{\theta_2'}{\theta_2} \right. \\ &\quad \left. + 47880 \xi^3 \frac{\theta_2'^2}{\theta_2^2} + 47880 \xi^3 \frac{\theta_2'^3}{\theta_2^3} + 2520 \xi^2 \frac{\theta_2''}{\theta_2} \right. \\ &\quad \left. + 7980 \xi^3 \frac{\theta_2'}{\theta_2} \frac{\theta_2''}{\theta_2} + 140 \frac{\theta_2'''}{\theta_2} \right), \end{aligned} \quad (25)$$

∴

The free energy per unit length of an infinitely long strip of width L at criticality has the finite-size scaling form [10]

$$F = fL + f^* + \frac{\Delta}{L} + \dots, \quad (26)$$

where f is the bulk free energy per unit area, $\frac{1}{2}f^*$ is the surface energy, L^{-1} is a scaling field, and Δ is a universal constant that depends only on the type of boundary conditions [11],

$$\Delta = -\frac{\pi}{12}, \quad \text{periodic boundary conditions,}$$

$$\Delta = \frac{\pi}{6}, \quad \text{antiperiodic boundary conditions,}$$

$$\Delta = -\frac{\pi}{48}, \quad \text{free boundary conditions,}$$

$$\Delta = -\frac{\pi}{48}, \quad \text{fixed } ++ \text{ boundary conditions,}$$

$$\Delta = \frac{23\pi}{48}, \quad \text{fixed } +- \text{ boundary conditions,}$$

$$\Delta = \frac{\pi}{24}, \quad \text{mixed boundary conditions.} \quad (27)$$

For fixed ++ (or +-) boundary conditions the spins are fixed to the same (or opposite) values on two sides of the strip. The mixed boundary conditions correspond to free boundary conditions on one side of the strip, and fixed boundary conditions on the other. Therefore, BK and the mixed boundary conditions are the same on one side of the long strip (fixed to + for all spins) and they are different on another side of the long strip (fixed to +-+ - . . . for BK boundary conditions and free boundary conditions for the mixed boundary conditions).

Using Kronecker's functions asymptotic form when $\xi \rightarrow 0$ and $\xi \rightarrow \infty$ we can obtain from Eq. (17) the free energy per unit length of an infinitely long strip of finite width. In the limit $\xi \rightarrow \infty$ (i.e., $\mathcal{M} \rightarrow \infty$) for fixed $2\mathcal{N}$ from Eq. (17) one obtains the free energy expansion for infinitely long cylinder of circumference $2\mathcal{N}$,

$$\begin{aligned} \lim_{\mathcal{M} \rightarrow \infty} \frac{F}{\mathcal{M}} &= 2\mathcal{N}f_{bulk} - \frac{\pi}{24\mathcal{N}} \\ &+ 2 \sum_{p=1}^{\infty} \left(\frac{\pi}{2\mathcal{N}} \right)^{2p+1} \frac{\lambda_{2p} B_{2p+2}^{1/2}}{(2p)!(2p+2)} \\ &= 2\mathcal{N} \left(-\frac{2G}{\pi} - \frac{1}{2} \ln 2 \right) - \frac{\pi}{12} \left(\frac{1}{2\mathcal{N}} \right) - \frac{7\pi^3}{1440} \left(\frac{1}{2\mathcal{N}} \right)^3 \\ &- \frac{31\pi^5}{24 \cdot 192} \left(\frac{1}{2\mathcal{N}} \right)^5 - \frac{10033\pi^7}{9 \cdot 676 \cdot 800} \left(\frac{1}{2\mathcal{N}} \right)^7 - \dots \end{aligned} \quad (28)$$

This result coincides with that obtained in [14] with the leading finite-size correction to free energy $-\pi/12(2\mathcal{N})^{-1}$. In the limit $\xi \rightarrow 0$ (i.e. $\mathcal{N} \rightarrow \infty$) for fixed \mathcal{M} we obtain the expansion of free energy of infinitely long strip with BK boundary condition of the width \mathcal{M} ,

$$\begin{aligned} \lim_{\mathcal{N} \rightarrow \infty} \frac{F}{2\mathcal{N}} &= \mathcal{M}f_{bulk} + f_1 + \frac{\pi}{24(\mathcal{M}+1)} \\ &+ \sum_{p=1}^{\infty} \left[\frac{\pi}{2(\mathcal{M}+1)} \right]^{2p+1} \frac{\lambda_{2p} B_{2p+2}}{(2p)!(2p+2)} \\ &= \mathcal{M} \left(-\frac{2G}{\pi} - \frac{1}{2} \ln 2 \right) + \frac{1}{2} \ln(1 + \sqrt{2}) - \frac{2G}{\pi} \\ &+ \frac{\pi}{24} \frac{1}{\mathcal{M}} - \frac{\pi}{24} \frac{1}{\mathcal{M}^2} + \left(\frac{\pi}{24} + \frac{\pi^3}{2800} \right) \end{aligned}$$

$$\times \frac{1}{\mathcal{M}^3} - \left(\frac{\pi}{24} + \frac{\pi^3}{960} \right) \frac{1}{\mathcal{M}^4} + \dots \quad (29)$$

Here the leading finite-width correction to free energy is $\pi/24\mathcal{M}^{-1}$. From Eqs. (26)–(29) one can see that

$$L = 2\mathcal{N}, \quad f = f_{bulk}, \quad f^* = 0, \quad \Delta = -\frac{\pi}{12}, \quad (30)$$

$$L = \mathcal{M}, \quad f = f_{bulk}, \quad f^* = f_1, \quad \Delta = \frac{\pi}{24}. \quad (31)$$

Our results are consistent with the conformal field theory prediction for the mixed boundary condition [see Eq. (27)] although the mixed boundary condition and the BK boundary condition are different on one side of the long strip.

