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Exact finite-size-scaling corrections to the critical two-dimensional Ising model on a torus: II. Triangular and hexagonal lattices

Jesús Salas

Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, Zaragoza 50009, Spain

E-mail: jesus@melkweg.unizar.es

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Abstract
We compute the finite-size corrections to the free energy, internal energy and specific heat of the critical two-dimensional spin-$1/2$ Ising model on triangular and hexagonal lattices wrapped on a torus. We find the general form of the finite-size corrections to these quantities, as well as explicit formulae for the first coefficients of each expansion. We analyse the implications of these findings for the renormalization-group description of the model.

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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 $V = L^d$ grows, yielding the critical singularities in the limit $L \to \infty$. For bulk experimental systems (containing $V \sim 10^{23}$ particles), the finite-size rounding of the phase transition is usually beyond the experimental resolution; but in Monte Carlo simulations ($V \lesssim 10^6 - 10^7$) 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 coming 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 T and magnetic field h (i.e., μ_t and μ_h, respectively) are independent of L [11].
(c) The scaling field μ_L associated with the lattice size equals L^{-1} exactly, with no corrections $L^{-2}, L^{-3}, \ldots$ [4].

Moreover, in the nearest-neighbour spin-1/2 two-dimensional Ising model, it was further assumed for many years that there are no irrelevant operators [12, 13]; indeed this assumption was confirmed numerically through order $(T - T_c)^3$, at least as regards the bulk behaviour of the susceptibility in the isotropic square-lattice Ising model [13]. However, several authors have recently found overwhelming evidence that there are indeed irrelevant operators playing a role in the two-dimensional Ising model [14–20]. In particular, for the square-lattice Ising model they have found by studying the bulk magnetic susceptibility that there is one irrelevant operator contributing to order $(T - T_c)^4$ and there is (at least) one irrelevant operator contributing to order $(T - T_c)^6$.

An interesting way to test assumptions (a)–(c) and see the effect of the irrelevant operators is to compute the asymptotic expansion (in powers of L^{-1}) of the free energy and its derivatives with respect to the temperature at the critical point. The square-lattice Ising model is the best understood case.

In a classic paper, Ferdinand and Fisher [21] considered the energy and the specific heat of the square-lattice Ising model on a torus of width L and aspect ratio ρ, and obtained the first two (respectively three) terms of the large-L asymptotic expansion of the energy (respectively specific heat) at fixed $x \equiv L(T - T_c)$ (this is the finite-size-scaling regime) and fixed ρ. In particular, at criticality ($T = T_c$) they computed the finite-size corrections to both quantities to order L^{-1}. Their results have been improved at the critical point by several authors [22–25]. Their results can be summarized as follows:

$$f_c^{\rm sq}(L,\rho) = f_{\rm bulk}^{\rm sq} + \sum_{m=1}^{\infty} \frac{f_{2m}^{\rm sq}(\rho)}{L^{2m}} \tag{1.1a}$$

$$E_c^{\rm sq}(L,\rho) = E_0 + \sum_{m=0}^{\infty} \frac{E_{2m+1}^{\rm sq}(\rho)}{L^{2m+1}} \tag{1.1b}$$

$$C_{H,c}^{\rm sq}(L,\rho) = C_{00}^{\rm sq} \log L + C_0^{\rm sq}(\rho) + \sum_{m=1}^{\infty} \frac{C_m^{\rm sq}(\rho)}{L^m} \tag{1.1c}$$

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

where f_c, E_c and $C_{H,c}$ are, respectively, the critical free energy, internal energy and specific heat[3].

The first important observation is that there are no logarithmic corrections except for the specific-heat leading term $C_{00}^{\mathrm{sq}} \log L$. Secondly, the finite-size corrections are integer powers of L^{-1}, which is consistent with the irrelevant operators taking integer exponents. Furthermore, not all the powers of L^{-1} occur; in the large-L expansion of the free energy (respectively internal energy) only even (respectively odd) powers of L^{-1} can occur. In the specific-heat expansion all powers of L^{-1} can appear. In addition, the coefficients C_m^{sq} and E_m^{sq} satisfy the relation

$$\frac{E_m^{\mathrm{sq}}(\rho)}{C_m^{\mathrm{sq}}(\rho)} = \begin{cases} -1/\sqrt{2} & \text{for } m \text{ odd} \\ 0 & \text{for } m \text{ even.} \end{cases} \tag{1.2}$$

The authors of [20] classified (using conformal field theory) all possible irrelevant operators that may occur in the two-dimensional Ising model and found that all their results (in the thermodynamic limit and at criticality on a finite torus) can be explained in terms of the following conjecture:

Conjecture 1.1 ([20], conjecture (d2)). *The only irrelevant operators which appear in the two-dimensional nearest-neighbour Ising model are those due to the lattice breaking of the rotational symmetry.*

In particular, for the square-lattice Ising model the first operator that breaks rotational invariance is the spin-four operator $T^2 + \bar{T}^2$ (where here T is the energy–momentum operator) whose renormalization-group exponent is $y = -2$. In [20] they showed that this operator can give rise to all the observed corrections in (1.1)[4].

In this paper we extend the above results to the triangular and hexagonal lattices. We will obtain the large-L asymptotic expansions for the critical free energy, internal energy and specific heat for such lattices wrapped on a torus of width L and fixed aspect ratio ρ. The interest of this computation is three-fold. First, we can make a new test of conjecture 1.1. In the triangular lattice, the first irrelevant operator (belonging to the identity family) that breaks rotational invariance is $T^3 + \bar{T}^3$ with $y = -6$ [20]. If conjecture 1.1 is true, then several coefficients in the finite-size-scaling expansions (1.1) should vanish. Second, we can directly check whether the ratio (1.2) is universal or not, that is, if (1.2) depends or not on the microscopic details of the lattice. Finally, the asymptotic expansions could be useful to check Monte Carlo simulations.

A first study of the triangular-lattice Ising model partition function on a finite torus was done by Nash and O'Connor [32]. They obtained (among other interesting results) the exact expression of such a partition function with anisotropic nearest-neighbour couplings and extracted its scaling limit. They computed the bulk contribution to the free energy f_{bulk} and the first finite-size correction $f_2(\rho)$. Here we will extend their results at the critical point.

[3] Janke and Kenna [26] have studied similar expansions for the square-lattice Ising model with Branscamp–Kunz boundary conditions. The analytic structure is similar to (1.1) but additional terms arise due to the boundary conditions. For instance, there is a term $\sim \log L/L$ in the specific heat. On the other hand, Lu and Wu [27] studied the critical free energy for the square-lattice Ising model on non-orientable surfaces (namely, the Möbius strip and the Klein bottle). They found the first terms of the large-L expansion of $f_c(L, \rho)$; although they did not give details about the analytic structure of such expansion. In particular, there is an additional term $\sim L^{-1}$ in the expansion for the Möbius strip (due to 'surface' effects) which is absent in the Klein bottle. They also explicitly showed that the coefficient $f_2^{\mathrm{sq}}(\rho)$ depends on the boundary conditions (even if the expansion (1.1*a*) holds true).

[4] A similar finite-size scaling analysis was carried out for the one-dimensional Ising quantum chain which belongs to the same universality class of the two-dimensional Ising model [28–31].

The main results of this paper can be summarized as follows

$$f_c(L,\rho) = f_{\rm bulk} + \sum_{m=1}^{\infty} \frac{f_{2m}(\rho)}{L^{2m}} \tag{1.3a}$$

$$E_c(L,\rho) = E_0 + \sum_{m=0}^{\infty} \frac{E_{2m+1}(\rho)}{L^{2m+1}} \tag{1.3b}$$

$$C_{H,c}(L,\rho) = C_{00}\log L + C_0(\rho) + \sum_{m=1}^{\infty} \frac{C_m(\rho)}{L^m} \tag{1.3c}$$

$$f_c^{(3)}(L,\rho) = \mathcal{A}_1(\rho)L + A_{00}\log L + A_0(\rho) + \sum_{m=1}^{\infty} \frac{A_m(\rho)}{L^m} \tag{1.3d}$$

$$f_{c,\log}^{(4)}(L,\rho) = B_{00}\log L \tag{1.3e}$$

where $f_c^{(3)}$ (respectively $f_{c,\log}^{(4)}$) is the third derivative (respectively the logarithmic contribution to the fourth derivative) of the free energy with respect to the inverse temperature β evaluated at the critical point. We have also found explicit formulae for the coefficients $f_2(\rho)$, $f_6(\rho)$, $E_1(\rho)$, $E_5(\rho)$, C_{00}, $C_0(\rho)$, $C_1(\rho)$, $C_4(\rho)$, $C_5(\rho)$, $\mathcal{A}_1(\rho)$, A_{00}, $A_0(\rho)$, $A_1(\rho)$ and B_{00} (indeed, $f_4 = f_8 = E_3 = E_7 = C_2 = C_3 = A_2 = 0$).

Our results on the general analytic structure of the finite-size corrections to these models are:

- The analytic structure of the finite-size-scaling corrections of the quantities considered here is exactly the same for the triangular and the hexagonal lattices.
- The finite-size corrections to the free energy, internal 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 free energy, only *even* integer powers of L^{-1} occur. The only exceptions are the powers L^{-4} and L^{-8} whose coefficients vanish.
- In the finite-size expansion of the energy, we only find *odd* integer powers of L^{-1}. In this case, the coefficients associated with the powers L^{-3} and L^{-7} vanish.
- In the finite-size expansion of the specific heat, any integer powers of L^{-1} can occur, except the terms L^{-2} and L^{-3}. In addition, the non-zero coefficients of the odd powers of L^{-1} in this expansion are proportional to the corresponding coefficients in the internal energy expansion as in the square lattice.
- In the finite-size expansion of $f_c^{(3)}$ we find that the expected leading term $L\log L$ is missing, and the actual leading term is simply L. We find that all powers of L^{-1} appear in such expansion, except L^{-2}.
- In the finite-size expansion of the fourth derivative of the free energy $f_c^{(4)}$ we find that there is only a logarithmic term $\sim\log L$, even though we expect two additional logarithmic contributions of order $L\log L$ and $L^2\log L$, respectively.

The above results are very useful to gain new insights into the renormalization-group description of the two-dimensional Ising model. Our conclusions on this topic are:

- Some irrelevant operators should vanish at criticality. This happens, in particular, to the less irrelevant one $T\bar{T}$ with renormalization-group exponent $y = -2$.
- In order to give account of all the finite-size corrections, we should include *at least* two irrelevant operators, in agreement with the results of [17, 18].

- The scaling function $\hat{W}(x)$ (which is responsible for the logarithmic corrections to the derivatives of the free energy) vanishes at criticality $x = 0$. Its first derivatives at criticality satisfy

$$\left.\frac{\partial^n W(x)}{\partial x^n}\right|_{x=0} = \begin{cases} 0 & \text{for } n = 1, 3, 4 \\ 1/(\lambda\pi\sqrt{3}) & \text{for } n = 2 \end{cases} \tag{1.4}$$

where $\lambda = 1$ (respectively 2) for the triangular (respectively hexagonal) lattice. These equations motivate the conjecture that $\hat{W}(x) = x^2/(2\lambda\pi\sqrt{3})$.

- The non-linear scaling field associated with the temperature can be computed for both lattices and it is given by

$$\mu_t(\tau) = \tau - \tfrac{1}{24}\tau^3 + \mathcal{O}(\tau^5). \tag{1.5}$$

This result provides a cross-check of the analysis of infinite-volume quantities [20].

The plan of this paper is as follows: in section 2, we present our definitions and notation. In sections 3–6 we present the computation of the asymptotic expansions for the free energy, internal energy, specific heat and higher derivatives of the free energy, respectively. In section 7, we discuss the consequences of our results on the renormalization-group description of the models. In particular, we will focus on the irrelevant operators of the model and on the finite-size-scaling functions. Finally, in section 8, we present our conclusions and discuss the results. We have summarized the technical details in the appendixes: in appendix A we recall the Euler–MacLaurin formula, and in appendix B (respectively appendix C) we collect the definitions and properties of the θ-functions (respectively Kronecker's double series).

2. Basic definitions

Let us first consider an Ising model on a triangular lattice wrapped on a torus of size $N \times M$ at zero magnetic field. The Hamiltonian is given by

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

The partition function is given by

$$Z_{NM}(\beta) = \sum_{\{\sigma=\pm 1\}} \mathrm{e}^{-\mathcal{H}}. \tag{2.2}$$

The dual of such triangular lattice is an hexagonal lattice wrapped on a torus of size $N \times M$ and containing $2NM$ sites (i.e., the hexagonal lattice can be viewed as a triangular lattice with a two-point basis). The Hamiltonian and the partition functions of the Ising model on this lattice are also given by (2.1) and (2.2).

If one brushes aside some subtleties about boundary conditions, one can relate the partition function (2.2) of a triangular-lattice Ising model at coupling β to the partition function of the Ising model on the dual (i.e., hexagonal) lattice at a 'dual' coupling $\beta^\star$ [33, 34]:

$$Z_{NM}^{\mathrm{tri}}(\beta) = Z_{2NM}^{\mathrm{hc}}(\beta^\star) 2^{1-2NM} (2\sinh 2\beta)^{3NM/2} \tag{2.3}$$

where $\beta^\star$ is defined by

$$\tanh \beta^\star = \mathrm{e}^{-2\beta}. \tag{2.4}$$

Using equation (2.3) and the star-triangle equation [35] we can obtain the critical values of the couplings for both models

$$\beta_c = \begin{cases} \frac{1}{4}\log 3 & \text{triangular} \\ \frac{1}{2}\log(2+\sqrt{3}) & \text{hexagonal.} \end{cases} \tag{2.5}$$

However, this argument is strictly valid only in the infinite-volume limit; it gives the correct relation

$$f^{\mathrm{tri}}(\beta) = 2f^{\mathrm{hc}}(\beta^\star) - 2\log 2 + \tfrac{3}{2}\log(2\sinh 2\beta) \tag{2.6}$$

between infinite-volume free energies and the correct critical points (2.5), but identity (2.3) for finite-lattice partition functions does *not*, in general, hold. This is because a periodic lattice is non-planar, so that the correct duality formula also involves a pair of 'homological' modes arising from the two directions of winding around the torus [36]. Or put it another way: high-temperature graphs that wind around the lattice do *not* necessarily correspond to low-temperature graphs on the dual lattice. Therefore, on a finite lattice—which is the subject of this paper—we need to be more careful[5].

We begin by computing the exact partition function of both models on a torus of size $N \times M$. One way to do this is by relating the Ising model to a dimer model [37]. The same computation leading to the square-lattice partition function can be used to obtain the hexagonal-lattice partition function [38] by changing the weights of the different dimer configurations. Though the triangular-lattice Ising partition function cannot be derived from the hexagonal-lattice partition function using duality (2.3), for the reasons given above, we can instead use the star-triangle transformation [35]. Then, the triangular-lattice partition function Z^{tri}_{MN} is related to the hexagonal-lattice partition function Z^{hc}_{2MN} (containing twice as much sites) by the formula

$$Z^{\mathrm{tri}}_{MN}(\beta) = R(\beta)^{-MN} Z^{\mathrm{hc}}_{2MN}(\tilde{\beta}) \tag{2.7}$$

where the $\tilde{\beta}$ and $R(\beta)$ are given by [35]

$$\sinh 2\tilde{\beta} = \frac{1}{\kappa(\beta)}\frac{1}{\sin 2\beta} \tag{2.8a}$$

$$R(\beta)^2 = \frac{2}{\kappa(\beta)^2 \sinh^3 2\beta} \tag{2.8b}$$

and κ (which depends on β through the parameter $v = \tanh\beta$) is equal to [35]

$$\kappa(\beta) = \frac{(1-v^2)^3}{4\sqrt{(1+v^3)v^3(1+v)^3}}. \tag{2.9}$$

After straightforward (but lengthy) algebra we find that the partition function for both lattices can be written in a very similar way in the ferromagnetic regime:

$$Z_V(\beta) = \frac{1}{2}(2\sin 2\beta)^{V/2} \sum_{\alpha,\beta=0,1/2} Z_{\alpha,\beta}(\mu) \tag{2.10}$$

where V is the number of spins in the lattice (e.g., $V = NM$ in the triangular lattice and $V = 2NM$ in the hexagonal lattice). The functions $Z_{\alpha,\beta}(\mu)$ are given by

$$\begin{aligned} Z_{\alpha,\beta}(\mu)^2 = \prod_{n=0}^{N-1}\prod_{m=0}^{M-1} 4\left\{\sin^2\left(\frac{\pi(n+\alpha)}{N}\right) + \sin^2\left(\frac{\pi(m+\beta)}{M}\right)\right. \\ \left. + \sin^2\left(\frac{\pi(m+\beta)}{M} - \frac{\pi(n+\alpha)}{N}\right) + 2\sinh^2\mu\right\} \end{aligned} \tag{2.11}$$

where the 'mass' term μ is given by

$$e^{2\mu} = \begin{cases} \frac{1}{2}(e^{4\beta}-1) & \text{triangular} \\ 2\sinh^2\beta & \text{hexagonal.} \end{cases} \tag{2.12}$$

The critical point corresponds to the vanishing of the mass, thus giving (2.5).

