Universal and nonuniversal amplitude ratios for scaling corrections on Ising strips

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We consider strips of Ising spins at criticality. For strips of width N sites, subdominant (additive) finite-size corrections to scaling are assumed to be of the form a_k/N^k for the free energy, and b_k/N^k for inverse correlation length, with integer values of k. We investigate the set $\{a_k,b_k\}$ ($k \geqslant 2$) by exact evaluation and numerical transfer-matrix diagonalization techniques, and their changes upon varying anisotropy of couplings, spin quantum number S, and (finite) interaction range, in all cases for both periodic (PBCs) and free (FBCs) boundary conditions across the strip. We find that the coefficient ratios b_k/a_k remain constant upon varying coupling anisotropy for $S = 1/2$ and first-neighbor couplings, for both PBCs and FBCs (albeit at distinct values in either case). Such apparently universal behavior is not maintained upon changes in S or interaction range.

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I. INTRODUCTION

In this paper we investigate corrections to scaling in critical Ising systems on a strip geometry. Consider a square lattice with N lines and M columns, in the limit $M \to \infty$. Other two-dimensional lattices, such as triangular or honeycomb, can be brought into a squarelike shape by suitable bond additions or deletions. From the largest (Λ_0) and second-largest (Λ_1) eigenvalues of the column-to-column transfer-matrix (TM), one obtains the free energy per spin f_N (in units of k_BT) and spin-spin correlation length ξ_N via [1]

$$N\, f_N = \zeta\, \ln \Lambda_0; \qquad \xi_N^{-1} = \zeta\, \ln \frac{\Lambda_0}{|\Lambda_1|}. \tag{1}$$

The factor ζ is unity for the square lattice and, in triangular and honeycomb geometries (also for the square lattice when the TM progresses along the diagonal [2,3]), corrects for the fact that the physical length added upon each application of the TM differs from one lattice spacing [4]. In all cases of interest here, i.e., ferromagnetic systems, Λ_0 and Λ_1 are both real and positive.

At the critical point T_c where a second-order transition takes place, conformal invariance [5] gives the following relations regarding universal quantities c, the conformal anomaly [6], and the spin scaling dimension x_1 [7]:

$$\lim_{N\to\infty} N^2\,(f_N - f_\infty) - 2N\, f_{\rm surf} = \alpha\pi c; \tag{2}$$

$$\lim_{N\to\infty} N\,\xi_N^{-1} = \beta\pi x_1. \tag{3}$$

In Eq. (2), where $c = 1/2$ for models in the Ising universality class, $f_{\rm surf} = 0$ for strips with periodic boundary conditions (PBCs) across, and nonzero for free (FBCs) or fixed BCs; $\alpha = \frac{1}{6}$ for PBCs, and $\frac{1}{24}$ for FBCs [6]. In Eq. (3), where the exponent x_1 for the Ising universality class is $x_1^b = \frac{1}{8}$ in the bulk, and $x_1^s = \frac{1}{2}$ for the ordinary surface transition, one has $x_1 = x_1^b$, $\beta = 2$ for PBCs, and $x_1 = x_1^s$, $\beta = 1$ for FBCs [7].

Since Eqs. (2) and (3) are expected to be exact only asymptotically, it is of interest to develop a systematic understanding of the corresponding finite-N corrections. We write

$$N\,(f_N - f_\infty) - 2\, f_{\rm surf} = \sum_{k=1}^{\infty} \frac{a_k}{N^k}, \tag{4}$$

$$\xi_N^{-1} = \sum_{k=1}^{\infty} \frac{b_k}{N^k}, \tag{5}$$

where $a_1 = \alpha\pi c$, $b_1 = \beta\pi x_1$. Assuming only integer powers of N^{-1} in Eqs. (4) and (5) is believed to be warranted as long as one is dealing with models in the Ising universality class [8]. We revisit this assumption in Secs. IV and V below. Our task here will be to learn as much as possible about the coefficients $\{a_k, b_k\}$, $k \geqslant 2$, as well as (for reasons explained below) their ratios b_k/a_k. We are interested in their respective universality, or lack thereof, upon changes in boundary conditions, degree of spatial anisotropy of interactions, spin quantum number S, and (finite) interaction range. We restrict ourselves to the square lattice.

In Sec. II we investigate $S = 1/2$ strips with PBCs, first-neighbor interactions, and varying degrees of spatial anisotropy; in Sec. III, we examine systems with FBCs, again with varying anisotropy; Sec. IV deals with the spin-1 case, and isotropic couplings only; in Sec. V we return to $S = 1/2$ and introduce next-nearest-neighbor couplings (keeping to isotropic interactions). Finally, in Sec. VI, concluding remarks are made.

II. PERIODIC BOUNDARY CONDITIONS

A. Preliminaries: Isotropic systems

We recall results for strips cut along the x direction, with N lines and $M \to \infty$ columns, and PBCs across. All eigenvalues of the TM can be written in closed form [1]. With $K_i \equiv J_i/k_BT$ being the interactions respectively along x ($i = 1$) and y ($i = 2$), Λ_0 and Λ_1 are

$$\ln \Lambda_0 - \frac{1}{2} N \ln(2\sinh 2K_1) = \frac{1}{2}\sum_{r=0}^{N-1} \gamma_{2r+1}, \tag{6}$$

$$\ln \Lambda_1 - \frac{1}{2} N \ln(2\sinh 2K_1) = \frac{1}{2}\sum_{r=0}^{N-1} \gamma_{2r}, \tag{7}$$

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where

$$\cosh \gamma_r = \cosh 2K_1^* \cosh 2K_2 - \sinh 2K_1^* \sinh 2K_2 \cos \omega_r; \tag{8}$$

the dual couplings K_i^* are defined by $\tanh K_i^* = \exp(-2K_i)$, and the allowed frequencies are $\omega_r = r\pi/N$.

