Exact finite-size scaling with corrections in the two-dimensional Ising model with special boundary conditions

W. Janke[a] and R. Kenna[b]

[a]Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

[b]School of Mathematics, Trinity College Dublin, Ireland

The two-dimensional Ising model with Brascamp-Kunz boundary conditions has a partition function more amenable to analysis than its counterpart on a torus. This fact is exploited to *exactly* determine the full finite-size scaling behaviour of the Fisher zeroes of the model. Moreover, exact results are also determined for the scaling of the specific heat at criticality, for the specific-heat peak and for the pseudocritical points. All corrections to scaling are found to be analytic and the shift exponent λ does not coincide with the inverse of the correlation length exponent $1/\nu$.

1. INTRODUCTION

Finite-size scaling (FSS) is a well established technique for the extraction of critical exponents from finite volume analyses [1]. Such exponents characterise critical phenomena at a second-order phase transition. The simplest model exhibiting such a transition is the Ising model in two dimensions, which, despite a long history and extensive study, still offers new results and insights. Here, we study the model under the special boundary conditions of Brascamp and Kunz [2] to extract new information and to help resolve some hitherto puzzling features of FSS.

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 the location of its peak, β_L, its height $C_L(\beta_L)$ and its value at the infinite-volume critical point $C_L(\beta_c)$. The peak position, β_L, is a pseudocritical point which typically approaches β_c as $L \to \infty$ as

$$|\beta_L - \beta_c| \sim L^{-\lambda}, \tag{1}$$

where λ is the shift exponent. In two dimensions, the Ising specific heat scales as $\ln L$. Of further interest is the FSS of the complex Fisher zeroes of the partition function [3]. The leading behaviour of the imaginary part of a Fisher zero is [4]

$$\mathrm{Im} z_j(L) \sim L^{-1/\nu}, \tag{2}$$

where z stands generically for an appropriate function of temperature, the subscript j labels the zeroes, and ν is the correlation length critical exponent. The real part of the lowest zero may be viewed as another effective critical or pseudocritical point, scaling as

$$|\mathrm{Re} z_1(L) - z_c| \sim L^{-\lambda_{\mathrm{zero}}}, \tag{3}$$

where $z = z_c$ at $\beta = \beta_c$. Usually the shift exponents, λ and λ_{zero}, coincide with $1/\nu$, but this is not a consequence of FSS and is not always true.

The following results have been obtained for FSS in the two-dimensional Ising model.

Exact Analytical Results: For toroidal lattices the specific-heat FSS has been determined exactly to order L^{-3} at the infinite-volume critical point in [5–7]. Only integer powers of L^{-1} occur, with no logarithmic modifications (except for the leading term), i.e.,

$$C_L(\beta_c) = C_{00} \ln L + C_0 + \sum_{k=1}^{\infty} \frac{C_k}{L^k}. \tag{4}$$

For these periodic boundary conditions the shift exponent for the specific heat is $\lambda = 1 = 1/\nu$, except for special values of the ratio of the lengths of the lattice edges, in which case pseudocritical specific-heat scaling was found to be of the form $L^{-2} \ln L$ [5].

Numerical Results: For spherical lattices the shift exponent of the specific heat was found to be significantly away from $1/\nu = 1$, with λ ranging from approximately 1.75 to 2 (with the possibility of logarithmic corrections) [8]. Therefore the FSS of the specific-heat pseudocritical point does not appear to match the correlation length scaling.

In another study [9], FSS of Fisher zeroes for square periodic lattices yielded a value of ν which appeared to approach the exact value (unity) as the thermodynamic limit is approached. Small lattices appeared to yield an effective correction-to-scaling exponent $\omega \approx 1.8$ while closer to the thermodynamic limit, these corrections tended to be analytic with $\omega = 1$. A certain formal limit of conformal field theory suggests a correction exponent $\omega = 4/3$ [10]. However, the validity of this limit has long been unclear [11] and the question of the absence of a subleading operator corresponding to $\omega = 4/3$ in the standard Ising model in two dimensions was recently addressed in depth in [12] (see also [13]).

