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Exact finite-size-scaling corrections to the critical two-dimensional Ising model on a torus

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Abstract

We analyse the finite-size corrections to the energy and specific heat of the critical two-dimensional spin-$\frac{1}{2}$ Ising model on a torus. We extend the analysis of Ferdinand and Fisher to compute the correction of order L^{-3} to the energy and the corrections of order L^{-2} and L^{-3} to the specific heat. We also obtain general results on the form of the finite-size corrections to these quantities: only integer powers of L^{-1} occur, unmodified by logarithms (except of course for the leading $\log L$ term in the specific heat); and the energy expansion contains only odd powers of L^{-1}. In the specific-heat expansion any power of L^{-1} can appear, but the coefficients of the odd powers are proportional to the corresponding coefficients of the energy expansion.

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1. Introduction

It is well known that phase transitions in statistical–mechanical systems can occur only in the infinite-volume limit. In any finite system, all thermodynamic quantities (such as the magnetic susceptibility and the specific heat) are analytic functions of all parameters (such as the temperature and the magnetic field); but near a critical point they display peaks whose height increases and whose width decreases as the volume $N = L^d$ grows, yielding the critical singularities in the limit $L \to \infty$. For bulk experimental systems (containing $N \sim 10^{23}$ particles) the finite-size rounding of the phase transition is usually beyond the experimental resolution; but in Monte Carlo simulations ($N \lesssim 10^6$–10^7) it is visible and is often the dominant effect.

Finite-size scaling theory [1–4] provides a systematic framework for understanding finite-size effects near a critical point. The idea is simple: the only two relevant length scales are the system linear size L and the correlation length ξ_∞ of the bulk system at the same parameters, so everything is controlled by the single ratio ξ_∞/L[1]. If $L \gg \xi_\infty$, then finite-size effects are

[1] This is true only for systems below the upper critical dimension d_c. For Ising models with short-range interaction, $d_c = 4$.

negligible; for $L \sim \xi_\infty$, thermodynamic singularities are rounded and obey a scaling ansatz $\mathcal{O} \sim L^{p_\mathcal{O}} F_\mathcal{O}(\xi_\infty/L)$ where $p_\mathcal{O}$ is a critical exponent and $F_\mathcal{O}$ is a scaling function. Finite-size scaling is the basis of the powerful phenomenological renormalization group method (see [3] for a review); and it is an efficient tool for extrapolating finite-size data from Monte Carlo simulations so as to obtain accurate results on critical exponents, universal amplitude ratios and subleading exponents ([5–8], and references therein[2]). In particular, in systems with multiplicative and/or additive logarithmic corrections (such as the two-dimensional four-state Potts model [10]), a good understanding of finite-size effects is crucial for obtaining reliable estimates of the physically interesting quantities.

In finite-size-scaling theory for systems with periodic boundary conditions, three simplifying assumptions have frequently been made:

(a) The regular part of the free energy, $f_{\rm reg}$, is independent of the lattice size L [4] (except possibly for terms that are exponentially small in L).
(b) The scaling fields associated with the temperature and magnetic field (i.e. g_t and g_h, respectively) are independent of L [11].
(c) The scaling field g_L associated with the lattice size is equal to L^{-1} exactly, with no corrections L^{-2}, L^{-3}, ... [4].

Moreover, in the nearest-neighbour spin-$\frac{1}{2}$ 2D Ising model, it has further been assumed that:

(d) There are no irrelevant operators [12, 13].

Unfortunately, the combination of these four assumptions implies that the asymptotic expansions for the energy and specific heat for the Ising model at criticality terminate at order $1/L$ (see [14]). However, the numerical results presented in [7, 14] (as well as the analytic results presented in this paper) show this to be false. The problem, therefore, is to determine which one(s) of these assumptions are invalid, and why. Assumption (c) is extremely plausible from renormalization-group considerations, at least for periodic boundary conditions; and assumption (d) has been confirmed numerically to order $(T - T_{\rm c})^3$ at least as regards the bulk behaviour of the susceptibility [13]. However, both numerical [15, 16] and theoretical [17] evidence has recently emerged suggesting that irrelevant operators do contribute to the susceptibility at order $(T - T_{\rm c})^4$.

In a classic paper, Ferdinand and Fisher [18] considered the energy and the specific heat of the two-dimensional Ising model on a torus of length L and aspect ratio ρ, and obtained the first two (three) terms of the large-L asymptotic expansion of the energy (specific heat) at fixed $x \equiv L(T - T_{\rm c})$ (this is the finite-size-scaling regime) and fixed ρ[3]. In particular, at criticality ($T = T_{\rm c}$) they computed the finite-size corrections to both quantities to order L^{-1}. In 1999, Hu *et al* [22] published (without details) the correction of order L^{-3} to the energy and showed that the L^{-2} correction is absent[4]. In this paper we compute explicitly the following finite-size corrections:

- The correction of order L^{-3} to the energy.
- The corrections of order L^{-2} and L^{-3} to the specific heat.

[2] Finite-size scaling has also been successfully applied to data from transfer-matrix computations [9].

[3] Ferdinand and Fisher [18] also obtained the position of the maximum of the specific heat $x_{\rm max}(\rho)$ which depends on the torus aspect ratio ρ. Furthermore, Kleban and Akinci [19, 20] showed that an excellent approximation can be obtained by keeping only the two largest eigenvalues of the transfer matrix, and they interpreted their results in terms of domain-wall energies. This approximation is already good at $\rho = 1$ and becomes exponentially better with increasing ρ. This method could surely simplify the computations presented in this paper; but here we are interested in the *exact* values of the finite-size-scaling corrections. These results are used as theoretical inputs in [14, 21].

[4] The published version of [22] contains several misprints in the crucial formula (3.23). Version 2 of this paper in the Los Alamos preprint archive cond-mat contains the correct formula.

Furthermore, we also find new insights into the general analytic structure of the finite-size corrections to this model. We show that in the critical two-dimensional Ising model:

- The finite-size corrections to the energy and specific heat are always integer powers of L^{-1}, *unmodified by logarithms* (except of course for the leading $\log L$ term in the specific heat).
- In the finite-size expansion of the energy, only *odd* integer powers of L^{-1} occur.
- In the finite-size expansion of the specific heat, any integer powers of L^{-1} can occur. However, the coefficients of the odd powers of L^{-1} in this expansion are proportional to the corresponding coefficients in the energy expansion.

These results can be compared to the general renormalization-group expression for the finite-size corrections to the energy and the specific heat [14], in which arbitrary powers of L^{-1} and terms of the type $L^{-1+p}\log L$ (where p is some real number) can occur. The implications of these results for understanding which one(s) of the assumptions (a)–(d) are invalid will be analysed elsewhere [21].

The plan of this paper is as follows: in section 2 we present our definitions and notation (generally following [18]). In sections 3 and 4 we present the computation of the next terms in the asymptotic expansions for the energy and specific heat, respectively. Finally, in section 5 we present our arguments about the type of finite-size-scaling correction that can occur in these two expansions. We have summarized in appendix A the basic definitions and properties of the θ-functions that will be needed in this paper. In appendix B we recall the Euler–MacLaurin formula.

Remark. After the completion of this paper, we learned that similar results have been independently obtained by Izmailian and Hu [23].

2. Basic definitions

Let us consider an Ising model on a torus of size $m \times n$ at zero magnetic field. The Hamiltonian is given by[5]

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} \sigma_i \sigma_j. \tag{2.1}$$

The partition function can be written as

$$Z_{mn} = \sum_{\{\sigma\}} \mathrm{e}^{-\mathcal{H}} = \tfrac{1}{2}(2\sinh 2K)^{mn/2} \sum_{i=1}^{4} Z_i(K, n, m) \tag{2.2}$$

where the partial partition function Z_1 is given by

$$Z_1(K, n, m) = \prod_{r=0}^{n-1} 2\cosh\left(\frac{m\gamma_{2r+1}}{2}\right) \tag{2.3}$$

and the rest are defined analogously using the first three columns of the following table (the last two columns will be needed afterwards in (2.9)/(4.18)).

$$\begin{array}{lllll} Z_1: & 2r+1 & \cosh & \tanh & \mathrm{sech} \\ Z_2: & 2r+1 & \sinh & \coth & \mathrm{i}\,\mathrm{csch} \\ Z_3: & 2r & \cosh & \tanh & \mathrm{sech} \\ Z_4: & 2r & \sinh & \coth & \mathrm{i}\,\mathrm{csch}. \end{array} \tag{2.4}$$

[5] In this paper we are following basically the notation used by Ferdinand and Fisher in [18], with a few minor modifications.

The quantities $\gamma_l = \gamma_l(K, n)$ are defined by

$$\cosh\gamma_l \equiv c_l = \cosh 2K \coth 2K - \cos\left(\frac{l\pi}{n}\right). \tag{2.5}$$

In particular, we have

$$\gamma_0 = 2K + \log(\tanh K) \tag{2.6a}$$

$$\gamma_l = \log\left(c_l + \sqrt{c_l^2 - 1}\right) \qquad l \neq 0. \tag{2.6b}$$

The quantities γ_l (2.6) satisfy $\gamma_l = \gamma_{2n-l}$, and γ_l is a monotonically increasing function of l for $0 \leqslant l \leqslant n$.