[5] We thank Alan Sokal for useful clarifications about this point.

Remark. The fact that the partition function of both lattices depends on the same functions $Z_{\alpha,\beta}(\mu)$ can be explained by noting that the translational symmetry of both lattices is the same (i.e., they have the same underlying Bravais lattice). This issue explains why the finite-size expansions are so similar in both lattices.

The functions $Z_{\alpha,\beta}(\mu)$ can be expanded in powers of μ. In particular, when $(\alpha, \beta) \neq (0, 0)$ the functions are even in μ, while $Z_{0,0}(\mu)$ is an odd function of μ:

$$Z_{\alpha,\beta}(\mu) = Z_{\alpha,\beta}(0) + \frac{1}{2!} Z''_{\alpha,\beta}(0)\mu^2 + \cdots \qquad (\alpha, \beta) \neq (0, 0) \tag{2.13}$$

$$Z_{0,0}(\mu) = \mu Z'_{\alpha,\beta}(0) + \frac{1}{3!} Z'''_{\alpha,\beta}(0)\mu^3 + \cdots. \tag{2.14}$$

This is similar to what happens in the square-lattice Ising model [25].

We are interested in computing the asymptotic expansions for large N and M with fixed aspect ratio (e.g. length to width ratio):

$$\rho = \frac{M}{N} \tag{2.15}$$

of the free energy $f(\beta; N, \rho)$, internal energy $E(\beta; N, \rho)$ and specific heat $C_H(\beta; N, \rho)$ at the critical point $\beta = \beta_c$. These quantities are defined as follows:

$$f(\beta; N, \rho) = \frac{1}{V} \log Z_V(\beta) \tag{2.16a}$$

$$E(\beta; N, \rho) = -\frac{\partial}{\partial\beta} f(\beta; N, \rho) \tag{2.16b}$$

$$C_H(\beta; N, \rho) = \frac{\partial^2}{\partial\beta^2} f(\beta; N, \rho). \tag{2.16c}$$

In section 6 we will also consider higher derivatives of the free energy at criticality

$$f_c^{(k)}(N, \rho) = \left. \frac{\partial^k}{\partial\beta^k} f(\beta; N, \rho) \right|_{\beta=\beta_c} \tag{2.17}$$

with $k = 3, 4$.

Remark. The definition of the specific heat (2.16c) is somewhat non-standard as it does not contain the factor β^2.

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

Let us start with the basic quantity $Z_{\alpha,\beta}$ (2.11) and write it in the form

$$Z_{\alpha,\beta}(\mu) = \prod_{n=0}^{N-1} \prod_{m=0}^{M-1} 4 \left\{ \cosh 2\mu + \sin^2\left(\frac{\pi(n+\alpha)}{N}\right) - \cos\left(\frac{\pi(n+\alpha)}{N}\right) \cos\left(\frac{2\pi(m+\beta)}{M} - \frac{\pi(n+\alpha)}{N}\right) \right\}. \tag{3.1}$$

The product over m in (3.1) can exactly be performed with the help of the following identity [32]:

$$\prod_{m=0}^{M-1} \left[\zeta - \lambda \cos\left(\frac{2\pi(m+\beta)}{M}\right) \right] = \left(\frac{\lambda z_+}{2}\right)^M |1 - z_- \,\mathrm{e}^{-2\pi \mathrm{i}\beta}|^2 \tag{3.2}$$

where ζ and λ are any two real numbers such that $|\zeta/\lambda| \geqslant 1$ and the quantities $z_\pm$ are given by

$$z_\pm = \frac{\zeta}{\lambda} \pm \sqrt{\left(\frac{\zeta}{\lambda}\right)^2 - 1} \tag{3.3a}$$

$$z_+ z_- = 1. \tag{3.3b}$$

We can finally write $Z_{\alpha,\beta}(\mu)$ as

$$Z_{\alpha,\beta}(\mu) = 2^{NM/2} \prod_{n=0}^{N-1} \left(\cosh 2\mu + \sin^2\phi_{n+\alpha} + \sqrt{\left[\cosh 2\mu + \sin^2\phi_{n+\alpha}\right]^2 - \cos^2\phi_{n+\alpha}}\right)^{M/2} \times \prod_{n=0}^{N-1} \left|1 - z_-(n+\alpha, N, \mu)^M \, \mathrm{e}^{-2\pi \mathrm{i}\beta + M\mathrm{i}\phi_{n+\alpha}}\right| \tag{3.4}$$

where we have used the shorthand notation

$$z_\pm(k, N, \mu) = \frac{\cosh 2\mu + \sin^2\phi_k \pm \sqrt{\left[\cosh 2\mu + \sin^2\phi_k\right]^2 - \cos^2\phi_k}}{\cos\phi_k} \tag{3.5a}$$

$$\phi_k = \frac{\pi k}{N}. \tag{3.5b}$$

Let us now evaluate the functions $Z_{\alpha,\beta}(0)$ for $(\alpha, \beta) \neq (0, 0)$. We follow here the procedure used in [25], which proved to be very efficient for extracting the large-N asymptotic expansions of the quantities of interest. We first compute the sum

$$f_1 = \frac{M}{2} \sum_{n=0}^{N-1} \log\left[1 + \sin^2\phi_{n+\alpha} + \sin\phi_{n+\alpha}\sqrt{3 + \sin^2\phi_{n+\alpha}}\right] = \frac{M}{2} \sum_{n=0}^{N-1} \omega_1(\phi_{n+\alpha}) \tag{3.6}$$

where

$$\omega_1(k) = \log[1 + \sin^2 k + \sin k\sqrt{3 + \sin^2 k}] = \lambda k + \sum_{k=2}^{\infty} \frac{k^p}{p!}\lambda_p. \tag{3.7}$$

The function ω_1 and all its derivatives are integrable over $[0, \pi]$, and in addition,

$$\omega_1^{(k)}(\pi) - \omega_1^{(0)}(0) = \begin{cases} -2\omega_1^{(k)}(0) & k = 2, 6, 10, 12, 14, \ldots \\ 0 & \text{otherwise.} \end{cases} \tag{3.8}$$

We can now use the Euler–MacLaurin summation formula (A.6) to obtain

$$\frac{1}{N} \sum_{n=0}^{N-1} \omega_1(\phi_{n+\alpha}) = \frac{1}{\pi} \int_0^\pi \omega_1(x)\, \mathrm{d}x - \frac{\lambda}{\pi N^2} B_2(\alpha) - \sum_{m=1}^{\infty} \left(\frac{\pi}{N}\right)^{2m} \frac{B_{2m+2}(\alpha)}{(2m+2)!}\lambda_{2m+1}. \tag{3.9}$$

The first coefficients λ_k are

$$\lambda = \sqrt{3} \qquad \lambda_3 = \lambda_7 = 0 \qquad \lambda_5 = \frac{16}{\sqrt{3}} \qquad \lambda_9 = 1792\sqrt{3} \qquad \lambda_{11} = -\frac{51\,200}{\sqrt{3}}. \tag{3.10}$$

The final result for f_1 is

$$f_1 = \frac{NM}{2\pi} \int_0^\pi \omega_1(x)\, \mathrm{d}x - \frac{\pi\lambda\rho}{2} B_2(\alpha) - \pi\rho \sum_{m=1}^{\infty} \left(\frac{\pi}{N}\right)^{2m} \frac{B_{2m+2}(\alpha)}{(2m+2)!}\lambda_{2m+1}. \tag{3.11}$$

Let us now consider the quantity f_2

$$f_2 = \sum_{n=0}^{N-1} \log \left|1 - z_-(n+\alpha, N, 0)^M \, \mathrm{e}^{-2\pi \mathrm{i}\beta + M\mathrm{i}\phi_{n+\alpha}}\right|. \tag{3.12}$$

We first note that when $n + \alpha = N/2$, the factor $z_-(n+\alpha, N, 0) = 0$, so this term does not contribute to the sum (3.12). In the other cases $z_-(n+\alpha, N, 0)$ does not vanish and we can use (3.3*b*) to write (3.12) as

$$f_2 = \sum_{n=0}^{N-1}{}' \log \left|1 - \mathrm{e}^{-M\log z_+(n+\alpha,N,0) - 2\pi\mathrm{i}\beta + M\mathrm{i}\phi_{n+\alpha}}\right| \tag{3.13}$$

where $\sum'$ means that we have taken out the term with $n + \alpha = N/2$ (if such a term exists).

We now proceed as in [25]: we first write $\log|1 - \mathrm{e}^{-A}| = \mathrm{Re}\log(1 - \mathrm{e}^{-A})$ and then expand $\log(1 - \mathrm{e}^{-A})$ as a power series in e^{-A}:

$$f_2 = -\mathrm{Re} \sum_{p=1}^{\infty} \sum_{n=0}^{N-1}{}' \frac{1}{p} \mathrm{e}^{-2p[M(\log z_+(n+\alpha,N,0) - \mathrm{i}\phi_{n+\alpha})/2 + \pi\mathrm{i}\beta]}. \tag{3.14}$$

It is convenient to write the function $\log z_+(k, N, 0)$ as

$$\log z_+(k, N, 0) \equiv \omega_2(\phi_k) = \omega_1(\phi_k) - \log\cos\phi_k \tag{3.15}$$

where $\omega_1(k)$ is the function (3.7). We then split the sum over n into two parts: $n \in [0, \lfloor N/2 \rfloor - 1]$, and $n \in [\lfloor N/2 \rfloor, N-1]$. By making the substitution $n \to N - 1 - n$ in the second sum, we finally obtain

$$\begin{aligned} f_2 = -\mathrm{Re} \sum_{p=1}^{\infty} \sum_{n=0}^{\lfloor N/2 \rfloor - 1}{}' \frac{1}{p} \mathrm{e}^{-2p(M[w_2(\phi_{n+\alpha}) - \mathrm{i}\phi_{n+\alpha}] + \mathrm{i}\pi\beta)} \\ - \mathrm{Re} \sum_{p=1}^{\infty} \sum_{n=0}^{N - \lfloor N/2 \rfloor - 1}{}' \frac{1}{p} \mathrm{e}^{-2p(M[w_2(\phi_{n+1-\alpha}) - \mathrm{i}\phi_{n+\alpha}] - \mathrm{i}\pi\beta)}. \end{aligned} \tag{3.16}$$

We now expand the function $\omega_2(k)$ as a power series in k

$$\omega_2(k) = \lambda k + \sum_{m=1}^{\infty} \frac{\lambda_{2m+1}}{(2m+1)!} k^{2m+1} \tag{3.17}$$

where the λ_k are exactly those of the function ω_1 (3.10). We obtain an expression of the form

$$\begin{aligned} f_2 = -\mathrm{Re} \sum_{p=0}^{\infty} \frac{1}{p} \sum_{n=0}^{\lfloor N/2 \rfloor - 1}{}' \mathrm{e}^{-2p[\pi\tau_0\rho(n+\alpha) + \mathrm{i}\pi\beta]} \exp\left\{-\pi p\rho \sum_{m=1}^{\infty} \left(\frac{\pi}{N}\right)^{2m} \frac{\lambda_{2m+1}}{(2m+1)!} (n+\alpha)^{2m+1}\right\} \\ - \mathrm{Re} \sum_{p=0}^{\infty} \frac{1}{p} \sum_{n=0}^{N - \lfloor N/2 \rfloor - 1}{}' \mathrm{e}^{-2p[\pi\tau_0\rho(n+1+\alpha) - \mathrm{i}\pi\beta]} \\ \times \exp\left\{-\pi p\rho \sum_{m=1}^{\infty} \left(\frac{\pi}{N}\right)^{2m} \frac{\lambda_{2m+1}}{(2m+1)!} (n+1-\alpha)^{2m+1}\right\} \end{aligned} \tag{3.18}$$

where τ_0 is a complex number equal to

$$\tau_0 = \frac{\lambda - \mathrm{i}}{2} = \frac{\sqrt{3} - \mathrm{i}}{2} = \mathrm{e}^{-\mathrm{i}\pi/6}. \tag{3.19}$$

The next step consists in expanding the exponentials in powers of N^{-k}. By following the procedure introduced in [25, appendix B] we obtain

$$f_2 = -\mathrm{Re}\sum_{p=0}^{\infty}\frac{1}{p}\sum_{n=0}^{\lfloor N/2\rfloor-1}{}' \left\{1 - p\pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+1)!}(n+\alpha)^{2m+1}\right\} \mathrm{e}^{\{-2p[\pi\tau_0\rho(n+\alpha)+\mathrm{i}\pi\beta]\}}$$
$$- \mathrm{Re}\sum_{p=0}^{\infty}\frac{1}{p}\sum_{n=0}^{N-\lfloor N/2\rfloor-1}{}' \left\{1 - p\pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+1)!}(n+1-\alpha)^{2m+1}\right\}$$
$$\times\, \mathrm{e}^{\{-2p[\pi\tau_0\rho(n+1+\alpha)-\mathrm{i}\pi\beta]\}} \tag{3.20}$$

where the Λ_k are certain differential operators. The first ones are

$$\Lambda_3 = \Lambda_7 = 0 \tag{3.21a}$$
$$\Lambda_5 = \lambda_5 \tag{3.21b}$$
$$\Lambda_9 = \lambda_9 + \frac{63}{5}\lambda_5^2\frac{\partial}{\partial\lambda} \tag{3.21c}$$
$$\lambda_{11} = \lambda_{11}. \tag{3.21d}$$

We can now extend the sum over n to $n = \infty$ as the error is exponentially small. On the other hand, the contribution of the term with $n + \alpha = N/2$ is also exponentially small, so we can take out this constraint. Then, after rearranging the sums, we obtain

$$f_2 = \sum_{n=0}^{\infty}\log\left|1 - \mathrm{e}^{-2\pi[\rho\tau_0(n+\alpha)+\mathrm{i}\beta]}\right| + \sum_{n=0}^{\infty}\log\left|1 - \mathrm{e}^{-2\pi[\rho\tau_0(n+1-\alpha)-\mathrm{i}\beta]}\right|$$
$$+\pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+1)!}\,\mathrm{Re}\sum_{p=1}^{\infty}\sum_{n=0}^{\infty}\left\{(n+\alpha)^{2m+1}\,\mathrm{e}^{-2p\pi[\rho\tau_0(n+\alpha)+\mathrm{i}\beta]}\right.$$
$$\left. + (n+1-\alpha)^{2m+1}\,\mathrm{e}^{-2p\pi[\rho\tau_0(n+1-\alpha)+\mathrm{i}\beta]}\right\}. \tag{3.22}$$

The desired result can be obtained by plugging in (B.13)/(C.2):

$$f_2 = \log\left|\frac{\theta_{\alpha,\beta}(\mathrm{i}\tau_0\rho)}{\eta(\mathrm{i}\tau_0\rho)}\right| + \frac{\pi\lambda\rho}{2}B_2(\alpha)$$
$$+\pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+2)!}\left[B_{2m+2}(\alpha) - \mathrm{Re}\,K_{2m+2}^{\alpha,\beta}(\mathrm{i}\tau_0\rho)\right] \tag{3.23}$$

where the elliptic θ-function $\theta_{\alpha,\beta}$ and the Dedekind's η-function are defined in appendix B, the objects $B_p(\alpha)$ are Bernoulli polynomials defined in appendix A, and $K_{2m+2}^{\alpha,\beta}$ are Kronecker's double series defined in appendix C. Then, the value of $Z_{\alpha,\beta}(0)$ is given by

$$\log Z_{\alpha,\beta}(0) = \frac{NM}{2}\log 2 + \frac{NM}{2\pi}\int_0^{\pi}\omega_1(t)\,\mathrm{d}t + \log\left|\frac{\theta_{\alpha,\beta}(\mathrm{i}\tau_0\rho)}{\eta(\mathrm{i}\tau_0\rho)}\right|$$
$$-\pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+2)!}\,\mathrm{Re}\,K_{2m+2}^{\alpha,\beta}(\mathrm{i}\tau_0\rho). \tag{3.24}$$

