Exact Finite-Size Scaling and Corrections to Scaling in the Ising Model with Brascamp-Kunz Boundary Conditions

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Abstract

The Ising model in two dimensions with the special boundary conditions of Brascamp and Kunz is analysed. Leading and sub-dominant scaling behaviour of the Fisher zeroes are determined exactly. The finite-size scaling, with corrections, of the specific heat is determined both at the critical and pseudocritical points. The shift exponents associated with scaling of the pseudocritical points are not the same as the inverse correlation length critical exponent. All corrections to scaling are analytic.

1 Introduction

Second order critical phenomena are signaled by the divergence of an appropriate second derivative of the free energy along with the correlation length. For temperature driven phase transitions, this divergence is in the specific heat. Of central interest in the study of such phenomena is the determination of the critical exponents which characterize these divergences. Here, the concept of universality plays a fundamental role. The universality hypothesis asserts that critical behaviour is determined solely by the number of space (or space time) dimensions and by the symmetry properties of the order parameters of the model. The universality class is thus labeled by critical exponents describing the singular behaviour of thermodynamic functions in the infinite volume limit. In finite systems the counterparts of these singularities are smooth peaks the shapes of which depend on the critical exponents. Finite-size scaling (FSS) is a well established technique for the numerical or analytical extraction of these exponents from finite volume analyses [1, 2, 3, 4].

In particular, let $C_L(\beta)$ be the specific heat at inverse temperature β for a system of linear extent L. FSS of the specific heat is characterized by *(i)* the location of its peak, β_L, *(ii)* its height $C_L(\beta_L)$ and *(iii)* its value at the infinite volume critical point $C_L(\beta_c)$. The position of the specific heat peak, β_L, is a pseudocritical point which approaches β_c as $L \rightarrow \infty$ in a manner dictated by the shift exponent λ,

$$|\beta_L - \beta_c| \sim L^{-\lambda} \quad . \tag{1.1}$$

Finite-size scaling theory also gives that if the specific heat divergence is of a power-law type in the thermodynamic limit, $C_L \sim |\beta - \beta_c|^{-\alpha}$, then its peak behaves with L as

$$C_L(\beta_L) \sim L^{\alpha/\nu} \quad , \tag{1.2}$$

in which ν is the correlation length critical exponent. When $\alpha = 0$, which is the case in the Ising model in two dimensions, this behaviour is modified to

$$C_L(\beta_L) \sim \ln L \quad . \tag{1.3}$$

In most models the shift exponent λ coincides with $1/\nu$, but this is not a direct conclusion of finite-size scaling and is not always true. If the shift exponent obeys $\lambda \geq 1/\nu$ then (1.2) also holds if the pseudocritical temperature β_L is replaced by the critical one β_c. If, on the other hand, $\lambda < 1/\nu$, one has $C_L(\beta_c) \sim L^{\lambda\alpha}$ in the power-law case [2].

The leading FSS behaviour of a wide range of models is by now well understood. Recently, attention has focused on the determination of corrections to scaling [5, 6, 7, 8, 9, 10, 11, 12]. These corrections may arise from irrelevant scaling fields or be analytic in L^{-1}. Typically, numerically based or experimental studies involve systems of limited size where these corrections to leading FSS behaviour cannot be dismissed. A better knowledge of universal sub-dominant behaviour would therefore be of great benefit in FSS extrapolation procedures [13, 14, 15, 16, 17, 18, 19, 20, 21, 22].

The Ising model in two dimensions is the simplest statistical physics model displaying critical behaviour. Although solved in the absence of an external field [23], it remains a very useful testing ground in which new techniques can be explored in the hope of eventual application to other, less understood, models in both statistical physics and in lattice field theory.

Exploiting the exactly known partition function of the two dimensional Ising model on finite lattices with toroidal boundary conditions [13], Ferdinand and Fisher [14] analytically determined the specific heat FSS to order L^{-1}. At the infinite volume critical point this was recently extended to order L^{-3} by Izmailian and Hu [19] and independently by Salas [20]. It was found that only integer powers of L^{-1} occur, with no logarithmic modifications (except of course for the leading logarithmic term), i.e.,

$$C_L(\beta_c) = C_{00} \ln L + C_0 + \sum_{k=1}^{\infty} \frac{C_k}{L^k} \quad . \tag{1.4}$$

For the toroidal lattice, the coefficients C_{00}, C_0, C_1, C_2 and C_3 have been determined explicitly [14, 19, 20, 23]. Ferdinand and Fisher also determined the behaviour of the specific heat pseudocritical point, finding $\lambda = 1 = 1/\nu$ (except for special values of the ratio of the lengths of the lattice edges, in which case pseudocritical scaling was found to be of the form $L^{-2}\ln L$).

The specific heat of the Ising model has also recently been studied numerically on two dimensional lattices with other boundary conditions in Refs. [6, 7]. For lattices with spherical topology, the correlation length and shift exponents were found to be $\nu = 1.00 \pm 0.06$ and $\lambda = 1.745 \pm 0.015$, significantly away from $1/\nu$ [6]. This is compatible with an earlier study reporting $\lambda \approx 1.8$ [5]. Therefore the FSS of the specific heat pseudocritical point does not match the correlation length scaling behaviour. This is in contrast to the situation with toroidal boundary conditions, where $\lambda = 1/\nu = 1$ [14]. On the other hand, it was established in [6] that the critical properties on such a lattice are the same as for the torus.