The internal energy density E and the specific heat C_H are given by

$$E(K, m, n) = -\coth 2K - \frac{1}{mn}\left[\frac{\sum_{i=1}^4 Z_i'}{\sum_{i=1}^4 Z_i}\right] \tag{2.7}$$

$$C_\mathrm{H}(K, m, n) = -2\mathrm{csch}^2 2K + \frac{1}{mn}\left[\frac{\sum_{i=1}^4 Z_i''}{\sum_{i=1}^4 Z_i} - \left(\frac{\sum_{i=1}^4 Z_i'}{\sum_{i=1}^4 Z_i}\right)^2\right] \tag{2.8}$$

where the primes denote derivatives with respect to the coupling constant K. In computing observables (2.7)/(2.8), the following formulae, derived from (2.3), will be useful:

$$\frac{Z_1'}{Z_1} = \frac{m}{2}\sum_{r=0}^{n-1} \gamma_{2r+1}' \tanh\left(\frac{m\gamma_{2r+1}}{2}\right) \tag{2.9a}$$

$$\frac{Z_1''}{Z_1} = \left[\frac{m}{2}\sum_{r=0}^{n-1} \gamma_{2r+1}' \tanh\left(\frac{m\gamma_{2r+1}}{2}\right)\right]^2 + \frac{m}{2}\sum_{r=0}^{n-1} \gamma_{2r+1}'' \tanh\left(\frac{m\gamma_{2r+1}}{2}\right)$$
$$+ \left(\frac{m}{2}\right)^2 \sum_{r=0}^{n-1} \left[\gamma_{2r+1}' \mathrm{sech}\left(\frac{m\gamma_{2r+1}}{2}\right)\right]^2. \tag{2.9b}$$

The analogous ratios for $i = 2, 3, 4$ can be obtained from (2.9*a*)/(2.9*b*) by using (2.4) (Note that the third column of (2.4) does not play any role here.) The factor i in the entry i csch of (2.4) changes the sign of the last term of (2.9*b*) for Z_2'' and Z_4''.

The critical point of the Ising model corresponds to the self-dual point $\sinh 2K_\mathrm{c} = 1$. That is

$$K_\mathrm{c} = \tfrac{1}{2}\log(1 + \sqrt{2}). \tag{2.10}$$

In this paper we are concerned with the finite-size-scaling corrections to the energy and specific heat of the critical Ising model. We will express all our results in terms of the length n and the aspect ratio of the torus ρ[6]:

$$\rho = \frac{m}{n}. \tag{2.11}$$

Indeed, all our results are invariant under the transformation $n \leftrightarrow m$. Here we shall show that the energy and specific heat at criticality have asymptotic expansions of the form

$$-E(K_\mathrm{c}, m, n) \equiv -E_\mathrm{c}(n, \rho) = E_0 + \sum_{k=1}^{\infty} \frac{E_k(\rho)}{n^k} \tag{2.12}$$

$$C_\mathrm{H}(K_\mathrm{c}, n, m) \equiv C_{\mathrm{H,c}}(n, \rho) = C_{00}\log n + C_0(\rho) + \sum_{k=1}^{\infty} \frac{C_k(\rho)}{n^k}. \tag{2.13}$$

[6] In conformal-field-theory language, the modular parameter of the torus is $\tau = \mathrm{i}\rho$ [24], where this τ has nothing to do with the temperature-like parameter defined in (2.14).

The coefficients E_0 and C_{00} can be obtained from Onsager's solution [25]; E_1, C_0, and C_1 were computed by Ferdinand and Fisher [18] and, finally, the fact that $E_2 = 0$ and the expression for E_3 were given (without details) in [22]. Here we shall compute explicitly the terms E_3, C_2 and C_3, and shall show that $E_2 = E_4 = E_6 = \cdots = 0$.

Let us now see how γ_l and its derivatives behave close to the critical point (2.10). To do so, we introduce the finite-size-scaling parameter τ as in [18, equation (2.12)][7]:

$$\left(\frac{\tau}{n}\right)^2 = \frac{1}{2}\left(\sinh 2K + \frac{1}{\sinh 2K}\right) - 1. \tag{2.14}$$

Thus, $\tau = 0$ corresponds to the critical point $K = K_c$, and $\tau \neq 0$ fixed corresponds to the finite-size-scaling regime $n \to \infty$, $K \to K_c$ with $n(K - K_c)$ fixed. Hereafter, we will consider the behaviour of all quantities as a function of τ in the limit $\tau \to 0$. The value of γ_0 at $\tau = 0$ is zero; its behaviour close to the critical point is given by

$$\gamma_0(\tau, n) = -2\left(\frac{\tau}{n}\right) + \mathcal{O}\left[\left(\frac{\tau}{n}\right)^3\right]. \tag{2.15}$$

The derivatives of γ_0 with respect to K are non-vanishing at criticality:

$$\gamma_0'(0, n) \equiv \left.\frac{d\gamma_0}{dK}\right|_{T=T_c} = 4 \tag{2.16a}$$

$$\gamma_0''(0, n) \equiv \left.\frac{d^2\gamma_0}{dK^2}\right|_{T=T_c} = -4\sqrt{2}. \tag{2.16b}$$

(Note that prime continues to denote d/dK, *not* $d/d\tau$. However, the final result will be expressed in terms of τ (in the limit $\tau \to 0$), hence the notation $\gamma_0'(0, n)$.) For a generic $l \neq 0$ the critical value of γ_l is given by

$$\gamma_l(0, n) = 2\log\left[\sqrt{1 + \sin^2\left(\frac{l\pi}{2n}\right)} + \sin\left(\frac{l\pi}{2n}\right)\right] \tag{2.17}$$

while its derivatives with respect to K are given by

$$\gamma_l' = \frac{c_l'}{\sqrt{c_l^2 - 1}} \tag{2.18a}$$

$$\gamma_l'' = \frac{c_l''}{\sqrt{c_l^2 - 1}} - \frac{c_l (c_l')^2}{(c_l^2 - 1)^{3/2}} \tag{2.18b}$$

where the quantity c_l' vanishes at criticality as

$$c_l'(\tau, n) = c'(\tau, n) = -8\left(\frac{\tau}{n}\right) + \mathcal{O}\left[\left(\frac{\tau}{n}\right)^2\right] \tag{2.19}$$

and the quantity c_l'' gives a non-zero value

$$c_l''(0, n) = c''(0, n) = 16. \tag{2.20}$$

We can write the partial partition functions Z_i (cf (2.3)/(2.4)) in the following form:

$$Z_1(\tau, n, \rho) = P_1(\tau, n, \rho)\exp\left(\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r+1}\right) \tag{2.21a}$$

[7] The parameter τ plays the same role as the usual finite-size-scaling parameter $x \equiv L(T - T_c)$. Indeed, to leading order in $K - K_c$ we have $\tau = -2n(K - K_c)$.

$$Z_2(\tau, n, \rho) = P_2(\tau, n, \rho) \exp\left(\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r+1}\right) \tag{2.21b}$$

$$Z_3(\tau, n, \rho) = P_3(\tau, n, \rho) \exp\left(\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r}\right)[1 + e^{-m\gamma_0}] \tag{2.21c}$$

$$Z_4(\tau, n, \rho) = P_4(\tau, n, \rho) \exp\left(\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r}\right)[1 - e^{-m\gamma_0}] \tag{2.21d}$$

where the quantities $P_i(\tau, n, \rho)$ are given by

$$\log P_1(\tau, n, \rho) = \sum_{r=0}^{n-1} \log(1 + e^{-m\gamma_{2r+1}}) \tag{2.22a}$$

$$\log P_2(\tau, n, \rho) = \sum_{r=0}^{n-1} \log(1 - e^{-m\gamma_{2r+1}}) \tag{2.22b}$$

$$\log P_3(\tau, n, \rho) = \sum_{r=1}^{n-1} \log(1 + e^{-m\gamma_{2r}}) \tag{2.22c}$$

$$\log P_4(\tau, n, \rho) = \sum_{r=1}^{n-1} \log(1 - e^{-m\gamma_{2r}}). \tag{2.22d}$$

The functions (2.22) give non-vanishing constants in the limit $\tau \to 0$ [18]:

$$\log P_1(0, n, \rho) = \frac{\theta_3}{\theta_0} + \mathcal{O}(n^{-2}) \tag{2.23a}$$

$$\log P_2(0, n, \rho) = \frac{\theta_4}{\theta_0} + \mathcal{O}(n^{-2}) \tag{2.23b}$$

$$\log P_3(0, n, \rho) = \frac{1}{2}\frac{\theta_2}{\theta_0} e^{\pi\rho/4} + \mathcal{O}(n^{-2}) \tag{2.23c}$$

$$\log P_4(0, n, \rho) = \theta_0^2 + \mathcal{O}(n^{-2}) \tag{2.23d}$$

where the functions θ_i with $i = 2, 3, 4$ are the usual θ-functions (see appendix A), and θ_0 is defined in (A.2).