The free energy at the critical point can be computed directly from (2.10):

$$f_c(N, M) = -\frac{1}{V}\log 2 + \frac{1}{2}\log(2\sinh 2\beta_c) + \frac{1}{V}\log\sum_{\alpha,\beta}Z_{\alpha,\beta}(0). \tag{3.25}$$

Table 1. Values of the coefficients $f_2^{\mathrm{tri}}(\rho)$ and $f_6^{\mathrm{tri}}(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$f_2^{\mathrm{tri}}(\rho)$	$f_6^{\mathrm{tri}}(\rho)$
1	0.636 514 168 294 813	0.084 178 614 254 145
2	0.340 929 552 077 890	0.052 778 553 027 830
3	0.267 452 513 800 776	0.069 393 489 802 385
4	0.242 663 080 213 048	0.079 193 473 629 707
5	0.233 284 972 993 438	0.084 621 760 086 675
6	0.229 516 370 606 439	0.087 503 667 615 417
7	0.227 941 884 733 430	0.088 999 315 024 483
8	0.227 265 427 814 348	0.089 766 374 485 276
9	0.226 968 542 233 183	0.090 157 377 673 790
10	0.226 836 041 806 366	0.090 356 069 258 841
11	0.226 776 103 731 001	0.090 456 876 341 452
12	0.226 748 689 100 100	0.090 507 980 191 895
13	0.226 736 034 656 892	0.090 533 876 582 898
14	0.226 730 148 221 756	0.090 533 876 582 898
15	0.226 727 392 017 273	0.090 553 643 011 573
16	0.226 726 094 176 590	0.090 557 009 779 414
17	0.226 725 480 047 888	0.090 558 715 190 155
18	0.226 725 188 196 890	0.090 559 579 041 296
19	0.226 725 048 974 839	0.090 560 016 609 581
20	0.226 724 982 337 581	0.090 560 238 251 165
∞	0.226 724 920 529 277	0.090 560 465 757 793

The result (3.24) means that the free energy for both lattices can be written as

$$f_c(N,\rho) = f_{\mathrm{bulk}} + \sum_{m=1}^{\infty} \frac{f_{2m}(\rho)}{N^{2m}}. \tag{3.26}$$

Thus, only even powers of N^{-1} can occur, and in contrast to what happens in the square-lattice, we find some even powers whose coefficient vanishes (e.g., $f_4 = f_8 = 0$). The above result agrees with the formula found by Izmailian and Hu [41] for an Ising model on a $N \times \infty$ hexagonal (or triangular) lattice with periodic boundary conditions.

The first coefficients for the triangular lattice are given by

$$f_{\mathrm{bulk}}^{\mathrm{tri}} = \frac{1}{2}\log\frac{4}{\sqrt{3}} + \frac{1}{2\pi}\int_0^{\pi} \omega_1(t)\,\mathrm{d}t \approx 0.879\,585\,3861\ldots \tag{3.27a}$$

$$f_2^{\mathrm{tri}}(\rho) = \frac{1}{\rho}\log\frac{|\theta_2|+|\theta_3|+|\theta_4|}{2|\eta|} \tag{3.27b}$$

$$f_4^{\mathrm{tri}}(\rho) = f_8^{\mathrm{tri}}(\rho) = 0 \tag{3.27c}$$

$$f_6^{\mathrm{tri}}(\rho) = -\frac{\pi^5}{45\sqrt{3}}\,\mathrm{Re}\,\frac{|\theta_4|K_6^{\frac{1}{2},0} + |\theta_2|K_6^{0,\frac{1}{2}} + |\theta_3|K_6^{\frac{1}{2},\frac{1}{2}}}{|\theta_2|+|\theta_3|+|\theta_4|} \tag{3.27d}$$

where the θ_i are the standard θ-functions defined in (B.10) and the functions $K_6^{\alpha,\beta}$ are given in terms of θ-functions in (C.4). As explained in appendix B, all the functions θ_i, η and $K_p^{\alpha,\beta}$ are evaluated at $z = 0$ and $\tau = \mathrm{i}\tau_0\rho$ (B.11). The numerical values of these coefficients for several values of ρ can be found in table 1.

The coefficients of the hexagonal-lattice expansion are found to be

$$f_{\rm bulk}^{\rm hc} = \frac{1}{2}\log 2\sqrt{6} + \frac{1}{4\pi}\int_0^{\pi} \omega_1(t)\,{\rm d}t \approx 1.025\,059\,0964\ldots \tag{3.28a}$$

$$f_{2m}^{\rm hc}(\rho) = \tfrac{1}{2} f_{2m}^{\rm tri}(\rho). \tag{3.28b}$$

The numerical values of the coefficients $f_2^{\rm hc}$ and $f_6^{\rm hc}$ can be obtained from table 1 with the help of (3.28*b*).

Remarks.

1. The values of the bulk critical free energy (3.27*a*)/(3.28*a*) indeed coincide with the values obtained from the well-known results in the thermodynamic limit [39, 40, 38] when $\beta = \beta_c$:

$$f_{\rm bulk}^{\rm tri}(\beta) = \frac{1}{2}\int_0^{\pi}\int_0^{\pi} \frac{{\rm d}x\,{\rm d}y}{4\pi^2} \log[\cosh^3 2\beta + \sinh^3 2\beta - \omega(x,y)\sinh 2\beta] + \log 2 \tag{3.29a}$$

$$f_{\rm bulk}^{\rm hc}(\beta) = \frac{1}{4}\int_0^{\pi}\int_0^{\pi} \frac{{\rm d}x\,{\rm d}y}{4\pi^2} \log[1 + \cosh^3 2\beta - \omega(x,y)\sinh^2 2\beta] + \frac{3}{4}\log 2 \tag{3.29b}$$

where

$$\omega(x,y) = \cos x + \cos y + \cos(x-y). \tag{3.30}$$

2. The limiting values of the coefficients f_2 and f_6 as $\rho \to \infty$ are easily found to be (cf (B.12))

$$\lim_{\rho\to\infty} f_2^{\rm tri}(\rho) = \frac{\sqrt{3}\pi}{24} \tag{3.31a}$$

$$\lim_{\rho\to\infty} f_6^{\rm tri}(\rho) = \frac{31\pi^5}{60\,480\sqrt{3}}. \tag{3.31b}$$

The corresponding limiting values for the hexagonal lattice are one half of the above values (cf (3.28*b*)).

3. Using the properties of the θ-functions (B.20)/(B.21) and of the functions $K_6^{\alpha,\beta}$ (C.5)/(C.6) we can easily check that the terms (3.27*b*)/(3.27*d*) have the correct behaviour under the transformation $N \leftrightarrow M (\rho \to 1/\rho)$. In particular,

$$f_2(\rho) = \frac{f_2(1/\rho)}{\rho^2} \tag{3.32}$$

$$f_6(\rho) = \frac{f_6(1/\rho)}{\rho^6}. \tag{3.33}$$

4. From (3.24)/(3.21) we see that there is, in general, a non-zero contribution to $\log Z_{\alpha,\beta}(0)$ at any order N^{-2m} with $m \geqslant 4$. However, we cannot rule out cancellations leading to the vanishing of any of the coefficients $f_{2m}(\rho)$ with $m \geqslant 5$ in (3.26). Similar arguments apply to the other large-N expansions in the next sections.

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

Now we will deal with the internal energy (2.16*b*). Using (2.10)/(2.13) we can write the critical internal energy as follows:

$$-E_c(N,\rho) = \coth 2\beta_c + \frac{1}{V}\left.\frac{\mathrm{d}\mu}{\mathrm{d}\beta}\right|_{\beta=\beta_c} \frac{Z'_{0,0}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)}. \tag{4.1}$$

The derivative $\mathrm{d}\mu/\mathrm{d}\beta$ can easily be computed from equation (2.12). Thus, the only unknown object is $Z'_{0,0}(0)$, which can be written as

$$Z'_{0,0}(0) = 2M\, 2^{NM/2} \prod_{n=0}^{N-1}\left(1+\sin^2\phi_n + \sin\phi_n\sqrt{3+\sin^2\phi_n}\right)^{M/2} \prod_{n=1}^{N-1}\left|1 - z_-(n,N,0)^M\, \mathrm{e}^{M\mathrm{i}\phi_n}\right|. \tag{4.2}$$

By noting that the first product is nothing more than f_1 (3.6) with $\alpha = 0$, we can write (4.2) as

$$\log Z'_{0,0}(0) = \frac{NM}{2}\log 2 + \log 2M + \frac{NM}{2\pi}\int_0^\pi \omega_1(t)\,\mathrm{d}t - \frac{\pi\rho\lambda}{2}B_2(0)$$
$$- \pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{B_{2m+2}(0)}{(2m+2)!}\lambda_{2m+1} + \sum_{n=1}^{N-1}\log\left|1 - z_-(n,N,0)^M\,\mathrm{e}^{M\mathrm{i}\phi_n}\right|. \tag{4.3}$$

The last sum in (4.3) is equal to the definition of f_2 (3.12) with $\alpha = 0$, except for the fact that the sum in (4.3) starts at $n = 1$ rather than at $n = 0$. We can follow step by step the same procedure leading to (3.22): the result coincides with (3.22) when $\alpha = 0$ except that the first sum in (3.22) now starts at $n = 1$. Using (B.16)/(C.2) we obtain the final result

$$\log Z'_{0,0}(0) = \frac{NM}{2}\log 2 + \log 2M + \frac{NM}{2\pi}\int_0^\pi \omega_1(t)\,\mathrm{d}t + 2\log|\eta(\mathrm{i}\tau_0\rho)|$$
$$- \pi\rho\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+2)!}\,\mathrm{Re}\, K^{0,0}_{2m+2}(\mathrm{i}\tau_0\rho). \tag{4.4}$$

This equation implies that the critical internal energy can be written as a power series in N^{-1}:

$$-E_c(N,\rho) = E_0 + \sum_{m=0}^{\infty}\frac{E_{2m+1}(\rho)}{N^{2m+1}}. \tag{4.5}$$

For the triangular lattice we find that

$$E_0^{\mathrm{tri}} = 2 \tag{4.6a}$$

$$E_1^{\mathrm{tri}}(\rho) = \frac{3|\theta_2\theta_3\theta_4|}{|\theta_2| + |\theta_3| + |\theta_4|} \tag{4.6b}$$

$$E_3^{\mathrm{tri}}(\rho) = E_7^{\mathrm{tri}}(\rho) = 0 \tag{4.6c}$$

$$E_5^{\mathrm{tri}}(\rho) = -\frac{\pi^5\rho}{15\sqrt{3}}\frac{|\theta_2\theta_3\theta_4|}{(|\theta_2|+|\theta_3|+|\theta_4|)^2}\,\mathrm{Re}\left\{(|\theta_2|+|\theta_3|+|\theta_4|)K_6^{0,0}\right.$$
$$\left. - |\theta_4|K_6^{\frac{1}{2},0} - |\theta_2|K_6^{0,\frac{1}{2}} - |\theta_3|K_6^{\frac{1}{2},\frac{1}{2}}\right\} \tag{4.6d}$$

Table 2. Values of the coefficients $E_1^{\rm tri}(\rho)$ and $E_5^{\rm tri}(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$E_1^{\rm tri}(\rho)$	$E_5^{\rm tri}(\rho)$
1	1.017 408 797 595 956	−0.359 705 063 388 737
2	0.612 513 647 162 813	−0.178 088 378 079 924
3	0.345 040 108 164 264	−0.168 599 461 543 254
4	0.185 288 835 745 847	−0.127 979 167 922 216
5	0.096 804 501 605 795	−0.086 206 117 890 971
6	0.049 827 662 298 672	−0.054 108 487 929 080
7	0.025 447 703 091 251	−0.032 506 071 497 113
8	0.012 944 169 002 509	−0.018 975 959 727 317
9	0.006 570 580 061 525	−0.010 859 541 565 321
10	0.003 331 786 807 789	−0.006 125 084 912 961
11	0.001 688 570 266 906	−0.003 416 526 641 140
12	0.000 855 546 533 105	−0.001 888 941 526 185
13	0.000 433 419 665 204	−0.001 036 828 005 370
14	0.000 219 555 049 642	−0.000 565 662 233 279
15	0.000 111 214 898 315	−0.000 307 012 198 010
16	0.000 056 334 542 069	−0.000 165 883 847 105
17	0.000 028 535 313 425	−0.000 089 278 100 310
18	0.000 014 454 016 292	−0.000 047 882 460 122
19	0.000 007 321 388 062	−0.000 025 601 385 603
20	0.000 003 708 495 908	−0.000 013 650 380 771
∞	0	0

where we have used (B.15)/(C.4). The numerical values of these coefficients can be found in table 2. In the hexagonal-lattice case we obtain

$$E_0^{\rm hc} = \frac{2}{\sqrt{3}} \tag{4.7a}$$

$$E_{2m+1}^{\rm hc}(\rho) = \frac{E_{2m+1}^{\rm tri}(\rho)}{2\sqrt{3}}. \tag{4.7b}$$

The numerical values of the coefficients $E_1^{\rm hc}$ and $E_5^{\rm hc}$ can be obtained from table 2 by using (4.7b).

Remarks.

1. The limiting values of the coefficients E_1 and E_5 as $\rho \to \infty$ are easily found to be (cf (B.12))
$$\lim_{\rho\to\infty} E_1(\rho) = \lim_{\rho\to\infty} E_5(\rho) = 0. \tag{4.8}$$
This formula is valid for the triangular and hexagonal lattices. In particular, we expect that *all* the coefficients $E_{2m+1}(\rho)$ will vanish in the limit $\rho \to \infty$ due to the existence of the factor $|\theta_2\theta_3\theta_4|$ which vanishes exponentially fast. Thus, on an infinitely long torus, the internal energy for *any* finite width N is equal to the bulk value E_0 with no finite-size corrections.
2. Using the properties of the θ-functions (B.20)/(B.21) and of the functions $K_6^{\alpha,\beta}$ (C.5)/(C.6) we can easily check that the coefficients E_1 and E_5 (4.6b)/(4.6d)/(4.7b) have the correct behaviour under the transformation $\rho \to 1/\rho$. In particular,
$$E_1(\rho) = \frac{E_1(1/\rho)}{\rho} \tag{4.9}$$
$$E_5(\rho) = \frac{E_5(1/\rho)}{\rho^5}. \tag{4.10}$$

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

The specific heat at criticality is given by the following formula:

$$C_{H,c} = \frac{-2}{\sinh^2 2\beta_c} + \frac{1}{V} \left.\frac{\mathrm{d}^2\mu}{\mathrm{d}\beta^2}\right|_{\beta=\beta_c} \frac{Z'_{0,0}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)}$$

$$+ \frac{1}{V} \left.\frac{\mathrm{d}\mu}{\mathrm{d}\beta}\right|^2_{\beta=\beta_c} \left[\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)} - \left(\frac{Z'_{0,0}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)} \right)^2 \right]. \tag{5.1}$$

The main goal of this section is to compute the ratio

$$\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)} \tag{5.2}$$

where the sums go over $(\alpha, \beta) \neq (0, 0)$. After some algebra, we can write the derivative $Z''_{\alpha,\beta}(0)$ as follows

$$Z''_{\alpha,\beta}(0) = \frac{4MN}{\pi\sqrt{3}} Z_{\alpha,\beta}(0) \left[\mathcal{S}^{(1)}_{\alpha} + 2\mathcal{S}^{(2)}_{\alpha,\beta} + \frac{\pi\sqrt{3}}{4} \rho\, \delta_{\alpha,0} \right] \tag{5.3}$$

where the sums $\mathcal{S}^{(j)}$ are given by

$$\mathcal{S}^{(1)}_{\alpha} = \frac{\pi\sqrt{3}}{2N} \sum_{n=\delta_{\alpha,0}}^{N-1} \frac{1}{\sin\phi_{n+\alpha}\sqrt{3+\sin^2\phi_{n+\alpha}}} \tag{5.4a}$$

$$\mathcal{S}^{(2)}_{\alpha,\beta} = \frac{\pi\sqrt{3}}{2N} \operatorname{Re} \sum_{n=\delta_{\alpha,0}}^{N-1} \frac{1}{\sin\phi_{n+\alpha}\sqrt{3+\sin^2\phi_{n+\alpha}}} \frac{z_-^M\, \mathrm{e}^{-2\pi \mathrm{i}\beta + M\mathrm{i}\phi_{n+\alpha}}}{1 - z_-^M\, \mathrm{e}^{-2\pi\mathrm{i}\beta + M\mathrm{i}\phi_{n+\alpha}}}. \tag{5.4b}$$

The variables $\phi_{n+\alpha}$ and $z_- = z_-(n+\alpha, N, 0)$ are given by (3.5) and $\delta_{\alpha,0}$ is the usual Kronecker's delta.