The finite size behaviour of the specific heat is related to that of the complex temperature zeroes of the partition function, the so-called Fisher zeroes [24]. Indeed, the FSS of the latter provides further information on the critical exponents of the model. The leading FSS behaviour of the imaginary part of a Fisher zero is [25]

$$\mathrm{Im} z_j(L) \sim L^{-1/\nu} \quad , \tag{1.5}$$

while the real part of the lowest zero may be viewed as another pseudocritical point, scaling as

$$|\beta_c - \mathrm{Re} z_1(L)| \sim L^{-\lambda_{\rm zero}} \quad . \tag{1.6}$$

Hoelbling and Lang used a variety of cumulants as well as Fisher zeroes to study universality of the Ising model on sphere-like lattices [7]. They reported that the imaginary part of the first zero is an optimal quantity to determine the exponent ν which is in perfect agreement with unity for all lattices studied. Regarding the FSS of the pseudocritical point, the numerical results on a torus are in agreement with $\lambda = 1/\nu = 1$ [14]. The pseudocritical point (from specific heat, the real part of the lowest zero as well as from two other types of cumulant) is not, however, of the Ferdinand-Fisher type. I.e., the amplitude of any $\mathcal{O}(1/L)$ contribution is compatible with zero. While a shift exponent $\lambda = 1.76(7)$ is consistent with their numerical results, Hoelbling and Lang point out that this is not stringent and pseudocritical FSS of the form $L^{-2}\log L$ or even L^{-2} are also compatible with their data. Thus, while a possible leading L^{-1} term almost or completely vanishes and subleading terms are dominant, the precise nature of these corrections could not be unambiguously decided. In any case, FSS of the position of the specific heat peak does not accord with the correlation length exponent for spherical lattices and the thermodynamic limit is achieved faster there than on a toroidal lattice.

In another recent study [8] involving Fisher zeroes, Beale's [15] exact distribution function for the energy of the two dimensional Ising model was exploited to obtain the exact zeroes for square periodic lattices up to size $L = 64$. The FSS analysis in [8] yielded a value for the correlation length critical exponent, ν, which appeared to approach the exact value (unity) as the thermodynamic limit is approached. Small lattices appeared to yield a correction-to-scaling exponent in broad agreement with early estimates ($\omega \approx 1.8$ [26]). However, closer to the thermodynamic limit, these corrections appeared to be analytic with $\omega = 1$. On the other hand, in [17], the scaling behaviour of the susceptibility and related quantities was considered and evidence for $\omega = 1.75$ or, possibly, 2 was presented.

In the light of these recent analyses, we wish to present analytic results which may clarify the situation. To this end, we have selected the Ising model with special boundary conditions due to Brascamp and Kunz [27]. These boundary conditions permit an analytical approach to the determination of a number of thermodynamic quantities. Recently, Lu and Wu exploited this fact to determine the density of Fisher zeroes in the thermodynamic limit [28]. In this paper, we take a complimentary approach, exploiting FSS behaviour (i) to determine critical exponents, (ii) to determine corrections to leading scaling and (iii) to gain experience in the hope of eventual application to other, less transparent scenarios. The rest of this paper is organised as follows. In Section 2 the Brascamp-Kunz boundary conditions are introduced and the exact FSS of the Fisher zeroes calculated. The specific heat and its pseudocritical point are analysed in Section 3. Our conclusions are contained in Section 4 and the Appendix contains some calculations of relevance to the specific heat analysis of Section 3.

2 The Fisher Zeroes for Brascamp-Kunz Boundary Conditions

Brascamp and Kunz introduced special boundary conditions, for which the Fisher zeroes are known for any finite size lattice [27]. They considered a regular lattice with M sites in the x direction and $2N$ sites in the y direction. The special boundary conditions are periodic in the x direction and Ising spins fixed to $\dots +++ \dots$ and $\dots +-+-+- \dots$ along the edges in the y direction. For such a lattice, the Ising partition function can be rewritten as

$$Z_{M,2N} = 2^{2MN} \prod_{i=1}^{N} \prod_{j=1}^{M} \left[1 + z^2 - z(\cos\theta_i + \cos\phi_j) \right] \quad , \tag{2.1}$$

where $z = \sinh 2\beta$, $\theta_i = (2i-1)\pi/2N$ and $\phi_j = j\pi/(M+1)$ and where $\beta = 1/k_BT$ is the inverse temperature. The multiplicative form of (2.1) is of central importance to this paper.