IV. ASYMPTOTIC EXPANSION OF THE INTERNAL ENERGY AND THE SPECIFIC HEAT

The internal energy per spin and the specific heat per spin can be obtained from the partition function $Z_{\mathcal{M},2\mathcal{N}}$,

$$U = -\frac{1}{2\mathcal{M}\mathcal{N}} \frac{d}{dJ} \ln Z_{\mathcal{M},2\mathcal{N}} = -\frac{\sqrt{1+e^{-4\mu}}}{2\mathcal{M}\mathcal{N}} \frac{d}{d\mu} \ln Z_{\mathcal{M},2\mathcal{N}}, \quad (32)$$

$$\begin{aligned} C &= \frac{1}{2\mathcal{M}\mathcal{N}} \frac{d^2}{dJ^2} \ln Z_{\mathcal{M},2\mathcal{N}} \\ &= \frac{e^{-4\mu}}{\mathcal{M}\mathcal{N}} \left(\frac{1+e^{4\mu}}{2} \frac{d^2}{d\mu^2} \ln Z_{\mathcal{M},2\mathcal{N}} - \frac{d}{d\mu} \ln Z_{\mathcal{M},2\mathcal{N}} \right). \end{aligned} \quad (33)$$

Let us first consider the internal energy. At the critical point $T = T_c$ ($\mu = 0$) the internal energy is given by

$$U = -\sqrt{2} + \sqrt{2} \frac{d}{d\mu} \ln Z_{1/2,0}(0). \quad (34)$$

One can note that $Z_{1/2,0}(\mu)$ is an even function with respect to its argument μ , which implies immediately that $[dZ_{1/2,0}(\mu)/d\mu]_{\mu=0} = 0$. Thus we find that internal energy for the finite system is equal to its bulk values without any finite-size corrections, namely, $U = -\sqrt{2}$.

At the critical point $T = T_c$ ($\mu = 0$) the specific heat is given by

$$\begin{aligned} C &= -2 - \frac{4\mathcal{N}}{\mathcal{M}} - \frac{\sqrt{2}}{\mathcal{M}} \tanh[2\mathcal{M} \ln(1 + \sqrt{2})] \\ &+ \frac{1}{2\mathcal{M}\mathcal{N}} \frac{d^2}{d\mu^2} \ln Z_{1/2,0}(0). \end{aligned} \quad (35)$$

The analysis of the $Z''_{1/2,0}(0)$ is a little more involved. Taking the second derivative of Eq. (11) with respect to mass variable μ and then considering the limit $\mu \rightarrow 0$, we obtain

$$\begin{aligned}
 \frac{Z''_{1/2,0}(0)}{Z_{1/2,0}(0)} &= M \sum_{n=0}^{N-1} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) \text{cth}\left[M\omega_0\left(\frac{\pi(n+1/2)}{N}\right)\right] \\
 &= M \sum_{n=0}^{N-1} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) \\
 &\quad + 2M \sum_{n=0}^{N-1} \sum_{m=1}^{\infty} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) \\
 &\quad \times \exp\left\{-2m\left[M\omega_0\left(\frac{\pi(n+1/2)}{N}\right)\right]\right\}, \quad (36)
 \end{aligned}$$

where $M=2(\mathcal{M}+1)$, $N=2\mathcal{N}$, and $\omega_0''(x)$ is the second derivative of $\omega_\mu(x)$ with respect to μ at criticality

$$\omega_0''(x) = \frac{2}{\sin x \sqrt{1 + \sin^2 x}}.$$

Using Taylor's theorem, the asymptotic expansion of the $\omega_0''(x)$ can be written in the following form:

$$\omega_0''(x) = \frac{2}{x} \left\{ 1 + \sum_{p=1}^{\infty} \frac{\kappa_{2p}}{(2p)!} x^{2p} \right\},$$

where $\kappa_2 = -2/3$, $\kappa_4 = 172/15$, etc. The first sum in Eq. (36) we may transform as

$$\begin{aligned}
 M \sum_{n=0}^{N-1} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) \\
 = M \sum_{n=0}^{N-1} f\left(\frac{\pi(n+1/2)}{N}\right) + \frac{4S}{\pi} \sum_{n=0}^{N-1} \frac{1}{n+1/2}, \quad (37)
 \end{aligned}$$

where we have introduced the function $f(x) = \omega_0''(x) - 2/x - 2/(\pi - x)$. This function and all its derivatives are integrable over the interval $(0, \pi)$. Thus, for the first term in Eq. (37) we may use again the Euler-Maclaurin summation formula, and after a little algebra we obtain

$$\begin{aligned}
 M \sum_{n=0}^{N-1} f\left(\frac{\pi(n+1/2)}{N}\right) \\
 = \frac{S}{\pi} \int_0^\pi f(x) dx - 2\pi\xi \sum_{p=1}^{\infty} \left(\frac{\pi^2\xi}{S}\right)^{p-1} \\
 \times \frac{\kappa_{2p} B_{2p}^{1/2}}{p(2p)!} + \frac{2S}{\pi} \sum_{p=1}^{\infty} \frac{B_{2p}^{1/2}}{p} \frac{1}{N^{2p}}, \quad (38)
 \end{aligned}$$