The first step is to compute the sum $\mathcal{S}^{(1)}_{\alpha}$ (5.4*a*). We will follow a procedure similar to the one used in [24] for the square lattice. Let us define the function

$$\omega_3(k) = \frac{\sqrt{3}}{\sin k\sqrt{3+\sin^2 k}} - \frac{1}{k} + \frac{1}{k-\pi}. \tag{5.5}$$

This function and all its derivatives are integrable over the interval $[0, \pi]$, so we can apply the Euler–MacLaurin formula (A.6). The final result is

$$\mathcal{S}^{(1)}_{\alpha}(N) = \sum_{n=\delta_{\alpha,0}}^{N-1} \frac{1}{n+\alpha} + \frac{1}{2N}\delta_{\alpha,0} + \frac{1}{2}\int_0^{\pi} \omega_3(t)\,\mathrm{d}t - \sum_{m=1}^{\infty} \left(\frac{\pi}{N}\right)^{2m} \frac{B_{2m}(\alpha)}{(2m)!} \tilde{\gamma}_{2m-1} \tag{5.6}$$

where the coefficients $\tilde{\gamma}_{2m-1}$ come from the expansion of $\omega_3(k)$ in powers of k:

$$\omega_3(k) = \sum_{m=0}^{\infty} \frac{\tilde{\gamma}_m}{m!} k^m \tag{5.7a}$$

$$= -\sum_{m=0}^{\infty} \frac{k^m}{\pi^{m+1}} + \sum_{m=1}^{\infty} \frac{\gamma_{2m+1}}{(2m+1)!} k^{2m+1}. \tag{5.7b}$$

In general, the coefficient $\tilde{\gamma}_m$ contains two contributions: one comes from the term $1/(k-\pi)$ which gives the (trivial) coefficient $-\pi^{-(m+1)}m!$, and the other contribution comes from the first two terms in the lhs of (5.5). We will denote by γ_m this latter (non-trivial) contribution. In particular, only the coefficients γ_{2m+1} with $m = 1, 2, 3, \ldots$ are non-zero. The first non-vanishing coefficients γ_m are

$$\gamma_3 = \tfrac{8}{15} \qquad \gamma_5 = -\tfrac{80}{21} \qquad \gamma_7 = \tfrac{448}{5}. \tag{5.8}$$

On the other hand, the value of the integral in (5.6) is

$$\frac{1}{2}\int_0^\pi \omega_3(t)\,\mathrm{d}t = \log\frac{\sqrt{3}}{\pi}. \tag{5.9}$$

In computing the sums $\sum_{n=\delta_{\alpha,0}}^{N-1}(n+\alpha)^{-1}$ we will use the result (see, e.g., [42])

$$\sum_{n=1}^{N}\frac{1}{N} = \log N + \gamma_E + \frac{1}{2N} - \sum_{k=1}^{\infty}\frac{B_{2k}}{2k}\frac{1}{N^{2k}} \tag{5.10}$$

(where $\gamma_E \approx 0.577\,215\,6649$ is the Euler constant) and take into account that $\alpha = 0, 1/2$. In the simplest case $\alpha = 0$ we have

$$\mathcal{S}_0^{(1)}(N) = \log N + \gamma_E + \log\frac{\sqrt{3}}{\pi} - \sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{B_{2m}}{(2m)!}\tilde{\gamma}_{2m-1} + \frac{1}{2N}$$
$$+ \frac{1}{2(N-1)} + \log\left(1-\frac{1}{N}\right) - \sum_{m=1}^{\infty}\frac{B_{2m}}{2m}\frac{1}{(N-1)^{2m}}. \tag{5.11}$$

This expression can be simplified by expanding it in powers of N^{-1}, and then using formulae (A.9)/(A.10). A further simplification can be made if we take into account (5.7*b*). The final result for $\alpha = 0$ is

$$\mathcal{S}_0^{(1)}(N) = \log N + \gamma_E + \log\frac{\sqrt{3}}{\pi} - \sum_{m=2}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{B_{2m}}{(2m)!}\gamma_{2m-1}. \tag{5.12}$$

The value for $\alpha = 1/2$ can be obtained using similar arguments in addition to (A.3). The final result for $\mathcal{S}_\alpha^{(1)}$ is

$$\mathcal{S}_\alpha^{(1)}(N) = \log N + \gamma_E + \log\frac{4\sqrt{3}}{\pi} - \log 4\,\delta_{\alpha,0} - \sum_{m=2}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{B_{2m}(\alpha)}{(2m)!}\gamma_{2m-1}. \tag{5.13}$$

In the above result only the non-trivial Taylor coefficients of the function ω_3 enter.

The second step is to compute the sums $\mathcal{S}_{\alpha,\beta}^{(2)}$ (5.4*b*). The procedure is similar to those already done in sections 3 and 4. We first write

$$z_-(n+\alpha, N, 0)^M = \mathrm{e}^{-M\log z_-(n+\alpha,N,0)} = \mathrm{e}^{-M\omega_2(\phi_{n+\alpha})} \tag{5.14}$$

where the function ω_2 has been defined in (3.15). Then we split the sum $\sum_{n=\delta_{\alpha,0}}^{N-1}$ into two parts: $n \in [\delta_{\alpha,0}, \lfloor N/2\rfloor - 1]$ and $n \in [\lfloor N/2\rfloor, N-1]$. In the second sum we perform the change $n \to N-1-n$ and using the properties of ω_3 we arrive at

$$\mathcal{S}_{\alpha,\beta}^{(2)} = \frac{\pi\sqrt{3}}{2N}\,\mathrm{Re}\left[\sum_{n=\delta_{\alpha,0}}^{\lfloor N/2\rfloor-1}\frac{1}{\sin\phi_{n+\alpha}\sqrt{3+\sin^2\phi_{n+\alpha}}}\frac{\mathrm{e}^{-2[M(\omega_2(\phi_{n+\alpha})-\mathrm{i}\phi_{n+\alpha})/2+\pi\mathrm{i}\beta]}}{1-\mathrm{e}^{-2[M(\omega_2(\phi_{n+\alpha})-\mathrm{i}\phi_{n+\alpha})/2+\pi\mathrm{i}\beta]}}\right.$$
$$\left. + \sum_{n=0}^{N-\lfloor N/2\rfloor-1}\begin{pmatrix}\alpha\to 1-\alpha\\ \beta\to-\beta\end{pmatrix}\right] \tag{5.15}$$

where the second term is the same as the first one with (α, β) replaced by $(1-\alpha, -\beta)$. Now we perform several Taylor expansions: first, we expand the denominator $1 - e^{-2A}$ in powers of e^{-2A}:

$$\mathcal{S}^{(2)}_{\alpha,\beta} = \frac{\pi\sqrt{3}}{2N}\,\mathrm{Re}\left[\sum_{n=\delta_{\alpha,0}}^{\lfloor N/2\rfloor-1}\sum_{p=1}^{\infty}\frac{e^{-2p[M(\omega_2(\phi_{n+\alpha})-i\phi_{n+\alpha})/2+\pi i\beta]}}{\sin\phi_{n+\alpha}\sqrt{3+\sin^2\phi_{n+\alpha}}} + \sum_{n=0}^{N-\lfloor N/2\rfloor-1}\sum_{p=1}^{\infty}\frac{e^{-2p[M(\omega_2(\phi_{n+1-\alpha})-i\phi_{n+1-\alpha})/2-\pi i\beta]}}{\sin\phi_{n+1-\alpha}\sqrt{3+\sin^2\phi_{n+1-\alpha}}}\right]. \tag{5.16}$$

Secondly, we expand $e^{-2p(M\omega_2/2)}$ as we did in (3.18) and finally, we expand the function

$$\frac{\sqrt{3}}{\sin k\sqrt{3+\sin^2 k}} = \omega_3(k) + \frac{1}{k} - \frac{1}{k-\pi} = \frac{1}{k} + \sum_{m=1}^{\infty}\frac{\gamma_{2m+1}}{(2m+1)!}k^{2m+1} \tag{5.17}$$

in powers of k. After rearranging the series, extending the sums over n to ∞ (as the error is exponentially small) and using (B.14)/(C.2) we obtain

$$\begin{aligned}\mathcal{S}^{(2)}_{\alpha,\beta} = {} & -\mathrm{Re}\log\theta_{\alpha,\beta} + \left[\log 2 - \frac{\pi\rho\sqrt{3}}{8}\right]\delta_{\alpha,0} \\ & + \frac{1}{2}\sum_{k=1}^{\infty}\left(\frac{\pi}{N}\right)^{2k+2}\frac{\gamma_{2k+1}}{(2k+2)!}\left[B_{2k+2}(\alpha) - \mathrm{Re}\,K^{\alpha,\beta}_{2k+2}(i\tau_0\rho)\right] \\ & - \frac{\pi\rho}{2}\sum_{k,m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m+2k+2}\frac{\Lambda_{2m+1}}{(2m+1)!}\frac{\gamma_{2k+1}}{(2k+2)!}W^{\alpha,\beta}_{2m+2k+2}(i\tau_0\rho) \\ & - \frac{\pi\rho}{2}\sum_{m=1}^{\infty}\left(\frac{\pi}{N}\right)^{2m}\frac{\Lambda_{2m+1}}{(2m+1)!}W^{\alpha,\beta}_{2m}(i\tau_0\rho)\end{aligned} \tag{5.18}$$

where the function $W^{\alpha,\beta}_m(\tau)$ is defined as follows:

$$W^{\alpha,\beta}_m(\tau) = \mathrm{Re}\sum_{n=0}^{\infty}\left[(n+\alpha)^m\frac{e^{2\pi i(\tau(n+\alpha)-\beta)}}{\left(1-e^{2\pi i(\tau(n+\alpha)-\beta)}\right)^2} + (n+1-\alpha)^m\frac{e^{2\pi i(\tau(n+1-\alpha)+\beta)}}{\left(1-e^{2\pi i(\tau(n+1-\alpha)+\beta)}\right)^2}\right]. \tag{5.19}$$

The ratio $Z''_{\alpha,\beta}(0)/Z_{\alpha,\beta}(0)$ (5.3) can be written as a power series in N^{-1}:

$$\frac{1}{MN}\frac{Z''_{\alpha,\beta}(0)}{Z_{\alpha,\beta}(0)} = \frac{4}{\pi\sqrt{3}}\left[\log N + \gamma_E + \log\frac{4\sqrt{3}}{2} - 2\,\mathrm{Re}\log\theta_{\alpha,\beta}\right] + \sum_{m=2}^{\infty}\frac{\tilde{d}^{\alpha,\beta}_{2m}(\rho)}{N^{2m}}. \tag{5.20}$$

This series contains only *even* powers of N^{-1} and it starts at N^{-4} (i.e., $\tilde{d}^{\alpha,\beta}_2 = 0$). The first non-vanishing coefficient $\tilde{d}^{\alpha,\beta}_{2m}$ is

$$\tilde{d}^{\alpha,\beta}_4(\rho) = -\frac{\pi^4}{45}\,\mathrm{Re}\,K^{\alpha,\beta}_4(i\tau_0\rho) - \frac{2\pi^5\rho}{15\sqrt{3}}W^{\alpha,\beta}_4(i\tau_0\rho). \tag{5.21}$$

It is worth noticing that the terms with $\delta_{\alpha,0}$ in (5.3)/(5.13)/(5.18) cancel out exactly.

Table 3. Values of the coefficients $d_0(\rho)$ and $d_4(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$d_0(\rho)$	$d_4(\rho)$
1	0.993 000 152 525 293	−0.034 652 876 469 773
2	1.205 930 021 583 709	−0.084 727 027 938 228
3	1.233 520 243 783 654	−0.146 295 429 270 869
4	1.189 798 214 112 785	−0.167 434 330 275 211
5	1.134 144 577 781 982	−0.157 595 538 508 037
6	1.088 416 663 135 744	−0.134 596 242 800 881
7	1.056 420 958 518 946	−0.110 373 125 092 552
8	1.035 808 103 247 928	−0.090 138 741 047 513
9	1.023 167 108 495 542	−0.075 083 168 632 513
10	1.015 661 512 376 353	−0.064 637 113 563 536
11	1.011 305 166 086 030	−0.057 721 974 432 342
12	1.008 818 898 345 350	−0.053 296 998 167 206
13	1.007 418 256 678 703	−0.050 537 602 364 217
14	1.006 637 342 854 852	−0.048 851 578 543 533
15	1.006 205 629 259 680	−0.047 838 335 036 578
16	1.005 968 648 007 326	−0.047 237 747 222 882
17	1.005 839 340 365 928	−0.046 885 886 437 925
18	1.005 769 147 640 350	−0.046 681 800 486 309
19	1.005 731 215 221 337	−0.046 564 452 961 825
20	1.005 710 797 002 295	−0.046 497 492 807 615
∞	1.005 687 333 437 919	−0.046 411 250 116 879

The computation of the ratio (5.2) is straightforward from (3.24)/(5.20). The leading term grows like $\log N$ and the rest can be expressed as a power series in N^{-1} where only *even* powers of N^{-1} enter

$$\frac{1}{MN}\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)} = \frac{4}{\pi\sqrt{3}}\log N + d_0(\rho) + \sum_{m=2}^{\infty}\frac{d_{2m}(\rho)}{N^{2m}}. \tag{5.22}$$

The coefficient associated with N^{-2} vanishes, so the first two non-zero coefficients $d_m(\rho)$ are

$$d_0(\rho) = \frac{4}{\pi\sqrt{3}}\left[\gamma_E + \log\frac{4\sqrt{3}}{\pi} - 2\frac{\sum|\theta_i|\,\mathrm{Re}\log\theta_i}{\sum|\theta_i|}\right] \tag{5.23a}$$

$$\begin{aligned} d_4(\rho) = -\frac{4\pi^3}{45}\Bigg[\frac{2\pi\rho}{3}\Bigg\{&\frac{\left(\sum|\theta_i|\,\mathrm{Re}\log\theta_i\right)\left(\sum|\theta_{\alpha,\beta}|\,\mathrm{Re}\,K_6^{\alpha,\beta}\right)}{\left(\sum|\theta_i|\right)^2} \\ &- \frac{\sum|\theta_{\alpha,\beta}|\,\mathrm{Re}\,K_6^{\alpha,\beta}\,\mathrm{Re}\log\theta_{\alpha,\beta}}{\sum|\theta_i|}\Bigg\} \\ &+ \frac{1}{\sqrt{3}}\frac{\left(\sum|\theta_{\alpha,\beta}|\,\mathrm{Re}\,K_4^{\alpha,\beta}\right)}{\sum|\theta_i|} + 2\pi\rho\,\frac{\sum|\theta_{\alpha,\beta}|W_4^{\alpha,\beta}}{\sum|\theta_i|}\Bigg] \end{aligned} \tag{5.23b}$$

where we have denoted by θ_i the θ-functions in the standard notation (B.10). The numerical values of these coefficients can be found in table 3.

Remarks.