Brascamp and Kunz showed that the zeroes of the partition function (2.1) are located on the unit circle in the complex z plane (so that the critical point is $z = z_c = 1$). These are

$$z_{ij} = \exp\left(i\alpha_{ij}\right) \quad , \tag{2.2}$$

where

$$\alpha_{ij} = \cos^{-1}\left(\frac{\cos\theta_i + \cos\phi_j}{2}\right) \quad . \tag{2.3}$$

Setting $2N = \sigma M$ and using a computer algebra system such as Maple, one may expand (2.3) in M to determine FSS of any zero to any desired order. Indeed, the first few terms in the expansion for the first zero which is the one of primary interest, are

$$\begin{aligned}\alpha_{11} = & M^{-1}\frac{\pi\sqrt{1+\sigma^2}}{\sqrt{2}\sigma} - M^{-2}\frac{\pi\sigma}{\sqrt{2}\sqrt{1+\sigma^2}} \\ & + M^{-3}\frac{\pi\sqrt{2}}{(1+\sigma^2)^{5/2}}\left\{\frac{\sigma}{4}(1+\sigma^2)(3+2\sigma^2) - \frac{\pi^2}{96\sigma^3}(1-\sigma^4)^2\right\} \\ & - M^{-4}\frac{\pi\sqrt{2}}{\sigma(1+\sigma^2)^{5/2}}\left\{\frac{\sigma^2}{4}(4+5\sigma^2+2\sigma^4) + \frac{\pi^2}{96}(5+3\sigma^2)(1-\sigma^2)(1+\sigma^2)\right\} \\ & + \mathcal{O}\left(M^{-5}\right) \quad . \end{aligned} \tag{2.4}$$

Separating out the real and imaginary parts of the FSS of the first zero yields

$$\begin{aligned} & \mathrm{Re} z_{11} = \cos\alpha_{11} = \\ & 1 - M^{-2}\frac{\pi^2}{4}\left(1+\frac{1}{\sigma^2}\right) + M^{-3}\frac{\pi^2}{2} + M^{-4}\frac{\pi^2}{4}\left(-3+\frac{\pi^2}{12}\left(1+\frac{1}{\sigma^4}\right)\right) + \mathcal{O}\left(M^{-5}\right) \quad , \end{aligned} \tag{2.5}$$

and

$$\begin{aligned} \mathrm{Im} z_{11} = \sin\alpha_{11} = & \frac{\pi\sqrt{2}}{\sigma(1+\sigma^2)^{5/2}}\left\{M^{-1}\frac{(1+\sigma^2)^3}{2} - M^{-2}\frac{\sigma^2(1+\sigma^2)^2}{2}\right. \\ & + M^{-3}\frac{1}{96\sigma^2}\left[-\pi^2(1+\sigma^2)^2\left(5+6\sigma^2+5\sigma^4\right) + 24\sigma^4(1+\sigma^2)(3+2\sigma^2)\right] \\ & \left. + M^{-4}\left[-\frac{\sigma^2}{4}\left(4+5\sigma^2+2\sigma^4\right) + \frac{\pi^2}{96}(1+\sigma^2)(1+3\sigma^2)(7+5\sigma^2)\right]\right\} + \mathcal{O}\left(M^{-5}\right) \quad , \end{aligned} \tag{2.6}$$

respectively. From the leading term in (2.6) and from (1.5) one has, indeed, that the correlation length critical exponent is 1. Note, however, from (2.5) that the leading FSS behaviour of the pseudocritical point in the form of the real part of the lowest zero is

$$z_c - \mathrm{Re} z_{11} = 1 - \mathrm{Re} z_{11} \sim M^{-2} \quad , \tag{2.7}$$

giving shift exponent $\lambda_{\rm zero} = 2$. This value is consistent with the numerical results of [7] for spherical lattices. One further notes that all corrections are powers of M^{-1} and in this sense entirely analytic.

Setting $\sigma = 1$ gives the FSS behaviour of the first zero for a square $M \times M$ lattice to be

$$\alpha_{11} = \pi M^{-1} - \frac{\pi}{2}M^{-2} + \frac{5\pi}{8}M^{-3} - \frac{11\pi}{16}M^{-4} + \mathcal{O}\left(M^{-5}\right) \quad , \tag{2.8}$$

which, for the real and imaginary parts separately is

$$\text{Re}z_{11} = \cos\alpha_{11} = 1 - \frac{\pi^2}{2}M^{-2} + \frac{\pi^2}{2}M^{-3} - \frac{\pi^2}{4}\left(3 - \frac{\pi^2}{6}\right)M^{-4} + \mathcal{O}\left(M^{-5}\right) \quad , \qquad (2.9)$$

$$\text{Im}z_{11} = \sin\alpha_{11} = \pi M^{-1} - \frac{\pi}{2}M^{-2} - \frac{\pi}{2}\left(\frac{\pi^2}{3} - \frac{5}{4}\right)M^{-3} + \frac{\pi}{4}\left(\pi^2 - \frac{11}{4}\right)M^{-4} + \mathcal{O}\left(M^{-5}\right) \quad . \qquad (2.10)$$

In summary, we have observed that for the first zero, the shift exponent is not $1/\nu$ and that all corrections are analytic. Expansion of higher zeroes yields the same result.

3 The Specific Heat

In terms of the variable $z = \sinh 2\beta$, the specific heat is

$$C \equiv \frac{k_B\beta^2}{V}\frac{\partial^2 \ln Z}{\partial\beta^2} = \frac{4k_B\beta^2}{V}\left[(1+z^2)\frac{\partial^2 \ln Z}{\partial z^2} + z\frac{\partial \ln Z}{\partial z}\right] \quad , \qquad (3.1)$$

where V is the volume of the system. The singular behaviour comes from the first term only, the second being entirely regular. Thus we may split (3.1) into singular and regular parts and retain only the former. From (2.1), this singular part of the specific heat for an $M \times 2N$ lattice is (up to the factor $(1+z^2)4k_B\beta^2$)

$$C^{\text{sing.}}_{M,2N}(z) = \frac{1}{2MN}\sum_{i=1}^{N}\sum_{j=1}^{M}\left\{\frac{2}{1+z^2-z(\cos\theta_i+\cos\phi_j)} - \frac{[2z-(\cos\theta_i+\cos\phi_j)]^2}{[1+z^2-z(\cos\theta_i+\cos\phi_j)]^2}\right\} \quad . \qquad (3.2)$$

An alternative approach is to write the partition function as

$$Z_{M,2N} = A(z)\prod_{i=1}^{N}\prod_{j=1}^{M}(z-z_{ij})(z-\bar{z}_{ij}) \quad , \qquad (3.3)$$

where the product is taken over all zeroes. The non-vanishing function $A(z)$ contributes only to the regular part of the partition function, and from (2.2) and (2.3), the product term leads precisely to the singular expression (3.2).