With $s_i \equiv \sinh 2K_i$, one has $s_1 s_2 = 1$ at the critical temperature where the system is self-dual, and Eq. (8) becomes

$$\cosh \gamma_r = 1 + \frac{1}{s_1^2}(1 - \cos \omega_r) \qquad (T = T_c). \tag{9}$$

For isotropic systems, $s_1 = s_2 = 1$ at criticality. In this case, the sums in Eqs. (6) and (7) were tackled [9] by applying the extended Euler-MacLaurin summation formula [10,11]:

$$\sum_{n=0}^{N-1} F(a + nh + \alpha h) = \frac{1}{h}\int_a^b F(x)\,dx + \sum_{k=1}^{\infty} \frac{h^{k-1}}{k!} B_k(\alpha) \times [F^{(k-1)}(b) - F^{(k-1)}(a)], \tag{10}$$

where $h = (b - a)/N$, $F^{(j)}(x)$ is the jth derivative of $F(x)$, $0 < \alpha < 1$, and the $B_k(\alpha)$ are the periodic Bernoulli polynomials [related to the Bernoullli *numbers*, denoted simply by B_k, by $B_k = B_k(0)$].

It was found that only odd powers of N^{-1}, i.e., $k = 2j - 1$, $j \geqslant 1$ occur in Eqs. (4) and (5); this can be traced back to the fact that the Bernoulli numbers B_m obey $B_{2m-1} = 0$ $(m > 1)$. Also, relatively simple closed-form expressions were derived for all a_k and b_k. Such expressions reproduce previously known exact results (for a_1 [6], b_1 [7], and b_3 [12]), and are in very good agreement with numerically obtained ones [13]. Furthermore, although the coefficients themselves are nonuniversal (upon changing lattice structure, or considering quantum Ising chains [14–16] instead of their two-dimensional classical counterparts), their ratio is found to remain constant upon the same set of changes [9]:

$$\frac{b_k}{a_k} = \frac{2^{k+1} - 1}{2^k - 1} \qquad (k = 2j - 1,\ j \geqslant 1)\,[\text{PBC}]. \tag{11}$$

It should be noted that when one considers the TM running along the diagonal of the square lattice (as in Refs. [2] and [3]), one gets for isotropic systems with PBCs the same value for the ratio b_k/a_k as in Eq. (11). Furthermore, the coefficients themselves have the same absolute value as those found with the TM along x, only they alternate in sign: $a_k, b_k < 0$ for $k = 1$, positive for $k = 2$, etc. [17].

B. Anisotropic systems with PBCs

With $K_1/K_2 \equiv R \neq 1$, one gets [18,19] the corresponding forms of Eqs. (2) and (3) [specializing to Ising spins on strips with PBCs] as

$$\lim_{N\to\infty} N^2 (f_{N(i)} - f_\infty) = \frac{1}{s_i}\frac{\pi}{12}, \tag{12}$$

$$\lim_{N\to\infty} N \left[\xi_{N(1)}^{-1}\,\xi_{N(2)}^{-1}\right]^{1/2} = \frac{\pi}{4}, \tag{13}$$

where $f_{N(i)}$ and $\xi_{N(i)}$ are, respectively, free energy and correlation length at criticality, both calculated by iterating the TM along the direction with couplings K_i. Note [18] that f_∞ in Eq. (12) also depends on R. $s_1 \equiv \sinh 2K_c$ is the solution of $\sinh 2K_c \sinh 2RK_c = 1$.

As noted in Ref. [9], Eq. (9) can be rewritten as

$$\gamma(\omega) = 2\,\ln(u + \sqrt{1 + u^2}), \qquad u \equiv \frac{1}{s_1}\sin\frac{\omega}{2}. \tag{14}$$

In this form, it is immediate to see that anisotropy brings about a simple rescaling of the argument in the sums of Eqs. (6) and (7). Furthermore, in the Euler-Maclaurin formula, $\gamma(\omega)$ only occurs through its derivatives of nth order $\gamma^{(n)}$ at the end points $\omega = 0$ and π, which satisfy $\gamma^{(n)}(\pi) = -\gamma^{(n)}(0)$; see Eq. (14). This is enough to guarantee that any coefficient $a_k(R)$ [$b_k(R)$] will differ from its isotropic counterpart $a_k(1)$ [$b_k(1)$] by a multiplicative correction, $g_k(s_1)$. Thus it is predicted in Ref. [9] that the ratios given in Eq. (11) will remain unchanged. In this context, Eqs. (12) and (13) reflect the (easily checkable) fact that $g_1(s_1) = s_1^{-1}$, where for Eq. (13) one also uses $s_1 s_2 = 1$ at criticality.

In order to test the robustness of the theoretical framework just expounded, we evaluated the third-order correction. This is done by replacing the argument of Eqs. (6) and (7) by its generalized form, Eq. (14), and following the corresponding effects on the N^{-3} term in Eq. (10), which arise from the third-order derivatives indicated there. One finds

$$g_3(s_1) = \frac{1}{2s_1^2}\left(s_1 + \frac{1}{s_1}\right) = \frac{1}{2s_1 t_1^2}, \tag{15}$$

where $t_1 \equiv \tanh 2K_1$.