Finally, we introduce the ratios

$$R_i(\tau, n, \rho) = \frac{Z_i(\tau, n, \rho)}{Z_1(\tau, n, \rho)}. \tag{2.24}$$

Thus, from (2.21) we obtain

$$R_1(\tau, n, \rho) = 1 \tag{2.25a}$$

$$R_2(\tau, n, \rho) = \frac{P_2(\tau, n, \rho)}{P_1(\tau, n, \rho)} \tag{2.25b}$$

$$R_3(\tau, n, \rho) = 2\cosh\left(\frac{m\gamma_0}{2}\right) P_0(\tau, n, \rho) \frac{P_3(\tau, n, \rho)}{P_1(\tau, n, \rho)} \tag{2.25c}$$

$$R_4(\tau, n, \rho) = 2\sinh\left(\frac{m\gamma_0}{2}\right) P_0(\tau, n, \rho) \frac{P_4(\tau, n, \rho)}{P_1(\tau, n, \rho)} \tag{2.25d}$$

where $P_0(\tau, n, \rho)$ is defined as

$$\log P_0(\tau, n, \rho) = \frac{m}{2}\left[\sum_{r=1}^{n-1}\gamma_{2r} - \sum_{r=0}^{n-1}\gamma_{2r+1}\right]. \tag{2.26}$$

The sum of the four ratios is denoted by R

$$R(\tau, n, \rho) = \sum_{i=1}^{4} R_i(\tau, n, \rho). \tag{2.27}$$

The ratios R_2 and R_3 have a non-vanishing value at the critical point [18]

$$R_2(0, n, \rho) = \frac{\theta_4}{\theta_3} + \mathcal{O}(n^{-2}) \tag{2.28a}$$

$$R_3(0, n, \rho) = \frac{\theta_2}{\theta_3} + \mathcal{O}(n^{-2}) \tag{2.28b}$$

while R_4 vanishes at $K = K_c$:

$$R_4(\tau, n, \rho) = -\sinh(\tau\rho)[\theta_2\theta_4 + \mathcal{O}(n^{-2})] + \mathcal{O}(\tau^2). \tag{2.29}$$

The sum of the four ratios at criticality is a non-zero constant

$$R(0, n, \rho) = \frac{\theta_2 + \theta_3 + \theta_4}{\theta_3} + \mathcal{O}(n^{-2}). \tag{2.30}$$

The function P_0 has also a non-vanishing limit at criticality:

$$P_0(0, n, \rho) = \mathrm{e}^{-\pi\rho/4}[1 + \mathcal{O}(n^{-2})]. \tag{2.31}$$

3. Finite-size-scaling corrections to the internal energy

The internal energy at the critical point E_c is equal to

$$-E_c(n, \rho) = -E(K_c, n, \rho) = \sqrt{2} + \lim_{\tau\to 0} \frac{1}{mnR} \sum_{i=1}^{4} \frac{Z_i'}{Z_i} R_i. \tag{3.1}$$

The terms Z_i'/Z_i with $i = 1, 2$ vanish trivially as all the γ_{2r+1}' vanish. The term Z_3'/Z_3 does not vanish due to the contribution of γ_0'; but its total contribution is also zero as it is multiplied by $\tanh(m\gamma_0/2)$, which vanishes at criticality. The only non-vanishing contribution comes from $i = 4$:

$$\frac{Z_4'}{Z_4} = \frac{m}{2}\gamma_0' \coth\left(\frac{m\gamma_0}{2}\right) \sim -2m\coth(\rho\tau) \qquad \text{as} \quad \tau \to 0. \tag{3.2}$$

So we obtain the formula

$$-E_c(n, \rho) = \sqrt{2} - \frac{2}{n} \lim_{\tau\to 0} \frac{R_4(\tau, n, \rho)}{R(0, n, \rho)} \coth(\rho\tau) \tag{3.3}$$

where $R(0, n, \rho)$ is given by (2.30). Note that, by (2.29), $R_4(\tau, n, \rho) \sim \tau$ as $\tau \to 0$, so $R_4(\tau, n, \rho)\coth(\rho\tau)$ gives rise to a non-zero result in this limit.

The goal of this section is to extend the Ferdinand–Fisher asymptotic expansion [18] to order n^{-4}. Let us first consider the quantity $\log P_4$ at criticality:

$$\log P_4(0, n, \rho) = \sum_{r=1}^{n-1} \log(1 - \mathrm{e}^{-m\gamma_{2r}}) = -2 \sum_{p=1}^{\infty} \frac{1}{p} \sum_{r=1}^{\lfloor \frac{n}{2} \rfloor} \mathrm{e}^{-mp\gamma_{2r}} \tag{3.4}$$

where $\lfloor x \rfloor$ is the largest integer $\leqslant x$. The sum over r can be split into two parts:

$$\sum_{r=1}^{\lfloor \frac{n}{2} \rfloor} = \sum_{r=1}^{s(n)-1} + \sum_{r=s(n)}^{\lfloor \frac{n}{2} \rfloor} \tag{3.5}$$

where $s(n)$ will be chosen afterwards. We can drop the second sum in (3.5), as it gives a contribution of order $\sim n|\log[1-\exp(-m\gamma_{2s})]| \sim n\exp[-2\pi\rho s(n)]$. Instead of the choice $s(n) = (3/2\pi\rho)\log n$ made by Ferdinand and Fisher, we shall use the choice

$$s(n) = \frac{M}{2\pi\rho}\log n \tag{3.6}$$

with M an arbitrary positive integer, to ensure that the total contribution of the second sum in (3.5) is as small as we want (namely, $\sim n^{-(M-1)}$).

We can use the following expression for γ_{2r} at criticality [18]:

$$\frac{1}{2}\gamma_{2r}(0,n) = \log\left[\sin\left(\frac{r\pi}{n}\right) + \sqrt{1+\sin^2\left(\frac{r\pi}{n}\right)}\right] \tag{3.7}$$

to obtain an asymptotic series of $m\gamma_{2r}$ in terms of n^{-1}:

$$m\gamma_{2r}(0,n) = 2\pi\rho r - \frac{2\rho\pi^3}{3}\frac{r^3}{n^2} + \frac{\rho\pi^5}{3}\frac{r^5}{n^4} + \mathcal{O}(n^{-6}). \tag{3.8}$$

We should recall that the choice of $s(n)$ (3.6) for *any* integer M guarantees that the ratio r/n is a small quantity for $0 \leqslant r \leqslant s(n)$ (as $r/n \leqslant s(n)/n \ll 1$ if n is large enough).

Remark. It is interesting to note that only even powers of n^{-1} occur in the expansion (3.8).

Plugging the expansion (3.8) into equation (3.4) we obtain

$$\log P_4(0,n,\rho) = -2\sum_{p=1}^{\infty}\frac{1}{p}\sum_{r=1}^{s(n)-1}\mathrm{e}^{-2\pi rp\rho} - \frac{4\pi^3\rho}{3}\sum_{p=1}^{\infty}\sum_{r=1}^{s(n)-1}\frac{r^3}{n^2}\mathrm{e}^{-2\pi rp\rho} + \mathcal{O}(n^{-4}). \tag{3.9}$$

We can extend the sums $\sum_{r=1}^{s(n)-1}$ to $\sum_{r=1}^{\infty}$ in (3.9) by introducing an error of order n^{-M}. The second term of the rhs of (3.9) can be expressed in terms of

$$\sum_{r=1}^{\infty} r^3\mathrm{e}^{-2\pi rp\rho} = \frac{1}{4}\left[\frac{1}{\sinh^2(\pi p\rho)} + \frac{3}{2}\frac{1}{\sinh^4(\pi p\rho)}\right]. \tag{3.10}$$

Finally, we can write $P_4(n,\rho)$ in the following form:

$$P_4(0,n,\rho) = \theta_0^2\left[1 - \frac{1}{n^2}\frac{p_1(\rho)}{2} + \mathcal{O}(n^{-4})\right] \tag{3.11}$$

which improves (2.23*d*). The function $p_1(\rho)$ is given by

$$p_1(\rho) = \frac{2\pi^3\rho}{3}\sum_{m=1}^{\infty}\left[\frac{1}{\sinh^2(m\pi\rho)} + \frac{3}{2}\frac{1}{\sinh^4(m\pi\rho)}\right]. \tag{3.12}$$