It is straightforward to perform the i- summation first in (3.2). Indeed, (A.3) and (A.4) yield the exact result, which is conveniently expressed as

$$C^{\text{sing.}}_{M,2N}(z) = \frac{1}{z^3}\frac{1}{M}\sum_{j=1}^{M}g_j(z) + \left(1 - \frac{1}{z^2}\right)\frac{1}{2M}\sum_{j=1}^{M}g_j^{(1)}(z) - \frac{1}{2z^2} \quad , \qquad (3.4)$$

where

$$g_j(z) = \frac{\tanh\left(N\cosh^{-1}\left(1/z+z-\cos\phi_j\right)\right)}{\sqrt{(1/z+z-\cos\phi_j)^2-1}} \quad , \qquad (3.5)$$

and where $g_j^{(k)}(z) = d^k g_j(z)/dz^k$.

It is convenient at this stage to introduce the sums

$$S_k = \frac{1}{M} \sum_{j=1}^{M} g_j^{(k)}(1) \quad , \tag{3.6}$$

and to make the observation that

$$g_j^{(1)}(1) = 0 \quad , \tag{3.7}$$

$$g_j^{(3)}(1) = -3 g_j^{(2)}(1) \quad . \tag{3.8}$$

Specific Heat at the Critical Point: At the infinite volume critical temperature, $z = z_c = 1$, the specific heat is, from (3.4),

$$C_{M,2N}^{\text{sing.}}(1) = S_0 - \frac{1}{2} \quad . \tag{3.9}$$

The sum S_0 is given in (A.25) in terms of the ratio ρ defined through

$$N = \rho(M+1) \quad . \tag{3.10}$$

This gives for the critical specific heat,

$$C_{M,2N}^{\text{sing.}}(1) = \frac{\ln M}{\pi}\left(1 + \frac{1}{M}\right) + c_0 + \frac{c_1}{M} + \frac{c_2}{M^2} + \frac{c_3}{M^3} + \mathcal{O}\left(\frac{1}{M^4}\right) \quad , \tag{3.11}$$

where

$$c_0 = \frac{1}{\pi}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi - 2W_1(\rho)\right) - \frac{1}{2} \quad , \tag{3.12}$$

$$c_1 = \frac{1}{\pi}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi + 1 - \frac{\pi}{4\sqrt{2}} - 2W_1(\rho)\right) \quad , \tag{3.13}$$

$$c_2 = \frac{1}{2\pi} + \frac{\pi}{144} + \frac{\pi}{6}W_2(\rho) - \frac{\rho\pi^2}{3}W_3(\rho) \quad , \tag{3.14}$$

$$c_3 = -\frac{1}{6\pi} - \frac{\pi}{144} - \frac{\pi}{6}W_2(\rho) + \frac{\rho\pi^2}{3}W_3(\rho) \quad , \tag{3.15}$$

where $\gamma_E \approx 0.577\,215\,664\,9\ldots$ is the Euler-Mascheroni constant and where the functions $W_k(\rho)$ are given in the appendix. Typical values of the constants c_0–c_3 are given in Table 1.

Table 1: Values of the coefficients c_0–c_3 for various values of the ratio $\rho = N/(M+1)$.

ρ	1/2	1	2
c_0	$-0.376\,674\,231\,4\ldots$	$-0.350\,879\,731\,2\ldots$	$-0.349\,694\,204\,8\ldots$
c_1	$0.264\,858\,959\,5\ldots$	$0.290\,653\,459\,7\ldots$	$0.291\,838\,986\,0\ldots$
c_2	$0.125\,896\,138\,1\ldots$	$0.175\,784\,346\,0\ldots$	$0.180\,950\,438\,8\ldots$
c_3	$-0.019\,792\,842\,7\ldots$	$-0.069\,681\,050\,6\ldots$	$-0.074\,847\,143\,4\ldots$

So for the critical specific heat, apart from the $\ln M/M$ term, the FSS is qualitatively the same as (but quantitatively different to) that of the torus topology (see (1.4)and [14, 19, 20]). We note that with the Brascamp-Kunz boundary conditions, it is far easier to extract the FSS behaviour. Indeed, determination of $\mathcal{O}(1/M^4)$ and higher terms proceeds is a similarly straightforward manner.

Specific Heat near the Critical Point: The pseudocritical point, $z_{M,2N}^{\rm pseudo}$, is the value of the temperature at which the specific heat has its maximum for a finite $M \times 2N$ lattice. One can determine this quantity as the point where the derivative of $C_{M,2N}(z)$ vanishes.