We numerically calculated f_N and ξ_N^{-1} from Eqs. (1), (6), and (7) for assorted values of R, and $N = 10j$, $j = 2,3\ldots 30$. The resulting sequences were adjusted to

$$f_N(R) = f_\infty(R) + \frac{1}{s_1}\frac{\pi}{12N^2} + \frac{a_3(R)}{N^4} + \frac{a_5(R)}{N^6}, \tag{16}$$

$$\xi_N^{-1}(R) = \frac{1}{s_1}\frac{\pi}{4N} + \frac{b_3(R)}{N^3} + \frac{b_5(R)}{N^5}, \tag{17}$$

where f_∞, $\{a_k\}$, and $\{b_k\}$ are adjustable parameters. It is important to keep the next-higher-order terms a_5 and b_5 in the truncated expansions above, in order to improve stability for the quantities a_3 and b_3, which are the main focus of interest here. The optimum range of N, large enough for higher-order terms to have negligible influence but not so large as to compromise the numerical accuracy of fits (since this depends crucially on differences between finite-N estimates of f_N and ξ_N^{-1}), was found to be $100 \leqslant N \leqslant 300$. In Fig. 1 we show $a_3(R)$ and $b_3(R)$, fitted via Eqs. (16) and (17), for several values of R spanning four orders of magnitude. The continuous lines depict Eq. (15), multiplied respectively by the isotropic values $a_3(1) = 7\pi^3/1440$, $b_3(1) = \pi^3/96$ [9,12,13]. The agreement is perfect, except for $a_3(R)$ at $R \gtrsim 30$ where reasonable convergence was only obtained upon adding the next higher-order term, $a_7(R)/N^8$, in Eq. (16).

Our results provide direct numerical evidence that the Euler-Maclaurin scheme used in Ref. [9] is indeed applicable to Ising systems with PBCs and any finite degree of (ferromagnetic) anisotropy. Similar conclusions were drawn for the anisotropic Ising model with Braskamp-Kunz boundary conditions [20].

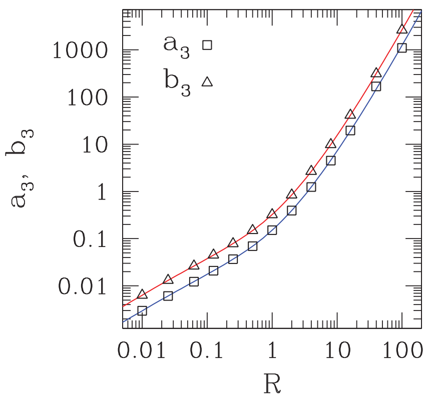

FIG. 1. (Color online) Points: results for $a_3(R)$, $b_3(R)$ defined in Eqs. (16) and (17), from fits of f_N, ξ_N^{-1} data evaluated for strips of widths $100 \leqslant N \leqslant 300$ and PBCs across, via Eqs. (1), (6), and (7). Uncertainties are smaller than symbol sizes. Full lines show $g_3(s_1)$ defined in Eq. (15), multiplied respectively by $a_3(1)$ (blue) and $b_3(1)$ (red) (see text).

It is interesting to consider the above results for $R \to \infty$. It is known [15,16,21,22] that the (zero-temperature) quantum Ising chain (QIC) in a transverse field [14] has a correspondence with this extreme anisotropic limit, via $f_\infty \leftrightarrow E_0$, $\xi^{-1} \leftrightarrow E_1 - E_0$, etc., where the E_i are the energy levels of the quantum system. In Ref. [9] the energy spectrum of the QIC with PBCs was studied directly with help of the Euler-Maclaurin formula, and the corresponding ratio b_k/a_k was found to obey Eq. (11). The latter result can also be extracted from the exact expressions Eqs. (17a) and (18a) of Ref. [21].

While the limit given in Eq. (13) is preserved as $R \to \infty$, the exponential divergence of the higher-order terms is not canceled:

$$\left[\xi_{N(1)}^{-1}\xi_{N(2)}^{-1}\right]^{1/2} = \frac{\pi}{4N} + \frac{1}{4}\left(s_1 + \frac{1}{s_1}\right)^2 \frac{\pi^3}{96N^3} + \cdots. \quad (18)$$

A similar effect (with the factor $1/s_1$) is already obvious in Eq. (12). In summary, although coefficient ratios b_k/a_k are preserved as $R \to \infty$, each term of the Euler-Maclaurin expansion for the two-dimensional Ising model with $R \gg 1$ is translated into its counterpart of the corresponding expansion for the QIC by means of a distinct anisotropy factor.

III. FREE BOUNDARY CONDITIONS

A. Isotropic systems

The eigenvalue spectrum of the TM has been obtained [23–25] for Ising $S = 1/2$ strips with nearest-neighbor couplings and free boundary conditions (FBCs) across. For a strip of width N sites, one has

$$\ln \Lambda_m = \frac{1}{2}\sum_{i=1}^{N} \pm\gamma(\omega_i), \quad m = 0, \ldots, 2^N - 1, \quad (19)$$

where the $\pm$ combinations run through all 2^N possibilities. A regular background term, $\frac{1}{2}N\ln(2\sinh 2K_1)$ [see Eqs. (6) and (7)], has been omitted. With all the $\gamma(\omega_i)$ real and positive for this case [23],

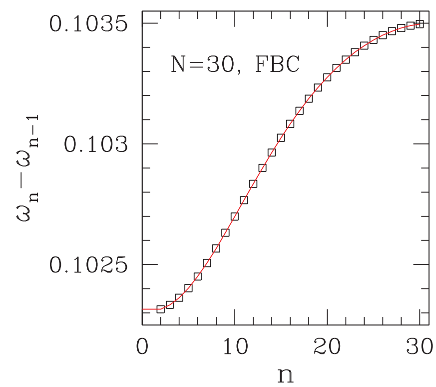

FIG. 2. (Color online) Ising strips with FBC and isotropic interactions, at T_c: differences $\omega_n - \omega_{n-1}$ ($n \geqslant 2$) between consecutive solutions of Eqs. (26) and (27), for strip of width $N = 30$ sites.