In the light of these analyses, we present exact results which help clarify the situation. To this end, we have selected the Ising model with Brascamp-Kunz boundary conditions [2].

2. FISHER ZEROES

The Brascamp-Kunz lattice has M sites in the x direction and $2N$ sites in the y direction. The boundary conditions are periodic in the y direction and the $2N$ spins along the left and right borders are fixed to $\ldots{+}{+}{+}\ldots$ and $\ldots{+}{-}{+}{-}{+}{-}\ldots$, respectively. The partition function is [2]

$$Z \propto \prod_{i=1}^{N}\prod_{j=1}^{M}\left[1 + z^2 - z(\cos\theta_i + \cos\phi_j)\right], \tag{5}$$

where $z = \sinh 2\beta$, $\theta_i = (2i-1)\pi/2N$ and $\phi_j = j\pi/(M+1)$. One notes that the partition function (5) is given as a double product. Determination of the Fisher zeroes of (5) is thus straightforward, as is the calculation of thermodynamic functions. For toroidal boundary conditions, on the other hand, the partition function is a sum of four such products [14]. There it is non-trivial to determine the zeroes or the thermodynamic functions.

The zeroes of (5) are on the unit circle in the complex-z plane (so the critical point is $z_c = 1$) [2]. These are $z_{ij} = \exp(i\alpha_{ij})$, where

$$\alpha_{ij} = \cos^{-1}\left(\frac{\cos\theta_i + \cos\phi_j}{2}\right). \tag{6}$$

One may expand (6) in M to determine the FSS of any zero to any desired order. Indeed, in terms of the shape parameter $\sigma = 2N/M$, the first zero is given by

$$\mathrm{Re}z_{11} = 1 - M^{-2}\frac{\pi^2}{4}\left(1 + \frac{1}{\sigma^2}\right) + \mathcal{O}\left(M^{-3}\right), \tag{7}$$

and

$$\mathrm{Im}z_{11} = \frac{\pi\sqrt{2}}{\sigma(1+\sigma^2)^{5/2}}\left[M^{-1}\frac{(1+\sigma^2)^3}{2} - M^{-2}\frac{\sigma^2(1+\sigma^2)^2}{2}\right] + \mathcal{O}\left(M^{-3}\right). \tag{8}$$

Higher order terms are straightforward to determine [15]. From the leading term in (8) and from (2), the correlation length critical exponent is indeed $\nu = 1$. Note, however, from (7) that the leading FSS behaviour of the pseudocritical point in the form of the real part of the lowest zero is

$$z_c - \mathrm{Re}z_{11} = 1 - \mathrm{Re}z_{11} \sim M^{-2}, \tag{9}$$

giving a shift exponent $\lambda_{\mathrm{zero}} = 2 \neq 1/\nu$. Note further that all corrections are powers of M^{-1} and thus analytic.

3. SPECIFIC HEAT

Since the partition function (5) is multiplicative, the free energy and hence the specific heat consists of two summations. These can be performed exactly (we refer the reader to [15] for details) and one finds the following results.

Specific Heat at the Critical Point: At the critical temperature the specific heat is, from (5),

$$C_{M,2N}^{\mathrm{sing.}}(1) = \frac{\ln M}{\pi}\left(1 + \frac{1}{M}\right) + \sum_{k=0}^{\infty}\frac{c_k}{M^k}. \tag{10}$$

The coefficients c_k can easily be determined exactly and those up to c_3 are explicitly given in [15]. So for the critical specific heat on a Brascamp-Kunz lattice, apart from a trivial $\ln M/M$ term (which could be removed by a redefinition of M [15]), the FSS is qualitatively the same as (but quantitatively different to) that of the torus topology in (4).