The specific heat is given in (3.4). This may now be expanded about the critical point $z = 1$. This Taylor expansion simplifies using (3.7) and (3.8). Indeed,

$$C_{M,2N}(z) = S_0 - \frac{1}{2} + (z-1)\left[-3S_0 + 1\right] + (z-1)^2 \left[\frac{3}{2}S_2 + 6S_0 - \frac{3}{2}\right] + (z-1)^3\left[-5S_2 - 10S_0 + 2\right] + \mathcal{O}\left((z-1)^4\right) \quad . \tag{3.16}$$

The sums S_0 and S_2 are given in (A.25) and (A.28) respectively.

From (3.16), the first derivative of the specific heat on a finite lattice near the infinite volume critical point is

$$\frac{dC_{M,2N}^{\rm sing.}(z)}{dz} = 1 - 3S_0 + 3(z-1)[S_2 + 4S_0 - 1] + 3(z-1)^2[-5S_2 - 10S_0 + 2] + O\left((z-1)^3\right) \quad . \tag{3.17}$$

Noting that, while S_2 is $\mathcal{O}\left(M^2\right)$, S_0 is $\mathcal{O}\left(\ln M\right)$, one sees that this derivative vanishes when

$$z - 1 = \frac{3S_0 - 1}{3\left[S_2 + 4S_0 - 1\right]} + \frac{\left[5S_2 + 10S_0 - 2\right]\left[3S_0 - 1\right]^2}{9\left[S_2 + 4S_0 - 1\right]^3} + \mathcal{O}\left((z-1)^3\right) \quad . \tag{3.18}$$

Expansion of (3.18) now gives the FSS of the pseudocritical point to be

$$z_{M,2N}^{\rm pseudo} = 1 + a_2\frac{\ln M}{M^2} + \frac{b_2}{M^2} + a_3\frac{\ln M}{M^3} + \frac{b_3}{M^3} + \mathcal{O}\left(\frac{(\ln M)^2}{M^4}\right) + \mathcal{O}\left(\frac{\ln M}{M^4}\right) + \mathcal{O}\left(\frac{1}{M^4}\right) \quad , \tag{3.19}$$

where

$$a_2 = -\frac{\pi^2}{2(\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho))} \quad , \tag{3.20}$$

$$b_2 = -\frac{\pi^2}{12}\frac{6\gamma_E + 9\ln 2 - 6\ln\pi - 2\pi - 12W_1(\rho)}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad , \tag{3.21}$$

$$a_3 = \frac{\pi^2}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad , \tag{3.22}$$

$$b_3 = -\frac{\pi^2}{2}\frac{1 - 2\gamma_E - 3\ln 2 + 2\ln\pi + \pi - \pi/(4\sqrt{2}) + 4W_1(\rho)}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad . \tag{3.23}$$

Again, the functions $W_k(\rho)$ are given in the appendix. Typical values of the coefficients are given in Table 2. Thus there is no leading $1/M$ or $\ln M/M$ term in the FSS of the specific heat pseudocritical point and the specific heat shift exponent does not coincide with $1/\nu = 1$. This is consistent with the result (2.7) for the finite-size scaling of the real part of the Fisher zeroes.

Table 2: Values of the coefficients a_2–d'_3 for various values of the ratio $\rho = N/(M+1)$.

ρ	1/2	1	2
a_2	−5.696 643 550 4 . . .	−4.200 054 895 9 . . .	−4.105 621 572 1 . . .
a_3	11.393 287 100 7 . . .	8.400 109 791 7 . . .	8.211 243 144 1 . . .
b_2	3.758 407 422 6 . . .	2.430 665 892 0 . . .	2.360 724 066 8 . . .
b_3	−16.015 279 517 2 . . .	−11.127 129 852 1 . . .	−10.846 367 057 9 . . .
c'_0	−0.376 674 233 5 . . .	−0.350 879 733 3 . . .	−0.349 694 207 0 . . .
c'_1	0.264 858 957 4 . . .	0.290 653 45 76 . . .	0.291 838 983 9 . . .
c'_2	1.309 837 121 4 . . .	0.847 424 969 7 . . .	0.829 066 715 2 . . .
c'_3	−6.557 959 374 1 . . .	−4.204 047 250 7 . . .	−4.086 049 903 8 . . .
d_2	−3.589 014 676 5 . . .	−2.321 114 940 5 . . .	−2.254 325 418 5 . . .
d_3	11.704 450 471 3 . . .	8.304 511 256 4 . . .	8.103 192 065 9 . . .
d'_2	2.719 946 882 3 . . .	2.005 378 462 3 . . .	1.960 289 872 9 . . .
d'_3	−2.719 946 882 3 . . .	−2.005 378 462 3 . . .	−1.960 289 872 9 . . .