Using similar methods one can obtain the improved version of (2.23):

$$P_1(0,n,\rho) = \frac{\theta_3}{\theta_0}\left[1 - \frac{1}{n^2}\left(\tilde{p}_2 - \frac{\tilde{p}_1}{2}\right) + \mathcal{O}(n^{-4})\right] \tag{3.13a}$$

$$P_2(0,n,\rho) = \frac{\theta_4}{\theta_0}\left[1 + \frac{1}{n^2}\left(\frac{p_1}{2} - p_2\right) + \mathcal{O}(n^{-4})\right] \tag{3.13b}$$

$$P_3(0,n,\rho) = \frac{1}{2}\frac{\theta_2}{\theta_0}\mathrm{e}^{\pi\rho/4}\left[1 + \frac{1}{n^2}\frac{\tilde{p}_1}{2} + \mathcal{O}(n^{-4})\right] \tag{3.13c}$$

where p_2, $\tilde{p}_1$ and $\tilde{p}_2$ are defined by

$$\tilde{p}_1(\rho) = \frac{2\pi^3\rho}{3}\sum_{m=1}^{\infty}(-1)^{m+1}\left[\frac{1}{\sinh^2(m\pi\rho)} + \frac{3}{2}\frac{1}{\sinh^4(m\pi\rho)}\right] \tag{3.14a}$$

$$p_2(\rho) = \frac{\pi^3\rho}{24}\sum_{m=1}^{\infty}\left[\frac{1}{\sinh^2(m\pi\rho/2)} + \frac{3}{2}\frac{1}{\sinh^4(m\pi\rho/2)}\right] \tag{3.14b}$$

$$\tilde{p}_2(\rho) = \frac{\pi^3\rho}{24}\sum_{m=1}^{\infty}(-1)^{m+1}\left[\frac{1}{\sinh^2(m\pi\rho/2)} + \frac{3}{2}\frac{1}{\sinh^4(m\pi\rho/2)}\right]. \tag{3.14c}$$

Finally, we have to improve the expression of $\log P_0$ (2.31). Let us first consider the sum

$$\frac{m}{2}\sum_{r=1}^{n-1}\gamma_{2r}(0,n) = m\sum_{r=0}^{n-1}\log\left[\sin\left(\frac{r\pi}{n}\right) + \sqrt{1+\sin^2\left(\frac{r\pi}{n}\right)}\right]. \tag{3.15}$$

We can apply the Euler–MacLaurin formula (B.4) to the function $f(p) = \log(\sin p + \sqrt{1+\sin^2 p})$ with $L = 2n$ and $\alpha = 1/2$. The result is[8]

$$\frac{m}{2}\sum_{r=1}^{n-1}\gamma_{2r}(0,n) = \frac{2mn}{\pi}G - \frac{\pi\rho}{6} - \frac{\pi^3\rho}{180}\frac{1}{n^2} + \mathcal{O}(n^{-4}) \tag{3.16}$$

where $G \approx 0.915\,965\,594\,177\,219$ is Catalan's constant. Using similar methods we obtain the other sum appearing in (2.31)[9]:

$$\frac{m}{2}\sum_{r=0}^{n-1}\gamma_{2r+1}(0,n) = \frac{2mn}{\pi}G - \frac{\pi\rho}{12} - \frac{7\pi^3\rho}{1440}\frac{1}{n^2} + \mathcal{O}(n^{-4}). \tag{3.17}$$

Putting (3.16) and (3.17) together we obtain the improved version of (2.31)

$$P_0(0,n,\rho) = \mathrm{e}^{-\pi\rho/4}\left[1 - \frac{p_3(\rho)}{n^2} + \mathcal{O}(n^{-4})\right] \tag{3.18}$$

where $p_3(\rho)$ is defined as

$$p_3(\rho) = \frac{\pi^3}{96}\rho. \tag{3.19}$$

Improved expressions for the ratios $R_i(\tau{=}0,n,\rho)$ are easily obtained from equations (3.11)/(3.13)

$$R_2(0,n,\rho) = \frac{\theta_4}{\theta_3}\left[1 - \frac{1}{n^2}\left(p_2 - \frac{p_1}{2} + \tilde{p}_2 - \frac{\tilde{p}_1}{2}\right) + \mathcal{O}(n^{-4})\right] \tag{3.20a}$$

$$R_3(0,n,\rho) = \frac{\theta_2}{\theta_3}\left[1 + \frac{1}{n^2}(\tilde{p}_1 - \tilde{p}_2 - p_3) + \mathcal{O}(n^{-4})\right] \tag{3.20b}$$

$$R_4(0,n,\rho) = -\sinh(\rho\tau)\theta_2\theta_4\left[1 - \frac{1}{n^2}\left(\frac{p_1}{2} + \tilde{p}_2 - \frac{\tilde{p}_1}{2} + p_3\right) + \mathcal{O}(n^{-4})\right]. \tag{3.20c}$$

Plugging the formulae (3.20) into the expression for the critical energy density (3.1) we obtain

$$-E_c(n,\rho) = \sqrt{2} + \frac{E_1(\rho)}{n} + \frac{E_3(\rho)}{n^3} + \mathcal{O}\left(\frac{1}{n^5}\right) \tag{3.21}$$

[8] It is easy to verify that $f^{(3)}(p)$ is integrable over $[0,\pi]$. This means that the next term in the expansion (3.16) is of order $\mathcal{O}(n^{-4})$.

[9] The leading terms of equations (3.16)/(3.17) were obtained by Ferdinand [26].

Table 1. Values of the coefficient $E_3(\rho)$ from (3.23) for several values of the torus aspect ratio ρ.

ρ	$E_3(\rho)$
1	−0.206 683 145 336 864
2	−0.184 202 899 115 749
3	−0.153 247 694 215 529
4	−0.102 599 506 933 675
5	−0.061 201 301 359 728
6	−0.034 200 082 347 112
7	−0.018 369 506 074 164
8	−0.009 614 465 215 356
9	−0.004 941 568 941 314
10	−0.002 505 707 497 764
15	−0.000 074 110 828 658
20	−0.000 001 946 957 522
∞	0

where $E_1(\rho)$ [18] and $E_3(\rho)$ are given by the expressions

$$E_1(\rho) = \frac{2\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4} \tag{3.22}$$

$$E_3(\rho) = -\frac{2\theta_2\theta_3\theta_4}{(\theta_2+\theta_3+\theta_4)^2}\left\{p_1(\rho)\left(\theta_4+\frac{\theta_2+\theta_3}{2}\right) - p_2(\rho)\theta_4 + \tilde{p}_1(\rho)\left(\frac{\theta_2-\theta_3}{2}\right) + \tilde{p}_2(\rho)\theta_3 + p_3(\rho)\left(\theta_3+\theta_4\right)\right\}. \tag{3.23}$$

The numerical values of the function $E_3(\rho)$ are given in table 1.

Remarks. (1) After the completion of this work, Professor Izmailian informed us that the correct expression for the coefficient $E_3(\rho)$ had been published in the revised version of [22] (which can be found in the Los Alamos preprint archive cond-mat). Their expression is surprisingly simple,

$$E_3(\rho) = -\frac{\pi^3\rho}{48}\frac{\theta_2\theta_3\theta_4}{(\theta_2+\theta_3+\theta_4)^2}\left[\theta_2^9+\theta_3^9+\theta_4^9\right]. \tag{3.24}$$

Indeed, the numerical value of (3.24) coincides with our result (3.23). It would be interesting to find the analytic identities proving the equivalence of (3.23) and (3.24).

(2) Let us check that (3.23) has the correct behaviour under $m \leftrightarrow n$ ($\rho \leftrightarrow 1/\rho$). Indeed, the (trivial) fact that $E_c(n, m) = E_c(m, n)$ implies that we should have

$$E_1(\rho) = \frac{E_1(1/\rho)}{\rho} \tag{3.25a}$$

$$E_3(\rho) = \frac{E_3(1/\rho)}{\rho^3}. \tag{3.25b}$$

The first equation (3.25*a*) can be easily proved by using Jacobi's imaginary transformation of the θ-functions (A.4). Using these transformations one can easily show that the second equation (3.25) holds for (3.24). We have also verified numerically that (3.25) holds for our result (3.23) to high accuracy using MATHEMATICA.

(3) There is another simple way to test our results: We can first compute the *exact* value of the critical energy density $E_c(n, \rho)$ for several values of n and a fixed value of ρ by using (2.7)/(2.3)/(2.4). Then, we subtract the first two terms of the expansion (3.21) and fit

Table 2. Fits of the function $-E_c(n,\rho) - \sqrt{2} - E_1(\rho)/n$ (cf (3.22)) to the ansatz $B_3 n^{-3} + B_5 n^{-5} + B_7 n^{-7}$ for several values of the torus aspect ratio ρ.

	$\rho = 1$	$\rho = 2$	$\rho = 3$
B_3	−0.206 683 145 3369	−0.184 202 899 1157	−0.153 247 694 2155
B_5	−0.730 182 312 35	−0.416 996 817	−0.316 738 073
B_7	−4.936 2	−3.405	−2.693

the resulting function to the ansatz $B_3 n^{-3} + B_5 n^{-5} + B_7 n^{-7}$. In table 2 we show the numerical results for such fits with $\rho = 1, 2$ and 3. For $\rho = 1$ we have used in the fits 1309 different values between $n = 16$ and 4096. For $\rho = 2, 3$ we have used ten different values corresponding to $n = 2^p$, $p = 2, \ldots, 11$ (that is why our estimates are more accurate for $\rho = 1$ than for $\rho = 2, 3$). We find an excellent agreement among the numerical estimates for B_3 and the exact values of E_3 quoted in table 1. The value of B_5 for $\rho = 1$ also agrees well with the value $\approx -0.730\,1823$ obtained by Izmailian [27] using analytic means.