where $\int_0^\pi f(x) dx = 2 \ln 2 - 4 \ln \pi$. The second sum in Eq. (37) can be written in terms of the digamma function $\psi(x)$,

$$\sum_{n=0}^{N-1} \frac{1}{n+1/2} = \psi(N+1/2) - \psi(1/2). \quad (39)$$

The asymptotic expansion of the digamma function $\psi(x)$ is given by (see Appendix D)

$$\psi(N+1/2) = \ln N - \sum_{p=1}^{\infty} (-1)^p \frac{B_p^{1/2}}{p} \frac{1}{N^p}. \quad (40)$$

Using the property of the Bernoulli polynomials $B_p^{1/2}$, namely, $B_{2p+1}^{1/2} = 0$, Eq. (39) can be rewritten as

$$\sum_{n=0}^{N-1} \frac{1}{n+1/2} = \ln N - \sum_{p=1}^{\infty} \frac{B_{2p}^{1/2}}{2p} \frac{1}{N^{2p}} - \psi(1/2). \quad (41)$$

Plugging Eqs. (38) and (41) back in Eq. (37), We finally obtain

$$\begin{aligned}
 M \sum_{n=0}^{N-1} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) &= \frac{4S}{\pi} \left\{ \ln N + \frac{1}{2} \ln 2 - \ln \pi - \psi(1/2) \right\} \\
 &\quad - 2\pi\xi \sum_{p=1}^{\infty} \left(\frac{\pi^2\xi}{S}\right)^{p-1} \frac{\kappa_{2p} B_{2p}^{1/2}}{p(2p)!}. \quad (42)
 \end{aligned}$$

Let us now consider the second sum in Eq. (36). Note that function $\omega_0''(x)$ can be represented as

$$\omega_0''(x) = \frac{2}{x} \exp\left\{ \sum_{p=1}^{\infty} \frac{\varepsilon_{2p}}{(2p)!} x^{2p} \right\}, \quad (43)$$

where coefficients ε_{2p} and κ_{2p} are related to each other through relation between moments and cumulants (Appendix B). Following the same lines as in Sec. III, the second sum in Eq. (36) can be written as

$$\begin{aligned}
 2M \sum_{n=0}^{N-1} \sum_{m=1}^{\infty} \omega_0''\left(\frac{\pi(n+1/2)}{N}\right) \exp\left[-2mM\omega_0\left(\frac{\pi(n+1/2)}{N}\right)\right] \\
 = \frac{4S}{\pi} \{R_{1/2,0}(\xi) + \psi(1/2)\} + \left(\kappa_2 \xi \frac{\partial}{\partial \xi} + \lambda_2 \xi^2 \frac{\partial^2}{\partial \xi^2} \right) \\
 \times \ln \frac{\theta_4(\xi)}{\eta(\xi)} - 2\pi\xi \sum_{p=2}^{\infty} \frac{\Omega_{2p}}{p(2p)!} \left(\frac{\pi^2\xi}{S}\right)^{p-1} \text{Re}K_{2p}^{1/2,0}(i\lambda\xi) \\
 + 2\pi\xi \sum_{p=1}^{\infty} \frac{\kappa_{2p} B_{2p}^{1/2}}{p(2p)!} \left(\frac{\pi^2\xi}{S}\right)^{p-1}, \quad (44)
 \end{aligned}$$

where

$$R_{1/2,0}(\xi) = -2 \ln \theta_4(\xi) + C_E + 2 \ln 2$$

and C_E is the Euler constant. The differential operators Ω_{2p} that have appeared here can be expressed via coefficients $\omega_{2p} = \varepsilon_{2p} + \lambda_{2p} \partial/\partial \lambda$ as

$$\Omega_2 = \omega_2,$$

$$\Omega_4 = \omega_4 + 3 \omega_2^2,$$

\vdots

Substituting Eqs. (42) and (44) into Eq. (36), we obtain exact asymptotic expansion of $Z''_{1/2,0}(0)$,

$$\begin{aligned} \frac{Z''_{1/2,0}(0)}{Z_{1/2,0}(0)} &= \frac{4S}{\pi} \left(\ln N + C_E + \ln \frac{2^{5/2}}{\pi} - 2 \ln \theta_4(\xi) \right) \\ &+ \left(\kappa_2 \xi \frac{\partial}{\partial \xi} + \lambda_2 \xi^2 \frac{\partial^2}{\partial \xi^2} \right) \ln \frac{\theta_4(\xi)}{\eta(\xi)} \\ &- 2 \pi \xi \sum_{p=2}^{\infty} \frac{\Omega_{2p}}{p(2p)!} \left(\frac{\pi^2 \xi}{S} \right)^{p-1} \text{Re} K_{2p}^{1/2,0}(i\lambda \xi). \end{aligned} \quad (45)$$