Inserting (3.19) for the pseudocritical point into (3.16) gives the FSS behaviour of the peak of the specific heat. This is

$$C^{\text{sing.}}_{M,2N}(z^{\text{pseudo}}_{M,2N}) = \frac{\ln M}{\pi}\left(1+\frac{1}{M}\right) + c'_0 + \frac{c'_1}{M} + d'_2\frac{(\ln M)^2}{M^2} + d_2\frac{\ln M}{M^2} + \frac{c'_2}{M^2} + d'_3\frac{(\ln M)^2}{M^3} + d_3\frac{\ln M}{M^3} + \frac{c'_3}{M^3} + \mathcal{O}\left(\frac{(\ln M)^2}{M^4}\right) \quad , \tag{3.24}$$

where

$$c'_0 = c_0 \quad , \tag{3.25}$$

$$c'_1 = c_1 \quad , \tag{3.26}$$

$$d'_2 = \frac{3\pi}{4}\frac{1}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad , \tag{3.27}$$

$$d_2 = \frac{\pi}{4}\frac{6\gamma_E + 9\ln 2 - 6\ln\pi - 2\pi - 12W_1(\rho)}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad , \tag{3.28}$$

$$c'_2 = c_2 + \frac{\pi}{48}\frac{(6\gamma_E + 9\ln 2 - 6\ln\pi - 2\pi - 12W_1(\rho))^2}{\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)} \quad , \tag{3.29}$$

$$d'_3 = -d'_2 \quad , \tag{3.30}$$

$$d_3 = \frac{\pi^2}{2(\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho))}\left(2 - \frac{3}{4\sqrt{2}} + \frac{3}{\pi}\left(1 - \gamma_E - \frac{3\ln 2}{2} + \ln\pi + 2W_1(\rho)\right)\right) \quad , \tag{3.31}$$

$$c'_3 = c_3 + \frac{\pi^3}{4(\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho))}\left\{-\frac{3}{\pi^2}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi - 2W_1(\rho)\right)^2 + \frac{1}{\pi}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi - 2W_1(\rho)\right)\left(4 + \frac{6}{\pi} - \frac{3}{2\sqrt{2}}\right) - 1 - \frac{2}{\pi} + \frac{1}{2\sqrt{2}}\right\} \quad . \tag{3.32}$$

Again, typical values for the coefficients are compiled in Table 2.

One remarks that, up to $\mathcal{O}(1/M)$, this is quantitatively the same at the critical specific heat scaling of (3.11). One further remarks that the higher order structure of (3.24) differs to that at the critical point as given by (3.11) in that there are logarithmic modifications to the subdominant terms.

4 Conclusions

We have derived exact expressions for the finite-size scaling of the Fisher zeroes for the Ising model with Brascamp-Kunz boundary conditions. The shift exponent, characterizing the scaling of the corresponding pseudocritical point is $\lambda = 2$ and is not the same as the correlation length critical exponent $\nu = 1$. This is consistent with numerical results for lattices with spherical topology [7]. Corrections to FSS can also be exactly determined and are found to be analytic. This is consistent with the large lattice numerical calculations of [8] for toroidal lattices.

A similar analysis applied to specific heat at criticality yields results qualitatively similar to those on a torus [14, 19, 20, 23]. These results complement the finite size scaling of the zeroes. I.e., apart from the leading logarithm, only analytic corrections appear.

The finite size scaling of the pseudocritical point, determined from the specific heat maximum is governed by a shift exponent $\lambda = 2$ with logarithmic corrections. This is again compatible with previous numerical results [5, 6, 7]. Finally, the first few terms for the FSS of the specific heat peak are derived. Again all corrections are analytic, but in contrast to the specific heat at the critical point, here they include logarithms.

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A Appendix

Consider, firstly, the sum

$$\frac{1}{N}\sum_{i=1}^{N}\frac{1}{(Z-\cos\theta_i)^k} \quad , \tag{A.1}$$

where $\theta_i = (2i-1)\pi/2N$, k is a positive integer and $Z > 1$ is independent of n. We firstly treat the case $k = 1$. We follow a similar calculation in [16] and construct

$$\mathcal{F}(z) = \frac{\cot\pi z}{Z - \cos\frac{(2z-1)\pi}{2N}} \quad . \tag{A.2}$$

Integrate $\mathcal{F}(z)$ along the rectangular contour bounded by Re$z = 1/2 + \epsilon$, Re$z = 2N + 1/2 + \epsilon$ and Im$z = \pm iR$ where R is some large real constant and ϵ is a small real number which we take to be positive. Because of the periodic nature of the integrand, the integrals along the left and right edges of the contour cancel. Further, due to the $\cot\pi z$ term, the integrand and hence the full integral vanishes in the limit of infinitely large R. Now, $\mathcal{F}(z)$ has $2N$ simple poles inside the contour along the real axis and a further two coming from the simple zeroes of its denominator. The residue theorem then gives the exact result

$$\frac{1}{N}\sum_{i=1}^{N}\frac{1}{Z-\cos\theta_i}=\frac{1}{\sqrt{Z^2-1}}\tanh\left(N\cosh^{-1}Z\right)\quad . \tag{A.3}$$

This result is also implicitly contained in [29]. Differentiation of (A.3) with respect to Z gives the sum (A.1) with larger values of k. In particular, we also find

$$\frac{1}{N}\sum_{i=1}^{N}\frac{1}{(Z-\cos\theta_i)^2}=\frac{Z\tanh\left(N\cosh^{-1}Z\right)}{(Z^2-1)^{3/2}}-\frac{N\mathrm{sech}^2\left(N\cosh^{-1}Z\right)}{Z^2-1}\quad . \tag{A.4}$$