$$\ln \Lambda_0 = \frac{1}{2}\sum_{n=1}^{N} \gamma(\omega_n); \quad (20)$$

$$\xi_N^{-1} = \gamma(\omega_1), \quad (21)$$

where ω_1 corresponds to the smallest γ. The relationship between the γ and the allowed frequencies ω_i is given by [23]

$$\cosh\gamma = \cosh 2K_1^* \cosh 2K_2 - \sinh 2K_1^* \sinh 2K_2 \cos\omega; \quad (22)$$

$$\sinh\gamma \cos\delta^* = \sinh 2K_2 \cosh 2K_1^* - \cosh 2K_2 \sinh 2K_1^* \cos\omega; \quad (23)$$

$$\sin\omega/\sinh\gamma = \sin\delta^*/\sinh 2K_1^*. \quad (24)$$

From Eqs. (22)–(24), one gets at the critical point, where $s_1 s_2 = 1$,

$$\cosh\gamma = 1 + \frac{1}{s_1^2}(1 - \cos\omega); \quad (25)$$

$$\tan\delta^* = t_1 \frac{\sin\omega}{(1 - \cos\omega)}, \quad (26)$$

again with $t_1 \equiv \tanh 2K_1$. From Eq. (25), the smallest γ corresponds to the lowest allowed ω. Note also that Eq. (25) is identical in form to Eq. (9), so it can also be rewritten as Eq. (14). Finally, the allowed frequencies ω_n can be determined from Eq. (26) combined with the quantization condition [23]:

$$e^{iN\omega} = \pm e^{i\delta^*}, \quad 0 \leqslant \omega \leqslant \pi, \quad (27)$$

by eliminating the auxiliary angle δ^*. For the remainder of this subsection, we shall consider only isotropic systems ($K_1 = K_2$), thus $s_1 = 1$, $t_1 = 1/\sqrt{2}$ in Eqs. (25) and (26).

The resulting frequencies are not equally spaced, as illustrated in Fig. 2. So the Euler-Maclaurin formula cannot be used in the same way as in Ref. [9] to calculate the free energy from Eq. (20). However, we show in the following that one can still make adaptations and extract some useful information. We

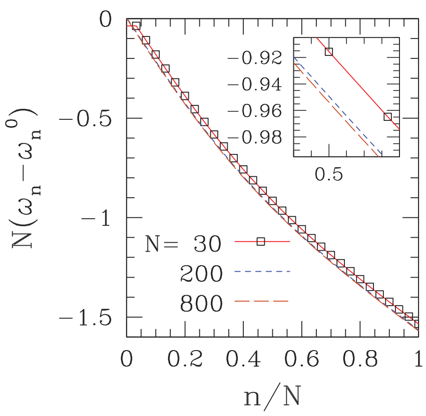

FIG. 3. (Color online) Ising strips with FBC and isotropic interactions, at T_c: illustrating the convergence of $N(\omega_n - \omega_n^0)$ toward $f(n/N)$ with increasing N; see Eq. (28). The inset is a blowup of the central section of the main figure.

found that for large N the ω_n approach the form

$$\omega_n = \omega_n^0 + \frac{1}{N}\, f\left(\frac{n}{N}\right), \quad \omega_n^0 \equiv \left(n - \frac{1}{2}\right)\frac{\pi}{N}, \quad 1 \leqslant n \leqslant N. \tag{28}$$

As shown in Fig. 3, $f(u)$ is a smoothly varying function of $u = n/N$. One has $f(0) = 0$, $\lim_{u\to 1} f(u) = -\pi/2$. Both limits can be understood by examination of the graphical solutions of Eqs. (26) and (27) [25]. The residual N dependence of $N(\omega_n - \omega_n^0)$ is highlighted in the inset of Fig. 3. This can be accounted for by an additive correction of the form $(1/N)\, f_2(n/N)$; f_2 is nearly constant, varying smoothly between ≈1.1 and 1.3 for $0 < n/N < 1$. We thus write

$$\gamma(\omega_n) = \gamma(\omega_n^0) + \sum_{j=1}^{\infty} \frac{1}{N^j}\, g^{(j)}(\omega_n^0), \tag{29}$$

with

$$g^{(1)}(\omega_n^0) \equiv \{f(\omega)\,\gamma^{(1)}(\omega)\}_{\omega_n^0},$$
$$g^{(2)}(\omega_n^0) \equiv \left\{f_2(\omega)\,\gamma^{(1)}(\omega) + \frac{1}{2!}\, f^2(\omega)\,\gamma^{(2)}(\omega)\right\}_{\omega_n^0} \ldots, \tag{30}$$

where $\gamma^{(m)} \equiv d^m\gamma/d\omega^m$, and the arguments of f and f_2 have been straightforwardly changed. Eq. (20) then becomes

$$\ln \Lambda_0 = \frac{1}{2}\sum_{n=1}^{N} \gamma(\omega_n^0) + \frac{1}{2N}\sum_{n=1}^{N} g^{(1)}(\omega_n^0) + \cdots \equiv \sum_{j=0}^{\infty} S_j. \tag{31}$$

So, each term [of order $j \geqslant 0$, with $g^{(0)}(\omega_n^0) \equiv \gamma(\omega_n^0)$] of the Taylor expansion indicated in Eq. (29) gives rise to a sum S_j of N terms, each of the latter evaluated at $\omega = \omega_n^0$ $(1 \leqslant n \leqslant N)$, i.e., at equally spaced intervals.

We investigated the feasibility of applying the Euler-Maclaurin formula, Eq. (10), to each S_j, with $x = \omega$, $h = \pi/N$, $a = 0$, $b = \pi$, $\alpha = 1/2$, so that the result would be of the form $S_j = \sum_{i=-1}^{\infty} a_i^j/N^{(i+j)}$ [where $i = -1$ corresponds to the integral in Eq. (10)]. S_j would then give contributions to $\ln \Lambda_0$ at all orders $N^{-(j+i)}$, $i \geqslant -1$. Note that $a_0^j \equiv 0$ because $B_1(1/2) = 0$ [10,11]. However, one would have to assume that the infinite sum implicit in each Taylor series commutes with the infinite sum present in each separate Euler-Maclaurin expansion [the form given in Eq. (10) assumes that the remainder term vanishes; see, e.g., Ref. [11]]. Having in mind that the expansion parameter of the Taylor series and the sampling interval of the Euler-Maclaurin formula can be of the same order (π/N), it is doubtful that such commutation can be guaranteed. With these words of caution in mind, here we evaluate only a few of the lowest-order terms which would occur in such a calculational framework.