Plugging Eq. (45) back in Eq. (35) we finally obtain exact asymptotic expansion of the specific heat

$$C = \frac{8}{\pi} \left(1 + \frac{1}{\xi \mathcal{N} - 1} \right) \ln 2\mathcal{N} + \sum_{p=0}^{\infty} \frac{C_p}{(2\mathcal{N})^p}, \quad (46)$$

where

$$\begin{aligned} C_0 &= \frac{8}{\pi} \left(C_E + \ln \frac{2^{5/2}}{\pi} - \frac{\pi}{4} \right) - \frac{4}{\xi} - \frac{16}{\pi} \ln \theta_4(\xi), \\ C_1 &= \frac{2}{\xi} (C_0 + 2 - \sqrt{2}), \\ C_2 &= \frac{2}{\xi} C_1 - \frac{\pi}{9} \left\{ \pi \xi \theta_3^4 \theta_4^4 + (\theta_2^4 + \theta_3^4) \left(1 + 4 \xi \frac{\theta_2'}{\theta_2} \right) \right\}, \\ C_3 &= \frac{2}{\xi} C_2, \\ C_4 &= \frac{2}{\xi} C_3 + \frac{\pi^5 \xi^4 \theta_4^4 \theta_3^4}{270} \left(\theta_2^8 - \frac{3}{2} \theta_4^4 \theta_2^4 - \frac{21}{4} \theta_4^8 \right) \\ &+ \frac{\pi^4 \xi^3 \theta_4^4 \theta_3^4}{54} \left(\theta_2^4 - \frac{7}{4} \theta_4^4 \right) \left(1 + 4 \xi \frac{\theta_2'}{\theta_2} \right) \\ &+ \frac{4 \pi^3 \xi^2}{135} \left(\theta_2^4 \theta_3^4 - \frac{7}{8} \theta_4^8 \right) \left(\frac{43}{40} + 5 \xi \frac{\theta_2'}{\theta_2} \right) \\ &+ 7 \xi^2 \frac{\theta_2'^2}{\theta_2^2} + \xi^2 \frac{\theta_2''}{\theta_2}, \\ C_5 &= \frac{2}{\xi} C_4, \\ &\vdots \end{aligned}$$

The $1/\mathcal{M}$ expansion of the specific heat has a form

$$C = \frac{8}{\pi} \left(1 + \frac{1}{\mathcal{M}} \right) \ln \mathcal{M} + \sum_{p=0}^{\infty} \frac{c_p}{\mathcal{M}^p}, \quad (47)$$

where

$$c_0 = C_0 - \frac{8}{\pi} \ln \frac{\xi}{2},$$

$$c_1 = \frac{\xi}{2} C_1 + \frac{8}{\pi} \left(1 - \ln \frac{\xi}{2} \right),$$

$$c_2 = \frac{\xi^2}{4} C_2 - \frac{\xi}{2} C_1 + \frac{4}{\pi},$$

$$c_3 = -\frac{\xi^2}{4} C_2 + \frac{\xi}{2} C_1 - \frac{4}{3\pi},$$

$$c_4 = \frac{\xi^4}{16} C_4 - \frac{\xi}{2} C_1 + \frac{2}{3\pi},$$

$$c_5 = -\frac{3\xi^4}{16} C_4 + \frac{\xi^2}{2} C_2 + \frac{\xi}{2} C_1 - \frac{2}{5\pi},$$

\vdots .

Typical values of the constants $c_0 - c_3$ are given in Table I, in which the coefficients are consistent with those obtained in [19].

Using Kronecker's functions asymptotic form when $\xi \rightarrow 0$ and $\xi \rightarrow \infty$ we can obtain from Eqs. (35) and (45) the specific heat per unit length of an infinitely long strip of finite width. In the limit $\xi \rightarrow \infty$ (i.e., $\mathcal{M} \rightarrow \infty$) for fixed $2\mathcal{N}$ the specific heat expansion for infinitely long cylinder of circumference $2\mathcal{N}$ can be written as

$$\begin{aligned} C &= \frac{8}{\pi} \ln 2\mathcal{N} + \frac{8}{\pi} \left(C_E + \ln \frac{2^{5/2}}{\pi} - \frac{\pi}{4} \right) \\ &- \sum_{p=1}^{\infty} \frac{4 \pi^{2p-1} \Omega_{2p} B_{2p}^{1/2}}{p(2p)!} \frac{1}{(2\mathcal{N})^{2p}} \\ &= \frac{8}{\pi} \ln 2\mathcal{N} + \frac{8}{\pi} \left(C_E + \ln \frac{2^{5/2}}{\pi} - \frac{\pi}{4} \right) - \frac{\pi}{9} \left(\frac{1}{2\mathcal{N}} \right)^2 \\ &- \frac{301 \pi^3}{10800} \left(\frac{1}{2\mathcal{N}} \right)^4 - \frac{29419 \pi^5}{1905120} \left(\frac{1}{2\mathcal{N}} \right)^6 \\ &- \frac{2759329 \pi^7}{145152000} \left(\frac{1}{2\mathcal{N}} \right)^8 - \dots \end{aligned} \quad (48)$$