The purpose of the remainder of this appendix is to calculate the two sums S_0 and S_2 where

$$S_k=\frac{1}{M}\sum_{j=1}^{M}g_j^{(k)}(1)\quad , \tag{A.5}$$

where $g_j^{(k)}(z)=d^k g_j(z)/dz^k$,

$$g_j(z)=\frac{\tanh\left(N\cosh^{-1}\left(1/z+z-\cos\phi_j\right)\right)}{\sqrt{(1/z+z-\cos\phi_j)^2-1}}\quad , \tag{A.6}$$

and where $\phi_j=\pi j/(M+1)$. It is convenient to rewrite $g_j(z)$ as

$$\begin{aligned}g_j(z)=&\frac{1}{\sqrt{(2+m^2-\cos\phi_j)^2-1}}\\&-2\frac{1}{\sqrt{(2+m^2-\cos\phi_j)^2-1}}\left\{\exp\left[2N\cosh^{-1}\left(2+m^2-\cos\phi_j\right)\right]+1\right\}^{-1}\quad ,\end{aligned} \tag{A.7}$$

where $m^2=1/z+z-2$. We consider, firstly, the sum

$$\sum_{j=1}^{M}\frac{1}{\sqrt{\left(2+m^2-\cos\phi_j\right)^2-1}}\quad , \tag{A.8}$$

and we are interested in the limit $m\to 0$. This may be calculated by direct application of the Euler-Maclaurin formula [30]. In fact, the more general summation (A.8) has been calculated in [16]. Writing $m=\eta/(M+1)$, that sum is given by

$$\begin{aligned}&\frac{1}{M+1}\sum_{j=1}^{M}\frac{1}{\sqrt{\left(2+\left(\frac{\eta}{M+1}\right)^2-\cos\phi_j\right)^2-1}}=\\&\frac{\ln(M+1)}{\pi}+\frac{1}{\pi}\left[\gamma_E-\ln\pi+\frac{3\ln 2}{2}+G_0\left(\frac{\sqrt{2}\eta}{\pi}\right)\right]-\frac{1}{M+1}\frac{1}{4\sqrt{2}}-\frac{\ln(M+1)}{(M+1)^2}\frac{\eta^2}{4\pi}\\&+\frac{1}{2}\frac{1}{(M+1)^2}\left[\frac{\pi}{6}\left(\frac{1}{12}-G_1\left(\frac{\sqrt{2}\eta}{\pi}\right)\right)+\frac{\eta^4}{3\pi^3}H_1\left(\frac{\sqrt{2}\eta}{\pi}\right)-\frac{\eta^2}{2\pi}\left(\gamma_E-\ln\pi+\frac{3\ln 2}{2}\right.\right.\\&\left.\left.+\frac{2}{3}G_0\left(\frac{\sqrt{2}\eta}{\pi}\right)-\frac{1}{3}\right)\right]+\frac{1}{(M+1)^3}\frac{3\sqrt{2}}{64}\eta^2+\mathcal{O}\left(\frac{\ln M}{(M+1)^4}\right)+\mathcal{O}\left(\frac{1}{(M+1)^4}\right)\quad ,\end{aligned} \tag{A.9}$$

where $\gamma_E \approx 0.577\,215\,664\,9\ldots$ is the Euler-Mascheroni constant [30] and where the remnant functions are

$$G_0(\alpha) = \sum_{n=1}^{\infty} (-1)^n \left(\begin{array}{c} 2n \\ n \end{array} \right) \zeta(2n+1) \left(\frac{\alpha}{2}\right)^{2n} \quad , \tag{A.10}$$

$$G_1(\alpha) = 2\sum_{n=1}^{\infty} \frac{(-1)^n}{n} \left(\begin{array}{c} 2n \\ n \end{array} \right) \zeta(2n+1) \left(\frac{\alpha}{2}\right)^{2n+2} \quad , \tag{A.11}$$

$$H_1(\alpha) = \sum_{n=1}^{\infty} (-1)^n (2n+1) \left(\begin{array}{c} 2n \\ n \end{array} \right) \zeta(2n+3) \left(\frac{\alpha}{2}\right)^{2n} \quad , \tag{A.12}$$

in which $\zeta(n)$ is a Riemann zeta function [30],

$$\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n} \quad . \tag{A.13}$$

Setting $\eta = 0$, one has the first component of the sum appearing in S_0,

$$\frac{1}{M+1} \sum_{j=1}^{M} \frac{1}{\sqrt{(2-\cos\phi_j)^2 - 1}} = \frac{\ln(M+1)}{\pi} + \frac{1}{\pi}\left[\gamma_E - \ln\pi + \frac{3\ln 2}{2}\right] - \frac{1}{M+1}\frac{1}{4\sqrt{2}} + \frac{1}{(M+1)^2}\frac{\pi}{144} + \mathcal{O}\left(\frac{1}{(M+1)^4}\right) \quad . \tag{A.14}$$

Next, we consider

$$\sum_{j=1}^{M} \frac{1}{\sqrt{\left(2 + \left(\frac{\eta}{M+1}\right)^2 - \cos\phi_j\right)^2 - 1}} \left\{\exp\left[2N\cosh^{-1}(2-\cos\phi_j)\right] + 1\right\}^{-1} \equiv \sum_{j=1}^{M} h_j(\eta) \quad . \tag{A.15}$$