We applied the Euler-Maclaurin formula to S_0 in Eq. (31). This differs from the sum indicated in its PBC counterpart, Eq. (6), in that the frequency spacing here is half that in the latter equation. For the corresponding integral of Eq. (10), this is compensated by the fact that the integration interval is cut in half as well, so from a_{-1}^0 one reobtains the bulk result $f_\infty - (1/2)\ln 2 = (2G/\pi)$, $G = 0.915\,965\,594\ldots$ (Catalan's constant) [1]. For the terms of Eq. (10) involving derivatives of the mth order, the corresponding term in S_0 has an extra factor $2^{-(1+m)}$ relative to its PBC analog [9]. One gets $a_1^0 = \pi/48$ as given by conformal invariance [6], $a_3^0 = 0.009\,42\ldots$ [9].

For S_1, we evaluated $I \equiv \int_0^\pi g^{(1)}(\omega)\,d\omega$ using finite-N approximations for $f(x)$ with $200 \leqslant N \leqslant 2000$, and extrapolating the resulting sequence against $1/N$. The final result is $I/2\pi = a_{-1}^1 = -0.181\,730\,9(1)$, to be compared with $2f_{\rm surf} = -0.181\,731\,48\ldots$ [27]. In the computation of higher-order terms, we ran into inconsistencies between results thus obtained and those coming from direct numerical evaluation of the free energy via Eq. (20). We conjecture that these difficulties stem from the conceptual problems in interchanging the order of infinite sums, referred to above.

As regards the correlation length, from Eq. (21) above, and combining Eqs. (3) and (14), one has for the finite-N estimate $\eta_1^s(N)$ of the decay-of-correlations exponent $\eta_1^s = 2x_1^s$

$$\eta_1^s(N) = \frac{2N}{\pi}\ln\left[y + \sqrt{y^2+1}\right], \quad y = 2 - \cos\omega_1. \tag{32}$$

By solving Eqs. (26) and (27) in the limit $\omega \to 0$, $\delta^* \to \pi/2$, and consequently taking $y \to 1$ in Eq. (32), one gets

$$\eta_1^s(N) = 1 - \frac{1}{\sqrt{2}}\frac{1}{N} + \left[\frac{1}{2} - \frac{\pi^2}{48}\right]\frac{1}{N^2} + \mathcal{O}(N^{-3}). \tag{33}$$

According to Eq. (33), both odd and even powers of N^{-1} are predicted to arise in the expansion of ξ_N^{-1} for this case. For Ising systems with FBCs, the occurrence of N^{-1} corrections to finite-N estimates of scaling powers was noted in Ref. [26]. We evaluated f_N and ξ_N for $N = 10j$, $j = 2,\ldots,30$, by numerically solving for the allowed frequencies and then plugging the results into Eq. (25) and, finally, Eq. (19).

We fitted free-energy data for $100 \leqslant N \leqslant 300$ to a truncated form of Eq. (4), with $k \leqslant 4$. After ensuring that known quantities were reproduced to good accuracy when allowed to vary freely, we fixed them at their known values, namely $f_\infty = (1/2)\ln 2 + (2G/\pi)$ [1]; $f_{\rm surf} = -0.090\,865\,7\ldots$ [27]; $a_1 = \pi/48$, with the results $a_2 = -0.046\,16(2)$, $a_3 = 0.024(1)$, $a_4 = 0.69W(6)$. Note that a_3 as given here differs from a_3^0 evaluated from S_0 above, in connection with Eq. (31). This is because a_3 gets additional contributions from higher-order sums S_k, $k > 0$ (not calculated there).

A fit of a subset ($100 \leqslant N \leqslant 300$) of the $\eta_1^s(N)$ thus obtained to the form $\eta_1^s(N) = \eta_1^s + \sum_{k=1}^4 b'_k N^{-k}$ gave $\eta_1^s = 1$ ($\pm 1 \times 10^{-10}$), $b'_1 = -0.707\,106\,80(3)$, $b'_2 = 0.294\,388(7)$, $b'_3 = 0.2274(7)$, $b'_4 = -0.68(3)$. By keeping η_1^s, b'_1, b'_2 fixed at the respective values predicted in Eq. (33), we obtained $b'_3 = 0.227\,972(6)$, $b'_4 = -0.7013(6)$. The above results both confirm the predictions of Eq. (33) for b'_1 and b'_2, and indicate that, in general, both even and odd powers of N^{-1} occur in the expansion whose lowest-order terms are given in that equation. We defer analysis of the ratios b_k/a_k thus obtained until the next subsection, where anisotropic systems with FBCs, and their connection to the QIC with free ends, are discussed.

B. Anisotropic systems with FBC

We first note that, even though Eq. (14) is valid here, the arguments given immediately below it do not seem to cover the present case, since for FBCs the ω_n depend on anisotropy in the nontrivial way given in Eqs. (26) and (27). Thus it is not obvious whether, e.g., Eq. (15) still applies to the free energy here.

We have directly examined the ω_n, for varying anisotropies, and have seen that their behavior is qualitatively similar to that for the isotropic case, depicted in Figs. 2 and 3. In particular, the limits $f(0) = 0$ and $f(1) = -\pi/2$ still hold [see the comments following Eq. (28)].