In the limit $\xi \rightarrow 0$ (i.e., $\mathcal{N} \rightarrow \infty$) for fixed \mathcal{M} we obtain the expression for specific heat of infinitely long strip with BK boundary condition of width \mathcal{M} ,

$$\begin{aligned} C &= \frac{8}{\pi} \frac{\mathcal{M}+1}{\mathcal{M}} \left(\ln(\mathcal{M}+1) + C_E + \ln \frac{2^{3/2}}{\pi} \right) - 2 - \frac{\sqrt{2}}{\mathcal{M}} \\ &- \sum_{p=1}^{\infty} \frac{2k_{2p} B_{2p}}{p(2p)!} \left(\frac{\pi}{2} \right)^{2p-1} \frac{1}{\mathcal{M}(\mathcal{M}+1)^{2p-1}} \\ &= \frac{8}{\pi} \left(1 + \frac{1}{\mathcal{M}} \right) \ln \mathcal{M} + \frac{8}{\pi} \left(C_E + \ln \frac{2^{3/2}}{\pi} - \frac{\pi}{4} \right) \\ &+ \frac{8}{\pi} \left(C_E + \ln \frac{2^{3/2}}{\pi} + 1 - \frac{\sqrt{2}\pi}{8} \right) \frac{1}{\mathcal{M}} + \left(\frac{4}{\pi} + \frac{\pi}{18} \right) \left(\frac{1}{\mathcal{M}} \right)^2 \\ &- \left(\frac{4}{3\pi} + \frac{\pi}{18} \right) \left(\frac{1}{\mathcal{M}} \right)^3 + \left(\frac{2}{3\pi} + \frac{\pi}{18} + \frac{43\pi^3}{21600} \right) \left(\frac{1}{\mathcal{M}} \right)^4 \end{aligned}$$

TABLE I. Values of the coefficients c_0-c_3 for various values of the ratio $\xi=(\mathcal{M}+1)/\mathcal{N}$. Presented here are $(c_0-2)/8$ and $c_i/8(i=1,2,3)$ for the convenience of comparison with the results of Janke and Kenna [19], in which $1/\rho$ is corresponding to ξ in the present paper.

ξ	1/2	1	2
$(c_0-2)/8$	-0.349 694 206 9 ...	-0.350 879 733 2 ...	-0.376 674 233 4 ...
$c_1/8$	0.291 838 983 9 ...	0.290 653 457 6 ...	0.264 858 957 4 ...
$c_2/8$	0.180 950 438 7 ...	0.175 784 345 6 ...	0.125 896 137 8 ...
$c_3/8$	-0.074 847 143 3 ...	-0.069 681 050 2 ...	-0.019 792 842 4 ...

$$-\left(\frac{2}{5\pi} + \frac{\pi}{18} + \frac{43\pi^3}{7200}\right)\left(\frac{1}{\mathcal{M}}\right)^5 + \dots \tag{49}$$

Note that the specific heat expansion for infinitely long cylinder contains only even powers of \mathcal{N}^{-1} (except, of course, the leading logarithmic term), while in the specific heat expansion for infinitely long strip with BK boundary condition any integer powers of \mathcal{M}^{-1} can occur.

In Fig. 2 we plot the aspect-ratio (ξ) dependence of the finite-size specific heat correction terms $C_0, C_1, C_2,$ and C_3 for the Ising model with BK boundary condition and those of the torus [15]. We use the logarithmic scales for the horizontal axis. For large enough $\xi(\gg 1)$, the finite-size properties of the Ising model with BK boundary condition and those of the torus become the same because the boundaries along the shorter direction determine the finite-size properties of the system; for both BK boundary condition and the torus, the boundary condition along the y axis is the periodic one.

V. SUMMARY AND DISCUSSION

In this paper, we have used the method of [20] to derive exact finite-size corrections for the free energy F and the specific heat C of the critical ferromagnetic Ising model on the $\mathcal{M}\times 2\mathcal{N}$ square lattice with Brascamp-Kunz (BK) boundary conditions [9]. We find that the finite-size corrections to the free energy and the specific heat are always integer powers of $\mathcal{N}^{-1}(\mathcal{M}^{-1})$ except, of course, the leading logarithmic term in the specific heat. In the finite-size expansion of the free energy given by Eq. (18), only even power of \mathcal{N}^{-1} occur, except for the term \mathcal{N} . In the finite-size expansion of the specific heat given by Eqs. (46) and (47), any integer powers of $\mathcal{N}^{-1}(\mathcal{M}^{-1})$ can occur.

We have compared our results with those under toroidal boundary conditions. When the ratio $\xi/2=(\mathcal{M}+1)/2\mathcal{N}$ is smaller than 1 the behaviors of finite-size corrections for C are quite different for BK and toroidal boundary conditions; when $\ln(\xi/2)$ is larger than 3, finite-size corrections for C in two boundary conditions approach the same value. In the limit $\mathcal{N}\rightarrow\infty$ we obtain the expansion of the free energy for infinitely long strip with BK boundary conditions. Our results are consistent with the conformal field theory prediction for the mixed boundary conditions by Cardy [11] although the definitions of boundary conditions in two cases are different on one side of the long strip. It is of interest to know under what conditions different boundary conditions could still give the same finite-size corrections.