It is natural to define an aspect ratio, ρ, through

$$N = \rho(M+1) \quad , \tag{A.16}$$

and introduce

$$X_j = \sqrt{2\eta^2 + \pi^2 j^2} \quad , \tag{A.17}$$

$$Y_j = \exp(2\rho X_j) + 1 \quad . \tag{A.18}$$

Dominant contributions to (A.15) come from the small j terms. The sum may thus replaced by [16]

$$\sum_{j=1}^{\infty} h_j(\eta) \quad , \tag{A.19}$$

where the expansion of the summand is

$$h_j(\eta) = \frac{M+1}{X_j Y_j} + \frac{1}{M+1}\left\{\frac{1}{24}\frac{\pi^4 j^4}{x_j^3 Y_j} - \frac{X_j}{8Y_j} + \frac{\rho}{12}\frac{Y_j - 1}{Y_j^2}\left(\frac{\pi^4 j^4}{X_j^2} + X_j^2\right)\right\} + \mathcal{O}\left(\frac{1}{(M+1)^3}\right) \quad . \tag{A.20}$$

Taking the limit of this quantity as $\eta \to 0$ gives the second component of the sum appearing in S_0,

$$\frac{1}{M+1} \sum_{j=1}^{M} \frac{1}{\sqrt{(2-\cos\phi_j)^2 - 1}} \left\{\exp\left[2N\cosh^{-1}(2-\cos\phi_j)\right] + 1\right\}^{-1} = \frac{1}{\pi}W_1(\rho) + \frac{1}{(M+1)^2}\left[-\frac{\pi}{12}W_2(\rho) + \frac{\rho\pi^2}{6}W_3(\rho)\right] + \mathcal{O}\left(\frac{1}{(M+1)^4}\right) \quad , \tag{A.21}$$

where

$$W_1(\rho) = \sum_{n=1}^{\infty} \frac{1}{n(e^{2\rho\pi n}+1)} \quad , \tag{A.22}$$

$$W_2(\rho) = \sum_{n=1}^{\infty} \frac{n}{(e^{2\rho\pi n}+1)} \quad , \tag{A.23}$$

$$W_3(\rho) = \sum_{n=1}^{\infty} \frac{n^2 e^{2\rho\pi n}}{(e^{2\rho\pi n}+1)^2} \quad . \tag{A.24}$$

The functions $W_k(\rho)$ are rapidly converging sums which may be computed numerically. For example, at $\rho = 1$, $W_1 \approx 0.001\,865\,707\,7\ldots$, $W_2 \approx 0.001\,870\,956\,1\ldots$ and $W_3 \approx 0.001\,874\,495\,5\ldots$. Finally, from (A.5), (A.7), (A.14) and (A.21), the desired result is

$$\begin{aligned} S_0 = & \frac{\ln M}{\pi} + \frac{1}{\pi}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi - 2W_1(\rho)\right) + \frac{\ln M}{M}\frac{1}{\pi} \\ & + \frac{1}{M}\frac{1}{\pi}\left(\gamma_E + \frac{3\ln 2}{2} - \ln\pi + 1 - \frac{\pi}{4\sqrt{2}} - 2W_1(\rho)\right) \\ & + \frac{1}{M^2}\left(\frac{1}{2\pi} + \frac{\pi}{144} + \frac{\pi}{6}W_2(\rho) - \frac{\rho\pi^2}{3}W_3(\rho)\right) \\ & - \frac{1}{M^3}\left(\frac{1}{6\pi} + \frac{\pi}{144} + \frac{\pi}{6}W_2(\rho) - \frac{\rho\pi^2}{3}W_3(\rho)\right) + \mathcal{O}\left(\frac{1}{M^4}\right) \quad . \end{aligned} \tag{A.25}$$

The sum S_2 is

$$S_2 = \frac{d^2}{dz^2}\frac{1}{M}\sum_{j=1}^{M} g_j(z)\bigg|_{z=1} \tag{A.26}$$

$$= \frac{d^2}{dz^2}\frac{1}{M}\sum_{j=1}^{M} \frac{1 - 2\left\{\exp\left[2N\cosh^{-1}(1/z + z - \cos\phi_j)\right] + 1\right\}^{-1}}{\sqrt{(1/z + z - \cos\phi_j)^2 - 1}}\Bigg|_{z=1} \quad . \tag{A.27}$$

The sums involved here are found by taking appropriate derivatives of (A.9) and (A.20). The result for S_2 is

$$\begin{aligned} S_2 = & M^2\frac{-2}{\pi^3}\left[\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)\right] \\ & + M\frac{-6}{\pi^3}\left[\zeta(3) - 2W_4(\rho) - 4\pi\rho W_5(\rho)\right] - \frac{\ln M}{2\pi} + \mathcal{O}(1) \quad , \end{aligned} \tag{A.28}$$

in which $\zeta(3) \approx 1.202\,056\,903\,2\ldots$ and

$$W_4(\rho) = \sum_{n=1}^{\infty} \frac{1}{n^3(\exp(2\rho\pi n)+1)} \quad , \tag{A.29}$$

$$W_5(\rho) = \sum_{n=1}^{\infty} \frac{\exp(2\rho\pi n)}{n^2(\exp(2\rho\pi n)+1)^2} \quad . \tag{A.30}$$

Typical values of these rapidly converging sums are $W_4 \approx 0.001\,864\,398\,1\ldots$ and $W_5 \approx 0.001\,861\,360\,1\ldots$ at $\rho = 1$.

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