1. The limiting values of the coefficients d_0 and d_4 as $\rho \to \infty$ are easily found to be (cf (B.12))

$$\lim_{\rho\to\infty} d_0(\rho) = \frac{4}{\pi\sqrt{3}}\left[\gamma_E + \log\frac{4\sqrt{3}}{\pi}\right] \tag{5.24a}$$

$$\lim_{\rho\to\infty} d_4(\rho) = -\frac{7\pi^3}{2700\sqrt{3}}. \tag{5.24b}$$

2. Using the properties of the θ-functions (B.20)/(B.21) we can easily verify that $d_0(\rho)$ has the right behaviour under the transformation $N \leftrightarrow M$ ($\rho \to 1/\rho$):

$$\frac{4}{\pi\sqrt{3}}\log\rho + d_0(1/\rho) = d_0(\rho). \tag{5.25}$$

The behaviour of $d_4(\rho)$ under this transformation can be checked numerically to be the right one

$$d_4(\rho) = \frac{d_4(1/\rho)}{\rho^4}. \tag{5.26}$$

The specific heat for the triangular and hexagonal lattices can be obtained from (5.1) and using the results of this section and of section 4. In particular, we can write for both lattices

$$C_{H,c}(N,\rho) = C_{00}\log N + C_0(\rho) + \sum_{m=1}^{\infty}\frac{C_m(\rho)}{N^m}. \tag{5.27}$$

For the triangular lattice the first coefficients are given by

$$C_{00}^{\mathrm{tri}} = \frac{12\sqrt{3}}{\pi} \tag{5.28a}$$

$$C_0^{\mathrm{tri}}(\rho) = 9d_0(\rho) - 6 - \rho E_1^{\mathrm{tri}}(\rho)^2 \tag{5.28b}$$

$$C_1^{\mathrm{tri}}(\rho) = -2E_1^{\mathrm{tri}}(\rho) \tag{5.28c}$$

$$C_2^{\mathrm{tri}}(\rho) = C_3^{\mathrm{tri}}(\rho) = 0 \tag{5.28d}$$

$$C_4^{\mathrm{tri}}(\rho) = 9d_4(\rho) - 2\rho E_1^{\mathrm{tri}}(\rho)\, E_5^{\mathrm{tri}}(\rho) \tag{5.28e}$$

$$C_5^{\mathrm{tri}}(\rho) = -2E_5^{\mathrm{tri}}(\rho) \tag{5.28f}$$

and for the hexagonal lattice the corresponding coefficients are

$$C_{00}^{\mathrm{hc}}(\rho) = \frac{2\sqrt{3}}{\pi} \tag{5.29a}$$

$$C_0^{\mathrm{hc}}(\rho) = \tfrac{3}{2}\, d_0(\rho) - \tfrac{2}{3} - 2\rho E_1^{\mathrm{hc}}(\rho)^2. \tag{5.29b}$$

$$C_1^{\mathrm{hc}}(\rho) = -\frac{2}{\sqrt{3}}\, E_1^{\mathrm{hc}}(\rho) \tag{5.29c}$$

$$C_2^{\mathrm{hc}}(\rho) = C_3^{\mathrm{hc}}(\rho) = 0 \tag{5.29d}$$

$$C_4^{\mathrm{hc}}(\rho) = \tfrac{3}{2}\, d_4(\rho) - 4\rho\, E_1^{\mathrm{hc}}(\rho)\, E_5^{\mathrm{hc}}(\rho) = \tfrac{1}{6} C_4^{\mathrm{tri}}(\rho) \tag{5.29e}$$

$$C_5^{\mathrm{hc}}(\rho) = -\frac{2}{\sqrt{3}}\, E_5^{\mathrm{hc}}(\rho). \tag{5.29f}$$

The numerical values of the coefficients C_0^{tri}, C_4^{tri} and C_0^{hc} can be found in table 4. The values of the coefficients C_1 and C_5 can be obtained from table 2, and the value of C_4^{hc} can be read from table 4 with the help of (5.29e).

Table 4. Values of the coefficients $C_0^{\text{tri}}(\rho)$, $C_4^{\text{tri}}(\rho)$ and $C_0^{\text{hc}}(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$C_0^{\text{tri}}(\rho)$	$C_4^{\text{tri}}(\rho)$	$C_0^{\text{hc}}(\rho)$
1	1.901 880 711 301 990	0.420 058 303 835 062	0.650 313 451 883 665
2	4.103 024 258 331 998	−0.326 217 003 543 879	1.017 170 709 722 000
3	4.744 524 165 326 869	−0.967 617 404 753 895	1.124 087 360 887 811
4	4.570 856 116 406 857	−1.317 204 084 284 658	1.095 142 686 067 810
5	4.160 445 642 382 107	−1.334 908 443 794 273	1.026 740 940 397 018
6	3.780 853 192 640 795	−1.179 012 991 639 663	0.963 475 532 106 799
7	3.503 255 527 522 170	−0.981 777 257 847 270	0.917 209 254 587 028
8	3.320 932 517 142 029	−0.807 318 620 952 495	0.886 822 086 190 338
9	3.208 115 423 758 777	−0.674 464 154 921 458	0.868 019 237 293 130
10	3.140 842 603 353 847	−0.581 325 872 529 628	0.856 807 100 558 975
11	3.101 715 130 809 265	−0.519 370 850 894 424	0.850 285 855 134 878
12	3.079 361 301 589 703	−0.479 634 197 647 875	0.846 560 216 931 617
13	3.066 761 868 024 451	−0.454 826 737 355 134	0.844 460 311 337 408
14	3.059 735 410 831 789	−0.439 660 729 459 804	0.843 289 235 138 631
15	3.055 850 477 805 811	−0.430 543 990 999 289	0.842 641 746 300 969
16	3.053 717 781 288 642	−0.425 139 425 966 243	0.842 286 296 881 440
17	3.052 554 049 450 865	−0.421 972 891 323 654	0.842 092 341 575 144
18	3.051 922 325 002 618	−0.420 136 179 461 406	0.841 987 054 167 103
19	3.051 580 935 973 584	−0.419 080 069 533 795	0.841 930 155 995 597
20	3.051 397 172 745 595	−0.418 477 433 243 636	0.841 899 528 790 933
∞	3.051 186 000 941 275	−0.417 701 251 051 913	0.841 864 333 490 213

Remarks.

1. The fact that the coefficients C_1 and C_3 are proportional, respectively, to E_1 and E_5 for the triangular (5.28) and hexagonal (5.29) lattices is not accidental. In fact, from (5.1)/(5.22) we conclude that *all* the *odd* coefficients in the specific-heat expansion are proportional to the corresponding coefficients of the internal-energy expansion. In fact, the proportional constant is given by (see (5.1)/(4.1))
$$\frac{E_{2m+1}}{C_{2m+1}} = \left.\frac{d\mu}{d\beta}\right|_{\beta=\beta_c} \left(\left.\frac{d^2\mu}{d\beta^2}\right|_{\beta=\beta_c} \right)^{-1}. \tag{5.30}$$
Indeed, for $m = 1, 3$ this ratio is indeterminate as both coefficients vanish.
2. The limiting values of the coefficients $C_m(\rho)$ as $\rho \to \infty$ are easily found to be (cf (B.12))
$$\lim_{\rho\to\infty} C_0^{\text{tri}}(\rho) = \frac{12\sqrt{3}}{\pi}\left[\gamma_E + \log\frac{4\sqrt{3}}{\pi} - \frac{\pi}{2\sqrt{3}}\right] \tag{5.31a}$$
$$\lim_{\rho\to\infty} C_1^{\text{tri}}(\rho) = \lim_{\rho\to\infty} C_5^{\text{tri}}(\rho) = 0 \tag{5.31b}$$
$$\lim_{\rho\to\infty} C_4^{\text{tri}}(\rho) = -\frac{7\pi^3}{300\sqrt{3}} \tag{5.31c}$$
$$\lim_{\rho\to\infty} C_0^{\text{hc}}(\rho) = \frac{2\sqrt{3}}{\pi}\left[\gamma_E + \log\frac{4\sqrt{3}}{\pi} - \frac{\pi}{3\sqrt{3}}\right] \tag{5.32a}$$

$$\lim_{\rho\to\infty} C_1^{\rm hc}(\rho) = \lim_{\rho\to\infty} C_5^{\rm hc}(\rho) = 0 \tag{5.32b}$$

$$\lim_{\rho\to\infty} C_4^{\rm hc}(\rho) = -\frac{7\pi^3}{1800\sqrt{3}}. \tag{5.32c}$$

3. The behaviour of the coefficients $C_m(\rho)$ under the transformation $\rho \to 1/\rho$ is that expected

$$C_0(\rho) = C_{00}\log\rho + C_0(1/\rho) \tag{5.33a}$$

$$C_m(\rho) = \frac{C_m(1/\rho)}{\rho^m} \qquad \text{for } m \geqslant 1. \tag{5.33b}$$

4. From table 4 it is clear that $C_4^{\rm tri}$ should vanish at a value between 1 and 2. Actually, due to (5.29e), $C_4^{\rm hc}$ should also vanish at the same value of ρ. We have found numerically that C_4 vanishes at

$$\rho_{\rm min} \approx 1.468\,889\,7779. \tag{5.34}$$

Indeed, due to the transformation properties of $C_4(\rho)$ under the transformation $\rho \to 1/\rho$, C_4 also vanishes at $\rho_{\rm min}^{-1} \approx 0.680\,786\,2748$. This is similar to what happens in the square lattice [24].

6. Higher derivatives of the free energy

6.1. Finite-size-scaling corrections to $f_c^{(3)}$

In this section we will consider the third derivative of the free energy (2.17) at criticality. Even though this observable is not relevant in practice, its computation is interesting as it provides new insights into the finite-size-scaling function $\hat{W}$ defined in section 7. The observable $f_c^{(3)}$ (2.17) can be written as follows:

$$\begin{aligned} f_c^{(3)} = {} & \frac{8\cosh 2\beta_c}{\sinh^3\beta_c} + \frac{1}{V}\left.\frac{{\rm d}^3\mu}{{\rm d}\beta^3}\right|_{\beta=\beta_c} \frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)} + \frac{1}{V}\left(\frac{{\rm d}\mu}{{\rm d}\beta}\right)^3_{\beta=\beta_c} \\ & \times\left[\frac{Z'''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)} - 3\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)}\frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)} + 2\left(\frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)}\right)^3\right] \\ & + \frac{3}{V}\left.\frac{{\rm d}^2\mu}{{\rm d}\beta^2}\right|_{\beta=\beta_c}\left.\frac{{\rm d}\mu}{{\rm d}\beta}\right|_{\beta=\beta_c}\left[\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)} - \left(\frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)}\right)^2\right]. \end{aligned} \tag{6.1}$$

The only unknown object is the derivative $Z'''_{0,0}(0)$, which can be written in the following way

$$\frac{Z'''_{0,0}(0)}{Z'_{0,0}(0)} = M^2 + \frac{12MN}{\pi\sqrt{3}}\left[\mathcal{S}_0^{(1)} + 2\mathcal{S}_{0,0}^{(2)}\right] \tag{6.2}$$

where the sums $\mathcal{S}^{(j)}$ were defined in (5.4). By following step by step the procedure developed in section 5 and leading to (5.20), we can compute the finite-size expansion of the ratio (6.2)

$$\frac{1}{MN}\frac{Z'''_{0,0}(0)}{Z'_{0,0}(0)} = \frac{12}{\pi\sqrt{3}}\log N + \tilde{A}(\rho) + \sum_{m=2}^{\infty}\frac{\tilde{A}_{2m}}{N^{2m}}. \tag{6.3}$$

By plugging in (6.1) the above result (6.3) and the results already obtained in sections 4 and 5, we obtain

$$f_c^{(3)}(N,\rho) = \mathcal{A}_1(\rho)N + A_{00}\log N + A_0(\rho) + \sum_{m=1}^{\infty}\frac{A_m(\rho)}{N^m}. \tag{6.4}$$

In this expansion, the coefficient A_2 is identically zero.

The most important result contained in (6.4) is that the coefficient associated with the expected leading term $\sim L \log L$ vanishes. This is a highly non-trivial fact and we will discuss its physical meaning in section 7. We have obtained the first four non-vanishing coefficients for the triangular lattice

$$\mathcal{A}_1^{\rm tri}(\rho) = 2\rho E_1^{\rm tri}(\rho)\left[\rho E_1^{\rm tri}(\rho)^2 + \frac{36\sqrt{3}}{\pi}\left(\frac{\sum|\theta_j|\,\mathrm{Re}\log\theta_j}{\sum|\theta_j|} - \log 2|\eta|\right)\right] \tag{6.5a}$$

$$A_{00}^{\rm tri} = -\frac{216}{\pi\sqrt{3}} \tag{6.5b}$$

$$A_0^{\rm tri}(\rho) = 48 - 54 d_0(\rho) + 6\rho E_1^{\rm tri}(\rho)^2 \tag{6.5c}$$

$$A_1^{\rm tri}(\rho) = 16 E_1^{\rm tri}(\rho) \tag{6.5d}$$

where the function $d_0(\rho)$ is defined in (5.23*a*). The numerical values of $\mathcal{A}_1^{\rm tri}$ and $A_0^{\rm tri}$ can be found in table 5, while the numerical values of $A_1^{\rm tri}$ can be computed from table 2. The coefficients for the hexagonal lattice are

$$\mathcal{A}_1^{\rm hc}(\rho) = 2\rho E_1^{\rm hc}(\rho)\left[4\rho E_1^{\rm hc}(\rho)^2 + \frac{36}{\pi\sqrt{3}}\left(\frac{\sum|\theta_j|\,\mathrm{Re}\log\theta_j}{\sum|\theta_j|} - \log 2|\eta|\right)\right] \tag{6.6a}$$

$$A_{00}^{\rm hc} = -\frac{12}{\pi} \tag{6.6b}$$

$$A_0^{\rm hc}(\rho) = \frac{16}{3\sqrt{3}} - 3\sqrt{3} d_0(\rho) + 4\sqrt{3}\rho E_1^{\rm hc}(\rho)^2 \tag{6.6c}$$

$$A_1^{\rm hc}(\rho) = 4 E_1^{\rm hc}(\rho) \tag{6.6d}$$

and their numerical values can be found in table 6.

Remarks.

1. The coefficients (6.5)/(6.6) have the right behaviour under the transformation $\rho \to 1/\rho$. In particular, they satisfy

$$\mathcal{A}_1(\rho) = \rho \mathcal{A}_1(1/\rho) \tag{6.7a}$$

$$A_0(\rho) = A_{00}\log\rho + A_0(1/\rho) \tag{6.7b}$$

$$A_1(\rho) = \frac{A_1(1/\rho)}{\rho}. \tag{6.7c}$$

2. In the limit $\rho \to \infty$, both $\mathcal{A}_1(\rho)$ and $A_1(\rho)$ go to zero as in this limit $E_1(\rho) \to 0$ exponentially fast. The limit of the coefficients $A_0(\rho)$ can be computed from (6.5*c*)/(6.6*c*) and (5.24*a*)

$$\lim_{\rho\to\infty} A_0^{\rm tri}(\rho) = 48 - \frac{72\sqrt{3}}{\pi}\left(\gamma_E + \log\frac{4\sqrt{3}}{\pi}\right) \tag{6.8a}$$

$$\lim_{\rho\to\infty} A_0^{\rm hc}(\rho) = \frac{16}{3\sqrt{3}} - \frac{12}{\pi}\left(\gamma_E + \log\frac{4\sqrt{3}}{\pi}\right). \tag{6.8b}$$

3. From table 5 we see that $\mathcal{A}_1^{\rm tri}(\rho)$ vanishes at a value $\rho_{\min}$ between 3 and 4.

Table 5. Values of the coefficients $\mathcal{A}_1^{\rm tri}(\rho)$ and $A_0^{\rm tri}(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$\mathcal{A}_1^{\rm tri}(\rho)$	$A_0^{\rm tri}(\rho)$
1	−16.556 352 382 598 901	0.588 715 732 188 061
2	−16.439 945 008 735 128	−12.618 145 549 991 986
3	6.161 165 303 236 093	−16.467 144 991 961 212
4	2.808 024 778 142 930	−15.425 136 698 441 144
5	6.829 759 193 109 778	−12.962 673 854 292 640
6	7.259 238 447 062 151	−10.685 119 155 844 771
7	6.078 697 042 860 241	−9.019 533 165 133 020
8	4.522 637 873 985 072	−7.925 595 102 852 174
9	3.134 987 142 065 343	−7.248 692 542 552 664
10	2.072 903 487 004 694	−6.845 055 620 123 084
11	1.324 966 640 033 683	−6.610 290 784 855 592
12	0.825 436 595 929 018	−6.476 167 809 538 218
13	0.503 936 252 639 239	−6.400 571 208 146 704
14	0.302 641 624 812 243	−6.358 412 464 990 734
15	0.179 285 740 783 859	−6.335 102 866 834 869
16	0.104 987 265 970 099	−6.322 306 687 731 851
17	0.060 870 848 500 045	−6.315 324 296 705 190
18	0.034 988 709 413 814	−6.311 533 950 015 708
19	0.019 959 520 236 906	−6.309 485 615 841 503
20	0.011 309 756 764 775	−6.308 383 036 473 573
∞	0	−6.307 116 005 647 652

Table 6. Values of the coefficients $\mathcal{A}_1^{\rm hc}(\rho)$ and $A_0^{\rm hc}(\rho)$ for several values of the torus aspect ratio ρ.