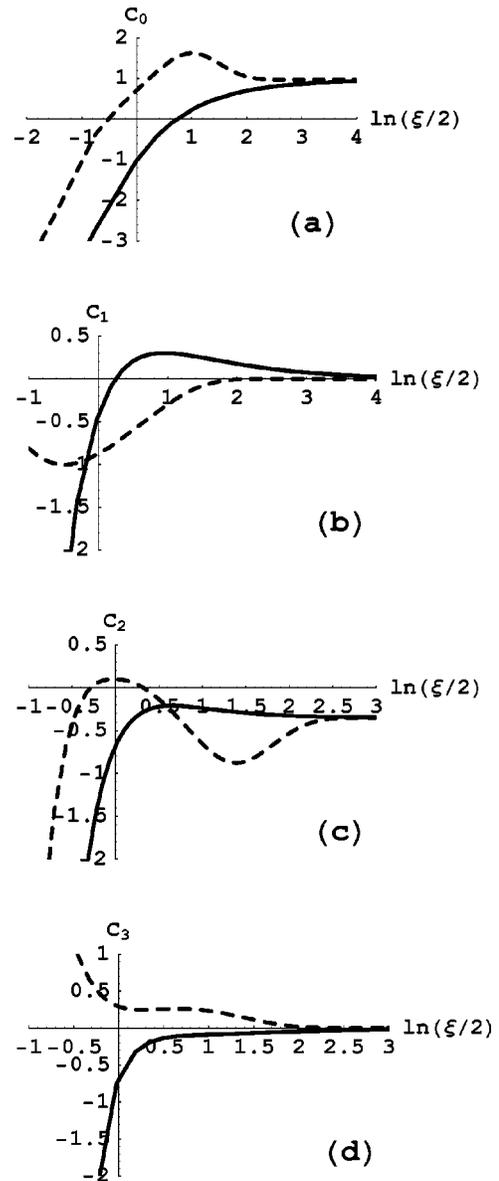


FIG. 2. Aspect-ratio (ξ) dependence of finite-size correction terms for the specific heat of the square lattice Ising model with Brascamp-Kunz boundary conditions (solid lines) and toroidal boundary conditions (dashed lines): (a) C_0 , (b) C_1 , (c) C_2 , and (d) C_3 .

The results of this paper show that the method of Ref. [20] is quite useful for calculating exact finite-size corrections for critical systems. It is of interest to apply this method to calculate exact finite-size corrections for the Ising model and other free models [20] on various lattices with various boundary conditions so that some general features of such finite-size corrections could be found.

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APPENDIX A: KRONECKER'S DOUBLE SERIES

Kronecker's double series can be defined as [22]

$$K_p^{1/2,0}(\tau) = -\frac{p!}{(-2\pi i)^p} \sum_{\substack{m,n \in \mathbb{Z} \\ (m,n) \neq (0,0)}} \frac{e^{-\pi i n}}{(n + \tau m)^p}.$$

In this form, however, they cannot be directly applied to our analysis. We need to cast them in a different form. To this end, let us separate from the double series a subseries with $m=0$,

$$K_p^{1/2,0}(\tau) = -\frac{p!}{(-2\pi i)^p} \sum_{n \neq 0} \frac{e^{-\pi i n}}{n^p} - \frac{p!}{(-2\pi i)^p} \sum_{m \neq 0} \sum_{n \in \mathbb{Z}} \frac{e^{-\pi i n}}{(n + \tau m)^p}.$$

Here the first sum gives nothing but Fourier representation of Bernoulli polynomials

$$B_p^\alpha = -\frac{p!}{(-2\pi i)^p} \sum_{n \neq 0} \frac{e^{-2\pi i n \alpha}}{n^p}. \quad (\text{A1})$$

The second sum can be rearranged with the help of the identity

$$\frac{p!}{(-2\pi i)^p} \sum_{n \in \mathbb{Z}} \frac{e^{-\pi i n}}{(z+n)^p} = p \sum_{n=0}^{\infty} (n+1/2)^{p-1} e^{2\pi i z(n+1/2)},$$

which can easily be derived from the following equation by differentiating it p times:

$$\frac{e^{2\pi i z \alpha}}{e^{2\pi i z} - 1} = -\sum_{n=0}^{\infty} e^{2\pi i z(n+\alpha)} = \frac{1}{2\pi i} \sum_{n=-\infty}^{+\infty} \frac{e^{-2\pi i n \alpha}}{z+n}. \quad (\text{A2})$$

The final result of our resummation of the double Kronecker sum is

$$K_p^{1/2,0}(\tau) = B_p^{1/2} - p \sum_{m \neq 0} \sum_{n=0}^{\infty} (n+1/2)^{p-1} e^{2\pi i m \tau(n+1/2)}.$$

Considering the Kronecker sums with pure imaginary aspect ratio, $\tau = i\xi$, we can further rearrange this expression to get summation only over positive $m \geq 1$,

$$B_{2p}^{1/2} - K_{2p}^{1/2,0}(i\xi) = 4p \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} (n+1/2)^{2p-1} e^{-2\pi m \xi(n+1/2)}. \quad (\text{A3})$$

APPENDIX B: RELATION BETWEEN MOMENTS AND CUMULANTS

Moments Z_{2k} and cumulants F_{2k} which enter the expansion of exponent

$$\exp\left\{\sum_{k=1}^{\infty} \frac{x^{2k}}{(2k)!} F_{2k}\right\} = 1 + \sum_{k=1}^{\infty} \frac{x^{2k}}{(2k)!} Z_{2k},$$

are related to each other as [25]

$$\begin{aligned} Z_2 &= F_2, \\ Z_4 &= F_4 + 3F_2^2, \\ Z_6 &= F_6 + 15F_2F_4 + 15F_2^3, \\ Z_8 &= F_8 + 28F_2F_6 + 35F_4^2 + 210F_2^2F_4 + 105F_2^4 \\ &\vdots \\ Z_k &= \sum_{r=1}^k \sum \binom{F_{k_1}}{k_1!}^{i_1} \cdots \binom{F_{k_r}}{k_r!}^{i_r} \frac{k!}{i_1! \cdots i_r!}, \end{aligned}$$

where summation is over all positive numbers $\{i_1 \cdots i_r\}$ and different positive numbers $\{k_1, \dots, k_r\}$ such that $k_1 i_1 + \dots + k_r i_r = k$.