(4) In the limit $\rho \to \infty$ of an infinitely long torus (i.e. a cylinder) we have

$$E_1(\infty) = E_3(\infty) = 0 \tag{3.26}$$

as $\lim_{\rho\to\infty} \rho\theta_2 = 0$, and $\lim_{\rho\to\infty} \theta_3 = \lim_{\rho\to\infty} \theta_4 = 1$ (cf (A.1)).

4. Finite-size-scaling corrections to the specific heat

The goal of this section is to extend the asymptotic series of Ferdinand and Fisher [18] for the specific heat to order n^{-3}. Let us start with the definition (2.8) and see which terms contribute to the critical value of C_H. The first term in (2.8) is just a constant ($=-2$); while the third term is quite similar to that already obtained for the energy density (3.3) $[= -4\rho R^{-2} R_4^2 \coth^2(\tau\rho)]$. The most involved term is the second one. Using the analysis of Ferdinand and Fisher, we can obtain the final expression for the critical specific heat $C_{H,c}(n,\rho) = C_H(K_c, n, \rho)$:

$$\begin{aligned} C_{H,c}(n,\rho) = {} & -2 + 4Q_{1,-} - \frac{4R_3(0,n,\rho)}{R(0,n,\rho)}[Q_{1,+} - Q_{1,-}] + 4\rho\frac{R_3(0,n,\rho)}{R(0,n,\rho)} \\ & - \frac{4}{R(0,n,\rho)}\sum_{i=1}^{3} R_i(0,n,\rho) Q_{1,i} + \frac{2\sqrt{2}}{n}\lim_{\tau\to 0}\frac{R_4(\tau,n,\rho)}{R(0,n,\rho)}\coth\tau\rho \\ & - 4\rho\lim_{\tau\to 0}\left(\frac{R_4(\tau,n,\rho)}{R(0,n,\rho)}\coth\tau\rho\right)^2 \end{aligned} \tag{4.1}$$

where the $Q_{1,\pm}$ and $Q_{1,i}$ are those defined in [18] evaluated at $\tau = 0$:

$$Q_{1,1}(n,\rho) = \frac{1}{n}\sum_{r=0}^{n-1}\frac{1 - \tanh(\frac{m\gamma_{2r+1}}{2})}{\sin(\frac{(r+1/2)\pi}{n})[1 + \sin^2(\frac{(r+1/2)\pi}{n})]^{1/2}} \tag{4.2a}$$

$$Q_{1,2}(n,\rho) = \frac{1}{n}\sum_{r=0}^{n-1}\frac{1 - \coth(\frac{m\gamma_{2r+1}}{2})}{\sin(\frac{(r+1/2)\pi}{n})[1 + \sin^2(\frac{(r+1/2)\pi}{n})]^{1/2}} \tag{4.2b}$$

$$Q_{1,3}(n,\rho) = \frac{1}{n}\sum_{r=1}^{n-1}\frac{1 - \tanh(\frac{m\gamma_{2r}}{2})}{\sin(\frac{r\pi}{n})[1 + \sin^2(\frac{r\pi}{n})]^{1/2}} \tag{4.2c}$$

$$Q_{1,4}(n,\rho) = \frac{1}{n}\sum_{r=1}^{n-1}\frac{1 - \coth(\frac{m\gamma_{2r}}{2})}{\sin(\frac{r\pi}{n})[1 + \sin^2(\frac{r\pi}{n})]^{1/2}} \tag{4.2d}$$

$$Q_{1,-}(n,\rho) = \frac{1}{n}\sum_{r=0}^{n-1} \frac{1}{\sin(\frac{(r+1/2)\pi}{n})[1+\sin^2(\frac{(r+1/2)\pi}{n})]^{1/2}} \tag{4.2e}$$

$$Q_{1,+}(n,\rho) = \frac{1}{n}\sum_{r=1}^{n-1} \frac{1}{\sin(\frac{r\pi}{n})[1+\sin^2(\frac{r\pi}{n})]^{1/2}}. \tag{4.2f}$$

The terms with the factors R_i/R ($i = 3, 4$) can be obtained easily using the results of section 3. Let us first consider the quantity $Q_{1,+}(n,\rho)$ (4.2*f*). The first step consists in expanding the factor $[1+\sin^2(r\pi/n)]^{-1/2}$ in equation (4.2*f*) in power series of $\sin(r\pi/n)$:

$$Q_{1,+} = \frac{1}{n}\sum_{r=1}^{n-1}\frac{1}{\sin(\frac{r\pi}{n})} + \frac{1}{n}\sum_{r=1}^{n-1}\sum_{k=1}^{\infty}\binom{-1/2}{k}\sin^{2k-1}\left(\frac{r\pi}{n}\right) \tag{4.3}$$

$$\equiv Q_{1,+}^{(1)} + Q_{1,+}^{(2)}. \tag{4.4}$$

The computation of $Q_{1,+}^{(2)}$ is done by applying the Euler–MacLaurin formula (B.4) to the function $f(p) = \sin^{2k-1}(p)$ with $L = 2n$ and $\alpha = 1/2$. The result is

$$Q_{1,+}^{(2)}(n,\rho) = -\frac{\log 2}{\pi} + \frac{\pi}{12}\frac{1}{n^2} + \mathcal{O}(n^{-4}). \tag{4.5}$$

The computation of the divergent part $Q_{1,+}^{(1)}$ is a little more involved. The idea is to apply the Euler–MacLaurin formula (B.4) to the function $f(p) = \sin^{-1}(p) - 1/p + 1/(p-\pi)$ with $L = 2n$ and $\alpha = 1/2$:

$$\frac{1}{n}\sum_{r=0}^{n-1}\left[\sin^{-1}\left(\frac{r\pi}{n}\right) - \frac{n}{r\pi} + \frac{n}{\pi(r-n)}\right] = \frac{2}{\pi}\log\frac{2}{\pi} + \frac{\pi}{6n^2}\left(\frac{1}{\pi^2}-\frac{1}{6}\right) + \mathcal{O}(n^{-4})$$

$$= Q_{1,+}^{(1)} - \frac{2}{\pi}\sum_{r=1}^{n-1}\frac{1}{r} - \frac{1}{\pi n}. \tag{4.6}$$

Using the well known asymptotic expansion [28] (see also (5.5))

$$\sum_{r=1}^{L}\frac{1}{r} = \log L + \gamma_E + \frac{1}{2L} - \frac{1}{12L^2} + \mathcal{O}(L^{-4}) \tag{4.7}$$

(where $\gamma_E \approx 0.577\,215\,6649$ is the Euler constant) we finally obtain

$$Q_{1,+}^{(1)}(n,\rho) = \frac{2}{\pi}\left[\log n + \gamma_E + \log\frac{2}{\pi} - \frac{\pi^2}{72n^2} + \mathcal{O}(n^{-4})\right]. \tag{4.8}$$

Putting together (4.5)/(4.8) we arrive at the final result

$$Q_{1,+}(n,\rho) = \frac{2}{\pi}\left[\log n + \gamma_E + \log\frac{2^{1/2}}{\pi} + \frac{\pi^2}{36n^2} + \mathcal{O}(n^{-4})\right]. \tag{4.9}$$

Using similar methods we obtain[10]

$$Q_{1,-}(n,\rho) = \frac{2}{\pi}\left[\log n + \gamma_E + \log\frac{2^{5/2}}{\pi} - \frac{\pi^2}{72n^2} + \mathcal{O}(n^{-4})\right]. \tag{4.10}$$

The last part consists in evaluation of the $Q_{1,i}$ (with $i = 1, 2, 3$) in (4.2). For brevity we will perform explicitly the simplest case $Q_{1,4}(n,\rho)$ (4.2*d*). The first step is to expand the term $1 - \coth(m\gamma_{2r}/2)$ as a power series in $\exp(-m\gamma_{2r})$

$$Q_{1,4}(n,\rho) = \frac{2}{n}\sum_{r=1}^{\lfloor\frac{n}{2}\rfloor}\sum_{p=1}^{\infty}\frac{e^{-mp\gamma_{2r}}}{\sin(\frac{r\pi}{n})\sqrt{1+\sin^2(\frac{r\pi}{n})}}. \tag{4.11}$$

[10] The leading term of this equation was obtained by Onsager [25].