ρ	$\mathcal{A}_1^{\rm hc}(\rho)$	$A_0^{\rm hc}(\rho)$
1	2.204 248 900 857 568	5.090 947 597 599 750
2	1.260 776 176 148 286	2.011 554 369 485 771
3	0.657 422 819 248 581	−0.855 894 359 177 661
4	1.682 404 023 579 180	−2.151 736 456 053 733
5	2.442 900 124 268 499	−2.489 361 833 956 631
6	2.452 406 095 152 028	−2.473 169 556 688 759
7	2.032 154 004 962 206	−2.378 716 655 165 567
8	1.508 563 855 204 567	−2.293 728 702 105 723
9	1.045 164 213 119 409	−2.234 638 841 885 926
10	0.690 994 951 708 971	−2.197 561 506 291 189
11	0.441 659 818 805 435	−2.175 477 057 251 966
12	0.275 146 193 270 710	−2.162 714 473 030 565
13	0.167 978 851 785 044	−2.155 480 460 188 504
14	0.100 880 556 816 132	−2.151 434 956 603 961
15	0.059 761 915 864 342	−2.149 195 097 142 150
16	0.034 995 755 659 000	−2.147 964 640 036 792
17	0.020 290 282 882 592	−2.147 292 993 714 472
18	0.011 662 903 145 113	−2.146 928 331 463 238
19	0.006 653 173 413 341	−2.146 731 247 829 992
20	0.003 769 918 921 741	−2.146 625 156 802 025
∞	0	−2.146 503 238 450 814

Actually, $\mathcal{A}_1^{\rm tri}$ is zero at

$$\rho_{\rm min,1}^{\rm tri} \approx 3.624\,926\,4261. \tag{6.9}$$

We also find that $A_0^{\rm tri}(\rho)$ vanishes at

$$\rho_{\rm min,2}^{\rm tri} \approx 1.030\,077\,3853. \tag{6.10}$$

In the hexagonal lattice, $\mathcal{A}_1^{\rm hc}(\rho)$ only vanishes in the limit $\rho \to \infty$, while $A_0^{\rm hc}$ is zero at

$$\rho_{\rm min,2}^{\rm hc} \approx 2.636\,769\,1963. \tag{6.11}$$

6.2. Logarithmic finite-size corrections to $f_c^{(4)}$

The full finite-size-scaling corrections to the fourth derivative of the free energy at criticality $f_c^{(4)}$ are rather cumbersome to compute. However, we can extract with much less effort the terms including logarithms. This is what we really need in the renormalization-group analysis of section 7.

The first step is the computation of the full expression for $f_c^{(4)}$ in terms of the derivatives of the basic objects $Z_{\alpha,\beta}$. We should keep only those terms in which $Z''_{\alpha,\beta}(0)$, $Z'''_{00}(0)$ or $Z^{(4)}_{\alpha,\beta}(0)$ enter. There are three possible contributions

$$f_{c,\log,1}^{(4)} = \frac{1}{V}\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)}[4\mu'\mu''' + 3(\mu')^2] \tag{6.12a}$$

$$f_{c,\log,2}^{(4)} = \frac{6}{V}(\mu')^2\mu''\frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)}\left[\frac{Z'''_{00}(0)}{Z'_{00}(0)} - 3\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)}\right] \tag{6.12b}$$

$$\begin{aligned} f_{c,\log,3}^{(4)} = \frac{1}{V}(\mu')^4 &\left[\frac{\sum Z^{(4)}_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)} - 3\left(\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)}\right)^2\right. \\ &\left. - 4\,\frac{Z'_{00}(0)}{\sum Z_{\alpha,\beta}(0)}\left(\frac{Z'''_{00}(0)}{Z'_{00}(0)} - 3\frac{\sum Z''_{\alpha,\beta}(0)}{\sum Z_{\alpha,\beta}(0)}\right)\right] \end{aligned} \tag{6.12c}$$

where the derivatives of μ with respect to β have been represented, for short, by μ', μ'', etc. The first contribution (6.12a) is clearly non-zero and of order $\log N$. The second contribution (6.12b) does not actually contain any logarithm, as the logarithmic contributions of $Z'''_{00}(0)/Z'_{00}(0)$ and $-3\sum Z_{\alpha,\beta}(0)''\big/\sum Z_{\alpha,\beta}(0)$ cancel out exactly (see, e.g., (5.22)/(6.3)). The same argument applies to the second line of (6.12c).

In order to compute the contribution of the first two terms in (6.12c), we have to consider the fourth derivative of $Z_{\alpha,\beta}(\mu)$ at $\mu = 0$ when $(\alpha,\beta) \neq (0,0)$. After some algebra, we find that the logarithmic contributions to that derivative are

$$Z^{(4)}_{\alpha,\beta,\log}(0) = \frac{12MN}{\pi\sqrt{3}}Z''_{\alpha,\beta}(0)\left(\mathcal{S}^{(1)}_{\alpha} + 2\mathcal{S}^{(2)}_{\alpha,\beta}\right) + M^2 Z''_{\alpha,\beta}(0)\delta_{\alpha,0} + \frac{8M^3N}{\pi\sqrt{3}}Z_{\alpha,\beta}(0)\log N\delta_{\alpha,0} \tag{6.13}$$

where the sums $\mathcal{S}^{(j)}$ are defined in (5.4). After some more algebra we find that the contribution of (6.12c) does *not* contain any logarithms.

In conclusion, we find that the finite-size-scaling expansion for the observable $f_c^{(4)}$ contains a *single* logarithmic term

$$f_{c,\log}^{(4)} = B_{00}\log N \tag{6.14}$$

where B_{00} can be read from (6.12a). Its numerical value is

$$B_{00} = \begin{cases} 2736/(\pi\sqrt{3}) & \text{triangular} \\ 120/(\pi\sqrt{3}) & \text{hexagonal.} \end{cases} \tag{6.15}$$

The leading term in the large-N expansion of $f_c^{(4)}$ is expected to be $\sim N^2$, and we also expect a term of order $\sim N$.

7. Irrelevant operators in the two-dimensional Ising model

Let us first collect the main results of the previous sections

$$f_c(N,\rho) = f_{\text{bulk}} + \sum_{m=1}^{\infty} \frac{f_{2m}(\rho)}{N^{2m}} \tag{7.1a}$$

$$E_c(N,\rho) = E_0 + \sum_{m=0}^{\infty} \frac{E_{2m+1}(\rho)}{N^{2m+1}} \tag{7.1b}$$

$$C_{H,c}(N,\rho) = C_{00}\log N + C_0(\rho) + \sum_{m=1}^{\infty} \frac{C_m(\rho)}{N^m} \tag{7.1c}$$

$$f_c^{(3)}(N,\rho) = \mathcal{A}_1(\rho)N + A_{00}\log N + A_0(\rho) + \sum_{m=1}^{\infty} \frac{A_m(\rho)}{N^m} \tag{7.1d}$$

$$f_{c,\log}^{(4)}(N,\rho) = B_{00}\log N. \tag{7.1e}$$

It is also important to mention that the coefficients f_4, f_8, E_3, E_7, C_2, C_3 and A_2 vanish. In this section we will use these results to study the irrelevant operators in the two-dimensional Ising model and the finite-size-scaling function $\tilde{W}$ defined below. The results will be applicable to both the triangular and hexagonal lattices as the analytic structure of the corresponding asymptotic expansions is the same. To our knowledge, there are no predictions based on conformal field theory for the hexagonal-lattice Ising model. In this section we will follow basically the notation of [20].

Let us start with the basic finite-size-scaling ansatz for a system defined on a torus of linear size L (the aspect ratio is also fixed and plays no role in this discussion), zero magnetic field and reduced temperature τ [20, 44]

$$f(\tau; L) = f_b(\tau) + \frac{1}{L^2} W\left(\left\{\mu_j(\tau)L^{y_j}\right\}\right) + \frac{\log L}{L^2}\tilde{W}\left(\left\{\mu_j(\tau)L^{y_j}\right\}\right) \tag{7.2}$$

where $f_b(\tau)$ is a regular function of τ and the scaling functions W and $\tilde{W}$ depend on the non-linear scaling fields $\mu_j(\tau)$ belonging to the identity and energy conformal families. Among them the only relevant field is the one associated with the temperature $\mu_t(\tau)$ (see table 7). In this ansatz we have explicitly used the assumptions (a)–(c) introduced in section 1.

The reduced temperature τ measures the distance to the critical point[6] and it is defined such that $\tau = 0$ at $\beta = \beta_c$ and $\tau > 0$ (respectively $\tau < 0$) for $\beta < \beta_c$ (respectively $\beta > \beta_c$). In the Ising model on the triangular and hexagonal lattices this parameter takes the form

$$\tau = \begin{cases} \dfrac{1 + v^2 - 4v}{(1-v)\sqrt{2v}} & \text{triangular} \\ \dfrac{1 - 3v^2}{v\sqrt{2(1-v^2)}} & \text{hexagonal} \end{cases} \tag{7.3}$$

[6] This parameter should not be confused with the torus modular parameter. In this section τ will mean the reduced temperature, while in the rest of the paper it will denote the usual modular parameter.

Table 7. Operators in the two-dimensional Ising model according to [20]. For each conformal family, we have listed the primary and quasiprimary fields belonging to it. For each scaling field μ_j, we show the notation used in [20], its spin s and its renormalization-group exponent y. We have included the most relevant fields (i.e., $y \geqslant -10$) with spin $s = 6\,\mathbb{N}$. We have omitted the conformal family $[\sigma]$ as it is irrelevant in this discussion. Only the primary fields I and ϵ are relevant.

Family	j	μ_j	s	y
$[I]$	0	I	0	2
	1	$T\bar{T}$	0	-2
	2	$T^3+\bar{T}^3$	6	-4
	3	$Q_4^I\bar{Q}_4^I$	0	-6
	4	$\bar{Q}_2^I Q_8^I + Q_2^I\bar{Q}_8^I$	6	-8
	5	$Q_{12}^I+\bar{Q}_{12}^I$	12	-10
$[\epsilon]$	t	ϵ	0	1
	6	$Q_6^\epsilon+\bar{Q}_6^\epsilon$	6	-5
	7	$Q_4^\epsilon\bar{Q}_4^\epsilon$	0	-7

where as usual $v = \tanh\beta$. Under the transformations that map the high-temperature phase onto the low-temperature phase and *vice versa*

$$v \to v' = \begin{cases} \left(\dfrac{\sqrt{1-v+v^2}-\sqrt{v}}{1-v}\right)^2 & \text{triangular} \\ \sqrt{\dfrac{1-v^2}{1+3v^2}} & \text{hexagonal} \end{cases} \tag{7.4}$$

the reduced temperature simply maps as $\tau \to -\tau$. Equations (7.3)/(7.4) in the triangular-lattice case were introduced in [20].

The non-linear scaling fields $\mu_j(\tau)$ can be written as a power series in τ

$$\mu_j(\tau) = \mu_j(0) + \tau\mu_{1,j} + \tfrac{1}{2}\tau^2\mu_{2,j} + \cdots \tag{7.5}$$

and we usually take the normalization $\mu_j(0) = 1$ for the identity-family fields, and $\mu_{1,j} = 1$ for the energy-family fields. (These latter scaling fields are odd under the transformation $\tau \to -\tau$, thus they satisfy $\mu_j(0) = 0$.)

As explained in [20], both scaling functions satisfy

$$W\left(\left\{\mu_j(-\tau)(-L)^{y_j}\right\}\right) = W\left(\left\{\mu_j(\tau)L^{y_j}\right\}\right) \tag{7.6}$$

(and analogously for $\tilde{W}$). Thus, even (respectively odd) derivatives of W and $\tilde{W}$ with respect to τ will contain only even (respectively odd) powers of L. This fact explains the structure found for the internal-energy and specific-heat expansions:

$$-E_c(L) = \left.\frac{\partial\tau}{\partial\beta}\right|_{\beta=\beta_c} \left.\frac{\partial f}{\partial\tau}\right|_{\tau=0} \tag{7.7a}$$

$$C_{H,c}(L) = \left.\frac{\partial^2\tau}{\partial\beta^2}\right|_{\beta=\beta_c} \left.\frac{\partial f}{\partial\tau}\right|_{\tau=0} + \left.\frac{\partial\tau}{\partial\beta}\right|_{\beta=\beta_c} \left.\frac{\partial f^2}{\partial\tau^2}\right|_{\tau=0}. \tag{7.7b}$$

In particular, (7.7) shows why the odd powers of the specific-heat expansion are related to those of the internal energy. We will also make the following assumption, which is motivated by the absence of terms $L^{-m}\log L$ for any $m > 0$ in the expansions (7.1)

(d) The scaling function $\tilde{W}$ only depends on the scaling field associated with the temperature

$$\tilde{W}\left(\left\{\mu_j(\tau)L^{y_j}\right\}\right) = \hat{W}(\mu_t(\tau)L). \tag{7.8}$$

As we know that there are no logarithmic contributions to the free and internal energies (7.1a)/(7.1b), the scaling function $\hat{W}$ should satisfy

$$\hat{W}(0) = \left.\frac{\partial \hat{W}(x)}{\partial x}\right|_{x=0} = 0. \tag{7.9}$$

Conformal field theory [20] provides a list of irrelevant operators that may appear in the two-dimensional Ising model (see table 7). By comparing the finite-size-scaling ansätze for the free energy, internal energy and specific heat obtained from (7.2) to the corresponding exact results (7.1) we may get new insights about the operator content of the model.

Let us start with the free energy. At the critical point $\tau = 0$ this can be written as

$$f_c(L) = f_b(0) + \frac{1}{L^2} W(\{x_j\}) \tag{7.10}$$

where W depends only on the identity-family fields through the variables $x_j = \mu_j(0)L^{y_j}$, as the energy-family scaling fields vanish at criticality. This expression can be Taylor expanded for large L, so we obtain a power series in L^{-1}. The exact result (7.1a) tells us that only corrections of order L^{2m} can occur, except for the terms of order L^{-4} and L^{-8}. From table 7, we see that the scaling fields $T\bar{T}$ and μ_3 precisely give corrections of order L^{-4} and L^{-8} to the expansion of (7.10). Hence, we need to impose the conditions

$$\mu_{T\bar{T}}(0) = \mu_3(0) = 0. \tag{7.11}$$

The derivative of the free energy with respect to τ can be written as [20]

$$\left.\frac{\partial f}{\partial \tau}\right|_{\tau=0} = \left.\frac{\partial f_b}{\partial \tau}\right|_{\tau=0} + \frac{1}{L^2}\sum_{j\in[\epsilon]} L^{y_j}\mu_{1,j} W_j(\{x_k\}) \tag{7.12a}$$

$$= \left.\frac{\partial f_b}{\partial \tau}\right|_{\tau=0} + \frac{1}{L}\mu_{1,t} W_t(\{x_k\}) + \frac{1}{L^7}\mu_{1,6} W_6(\{x_k\}) + \frac{1}{L^9}\mu_{1,7} W_7(\{x_k\}) + \cdots. \tag{7.12b}$$

Each function $W_j(\{x_k\})$ can be expanded as we did for the free energy, giving a power series in L^{-2m} with no contribution to orders L^{-4} and L^{-8}. From the exact solution (7.1b), we see that only corrections of the type L^{-2m-1} can appear except for the powers L^{-3} and L^{-7}. This implies that the scaling field μ_6 cannot play any role, thus

$$\mu_{1,6} = 0. \tag{7.13}$$

The second derivative of the free energy at criticality is given by [20]:

$$\left.\frac{\partial^2 f}{\partial \tau^2}\right|_{\tau=0} = \left.\frac{\partial^2 f_b}{\partial \tau^2}\right|_{\tau=0} + \frac{1}{L^2}\sum_{i,j\in[\epsilon]} L^{y_i+y_j} W_{ij}(\{x_k\})$$
$$+ \frac{1}{L^2}\sum_{j\in[I]} \mu_{2,j} L^{y_j} W_j(\{x_k\}) + 2\log L \left.\frac{\partial^2 \hat{W}(x)}{\partial x^2}\right|_{x=0} \tag{7.14}$$

where we have used the standard normalization. The second term in the rhs of (7.14) can be written as

$$\frac{1}{L^2}\sum_{i,j\in[\epsilon]} L^{y_i+y_j} W_{ij}(\{x_k\}) = W_{tt}(\{x_k\}) + \frac{1}{L^6} W_{t7}(\{x_k\}) + \cdots. \tag{7.15}$$

These two terms alone give all even powers of L^{-1} except L^{-2} in agreement with the exact expansion (7.1c). The third term in the rhs of (7.14) is equal to

$$\frac{1}{L^2}\sum_{j\in[I]} \mu_{2,j} L^{y_j} W_j(\{x_k\}) = \frac{1}{L^4}\mu_{2,1} W_1(\{x_k\}) + \frac{1}{L^6}\mu_{2,2} W_2(\{x_k\}) + \cdots. \tag{7.16}$$

Again, this is a power series containing all even powers of L^{-1} except L^{-2} in agreement with (7.1*c*).