APPENDIX C: REDUCTION OF KRONECKER'S DOUBLE SERIES TO θ FUNCTIONS

Let us consider a Laurent expansion of the Weierstrass function

$$\begin{aligned} \wp(z) &= \frac{1}{z^2} + \sum_{(n,m) \neq (0,0)} \left[\frac{1}{(z-n-\tau m)^2} - \frac{1}{(n+\tau m)^2} \right] \\ &= \frac{1}{z^2} + \sum_{p=2}^{\infty} a_p(\tau) z^{2p-2}. \end{aligned}$$

The coefficients $a_p(\tau)$ of the expansion can all be written in terms of the elliptic θ functions with the help of the recursion relation [26]

$$a_p = \frac{3}{(p-3)(2p+1)} (a_2 a_{p-2} + a_3 a_{p-3} + \cdots + a_{p-2} a_2),$$

where the first terms of the sequence are

$$a_2 = \frac{\pi^4}{15} (\theta_2^4 \theta_3^4 - \theta_2^4 \theta_4^4 + \theta_3^4 \theta_4^4),$$

$$a_3 = \frac{\pi^6}{189} (\theta_2^4 + \theta_3^4) (\theta_4^4 - \theta_2^4) (\theta_3^4 + \theta_4^4),$$

$$\begin{aligned}
 a_4 &= \frac{1}{3} a_2^2, \\
 a_5 &= \frac{3}{11} (a_2 a_3), \\
 a_6 &= \frac{1}{39} (2a_2^3 + 3a_3^2), \\
 &\vdots
 \end{aligned}$$

Kronecker functions $K_{2p}^{0,0}(\tau)$ are related directly to the coefficients $a_p(\tau)$

$$K_{2p}^{0,0}(\tau) = -\frac{(2p)!}{(-4\pi^2)^p} \frac{a_p(\tau)}{(2p-1)}.$$

Kronecker functions $K_{2p}^{1/2,0}(\tau)$ can in their turn be related to the function $K_{2p}^{0,0}(\tau)$ by means of simple resummation of Kronecker's double series

$$K_p^{1/2,0}(\tau) = 2^{1-p} K_p^{0,0}(\tau/2) - K_p^{0,0}(\tau).$$

Thus, Kronecker functions $K_{2p}^{1/2,0}(\tau)$ can all be expressed in terms of the elliptic θ functions only. For practical calculations the following identities are also helpful

$$\begin{aligned}
 2\theta_2^2(2\tau) &= \theta_3^2 - \theta_4^2, \\
 \theta_2^2(\tau/2) &= 2\theta_2\theta_3, \\
 2\theta_3^2(2\tau) &= \theta_3^2 + \theta_4^2, \\
 \theta_3^2(\tau/2) &= \theta_2^2 + \theta_3^2, \\
 2\theta_4^2(2\tau) &= 2\theta_3\theta_4, \\
 \theta_4^2(\tau/2) &= \theta_3^2 - \theta_2^2.
 \end{aligned}$$

From the formulas above we can easily write down the Kronecker functions that have appeared in our asymptotic expansions,

$$K_4^{1/2,0}(\tau) = \frac{1}{30} \left(\frac{7}{8} \theta_4^8 - \theta_2^4 \theta_3^4 \right),$$

$$K_6^{1/2,0}(\tau) = -\frac{1}{84} (\theta_2^4 + \theta_3^4) \left(\frac{31}{16} \theta_4^8 + \theta_2^4 \theta_3^4 \right).$$

Note that when $\xi \rightarrow \infty$ we have limits $\theta_2 \rightarrow 0, \theta_4 \rightarrow 1, \theta_3 \rightarrow 1$. The case $\xi \rightarrow 0$ can be obtained by using Jacobi's imaginary

transformation of the θ functions. In this case $\theta_2 \rightarrow 1/\sqrt{\xi}$, $\theta_4 \rightarrow 0$ and $\theta_3 \rightarrow 1/\sqrt{\xi}$ and the Kronecker's function can again be reduced to the Bernoulli polynomials.

APPENDIX D: ASYMPTOTIC EXPANSION OF THE DIGAMMA FUNCTION $\psi(N+\alpha)$

Let us start with the well known expansion of the digamma function $\psi(N)$ [23],

$$\psi(x) = \ln x - \frac{1}{2x} - \sum_{p=1}^{\infty} \frac{B_{2p}}{2p} \frac{1}{x^{2p}} = \ln x - \sum_{p=1}^{\infty} (-1)^p \frac{B_p}{p} \frac{1}{x^p}. \quad (D1)$$