Then we split the sum over r as in (3.5). The term including the sum $\sum_{r=s(n)}^{[n/2]}$ gives a total contribution of order $n^{-(M-1)}$ with the choice (3.6) for $s(n)$. The second step is to plug into (4.11) the expansion (3.8) for $m\gamma_{2r}$

$$Q_{1,4} = -\frac{4}{n}\sum_{p=1}^{\infty}\sum_{r=1}^{s-1}\frac{\mathrm{e}^{-2\pi rp\rho}}{\sin(\frac{r\pi}{n})\sqrt{1+\sin^2(\frac{r\pi}{n})}}$$

$$-\frac{8\pi^3\rho}{3n^3}\sum_{p=1}^{\infty}p\sum_{r=1}^{s-1}r^3\frac{\mathrm{e}^{-2\pi rp\rho}}{\sin(\frac{r\pi}{n})\sqrt{1+\sin^2(\frac{r\pi}{n})}} + \mathcal{O}(n^{-4}) \qquad (4.12a)$$

$$\equiv Q_{1,4}^{(a)} + Q_{1,4}^{(b)}. \qquad (4.12b)$$

The computation of $Q_{1,4}^{(b)}$ is quite easy. We expand the factors $\sin(r\pi/n)$ in powers of $r\pi/n$:

$$Q_{1,4}^{(b)} = -\frac{8\pi^2\rho}{3n^2}\sum_{p=1}^{\infty}p\sum_{r=1}^{s(n)-1}r^2\mathrm{e}^{-2\pi rp\rho} + \mathcal{O}(n^{-4}). \qquad (4.13)$$

Then we can extend the sum $\sum_{r=1}^{s(n)-1}$ to $\sum_{r=1}^{\infty}$ at an error of order $n^{-(M+2)}\log^2 n$. Using the fact that

$$\sum_{p=1}^{\infty}p\mathrm{e}^{-2\pi rp\rho} = \frac{\mathrm{e}^{-2\pi r\rho}}{(1-\mathrm{e}^{-2\pi r\rho})^2} = \frac{1}{4\sinh^2(\pi r\rho)} \qquad (4.14)$$

we have that

$$Q_{1,4}^{(b)} = -\frac{2\pi^2\rho}{3n^2}\sum_{p=1}^{\infty}\frac{r^2}{\sinh^2(\pi r\rho)}. \qquad (4.15)$$

The computation of $Q_{1,4}^{(a)}$ follows the same steps:

$$Q_{1,4}^{(a)} = -\frac{4}{\pi}\sum_{p=1}^{\infty}p\sum_{r=1}^{\infty}\frac{1}{r}\mathrm{e}^{-2\pi rp\rho} + \frac{4\pi}{3n^2}\sum_{p=1}^{\infty}p\sum_{r=1}^{\infty}r\mathrm{e}^{-2\pi rp\rho} + \mathcal{O}(n^{-4}). \qquad (4.16)$$

In this case the error introduced by extending the sum $\sum_{r=1}^{s(n)-1}$ to $\sum_{r=1}^{\infty}$ is of order n^{-M}. Using (4.14) we find that

$$Q_{1,4}^{(a)} = \frac{2}{\pi}\sum_{r=1}^{\infty}\frac{1}{r}[1-\coth(\pi r\rho)] - \frac{2\pi}{3n^2}\sum_{r=1}^{\infty}r[1-\coth(\pi r\rho)] + \mathcal{O}(n^{-4}). \qquad (4.17)$$

Thus, we write the final result as

$$Q_{1,4}(n,\rho) = Q_{1,4}^{(0)}(\rho) + \frac{Q_{1,4}^{(2)}(\rho)}{n^2} + \mathcal{O}(n^{-4}) \qquad (4.18a)$$

$$Q_{1,4}^{(0)}(\rho) = \frac{2}{\pi}\sum_{r=1}^{\infty}\frac{1}{r}[1-\coth(\pi r\rho)] \qquad (4.18b)$$

$$Q_{1,4}^{(2)}(\rho) = -\frac{2\pi}{3}\left\{\sum_{r=1}^{\infty}r[1-\coth(\pi r\rho)] + \pi\rho\sum_{r=1}^{\infty}r^2[\mathrm{i}\,\mathrm{csch}(\pi r\rho)]^2\right\}. \qquad (4.18c)$$

The other three quantities $Q_{1,i}$ (4.2a)– (4.2c) can be computed in a similar way. The result can be written as (4.18) using the translations given by (2.4). (In this case, the third column of (2.4) does not play any role.) For $i = 1, 2$ we should make two slight modifications: (a) The

Table 3. Values of the coefficient $C_2(\rho)$ from (4.22) for several values of the torus aspect ratio ρ.

ρ	$C_2(\rho)$
1	0.097 119 896 855 337
2	−0.326 865 280 829 340
3	−0.748 187 561 687 100
4	−0.877 385 104 391 125
5	−0.809 168 407 448 959
6	−0.682 469 414 146 146
7	−0.567 445 479 079 586
8	−0.483 401 539 198 706
9	−0.428 249 598 449 714
10	−0.394 311 952 593 824
15	−0.351 150 319 692 501
20	−0.349 140 134 316 672
∞	−0.349 065 850 398 866

factor r in (4.18) should be replaced by $r + 1/2$, and (b) the sums over r in $Q_{1,1}$ and $Q_{1,2}$ start at $r = 0$ rather than at $r = 1$ (as in $Q_{1,3}$ and $Q_{1,4}$).

Putting all the pieces together we arrive at the final result

$$C_{\mathrm{H,c}}(n,\rho) = \frac{8}{\pi}\log n + C_0(\rho) + \frac{C_1(\rho)}{n} + \frac{C_2(\rho)}{n^2} + \frac{C_3(\rho)}{n^3} + \mathcal{O}\left(\frac{1}{n^4}\right) \tag{4.19}$$

where the coefficients $C_i(\rho)$ are given by

$$C_0(\rho) = \frac{8}{\pi}\left(\log\frac{2^{5/2}}{\pi} + \gamma_E - \frac{\pi}{4}\right) - \frac{4}{\theta_2+\theta_3+\theta_4}\left[\frac{4}{\pi}\sum_{\nu=2}^{4}\theta_\nu\log\theta_\nu + \rho\frac{\theta_2^2\theta_3^2\theta_4^2}{\theta_2+\theta_3+\theta_4}\right] \tag{4.20}$$

$$C_1(\rho) = -2\sqrt{2}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4} = -\sqrt{2}E_1(\rho) \tag{4.21}$$

$$\begin{aligned} C_2(\rho) = {}& -4\rho\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}E_3(\rho) - \frac{\pi}{9} - 4A_3(\rho)\frac{\theta_2}{\theta_2+\theta_3+\theta_4}\left(\rho - \frac{\log 16}{\pi}\right) \\ & + \frac{\pi}{3}\frac{\theta_2}{\theta_2+\theta_3+\theta_4} - \frac{16}{\pi}[A_2(\rho)\theta_4 + A_3(\rho)\theta_2]\frac{\sum_{\nu=2}^{4}\theta_\nu\log\theta_\nu}{(\theta_2+\theta_3+\theta_4)^2} - \frac{4}{\theta_2+\theta_3+\theta_4}G(\rho) \end{aligned} \tag{4.22}$$

$$C_3(\rho) = -\sqrt{2}E_3(\rho) \tag{4.23}$$

where

$$G(\rho) = Q_{1,1}^{(2)}\theta_3 + Q_{1,2}^{(2)}\theta_4 + Q_{1,3}^{(2)}\theta_2 - Q_{1,2}^{(0)}A_2(\rho)\theta_4 - Q_{1,3}^{(0)}A_3(\rho)\theta_2 \tag{4.24a}$$

$$A_2(\rho) = p_2(\rho) + \tilde{p}_2(\rho) - \tfrac{1}{2}[p_1(\rho) + \tilde{p}_1(\rho)] \tag{4.24b}$$

$$A_3(\rho) = p_3(\rho) + \tilde{p}_2(\rho) - p_1(\rho). \tag{4.24c}$$

The expressions for C_0 and C_1 were first obtained by Ferdinand and Fisher [18]. The results for C_2 and C_3 are new. In table 3 we show the values of the coefficient $C_2(\rho)$ for several values of the aspect ratio ρ.

Remarks. (1) As shown by Ferdinand and Fisher using the Jacobi transformations (A.4), the coefficient $C_0(\rho)$ satisfies the identity

$$C_0(\rho) = C_0(\rho^{-1}) + \frac{8}{\pi}\log\rho. \tag{4.25}$$

Table 4. Fits of the function $C_{\mathrm{H,c}}(n,\rho) - (8/\pi)\log n - C_0(\rho) - C_1(\rho)/n$ (cf (4.19)/(4.20)/(4.21)) to the ansatz $D_2 n^{-2} + D_3 n^{-3} + D_4 n^{-4} + D_5 n^{-5}$ for several values of the torus aspect ratio ρ.

	ρ=1	ρ=2	ρ=3
D_2	0.097 119 896 855	−0.326 865 2808	−0.748 187 5617
D_3	0.292 294 1107	0.260 5022	0.216 7250
D_4	0.014 792	−1.063 5	−1.866 8
D_5	1.0326	0.59	0.45

Indeed, from relations (4.21)/(4.23) we conclude that these two coefficients have the right behaviour under the transformation $\rho \to 1/\rho$ (cf (3.25*a*)/(3.25*b*)). Finally, we have tested numerically that

$$C_2(\rho) = \frac{C_2(1/\rho)}{\rho^2} \tag{4.26}$$

is satisfied. This is a non-trivial test of the correctness of our result.