By incorporating anisotropy into Eq. (32) via Eq. (14), one gets the generalized version of Eq. (33):

$$\eta_1^s(N) = \frac{1}{s_1}\left\{1 - \frac{1}{2t_1}\frac{1}{N} + \frac{1}{2t_1^2}\left[\frac{1}{2} - \frac{\pi^2}{48}\right]\frac{1}{N^2}\right\} + \cdots. \quad (34)$$

We numerically calculated f_N and ξ_N^{-1} from Eqs. (1), (20), and (21) for assorted values of R, and $N = 10j$, $j = 2,3\ldots30$. Bearing in mind the FBC-adapted forms of Eqs. (12) and (13) [18,19], the resulting sequences were adjusted to

$$N(f_N - f_\infty) = 2f_{\rm surf} + \frac{1}{s_1}\frac{\pi}{48N} + \sum_{k=2}^{4}\frac{a_k(R)}{N^k}, \quad (35)$$

$$\xi_N^{-1}(R) = \frac{1}{s_1}\frac{\pi}{2N} + \sum_{k=2}^{4}\frac{b_k(R)}{N^k}, \quad (36)$$

where f_∞, $f_{\rm surf}$ (both of which, as well as f_N, also depend on R), $\{a_k\}$, and $\{b_k\}$ are adjustable parameters. The b'_k, defined in connection with Eqs. (32) and (33) relate to the b_k of Eq. (36) by $b_k = (\pi/2)\,b'_{k-1}$. As done in Sec. II, we keep the next-higher-order terms a_4 and b_4 in the truncated expansions above, in order to improve stability for the quantities a_2, a_3, b_2, and b_3, which are the main focus of interest here. Similarly, the range of N used in our fits was $100 \leqslant N \leqslant 300$. In Fig. 4 we show $a_2(R)$, $a_3(R)$, $b_2(R)$, and $b_3(R)$, fitted via Eqs. (35) and (36), for several values of R spanning four orders of magnitude. The lines depict the anisotropy factors from Eq. (34), namely $g_2 \equiv (2s_1t_1)^{-1}$ (dashed) and $g_3 \equiv (2s_1t_1^2)^{-1}$ (full) multiplied by the pertinent values of $a_2(1)$ and $b_2(1)$ (for g_2) or $a_3(1)$ and $b_3(1)$(for g_3). Once again, the agreement is perfect. The only case for which the higher-order terms (a_4 or b_4) made any perceptible difference was for $a_3(R)$ at $R \gtrsim 30$.

Our results provide direct numerical evidence that the coefficient ratios $b_2/a_2 = 24.06(2)$ and $b_3/a_3 = 19.3(6)$

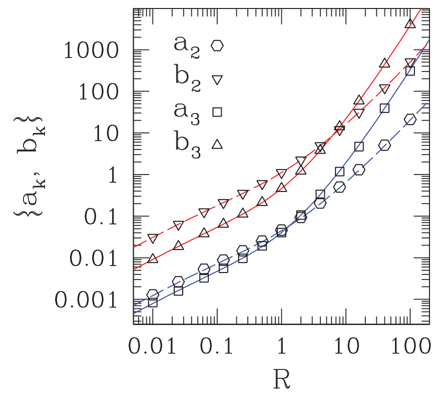

FIG. 4. (Color online) Points: results for $\{a_k(R), b_k(R)\}$ defined in Eqs. (35) and (36) [absolute values for $k = 2$], from fits of f_N, ξ_N^{-1} data evaluated for strips of widths $100 \leqslant N \leqslant 300$ and FBCs across. Uncertainties are smaller than symbol sizes. Lines show anisotropy factors defined in Eq. (34), multiplied respectively by $a_k(1)$ (blue) and $b_k(1)$ (red) ($k = 2,3$) (see text).

remain constant against any finite degree of (ferromagnetic) anisotropy. Note that b_3/a_3 differs substantially from the PBC value 15/7 [9]. It is remarkable that the free-energy coefficients depend on anisotropy in the same way as those for the correlation length. As stated in the first paragraph of this section, this is not obviously granted at the outset.

We consider the extreme anisotropic limit $R \to \infty$ of Ising strips with FBCs, and its connection to the QIC with FBCs at both ends [14,21]. In Ref. [28], the exact expressions for ground-state energy and energy gaps of the QIC, given in Ref. [14], were written as Euler-Maclaurin expansions; similarly to the PBC case, only odd powers of N^{-1} were found to occur in the corresponding forms of Eqs. (4) and (5). The counterpart to Eq. (11) in this case was shown to be

$$\frac{b_k}{a_k} = \frac{2(k+1)}{(2^k-1)\,B_{k+1}} \quad (k = 2j-1,\ j \geqslant 1)\ \text{(FBC)}. \quad (37)$$

For $k = 1$, this agrees with the conformal-invariance results of Eqs. (2) and (3); for $k = 3$, Eq. (37) gives $b_3/a_3 = -240/7$ [28].

Our results above for classical Ising spins differ from those for the QIC in that (i) both even and odd powers of N^{-1} occur, in free-energy as well as in correlation-length expansions; and (ii) $b_3/a_3 = +19.3(6)$, incompatible with the value given in Ref. [28]. Note however that, when one considers the two-dimensional classical Ising model with the TM running along the diagonal [3], in the corresponding version of FBCs, a picture closer to that found for PBCs emerges, namely [29] that only odd powers of N^{-1} occur in Eqs. (4) and (5), and the value $b_3/a_3 = -240/7$ is reproduced.

IV. $S = 1$

We considered $S = 1$ Ising systems on a square lattice, with both PBCs and FBCs, and isotropic couplings only. The critical temperature is known rather accurately [30], $J/k_BT_c = K_c = 0.590\,473(5)$.