Plugging in the above expansion $x=N+\alpha$ and expanding the resulting factors $\ln(1+\alpha/N), (1+\alpha/N)^{-p}$ in powers of N^{-1} we obtain

$$\begin{aligned}
 \psi(N+\alpha) &= \ln N - \sum_{p=1}^{\infty} (-1)^p \frac{\alpha^p}{pN^p} \\
 &\quad - \sum_{p=1}^{\infty} \sum_{k=0}^{\infty} (-1)^{k+p} B_p \frac{(p+k-1)!}{k!p!} \frac{\alpha^k}{N^{p+k}} \\
 &= \ln N - \sum_{p=1}^{\infty} (-1)^p \frac{\alpha^p}{pN^p} \\
 &\quad - \sum_{l=1}^{\infty} \sum_{p=1}^l (-1)^l B_p \frac{(l-1)!}{(l-p)!p!} \frac{\alpha^{l-p}}{N^l} \\
 &= \ln N - \sum_{l=1}^{\infty} \sum_{p=0}^l (-1)^l B_p \frac{(l-1)!}{(l-p)!p!} \frac{\alpha^{l-p}}{N^l}. \quad (D2)
 \end{aligned}$$

Using the relation between Bernoulli polynomials B_p^α and Bernoulli numbers B_p

$$B_l^\alpha = \sum_{p=0}^l B_p \frac{l!}{(l-p)!p!} \alpha^{l-p}, \quad (D3)$$

we finally obtain Eq. (40)

$$\psi(N+\alpha) = \ln N - \sum_{p=1}^{\infty} (-1)^p \frac{B_p^\alpha}{p} \frac{1}{N^p}. \quad (D4)$$

[1] M. E. Fisher, in *Critical Phenomena*, Proceedings of International School of Physics "Enrico Fermi," Course 51, 1970, edited by M. S. Green (Academic, New York, 1971).
 [2] M. N. Barber, in *Phase Transition and Critical Phenomena*, edited by C. Domb and J. L. Lebovits (Academic Press, New York, 1983), Vol. 8, p. 145.
 [3] V. Privman, *Finite Size Scaling and Numerical Simulation of*

Statistical Systems, edited by V. Privman (World Scientific, Singapore, 1990).

[4] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed. (Taylor and Francis, London, 1994).
 [5] L. Onsager, Phys. Rev. **65**, 117 (1944).
 [6] B. Kaufman, Phys. Rev. **76**, 1232 (1949).
 [7] A.E. Ferdinand and M.E. Fisher, Phys. Rev. **185**, 832 (1969).

- [8] B. W. McCoy and T. T. Wu, *The Two-Dimensional Ising Model* (Harvard University Press, Cambridge, MA, 1973).
- [9] H.J. Brascamp and H. Kunz, *J. Math. Phys.* **15**, 66 (1974).
- [10] H.W.J. Blote, J.L. Cardy, and M.P. Nightingale, *Phys. Rev. Lett.* **56**, 742 (1986).
- [11] J.L. Cardy, *Nucl. Phys. B* **275**, 200 (1986).
- [12] C.-K. Hu, C.-Y. Lin, and J.-A. Chen, *Phys. Rev. Lett.* **75**, 193 (1995); **75**, 2786(E) (1995); *Physica A* **221**, 80 (1995); C.-K. Hu and C.-Y. Lin, *Phys. Rev. Lett.* **77**, 8 (1996); F.-G. Wang and C.-K. Hu, *Phys. Rev. E*, **56**, 2310 (1997); C.-Y. Lin and C.-K. Hu, *ibid.* **58**, 1521 (1998); Y. Okabe, K. Kaneda, M. Kikuchi, and C.-K. Hu, *ibid.* **59**, 1585 (1999); Y. Tomita, Y. Okabe, and C.-K. Hu, *ibid.* **60**, 2716 (1999); H.-P. Hsu, S.-C. Lin, and C.-K. Hu, *ibid.* **64**, 016127 (2001); H. Watanabe *et al.*, *J. Phys. Soc. Jpn.* **70**, 1537 (2001); C.K. Hu, *J. Phys. A* **27**, L813 (1994).
- [13] C.K. Hu, J.A. Chen, N.Sh. Izmailian, and P. Kleban, *Phys. Rev. E* **60**, 6491 (1999); e-print cond-mat/9905203.
- [14] N.Sh. Izmailian and C.-K. Hu, *Phys. Rev. Lett.* **86**, 5160 (2001).
- [15] N.Sh. Izmailian and C.-K. Hu, *Phys. Rev. E* **65**, 036103 (2002); e-print cond-mat/0009024.
- [16] W.T. Lu and F.Y. Wu, *Phys. Rev. E* **63**, 026107 (2001).
- [17] J. Salas, *J. Phys. A* **34**, 1311 (2001).
- [18] K. Kaneda and Y. Okabe, *Phys. Rev. Lett.* **86**, 2134 (2001).
- [19] W. Janke and R. Kenna, *Phys. Rev. B* **65**, 064110 (2002); e-print cond-mat/0103332.
- [20] E. Ivashkevich, N.Sh. Izmailian, and Chin-Kun Hu, e-print cond-mat/0102470.
- [21] J. Salas, e-print cond-mat/0110287; *J. Phys. A* **35**, 1833 (2002).
- [22] A. Weil, *Elliptic Functions According to Eisenshtein and Kronecker* (Springer-Verlag, Berlin, 1976).
- [23] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1965).
- [24] G. H. Hardy, *Divergent Series* (Clarendon Press, Oxford, 1949).
- [25] Yu. V. Prohorov and Yu. A. Rozanov, *Probability Theory* (Springer-Verlag, New York, 1969).
- [26] G. A. Korn and T. M. Korn, *Mathematical Handbook* (McGraw-Hill, New-York, 1968).