The coefficient of the leading term should be equal to C_{00}

$$C_{00} = \left(\frac{\mathrm{d}\tau}{\mathrm{d}\beta}\bigg|_{\beta=\beta_c} \right)^2 \hat{W}''(0). \tag{7.17}$$

Hence we can determine the numerical value of $\hat{W}''(0)$ by using (5.28*a*)/(5.29*a*) and the definition of τ (7.3). The result is

$$\hat{W}''(0) = \begin{cases} 1/(\pi\sqrt{3}) & \text{triangular} \\ 1/(2\pi\sqrt{3}) & \text{hexagonal} \end{cases} \tag{7.18}$$

where we have considered the standard normalization for $\mu_t(\tau)$. The value (7.18) for the triangular lattice agrees with the result obtained in ([20], equation (3.34)).

Remarks.

1. The irrelevant scaling fields belonging to the identity family that may play a role have non-zero spin (namely, $s = 6,12$). The spin-zero fields belonging to this family should vanish at criticality (e.g., $\mu_j(0) = 0$). This result agrees with conjecture 1.1.
2. The vanishing of the field $\mu_1 = T\bar{T}$ at criticality supports conjecture (d0) of [20]. However, our results do not imply their stronger conjecture (d1): the scaling field $T\bar{T}$ decouples (i.e., $\mu_{T\bar{T}}(\tau) = 0$ for all τ)[7].
3. In the internal-energy analysis, we concluded that the irrelevant field μ_6 should vanish at criticality (7.13). This operator has spin six, therefore this result is *not* implied by conjecture 1.1. In other words, there are also cancellations in the non-scalar sector. On the other hand, we find no constraint on the spin-zero irrelevant field μ_7. However, if conjecture 1.1 is true, then we should have $\mu_{1,7} = 0$.
4. In order to obtain the exact solutions (7.1) we need to include *at least* two irrelevant operators. This result agrees with the findings of [17, 18] for the square-lattice model. It is worth noticing that we can formally obtain the exact solutions (7.1) by including the spin-6 irrelevant scaling field $\mu_2 = T^3 + \bar{T}^3$ with $y = -4$ and the spin-12 field μ_5 with $y = -10$,

$$f_c(L) = f_b(0) + \frac{1}{L^2} W\left(\mu_2(0)L^{-4}, \mu_5(0)L^{-10}\right) \tag{7.19a}$$

$$\frac{\partial f}{\partial \tau}\bigg|_{\tau=0} = \frac{\partial f_b}{\partial \tau}\bigg|_{\tau=0} + \frac{1}{L} W_t\left(\mu_2(0)L^{-4}, \mu_5(0)L^{-10}\right) \tag{7.19b}$$

$$\begin{aligned} \frac{\partial^2 f}{\partial \tau^2}\bigg|_{\tau=0} &= 2\hat{W}''(0)\log L + \frac{\partial^2 f_b}{\partial \tau^2}\bigg|_{\tau=0} + W_{tt}\left(\mu_2(0)L^{-4}, \mu_5(0)L^{-10}\right) \\ &\quad + \frac{1}{L^6}\mu_{2,2} W_2\left(\mu_2(0)L^{-4}, \mu_5(0)L^{-10}\right) \\ &\quad + \frac{1}{L^{12}}\mu_{2,5} W_5\left(\mu_2(0)L^{-4}, \mu_5(0)L^{-10}\right). \end{aligned} \tag{7.19c}$$

[7] It is worth mentioning that the authors of [20] showed by considering the large-distance behaviour of the triangular-lattice Ising model two-point function that $\mu_{T\bar{T}}(\tau) = o(\tau^4)$. This result strongly supports their conjecture (d1).

Let us now consider the observable $f_c^{(3)}$ (2.17). We are interested here only in the terms containing logarithms, which are directly related to the derivatives of the scaling function $\hat{W}(x)$. The contribution of this scaling function to this observable can be written as

$$f_{c,\log}^{(3)} = L \log L \ \hat{W}'''(0) \left(\frac{\partial \tau}{\partial \beta} \right)^3_{\beta=\beta_c} + 3 \log L \ \hat{W}''(0) \left. \frac{\partial \tau}{\partial \beta} \right|_{\beta=\beta_c} \left. \frac{\partial^2 \tau}{\partial \beta^2} \right|_{\beta=\beta_c}. \tag{7.20}$$

The exact result (6.4) shows that

$$\left. \frac{\partial^3 \hat{W}(x)}{\partial x^3} \right|_{x=0} = 0. \tag{7.21}$$

This result is consistent with the conjecture put forth by the authors of [20] who claimed that the scaling function $\hat{W}$ is quadratic in its argument (i.e., $\hat{W}(x) = Ax^2$).

On the other hand, the coefficient of the logarithmic term in $f_c^{(3)}$ (i.e., A_{00}) is proportional to $\hat{W}''(0)$. This observation provides another way to compute the quantity $\hat{W}''(0)$ and a direct means to test the predictions (7.18). By using the exact results (6.5*b*)/(6.6*b*)/(7.3), we arrive at the same values as in (7.18), supporting the correctness of our results.

Finally, we will discuss the observable $f_c^{(4)}$. The contribution of the scaling function $\hat{W}$ to this observable is given by

$$f_{c,\log}^{(4)} = L^2 \log L \ \hat{W}^{(4)}(0) \left(\frac{\partial \tau}{\partial \beta} \right) + 3 \log L \ \hat{W}''(0) \left[4 \frac{\partial \tau}{\partial \beta} \frac{\partial^3 \tau}{\partial \beta^3} + 3 \left(\frac{\partial^2 \tau}{\partial^2 \beta} \right)^2 + 4 \left(\frac{\partial^2 \tau}{\partial^2 \beta} \right)^4 \mu_{3,t} \right] \tag{7.22}$$

where all the derivatives of τ with respect to β should be evaluated at $\beta = \beta_c$. By comparing the above formula to (7.1*e*)/(6.15), we conclude that

$$\left. \frac{\partial^4 \hat{W}(x)}{\partial x^4} \right|_{x=0} = 0. \tag{7.23}$$

This result is compatible with $\hat{W}(x)$ being a quadratic function of x. On the other hand, as we know the numerical values of the derivatives of τ w.r.t. β for the triangular and hexagonal lattices, we can use equations (6.15)/(7.22) to deduce the value of $\mu_{3,t}$. The result is the same for both lattices $\mu_{3,t} = -1/4$, so the non-linear scaling field μ_t depends on τ in the following way:

$$\mu_t(\tau) = \tau - \tfrac{1}{24}\tau^3 + \mathcal{O}(\tau^5). \tag{7.24}$$

This relation coincides with the function $a(\tau)$ obtained in [20] for the triangular lattice[8]:

$$a(\tau) = \tau - \tfrac{1}{24}\tau^3 + \tfrac{47}{10\,368}\tau^5 - \tfrac{161}{248\,832}\tau^7 + \mathcal{O}(\tau^9). \tag{7.25}$$

The equality between $a(\tau)$ and $\mu_t(\tau)$ is important because it provides support to conjecture 1.1: if this conjecture is correct, then both functions should coincide [20].

We can summarize the results obtained on the scaling function $\hat{W}$ in the following conjecture (which is a natural extension of the conjecture $\hat{W}(x) = x^2/(2\pi)$ for the square-lattice model [20]):

[8] It is not hard to realize that the function $a(\tau)$ (7.25) is the same for the hexagonal lattice. The key observation is that the free energy for this lattice in the thermodynamic limit (3.29*b*) can be written as

$$f_{\rm bulk}^{\rm hc} = \frac{1}{4} \int_0^\pi \int_0^\pi \frac{{\rm d}x\,{\rm d}y}{4\pi^2} \log[3 + \tau^2 - \omega(x,y)] + \text{constant}$$

where τ is given by (7.3). This equation is equivalent to the definition used in [20] to define $a(\tau)$ for the triangular lattice.

Conjecture 7.1. *In the Ising model on the triangular and hexagonal lattices with toroidal boundary conditions, the scaling function* $\hat{W}$ *is a function solely of the argument* $x = \mu_t(\tau)L$ *and this function is equal to*

$$\hat{W}(x) = \begin{cases} x^2/(2\pi\sqrt{3}) & \textit{triangular} \\ x^2/(4\pi\sqrt{3}) & \textit{hexagonal.} \end{cases} \tag{7.26}$$

The coefficient of $\hat{W}$ should coincide with the constant A obtained in the infinite-volume limit analysis of the triangular-lattice model ([20], equation (2.34)). The agreement between those coefficients adds support to this conjecture.

8. Further remarks and conclusions

We have obtained the asymptotic expansions for the free energy, internal energy, specific heat and $f^{(3)}$ of a critical Ising model on the triangular and hexagonal lattices wrapped on a torus of width N and aspect ratio ρ. These expansions are given in (7.1). In particular, we have found the exact coefficients f_{bulk}, f_2, $f_4 = f_8 = 0$, f_6, E_0, E_1, $E_3 = E_7 = 0$, E_5, C_{00}, C_0, C_1, $C_2 = C_3 = 0$, C_4, C_5, $\mathcal{A}_1$, A_{00}, A_0, A_1, $A_2 = 0$ and B_{00} for both lattices.

The first important observation is that the analytic structure of the finite-size corrections of the observables considered in this paper is the same for the triangular- and the hexagonal-lattice models. The reason for this coincidence is that both lattices have the same underlying Bravais lattice. This agrees with the physical content of conjecture 1.1: as they have the same rotational symmetry group, they should have the same irrelevant operators, hence leading to the same finite-size corrections.

As can be seen in (7.1), all the corrections are integer powers of N^{-1}. The only exceptions are the logarithmic terms in the specific heat (7.1*c*), $f_c^{(3)}$ (7.1*d*) and $f_c^{(4)}$ (7.1*e*). In the first case, this term is the leading one, while in the other ones it is subleading. In the free-energy expansion (7.1*a*) only even powers of N^{-1} can occur, while in the internal-energy expansion (7.1*b*) only odd powers of N^{-1} appear. In the specific-heat expansion even and odd powers of N^{-1} occur. Furthermore, the odd coefficients in this latter expansion are proportional to the corresponding odd coefficients in the internal-energy expansion. The constant depends on how the mass μ (2.12) depends on the temperature (5.30). In the expansion of the observable $f^{(3)}$, we find corrections with all powers of N^{-1} except for the term N^{-2}. Indeed, the coefficients f_m, E_m, C_m and A_m do depend on the lattice structure of the model, hence they are not universal.

The fact that E_{2m+1}/C_{2m+1} is a ρ-independent number for the square lattice $(=-1/\sqrt{2})$ [24, 23], suggested the idea that this ratio might be universal (e.g., it does *not* depend on the lattice structure)[9]. However, our results show that this is not the case:

$$\frac{E_{2m+1}(\rho)}{C_{2m+1}(\rho)} = \begin{cases} -1/2 & \text{triangular} \\ -\sqrt{3}/2 & \text{hexagonal.} \end{cases} \tag{8.1}$$

Thus, the proportional constant *does* depend on the lattice structure, hence it is not universal. We can write (8.1) and the corresponding square-lattice relation (1.2) in an unified way by realizing that the constant is just $-1/E_0$.

[9] Izmailian and Hu [41] (see also [43]) computed the finite-size expansion of the free energy $f(N) = f_{\text{bulk}} + \sum_{k=1}^{\infty} f_k/N^{2k}$ and the inverse correlation length $\xi^{-1}(N) = \sum_{k=1}^{\infty} b_k/N^{2k-1}$ for a critical Ising model on several $N \times \infty$ lattices (i.e., square, hexagonal and triangular) with periodic boundary conditions. They found lattice-dependent coefficients f_k and b_k, but universal ratios $b_k/f_k = (2^{2k} - 1)/(2^{2k-1} - 1)$.

It is important to note[10] that one key ingredient in this discussion is the fact that there is an exact transformation (7.4) mapping the high-temperature phase onto the low-temperature phase, so we can define a parameter τ (7.3) transforming as $\tau \to -\tau$. It is not clear whether this transformation exists or not for an Ising model defined on a general lattice. However, if that transformation does exist, then we can define τ so equation (7.6) holds, leading to (7.7)/(8.1). We can summarize all these observations in the following conjecture:

Conjecture 8.1. *Let us consider a critical Ising system on a regular two-dimensional lattice with toroidal boundary conditions. Let us further assume that there is an exact mapping* $v \to v'$ *from the high-temperature phase onto the low-temperature phase such that* $\tau \to -\tau$. *Then, the internal energy and specific heat can be expanded in power series of* N^{-1} *as in (7.1b)/(7.1c) and the coefficients* $E_m(\rho)$ *and* $C_m(\rho)$ *satisfy*

$$\frac{E_m(\rho)}{C_m(\rho)} = \begin{cases} -1/E_0 & \text{for } m \text{ odd} \\ 0 & \text{for } m \text{ even} \end{cases} \tag{8.2}$$

where E_0 *is the bulk internal energy (see (7.1b)). Indeed, we understand that this ratio is not defined whenever* $E_m = 0$.

If this conjecture is true, then we could define the expansions

$$E_c(N,\rho) = E_0\left[1 + \sum_{m=0}^{\infty} \frac{\tilde{E}_{2m+1}(\rho)}{N^{2m+1}}\right] \tag{8.3a}$$

$$C_{H,c}(N,\rho) = E_0^2\left[\tilde{C}_{00}\log N + \tilde{C}_0(\rho) + \sum_{m=1}^{\infty}\frac{\tilde{C}_m(\rho)}{N^m}\right] \tag{8.3b}$$

and then the new ratios would be universal

$$\frac{\tilde{E}_m(\rho)}{\tilde{C}_m(\rho)} = \begin{cases} -1 & \text{for } m \text{ odd} \\ 0 & \text{for } m \text{ even.} \end{cases} \tag{8.4}$$

In section 1 we mentioned that the results contained in this paper could serve also to test Monte Carlo simulations. Indeed, the expressions (3.4)/(4.2)/(5.3) provide a way to compute the *exact* values of the internal energy and specific heat for any finite torus of size $N \times M$. For very large lattices one could also use the (easier to evaluate) asymptotic expansions (7.1*b*)/(7.1*c*).