In this case, no closed-form expressions for the TM eigenvalues are forthcoming, so one must rely on numerical

TABLE I. For $S = 1/2$ and 1, coefficients a_k, b_k from Eqs. (4) and (5), and their ratios b_k/a_k. Columns 2 and 4: calculated from fits of free-energy and correlation-length data for strips with PBCs across, and $10 \leqslant N \leqslant 16$, to truncated forms of those equations (see text). Quoted uncertainties refer exclusively to the fitting procedures, i.e., no account is taken of likely systematic errors. Column 3: exact values from Ref. [9].

Type	$S = 1/2$, fit	$S = 1/2$, exact	$S = 1$, fit
a_3	0.15082(1)	0.15073...	0.14772(2)
a_5	0.365(1)	0.39214...	0.313(3)
b_3	0.32305(1)	0.322982...	0.2212(2)
b_5	0.766(3)	0.79692...	0.11(5)
b_3/a_3	2.1420(3)	2.142857...	1.497(2)
b_5/a_5	2.098(3)	2.032258...	0.35(16)

diagonalization. The first consequence of this fact is that the assumption of only integer powers in Eqs. (4) and (5) must be reanalyzed. Indeed, while in Secs. II and III one could verify directly from the respective closed-form equations that no noninteger powers of N^{-1} were allowed, here this possibility does not arise. Furthermore, it has been shown for models very closely related to the standard Ising model that fractional powers occur in corrections to scaling [31,32]. It was conjectured that these would take the form $N^{-4/3}$, clearly a very important term in the current context. However, for the $S = 1$ Ising model on a square lattice, it has been numerically shown that the amplitude of a hypothetical $N^{-4/3}$ term is most likely zero [32], so in the current section at least, one can retain Eqs. (4) and (5) in their original form.

Second, the range of strip widths within practical reach is much restricted in comparison with $S = 1/2$ systems. We used $4 \leqslant N \leqslant 16$. Such a narrow range was, by far, the most quantitatively relevant source of systematic inaccuracies in our estimates of corrections to scaling, far outweighing, e.g., the uncertainties in T_c.

In order to assess the associated effects, we produced fits of free-energy and correlation-length data for sets of $S = 1/2$ data restricted to the same range of N. For PBCs, we took truncated forms of Eqs. (4) and (5) using the exact values of f_∞, a_1, and b_1, with $\{a_k,b_k\}$ as adjustable parameters for $k = 3,5,7$, and zero otherwise. The $k = 7$ terms were included in order to increase stability for the $k = 3$ and 5 ones. By further restricting the range of data fitted to $10 \leqslant N \leqslant 16$, we found very good agreement with the known values [9,13] of a_3, b_3, while for a_5 and b_5 deviations were of order 5% (see Table I).

Turning to $S = 1$ with PBCs, allowing for a_2, $b_2 \neq 0$ in Eqs. (4) and (5) gave fitted values of order 10^{-3}–10^{-4} (compared with a_3, b_3 of order 10^{-1}). We take this as signaling that, very likely, $a_2 = b_2 \equiv 0$. Taking a_4, $b_4 \neq 0$ produced uncertainties of 50% or more in the corresponding estimates. This latter fact does not provide as compelling an argument to assume $a_4 = b_4 = 0$ as the preceding one for a_2, b_2. However, in view of the limited number of data available for fitting, we decided that this was the most prudent route to take.

Using $10 \leqslant N \leqslant 16$ and proceeding as described above for $S = 1/2$, we found the results shown in the last column of Table I. Even assuming the systematic error in this case to be two orders of magnitude larger than that for $S = 1/2$, one gets $b_3/a_3 = 1.50(6)$, still at least 10 error bars away from encompassing the $S = 1/2$ value. We refrain from attaching much significance to the estimates of b_5/a_5, due to the large uncertainty in b_5.

For $S = 1$ systems with FBCs, we fixed $a_1 = \pi/48$ [6], $b_1 = \pi/2$ [7]. Upon extrapolation of both PBC and FBC data, the nonuniversal bulk free energy is estimated as $f_\infty = 1.317\,600(1)$. The surface free energy is $f_{\rm surf} = -0.095\,187(1)$. Although the latter quantities are immediate byproducts of TM calculations, their value for $S = 1$ Ising spins on a square lattice does not seem to be available in the published literature [33]. Free-energy fits assuming a_2, a_3, and a_4 as free parameters (the latter, for the purpose of stabilization of the former two), $a_k \equiv 0$ for $k \geqslant 5$, gave $a_2 = -0.0238(2)$, $a_3 = 0.019(3)$, i.e., both of the same order of magnitude, contrary to the corresponding case for PBCs. With similar assumptions for fits of correlation-length data, we obtained $b_2 = -0.5719(1)$, $b_3 = -0.562(1)$.

V. SECOND-NEIGHBOR COUPLINGS

For square-lattice $S = 1/2$ spins with nearest-neighbor (next-nearest-neighbor) couplings J (J'), we considered both interactions ferromagnetic and $J'/J = 1$. Again, the critical point is known to excellent accuracy [34], $K_c = 0.190\,192\,680\,7(2)$.

Once more, one must use numerical diagonalization of the TM since no closed-form expressions are available for the eigenvalues. We took $4 \leqslant N \leqslant 22$, a significantly broader range than was feasible for $S = 1$ in the preceding section, but not in any way comparable to the leeway one has for $S = 1/2$ with first-neighbor interactions only.

Similarly to Sec. IV, one must investigate whether noninteger powers show up in the corrections to scaling, $N^{-4/3}$ being a likely candidate [31,32]. We did this by fitting our PBC free-energy and correlation-length data, respectively, to

$$f_N = f_\infty + \frac{\pi}{12N^2} + \frac{a_{x_f}}{N^{x_f}};$$
$$\xi_N^{-1} = \frac{\pi}{4N} + \frac{b_{x_\xi}}{N^{x_\xi}}, \tag{38}$$

where the adjustable powers x_f, x_ξ represent the dominant nonuniversal corrections. From fits of data in the range $[N_0,22]$, we found $x_f = 3.83(2)$, $3.971(3)$, $3.981(3)$, respectively, for $N_0 = 4$, 12, and 16, and $x_\xi = 2.78(3)$, $2.921(6)$, and $2.937(3)$ for the same sequence of N_0. So it is apparent that $x_f \to 4$, $x_\xi \to 3$ with increasing N. Comparing with Eqs. (4) and (5), we conclude for the absence of fractional powers such as $N^{-4/3}$ here.