(2) We have also performed the following test: we have defined the function equal to the *exact* value of the specific heat $C_{\mathrm{H,c}}(n,\rho)$ minus the first three terms of the expansion (4.19). Then, we have fitted the result to several ansätze. In particular, we show in table 4 the results for the ansatz $D_2/n^2 + D_3/n^3 + D_4/n^4 + D_5/n^5$. We have used the same data as for the energy fits in section 3. The agreement between the values D_2, D_3 and the exact values (4.22)/(4.23)/(3.23) is very good. It is also interesting to note that $D_5(\rho) \approx -\sqrt{2}B_5(\rho)$, where $B_5(\rho)$ is the coefficient obtained in a similar fit to the energy (see table 2).

(3) By inspection from table 3, the function $C_2(\rho)$ should have a zero at a non-trivial value of the aspect ratio $\rho_{\min}$ between 1 and 2. We have evaluated numerically that value,

$$\rho_{\min} \approx 1.335\,440\,86. \tag{4.27}$$

By (4.26), there is another zero of $C_2(\rho)$ at $\rho_{\min}^{-1} \approx 0.748\,816\,39$.

(4) In the limit $\rho \to \infty$ the coefficients C_i tend to the following limits:

$$C_0(\infty) = \frac{8}{\pi}\left(\log\frac{2^{5/2}}{\pi} + \gamma_E - \frac{\pi}{4}\right) \tag{4.28a}$$

$$C_1(\infty) = 0 \tag{4.28b}$$

$$C_2(\infty) = -\frac{\pi}{9} \tag{4.28c}$$

$$C_3(\infty) = 0. \tag{4.28d}$$

Thus, only the coefficients associated with even powers of n^{-1} survive in this limit.

5. Further remarks and conclusions

The computation of the finite-size corrections to the energy and specific heat shows that, to order n^{-3}:

(a) All the corrections are integer powers of the quantity n^{-1}. In particular there are no multiplicative or additive logarithmic terms (except for the leading term in the specific heat).
(b) In the energy density we only find *odd* powers of n^{-1}. In particular, the corrections of order n^{-2} and n^{-4} are absent from (3.21).

(c) In the specific heat we find both even and odd powers of n^{-1}, but the coefficients of the corrections corresponding to odd powers of n^{-1} in (4.19) are proportional to the corresponding coefficients in the energy expansion (3.21): we found that $C_i(\rho) = -\sqrt{2}E_i(\rho)$ for $i = 1, 3$ (cf (4.21)/(4.23)), and the numerical test performed at the end of sections 3 and 4 shows that the same ratio holds for the next coefficients $C_5/E_5 \approx -\sqrt{2}$.

The natural question is whether these observations are general features that hold to all orders in n^{-1}. In this section, we will try to answer those questions.

Let us first analyse what happens to the energy. We first note that in the expansion (3.8) only even powers of n^{-1} occur. This expansion can be done to any finite order we want. The errors from neglecting the second sum in (3.5) and from extending the sums $\sum_{r=1}^{s(n)-1}$ to $\sum_{r=1}^{\infty}$ are at most of order $\mathcal{O}(n^{-(M-1)})$, and they can be made as small as we want by making M in the definition of $s(n)$ (3.6) as large as we need. This means that in the series expansions of the quantities $\log P_i$ ($i = 1, \ldots, 4$) (3.13) only even powers of n^{-1} appear. Secondly, we need to check that only even powers of n^{-1} occur in the expansion of $\log P_0$ (3.15). The argument is simple: all derivatives $f^{(k)}$ of the function $f(p) = \log(\sin p + \sqrt{1 + \sin^2 p})$ are integrable over the interval $[0, \pi]$. This implies that the Euler–MacLaurin formula (B.4) can be applied to any arbitrary order. As $f(0) = f(\pi)$, the correction of order n^{-1} vanishes and only corrections with even powers of n^{-1} can occur. The same conclusion applies to the expansion (3.15) and to the ratios R_i (3.20). Thus, from formula (3.3) we immediately conclude that only *odd* powers of n^{-1} appear in the finite-size corrections to the critical energy density. This result generalizes point (b) above. In particular, no logarithmic corrections occur in this expansion at any order.

Remark. The authors of [22] made an argument to explain the absence of the L^{-2} correction in the energy. They started with the Fortuin–Kasteleyn representation of the q-state Potts model on a graph G ($q = 2$ corresponds to the Ising model) [29, 30]:

$$Z_G(K) = \sum_{G' \subseteq G} v^{N_b(G')} q^{N_c(G')} \tag{5.1}$$

where N_b and N_c are respectively the number of bonds and connected clusters of the spanning subgraph $G' \subseteq G$, and $v = e^K - 1$. Then, they introduced the standard finite-size-scaling ansatz for the free energy assuming there are no irrelevant operators [4]:

$$f_G(K) = f_{reg}(K) + \frac{1}{L_x L_y} W(L_x^{1/\nu}(K - K_c)). \tag{5.2}$$

Here G is a square lattice of size $L_x \times L_y$, $f_{reg}(K)$ is the regular part of the free energy, ν is the usual critical exponent and $W(x)$ is an analytic function at $x = 0$. They expanded $W(x)$ around $x = 0$ and computed the mean values of N_c and N_b at criticality ($K = K_c$). They found that

$$\langle N_c \rangle = n_c L_x L_y + A L_x^{1/\nu} + B \tag{5.3a}$$

$$\langle N_b \rangle = n_b L_x L_y + C L_x^{1/\nu} \tag{5.3b}$$

with no constant correction to $\langle N_b \rangle$. The internal energy (2.7) is related linearly to N_b; thus, in the Ising model at criticality, we have $E_c = A_0 + A_1(\rho) L_x^{-1}$ with no higher-order corrections in L_x^{-1}. They concluded that the L_x^{-2} correction to the critical energy should vanish. Indeed, this argument also implies the stronger result that there are no corrections of any kind beyond order L_x^{-1}—a conclusion that is unfortunately false! So it is not clear that the ansatz (5.2) (even if we include irrelevant operators) is enough to reproduce the right finite-size expansion of the internal energy of the critical two-dimensional Ising model (3.21). A detailed discussion of this point will be published elsewhere [21] (see also [14, section 3] for preliminary results).

The analysis of the specific heat is a little more involved. Using the same procedure as for the energy, we conclude that the fourth ($\sim R_3/R$) and the last ($\sim R_4^2/R^2$) terms of (4.1) provide corrections with *even* powers of n^{-1}. Furthermore, the sixth term of (4.1) [$\sim R_4/(Rn)$] will give only *odd* powers of n^{-1}.

Let us see now what happens to the terms $Q_{1,i}$ (4.2*a*)–(4.2*d*). The argument for $Q_{1,4}$ (4.2*d*) is quite simple: the expansion of this quantity as a power series of $r\pi/n$ will only contain even powers of n^{-1}. Indeed, the errors from dropping the sum $\sum_{r=s(n)}^{\lfloor n/2\rfloor}$ in the beginning of the computation, and for extending the sum $\sum_{r=1}^{s(n)-1}$ to $\sum_{r=1}^{\infty}$ at the end of the computation, are both at most of order $\mathcal{O}(x^{-(M-1)})$ with the choice (3.6) for $s(n)$. Thus, the fifth term in (4.1) ($\sim \sum R_i Q_{1,i}/R$) will have only corrections with *even* powers of n^{-1}.

Finally, let us analyse the behaviour of $Q_{1,+}$ (4.2*f*). In the evaluation of $Q_{1,+}^{(2)}$ we had to apply the Euler–MacLaurin formula (B.4) to the function $f(p) = \sin^{2k-1} p$ with $k \geqslant 1$. The derivatives of this function are always integrable over the interval $[0,\pi]$, thus the expansion (4.5) only contains *even* powers of n^{-1}. In the evaluation of $Q_{1,+}^{(0)}$ we apply the Euler–MacLaurin formula (B.4) to the function $f(p) = 1/\sin p - 1/p + 1/(p-\pi)$. This function and all its derivatives are integrable over the interval $[0,\pi]$. Thus, equation (4.6) can be generalized to

$$Q_{1,+}^{(0)} = \frac{2}{\pi}\left\{\sum_{p=1}^{n-1}\frac{1}{p} + \frac{1}{2n} + \log\frac{2}{\pi} + \frac{\pi}{2}\sum_{k=1}^{\infty}\frac{B_{2k}}{2k}\left(\frac{\pi}{n}\right)^{2k}[f^{(2k-1)}(\pi) - f^{(2k-1)}(0)]\right\}. \tag{5.4}$$

This expansion contains in principle both even and odd powers of n^{-1}. We now plug in the well known result [28]

$$\sum_{p=1}^{L}\frac{1}{p} = \log L + \gamma_E + \frac{1}{2L} - \sum_{k=1}^{\infty}\frac{B_{2k}}{2k}L^{-2k} \tag{5.5}$$

with $L = n-1$, and expand the resulting factors $\log(1-1/n)$, $(1-1/n)^{-1}$ and $(1-1/n)^{-2k}$ in powers of n^{-1}. If we express the result as $\sum_k \alpha_k n^{-k}$, we immediately see that $\alpha_1 = 0$. The expression for the coefficients of the odd powers of n^{-1} is given by

$$\alpha_{2k+1} = \frac{1}{2} - \frac{1}{2k+1} - \sum_{m=1}^{k}\binom{2k}{2m-1}\frac{B_{2m}}{2m} \qquad k \geqslant 1. \tag{5.6}$$

To prove $\alpha_{2k+1} = 0$, we can apply the general Euler–MacLaurin formula (B.1) to the function $f(x) = x^{2k}$ with $n = 0$ and $m = 1$:

$$0 = \int_0^1 x^{2k}\,\mathrm{d}x - \frac{1}{2} + \sum_{m=1}^{k}\frac{B_{2m}}{(2m)!}\frac{(2k)!}{(2k-2m+1)!} = -\alpha_{2k+1}. \tag{5.7}$$

This implies that in the finite-size-scaling expansion of $Q_{1,+}$ only *even* powers of n^{-1} occur. The same holds for $Q_{1,-}$ (4.2*e*).