On the other hand, by taking the *exact* values of any observable for fixed aspect ratio ρ and several values of the torus width N, we can check whether the asymptotic expansions (7.1) are correct or not. In particular, by fitting the exact values to the corresponding ansatz, we can verify whether the numerical coefficients coincide with the estimates coming from the fits. We have performed such an analysis and have confirmed that the numerical values of the coefficients f_m, E_m, C_m and A_m for several values of ρ coincide with the estimates coming from the fits. In addition, this procedure allows us to obtain crude estimates of the next coefficients in each expansion. For instance, we obtain for $\rho = 1$ (which is the case most frequently considered in the literature) the following values:

$$f_{10}^{\text{tri}}(1) \approx 1.932 \qquad f_{10}^{\text{hc}}(1) \approx 0.966 \tag{8.5a}$$

$$E_9^{\text{tri}}(1) \approx -7.821 \qquad E_9^{\text{hc}}(1) \approx -2.258 \tag{8.5b}$$

$$C_6^{\text{tri}}(1) \approx -0.722 \qquad C_6^{\text{hc}}(1) \approx -0.120 \tag{8.5c}$$

$$A_3^{\text{tri}}(1) \approx 9.124 \qquad A_3^{\text{hc}}(1) \approx 0.878. \tag{8.5d}$$

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Appendix A. The Euler–MacLaurin formula

The Euler–MacLaurin formula is one important tool we need to compute asymptotic series. Here we will use the version of ([45], formula 23.1.32). Let $F(x)$ be a function whose first $2n$ derivatives are continuous in the interval (a, b). If we divide the interval into m equal parts (so that $h = (b - a)/m$), then we have

$$\sum_{k=0}^{m-1} F(a + kh + \alpha h) = \frac{1}{h}\int_a^b F(t)\,\mathrm{d}t + \sum_{k=1}^{p} \frac{h^{k-1}}{k!} B_k(\alpha)\left[F^{(k-1)}(b) - F^{(k-1)}(a)\right] - \frac{h^p}{p!}\int_0^1 \hat{B}_p(\alpha - t)\left\{\sum_{k=0}^{m-1} F^{(p)}(a + kh + th)\right\}\mathrm{d}t \tag{A.1}$$

where $p \leqslant 2n$, $0 \leqslant \alpha \leqslant 1$, $\hat{B}_n(x) = B_n(x - \lfloor x \rfloor)$ and $B_n(x)$ are the Bernoulli polynomials defined in terms of the Bernoulli numbers B_k by

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

Indeed, $B_n(0) = B_n$. The Bernoulli polynomials satisfy the identity ([45], equation 23.1.21):

$$B_n(1/2) = \left(\frac{1}{2^{n-1}} - 1\right) B_n. \tag{A.3}$$

We are mainly interested in sums of the form

$$\frac{1}{L}\sum_{n=0}^{\gamma L-1} F\left(\frac{2\pi}{L}(n + \alpha)\right). \tag{A.4}$$

The asymptotic expansion of the sum (A.4) in the limit $L \to \infty$ with γ fixed can be obtained from (A.1). If we assume that all the derivatives of $F(t)$ are integrable over the interval $[0, 2\pi\gamma]$ we can formally extend the sum in (A.1) to $k = \infty$ and drop the remainder term (namely, the integral in (A.1)). In this case, we can write the Euler–MacLaurin formula as follows:

$$\frac{1}{L}\sum_{n=0}^{\gamma L-1} F\left(\frac{2\pi}{L}(n + \alpha)\right) = \frac{1}{2\pi}\int_0^{2\pi\gamma} F(t)\,\mathrm{d}t + \frac{1}{2\pi}\sum_{k=1}^{\infty}\left(\frac{2\pi}{L}\right)^k \frac{B_k(\alpha)}{k!}\left[F^{(k-1)}(2\pi\gamma) - F^{(k-1)}(0)\right]. \tag{A.5}$$

In this paper, we need the above formula in the particular case $L = 2N$ and $\gamma = 1/2$. Then (A.5) reads

$$\frac{1}{N}\sum_{n=0}^{N-1} F\left(\frac{\pi}{N}(n + \alpha)\right) = \frac{1}{\pi}\int_0^{\pi} F(t)\,\mathrm{d}t + \frac{1}{\pi}\sum_{k=1}^{\infty}\left(\frac{\pi}{N}\right)^k \frac{B_k(\alpha)}{k!}\left[F^{(k-1)}(\pi) - F^{(k-1)}(0)\right]. \tag{A.6}$$

In the computation of the specific heat we also need formula (A.1) in the particular case $\alpha = 0$ and $h = 1$. In this case, we can formally write (A.1) for a function F whose derivatives are all integrable over $[a, b]$ in the following form [42]

$$\sum_{k=a}^{b-1} F(k) = \int_a^b F(t)\,\mathrm{d}t - \frac{1}{2}[F(b) - F(a)] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\left[F^{(2k-1)}(b) - F^{(2k-1)}(a)\right] \tag{A.7}$$

where we have used the fact that [45]

$$B_{2k+1} = \begin{cases} -\frac{1}{2} & k = 0 \\ 0 & k > 0. \end{cases} \tag{A.8}$$

As we did in [24], we can apply (A.7) to the function $F(x) = x^{2m}$ with $a = 0$ and $b = 1$. We then obtain the identity

$$\sum_{k=1}^{m} \frac{B_{2k}}{2k}\binom{2m}{2k-1} = \frac{1}{2} - \frac{1}{2m+1}. \tag{A.9}$$

If we apply (A.7) to the case $F(x) = x^{2m-1}$ with the same endpoints as before, we obtain

$$\sum_{k=1}^{m-1} \frac{B_{2k}}{2k}\binom{2m-1}{2k-1} = \frac{1}{2}\left(1 - \frac{1}{m}\right). \tag{A.10}$$

Appendix B. Theta functions

In this appendix, we gather all the definitions and properties of the Jacobi's θ-functions needed in this paper. We first introduce the object $\theta_{\alpha,\beta}(z,\tau)$ $(\alpha, \beta = 0, 1/2)$[11]

$$\theta_{\alpha,\beta}(z,\tau) = \sum_{n\in\mathbb{Z}} q^{(n+1/2-\alpha)^2} \exp\left\{2\pi\mathrm{i}\left(n + \frac{1}{2} - \alpha\right)\left(z + \beta - \frac{1}{2}\right)\right\} \tag{B.1}$$

where the nome q is defined in terms of the modular parameter τ as follows:

$$q = \mathrm{e}^{\pi\mathrm{i}\tau}. \tag{B.2}$$

Using the identity (proved in [46])

$$\prod_{n=0}^{\infty}[1 + q^{2n-1}t][1 + q^{2n-1}t^{-1}][1 - q^{2n}] = \sum_{n\in\mathbb{Z}} q^{n^2} t^n \tag{B.3}$$

we can write (B.1) as

$$\theta_{\alpha,\beta}(z,\tau) = \eta(\tau) q^{B_2(\alpha)}\,\mathrm{e}^{2\pi\mathrm{i}(1/2-\alpha)(z+\beta-1/2)} \prod_{n=0}^{\infty}\left[1 - q^{2(n+1-\alpha)}\,\mathrm{e}^{2\pi\mathrm{i}(z+\beta)}\right]\left[1 - q^{2(n+\alpha)}\,\mathrm{e}^{-2\pi\mathrm{i}(z+\beta)}\right] \tag{B.4}$$

where $\eta(\tau)$ is Dedekind η-function

$$\eta(\tau) = \mathrm{e}^{\pi\mathrm{i}\tau/12} \prod_{n=1}^{\infty}[1 - \mathrm{e}^{2\pi\mathrm{i}\tau n}] \tag{B.5}$$

[11] This object is almost identical to the one introduced in [25]. However, this latter one gives the wrong sign to $\theta_1(z,\tau)$ (cf (B.10)), although this is not important as we are only interested in the case $z = 0$ where $\theta_1(0,\tau) = 0$.

and $B_2(\alpha)$ is the Bernoulli polynomial (cf (A.2))

$$B_2(\alpha) = \alpha^2 - \alpha + \tfrac{1}{6}. \tag{B.6}$$

The relation of the functions $\theta_{\alpha,\beta}$ with the usual θ-functions $\theta_i(z,\tau)$, $i = 1,\ldots,4$ [47], is the following:

$$\theta_{0,0}(z,\tau) = \theta_1(z,\tau) = -\mathrm{i}\sum_{n\in\mathbb{Z}}(-1)^n\,\mathrm{e}^{2\pi\mathrm{i}z(n+1/2)+\pi\mathrm{i}\tau(n+1/2)^2} \tag{B.7}$$

$$\theta_{0,\frac{1}{2}}(z,\tau) = \theta_2(z,\tau) = \sum_{n\in\mathbb{Z}}\mathrm{e}^{2\pi\mathrm{i}z(n+1/2)+\pi\mathrm{i}\tau(n+1/2)^2} \tag{B.8}$$

$$\theta_{\frac{1}{2},0}(z,\tau) = \theta_4(z,\tau) = \sum_{n\in\mathbb{Z}}(-1)^n\,\mathrm{e}^{2\pi\mathrm{i}zn+\pi\mathrm{i}\tau n^2} \tag{B.9}$$

$$\theta_{\frac{1}{2},\frac{1}{2}}(z,\tau) = \theta_3(z,\tau) = \sum_{n\in\mathbb{Z}}\mathrm{e}^{2\pi\mathrm{i}zn+\pi\mathrm{i}\tau n^2}. \tag{B.10}$$

In this paper, we will only need these functions evaluated at $z = 0$ and $\tau = \mathrm{i}\tau_0\rho$ where τ_0 is given by (3.19). To simplify the notation we will use the shorthands

$$\theta_{\alpha,\beta} = \theta_{\alpha,\beta}(\mathrm{i}\tau_0\rho) = \theta_{\alpha,\beta}(z=0,\tau=\mathrm{i}\tau_0\rho) \tag{B.11a}$$

$$\theta_i = \theta_i(\mathrm{i}\tau_0\rho) = \theta_i(z=0,\tau=\mathrm{i}\tau_0\rho) \tag{B.11b}$$

$$\eta = \eta(\mathrm{i}\tau_0\rho) = \eta(\tau=\mathrm{i}\tau_0\rho). \tag{B.11c}$$

We also need the limits of the θ-functions in the limit $\rho\to\infty$. These limits are given by

$$\lim_{\rho\to\infty}\theta_3(\mathrm{i}\tau_0\rho) = \lim_{\rho\to\infty}\theta_4(\mathrm{i}\tau_0\rho) = 1 \tag{B.12a}$$

$$\lim_{\rho\to\infty}\theta_2(\mathrm{i}\tau_0\rho) = \lim_{\rho\to\infty}2\mathrm{e}^{-\pi\tau_0\rho/4} = 0. \tag{B.12b}$$

From equation (B.4) we arrive at the following identity valid when $(\alpha,\beta)\neq(0,0)$:

$$\log\left|\frac{\theta_{\alpha,\beta}(\mathrm{i}\tau_0\rho)}{\eta(\mathrm{i}\tau_0\rho)}\right| + \pi\rho\,\mathrm{Re}(\tau_0)B_2(\alpha) = \sum_{n=0}^{\infty}\left\{\log\left|1-\mathrm{e}^{-2\pi[\tau_0\rho(n+1-\alpha)-\mathrm{i}\beta]}\right|\right.$$
$$\left.+\log\left|1-\mathrm{e}^{-2\pi[\tau_0\rho(n+\alpha)+\mathrm{i}\beta]}\right|\right\}. \tag{B.13}$$

Another useful relation involving $\log\theta_{\alpha,\beta}(0,\tau)$ is the following:

$$\sum_{n=\delta_{\alpha,0}}^{\infty}\sum_{p=1}^{\infty}\frac{\mathrm{e}^{2\pi p\mathrm{i}(\tau(n+\alpha)-\beta)}}{n+\alpha} = -\left[\log\theta_{\alpha,\beta}(\tau) - \left(\frac{\mathrm{i}\pi\tau}{4}+\log 2\right)\delta_{\alpha,0}\right]. \tag{B.14}$$

We have proved this identity by considering each case $\alpha,\beta = 0, 1/2$ (with $(\alpha,\beta)\neq(0,0)$) separately and by a careful rearrangement of the corresponding series.

Dedekind's η-function satisfies the following identity:

$$\eta(\tau)^3 = \tfrac{1}{2}\theta_2(\tau)\theta_3(\tau)\theta_4(\tau). \tag{B.15}$$

The analogue of (B.13) when $(\alpha,\beta) = (0,0)$ is given in the particular case $\tau = \mathrm{i}\tau_0\rho$ by

$$\sum_{n=1}^{\infty}\log|1-\mathrm{e}^{-2\pi\tau_0\rho n}| = \log|\eta| + \frac{\pi\rho}{12}\mathrm{Re}(\tau_0). \tag{B.16}$$

We also need the behaviour of the θ functions under the Jacobi transformation

$$\tau\to\tau' = -1/\tau. \tag{B.17}$$

The result when $z = 0$ is given in [46]

$$\theta_3(0, \tau') = (-\mathrm{i}\tau)^{1/2}\theta_3(0, \tau) \tag{B.18a}$$

$$\theta_{2,4}(0, \tau') = (-\mathrm{i}\tau)^{1/2}\theta_{4,2}(0, \tau). \tag{B.18b}$$

In particular, if $\tau = \mathrm{i}\tau_0^\star\rho$ where

$$\tau_0^\star = \frac{\sqrt{3}+\mathrm{i}}{2} = \frac{1}{\tau_0} \tag{B.19}$$

is the complex conjugate of τ_0 (3.19), the θ-functions transform under (B.17) as follows:

$$\theta_3(0, \mathrm{i}\tau_0^\star/\rho) = (\tau_0\rho)^{1/2}\theta_3(0, \mathrm{i}\tau_0\rho) \tag{B.20a}$$

$$\theta_{2,4}(0, \mathrm{i}\tau_0^\star/\rho) = (\tau_0\rho)^{1/2}\theta_{4,2}(0, \mathrm{i}\tau_0\rho). \tag{B.20b}$$

Finally, we should mention that the absolute value of the above θ-functions does not depend on the sign of Im τ_0. Thus,

$$|\theta_i(0, \mathrm{i}\tau_0/\rho)| = |\theta_i(0, \mathrm{i}\tau_0^\star/\rho)|. \tag{B.21}$$

Appendix C. Kronecker's double series

In this appendix, we collect a few properties of the Kronecker's double series [48]. These series are defined as

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

The basic property we need is the following

$$B_{2p}(\alpha) - \mathrm{Re}\, K_{2p}^{\alpha,\beta}(\tau) = 2p\,\mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\big[(n+\alpha)^{2p-1}\,\mathrm{e}^{2\pi\mathrm{i}m[\tau(n+\alpha)-\beta]} + (n+1-\alpha)^{2p-1}\,\mathrm{e}^{2\pi\mathrm{i}m[\tau(n+1-\alpha)-\beta]}\big] \tag{C.2}$$

in the particular case $\tau = \mathrm{i}\tau_0\rho$ with $\tau_0 \in \mathbb{C}$ (cf (3.19)) and $\rho \in \mathbb{R}$. Equation (C.2) can easily be proved using the same arguments as in ([25], appendix D) where they consider the particular case $\tau = \mathrm{i}\rho$, $\rho \in \mathbb{R}$.

In this paper, we also need certain values of the $K_p^{\alpha,\beta}$ obtained in ([25], appendix E)

$$K_4^{0,\frac{1}{2}}(\tau) = \tfrac{1}{30}\left(\tfrac{7}{8}\theta_2^8 - \theta_3^4\theta_4^4\right) \tag{C.3a}$$

$$K_4^{\frac{1}{2},0}(\tau) = \tfrac{1}{30}\left(\tfrac{7}{8}\theta_4^8 - \theta_2^4\theta_3^4\right) \tag{C.3b}$$

$$K_4^{\frac{1}{2},\frac{1}{2}}(\tau) = \tfrac{1}{30}\left(\tfrac{7}{8}\theta_3^8 + \theta_2^4\theta_4^4\right) \tag{C.3c}$$

$$K_6^{0,0}(\tau) = \tfrac{1}{84}\left(\theta_2^4 + \theta_3^4\right)\left(\theta_4^4 - \theta_2^4\right)\left(\theta_3^4 + \theta_4^4\right) \tag{C.4a}$$

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

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

$$K_6^{\frac{1}{2},\frac{1}{2}}(\tau) = \tfrac{1}{84}\left(\theta_2^4 - \theta_4^4\right)\left(\tfrac{31}{16}\theta_3^8 - \theta_2^4\theta_4^4\right). \tag{C.4d}$$

The behaviour of the functions $K_6^{\alpha,\beta}$ under the Jacobi transformation (B.17) can be obtained using (B.20) and taking into account that $\tau_0^6 = -1$

$$K_6^{0,\frac{1}{2}}(0, \mathrm{i}\tau_0^\star/\rho) = \rho^6 K_6^{\frac{1}{2},0}(0, \mathrm{i}\tau_0\rho) \tag{C.5a}$$

$$K_6^{\frac{1}{2},0}(0, \mathrm{i}\tau_0^\star/\rho) = \rho^6 K_6^{0,\frac{1}{2}}(0, \mathrm{i}\tau_0\rho) \tag{C.5b}$$

$$K_6^{\frac{1}{2},\frac{1}{2}}(0, \mathrm{i}\tau_0^\star/\rho) = \rho^6 K_6^{\frac{1}{2},\frac{1}{2}}(0, \mathrm{i}\tau_0\rho) \tag{C.5c}$$

$$K_6^{0,0}(0, \mathrm{i}\tau_0^\star/\rho) = \rho^6 K_6^{0,0}(0, \mathrm{i}\tau_0\rho). \tag{C.5d}$$

Finally, we mention that the value of $\mathrm{Re}\, K_6^{\alpha,\beta}$ does not depend on the sign of $\mathrm{Im}\,\tau_0$:

$$\mathrm{Re}\, K_6^{\alpha,\beta}(0, \mathrm{i}\tau_0^\star/\rho) = \mathrm{Re}\, K_6^{\alpha,\beta}(0, \mathrm{i}\tau_0/\rho). \tag{C.6}$$

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