For strips with PBCs across, our analysis was then conducted along the lines described for $S = 1$ in Sec. IV. Contrary to the $S = 1$ case, allowing for a_7, $b_7 \neq 0$ did not improve stability of lower-order coefficients, and we decided to keep both to zero. The optimum range of widths for our fits was now $15 \leqslant N \leqslant 22$. We found $a_3 = -0.096\,26(6)$, $a_5 = 0.210(4)$; $b_3 = -0.3305(3)$, $b_5 = 1.96(1)$. From this, we estimate $b_3/a_3 = 3.43(1)$, which is again at variance with the $S = 1/2$ value [9] $15/7 = 2.142\,86\ldots$.

For FBCs, the known universal coefficients are $a_1 = \pi/48$ [6], $b_1 = \pi/2$ [7]. Combining PBC and FBC data, the extrapolated free energy per site is $f_\infty = 0.829\,264\,62(1)$, while the surface free energy is $f_{\rm surf} = -0.089\,538\,5(1)$. Estimates for these quantities are not quoted in published work on the next-nearest-neighbor $S = 1/2$ Ising model using TM techniques [33,34]. We attempted free-energy fits, at first using a_2, a_3, and a_4 as free parameters, and $a_k \equiv 0$ for $k \geqslant 5$. Similarly to the PBC case, allowing a_4 to vary did not improve stabilization of a_2 or a_3, so we set $a_4 \equiv 0$. We thus found $a_2 = 0.009\,94(2)$, $a_3 = -0.0096(1)$. From fits of correlation-length data, we obtained $b_2 = 0.232\,36(3)$, $b_3 = -0.529(1)$.

VI. DISCUSSION AND CONCLUSIONS

We have examined subdominant corrections to scaling for critical Ising systems on strip geometries. One of our main goals has been to check the extent to which the constant value of coefficient ratios, expressed in Eq. (11), remains valid within the broader Ising universality class.

In Sec. II we considered Ising $S = 1/2$ systems, on strips with PBCs across. We investigated the effects of anisotropic interactions, extending the framework introduced in Refs. [18] and [19], and providing numerical evidence that the nonuniversal coefficients a_3 and b_3 of Eqs. (4) and (5) indeed follow the prediction given by Eq. (15). As a byproduct, the validity of Eq. (11) has been directly verified within four orders of magnitude of anisotropy variation for this case.

In Sec. III, for strips of spin-1/2 systems with FBCs along one of the coordinate axes, we examined ways in which the nonconstant frequency spacing in the eigenvalue spectrum can be dealt with, in order to make the sum in Eq. (20) amenable to treatment via the Euler-Maclaurin summation formula. The lowest-order terms of the resulting expansion are shown to agree with known results.

From the correlation-length expression, Eq. (21), we showed directly that both odd and even powers of inverse strip width are expected in corrections to scaling, and explicitly evaluated the two lowest-order nonuniversal coefficients [see Eq. (33)]. Generalization to anisotropic systems is given in Eq. (34), where one can see that the first- and third-order anisotropy factors (respectively, $1/s_1$ and $1/2s_1t_1^2$) are the same as those for PBCs [see Eqs. (12), (13), and (15)]. We also found numerically that the amplitude ratios b_k/a_k remain constant, for $k = 2$ and 3, upon introduction of anisotropic couplings.

Sections IV and V deal, respectively, with $S = 1$ systems with first-neighbor interactions, and spin-1/2 ones with both first- and second-neighbor couplings. For PBCs we find that, in both cases, the ratio b_3/a_3 differs considerably from the value $15/7 = 2.142\,857\ldots$ found in Ref. [9] for $S = 1/2$, first-neighbor couplings only. We quote $b_3/a_3 = 1.50(6)$ for the former, and 3.43(1) for the latter. For FBCs, comparison of b_k/a_k ratios with those pertaining to $S = 1/2$ systems gives $b_2/a_2 = 24.0(2)$ ($S = 1$), 23.4(1) (next-nearest neighbor), 24.06(2) ($S = 1/2$, first neighbor). Although the error bars do not quite overlap, it appears that a constant value of this ratio cannot be definitely discarded. However, no such regularity is seen for b_3/a_3, its value being, respectively, $-30(5)$, $+55(1)$, and $+19.3(6)$ in each case.

Overall, it seems that both even and odd powers of N^{-1} always show up in Eqs. (4) and (5), for critical Ising strips with FBCs along one coordinate axis. On the other hand, for PBCs only odd ones occur. Concurring remarks can be found in the literature [12,26]; however, it seems difficult to prove such a statement rigorously. So far, one has to rely on case-by-case analyses, as was done here. As pointed out at the end of Sec. III, considering the version of FBCs with the TM running along the diagonal [3] is enough to restore a picture very similar to that holding for PBCs [29]. Thus the behavior of subdominant corrections to scaling is sensitive to what might appear to be a minor technical detail.

The constant value of amplitude ratios is maintained upon varying anisotropy for $S = 1/2$ systems with first-neighbor couplings, either with PBCs or FBCs; however, it does not seem to survive changes in spin S, or introduction of further neighbor interactions. We have thus established that the observed, apparently universal, constant amplitude ratios pertain to a limited subset of systems which are in the broader Ising universality class. It remains to be further investigated whether the close values found for b_2/a_2 with FBCs in the three cases are indeed an indication of an actual constant ratio.

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