Specific Heat near the Critical Point: The pseudocritical point of the specific heat, $z_{M,2N}^{\text{pseudo}}$, can be determined as the point where the derivative of $C_{M,2N}(z)$ vanishes. This gives [15]

$$z_{M,2N}^{\text{pseudo}} = 1 + a_2\frac{\ln M}{M^2} + \frac{b_2}{M^2} + a_3\frac{\ln M}{M^3} + \frac{b_3}{M^3} + \mathcal{O}\left(\frac{(\ln M)^2}{M^4}\right), \tag{11}$$

higher terms being of the form $\ln M/M^4$ and $1/M^4$. This implies $\lambda = 2 \neq 1/\nu$ (up to logarithmic corrections). For the specific-heat peak FSS we find [15]

$$C_{M,2N}^{\text{sing.}}(z_{M,2N}^{\text{pseudo}}) = \frac{\ln M}{\pi}\left(1 + \frac{1}{M}\right) + c_0' + \frac{c_1'}{M} + d_2'\frac{(\ln M)^2}{M^2} + \mathcal{O}\left(\frac{\ln M}{M^2}\right), \tag{12}$$

with $c_0' = c_0$ and $c_1' = c_1$. Higher order terms are of the form $1/M^2$, $(\ln M)^2/M^3$, $\ln M/M^3$ and $1/M^3$. Notice that, up to $\mathcal{O}(1/M)$, (12) is quantitatively the same as the critical specific-heat scaling (10). The higher order terms of (12) differ qualitatively from those in (10) in that there are logarithmic modifications of the form $(\ln M)^k/M^l$ (with integer k and l). Again, the values of the coefficients are given in [15].

4. CONCLUSIONS

For the two-dimensional Ising model with Brascamp-Kunz boundary conditions, we have derived exact expressions for the FSS of the Fisher zeroes to all orders. We have also determined the FSS of the critical specific heat, its pseudocritical point and its peak. The advantage of Brascamp-Kunz boundary conditions (over periodic ones) is that the partition function is a product and meliorates determination of higher order corrections.

The following are the main features we have found: All corrections to scaling are analytic (except for logarithms). The shift exponent λ does not coincide with $1/\nu$. The FSS of the specific-heat pseudocritical point and peak have logarithmic corrections. Apart from the leading term, this feature is absent in the critical specific heat.

REFERENCES

1. M.N. Barber, in: *Phase Transitions and Critical Phenomena*, Vol. 8, eds. C. Domb and J.L. Lebowitz (Academic Press, New York, 1983), p. 145.
2. H.J. Brascamp and H. Kunz, J. Math. Phys. 15 (1974) 65.
3. C.N. Yang and T.D. Lee, Phys. Rev. 87 (1952) 404; *ibid.* 410; M.E. Fisher, in: *Lectures in Theoretical Physics*, Vol. VIIC, ed. W.E. Brittin (Gordon and Breach, New York, 1968), p. 1.
4. C. Itzykson, R.B. Pearson, and J.B. Zuber, Nucl. Phys. B 220 (1983) 415.
5. A.E. Ferdinand and M.E. Fisher, Phys. Rev. 185 (1969) 832.
6. N.Sh. Izmailian and C.-K. Hu, Phys. Rev. E (in print) [cond-mat/0009024].
7. J. Salas, J. Phys. A 34 (2001) 1311.
8. J. González and M.A. Martín-Delgado, hep-th/9301057; O. Diego, J. González, and J. Salas, J. Phys. A 27 (1994) 2965; Ch. Hoelbling and C.B. Lang, Phys. Rev. B 54 (1996) 3434.
9. N.A. Alves, J.R. Drugowich de Felicio, and U.H.E. Hansmann, Int. J. Mod. Phys. C 8 (1997) 1063.
10. J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 3rd ed. (Clarendon Press, Oxford, 1996), p. 636.
11. G. Jug and B.N. Shalaev, J. Phys. A 32 (1999) 7249.
12. P. Calabrese, M. Caselle, A. Celi, A. Pelissetto, and E. Vicari, J. Phys. A 33 (2000) 8155.
13. M. Caselle, M. Hasenbusch, A. Pelissetto, and E. Vicari, cond-mat/0106372.
14. B. Kaufman, Phys. Rev. 76 (1949) 1232.
15. W. Janke and R. Kenna, Phys. Rev. B (in print) [cond-mat/0103332].