In summary, we have seen that in the finite-size-scaling expansion of the specific heat at criticality only integer powers of n^{-1} appear (except of course for the leading term $(8/\pi)\log n$). Furthermore, all contributions to the specific heat (4.1) give *even* powers of n^{-1}, except for one, namely, the sixth term in (4.1), which has the form

$$\frac{2\sqrt{2}}{n}\lim_{\tau\to 0}\frac{R_4(\tau,n,\rho)}{R(0,n,\rho)}\coth\tau\rho. \tag{5.8}$$

If we compare it to the expression for the energy (3.3) we conclude that the coefficients associated with *odd* powers of n^{-1} in the energy and specific-heat expansions are proportional.

In particular (cf, (2.12)/(2.13)), and recalling that $E_{2k} = 0$, we obtain

$$\frac{E_k(\rho)}{C_k(\rho)} = \begin{cases} -1/\sqrt{2} & \text{for } k \text{ odd} \\ 0 & \text{for } k \text{ even.} \end{cases} \tag{5.9}$$

This generalizes the results (4.21)/(4.23). Note in particular that the ratio $E_k(\rho)/C_k(\rho)$ is independent of the aspect ratio ρ.

Let us conclude with a brief discussion about the generality of the above results. It is clear that the leading-term coefficients E_0 and C_{00} in (2.12)/(2.13) do *not* depend on the boundary conditions, as they are bulk quantities. However, the finite-size-scaling coefficients $E_k(\rho)$ and $C_k(\rho)$ with $k \geqslant 1$ are expected to depend in general on the boundary conditions of the system. In particular, Lu and Wu [31] have obtained the finite-size expansion of the free energy for a critical Ising model with two different boundary conditions (namely, a Möbius strip and a Klein bottle). They found an expansion of the form

$$f_c(n,\rho) = f_0 + \frac{f_1(\rho)}{n} + \frac{f_2(\rho)}{n^2} + \cdots \tag{5.10}$$

where the coefficients $f_k(\rho)$ with $k = 1, 2$ *do* depend explicitly on the boundary conditions.

On the other hand, the fact that the ratio $E_k(\rho)/C_k(\rho)$ is a ρ-independent number suggests that it might be universal, i.e. independent of the details of the Hamiltonian. It would be very interesting to investigate this possibility. A first step in this direction has been achieved by Izmailian and Hu [32], who computed the finite-size expansion of the free energy per spin f_N and the inverse correlation length ξ_N^{-1} for a critical Ising model on several $N \times \infty$ lattices with periodic boundary conditions (namely, square, hexagonal and triangular). On each lattice they found expansions of the form

$$f_N - f_0 = \sum_{k=1}^{\infty} \frac{f_k}{N^{2k}} \tag{5.11a}$$

$$\xi_N^{-1} = \sum_{k=1}^{\infty} \frac{b_k}{N^{2k-1}} \tag{5.11b}$$

where the coefficients b_k and f_k *do* depend on the lattice. However, their ratio b_k/f_k is the same for all three lattices and equal to $b_k/f_k = (2^{2k}-1)/(2^{2k-1}-1)$. They also computed the corresponding expansions for a quantum spin chain belonging to the two-dimensional Ising model universality class. They found that the ratio b_k/f_k takes the same value as in the Ising case. This result supports the conjecture that this ratio is a universal quantity.

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Appendix A. Theta functions

In this appendix we gather all the definitions and properties of the Jacobi θ-functions needed in this paper. We follow the notation of [18], which was adapted from Whittaker and Watson [33].

We define the Jacobi θ-functions θ_i at $z = 0$ in the following way[11]:

$$\theta_2 \equiv \theta_2(0, \mathrm{e}^{-\pi\rho}) = 2\theta_0 \mathrm{e}^{-\pi\rho/4} \prod_{r=1}^{\infty} (1 + \mathrm{e}^{-2r\pi\rho})^2 \tag{A.1a}$$

$$\theta_3 \equiv \theta_3(0, \mathrm{e}^{-\pi\rho}) = \theta_0 \prod_{r=1}^{\infty} (1 + \mathrm{e}^{-(2r-1)\pi\rho})^2 \tag{A.1b}$$

$$\theta_4 \equiv \theta_4(0, \mathrm{e}^{-\pi\rho}) = \theta_0 \prod_{r=1}^{\infty} (1 - \mathrm{e}^{-(2r-1)\pi\rho})^2. \tag{A.1c}$$

The function $\theta_0(\rho)$ is defined as

$$\theta_0 = \theta_0(\rho) = \prod_{r=1}^{\infty} (1 - \mathrm{e}^{-2\pi r\rho}) \tag{A.2}$$

and it satisfies the following identity:

$$\theta_0 = \mathrm{e}^{\pi\rho/12} [\tfrac{1}{2}\theta_2\theta_3\theta_4]^{1/3}. \tag{A.3}$$

These θ-functions (A.1) satisfy the Jacobi imaginary transformation

$$\theta_2(0, \mathrm{e}^{-\pi/\rho}) = \rho^{1/2}\theta_4(0, \mathrm{e}^{-\pi\rho}) \tag{A.4a}$$

$$\theta_3(0, \mathrm{e}^{-\pi/\rho}) = \rho^{1/2}\theta_3(0, \mathrm{e}^{-\pi\rho}) \tag{A.4b}$$

$$\theta_4(0, \mathrm{e}^{-\pi/\rho}) = \rho^{1/2}\theta_2(0, \mathrm{e}^{-\pi\rho}). \tag{A.4c}$$

Appendix B. The Euler–MacLaurin formula

The Euler–MacLaurin formula (see e.g. [34, appendix B]) is the main tool we need to compute asymptotic series. The general form of this formula is given by

$$\sum_{k=n}^{m-1} f(k) = \int_n^m \mathrm{d}x\, f(x) - \tfrac{1}{2}[f(m) - f(n)] + \sum_{p=1}^{N} \frac{B_{2p}}{(2p)!}[f^{(2p-1)}(m) - f^{(2p-1)}(n)]$$
$$+ \frac{1}{(2N+1)!} \int_n^m \mathrm{d}x\, f^{(2N+1)}(x) B_{2N+1}(x - \lfloor x \rfloor) \tag{B.1}$$

where B_n are the Bernoulli numbers and $B_n(x)$ are the Bernoulli polynomials defined by

$$B_n(x) = \sum_{k=0}^{n} \binom{n}{k} B_k x^{n-k}. \tag{B.2}$$

In this paper we are mainly interested in sums of the form

$$\frac{1}{L} \sum_{n=0}^{\alpha L-1} f(p) \tag{B.3}$$

where $p = 2\pi n/L$. The asymptotic expansion of the sum (B.3) in the limit $L \to \infty$ with α fixed can be obtained from (B.1):

$$\frac{1}{L} \sum_{n=0}^{\alpha L-1} f(p) = \int_0^{2\pi\alpha} \frac{\mathrm{d}p}{2\pi} f(p) - \frac{1}{2L}[f(2\pi\alpha) - f(0)]$$

[11] In this particular case, $\theta_1(0, \mathrm{e}^{-\pi\rho}) = 0$.

$$+\frac{1}{2\pi}\sum_{k=1}^{N}\frac{B_{2k}}{(2k)!}\left(\frac{2\pi}{L}\right)^{2k}[f^{(2k-1)}(2\pi\alpha) - f^{(2k-1)}(0)]$$

$$+\frac{1}{(2N+1)!}\left(\frac{2\pi}{L}\right)^{2N+1}\int_0^{2\pi\alpha}\frac{\mathrm{d}p}{2\pi}f^{(2N+1)}(p)\hat{B}_{2N+1}(p) \qquad \text{(B.4)}$$

where

$$\hat{B}_n(p) = B_n\left(\frac{Lp}{2\pi} - \left\lfloor\frac{Lp}{2\pi}\right\rfloor\right). \qquad \text{(B.5)}$$

The expression (B.4) gives the asymptotic expansion of the sum (B.3) in powers of L^{-1} up to order L^{-2N} *if* the last integral in (B.4) is finite (i.e. if $f^{(2N+1)}(p)$ is integrable in the interval $[0, 2\alpha\pi]$). If $f(0) = f(2\pi\alpha)$, then only *even* powers of L^{-1} occur in the expansion (B.4).

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