Finite-size effects for the Ising model on helical tori

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We analyze the exact partition function of the Ising model on a square lattice under helical boundary conditions obtained by Liaw *et al.* [Phys. Rev. E **73**, 055101(R) (2006)]. Based on such an expression, we then extend the algorithm of Ivashkevich, Izmailian, and Hu [J. Phys. A **35**, 5543 (2002)] to derive an exact asymptotic expansion of the logarithm of the partition function and its first to fourth derivatives at the critical point. From such results, we find that the shift exponent for the specific heat is $\lambda=1$ for all values of the helicity factor d. We also find that finite-size corrections for the free energy, the internal energy, and the specific heat of the model in a crucial way depend on the helicity factor of the lattice.

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I. INTRODUCTION

Finite-size scaling [1,2] and finite-size corrections for critical lattice [3–6] have attracted much attention in recent decades. Based on the exactly known partition function of the two-dimensional (2D) Ising model [3,4] on the $M\times N$ square (SQ) lattice with torus boundary conditions, in 1969 Ferdinand and Fisher [5] calculated finite-size corrections for the free energy, the internal energy, and the specific heat of the Ising model for the fixed aspect ratio $\rho=M/N$ up to order $1/N^2$, $1/N$, and $1/N$, respectively. In 1967, Ferdinand [6] calculated finite-size corrections for the dimer model on finite SQ lattice with torus boundary conditions. Based on the subgraph expansion of the Ising model in the external field, in 1984, Hu [7] proposed finite-size scaling of the magnetic susceptibility for the Ising model on $\infty\times N$ lattices. Blote, Cardy, and Nightingale showed that for conformally invariant two-dimensional systems, the amplitude of the finite-size corrections to the free energy of an $\infty\times N$ system at criticality is linearly related to the conformal anomaly number c, for various boundary conditions [8].

In 1984, Privman and Fisher [9] proposed the idea of universal finite-size scaling functions (UFSSFs). Using a histogram Monte Carlo simulation method [10], in 1995–1998, Hu, Lin, and Chen calculated UFSSFs of the existence probability E_p, the percolation probability P, and the probability for the appearance of n percolation clusters for bond and site percolation models on SQ, honeycomb (HC), and plane triangular (PT) lattices [11] and some 3D lattices [12]. Using other Monte Carlo methods, Okabe *et al.* [13] calculated FSSFs for the Ising model on the SQ lattice with tilted (helical) boundary conditions, Tomita, Okabe, and Hu [14] found UFSSs of some static quantities for the Ising model on SQ, HC, and PT lattices, and Wang and Hu [15] obtained universal dynamic critical exponent and dynamic UFSSFs for the Ising model and SQ, HC, and PT lattices.

In 1997, Ziff, Finch, and Adamchik [16] calculated the number of finite clusters of percolation models on two-dimensional finite lattices. They found that the excess number of clusters over the bulk value is a universal quantity, dependent upon the system shape but independent of the lattice and percolation type [16]. Based on the connection between the q-state Potts model and a q-state bond-correlated percolation model (QBCPM) [7], Hu *et al.* [17] used a Monte Carlo method to calculate the excess number of clusters over the bulk value for the QBCPM. To obtain an analytic equation for the Ising model for comparing with the numerical data, they extended Ferdinand and Fisher's calculations [5] for finite-size corrections to higher orders [17]. After this work, Izmailian and collaborators studied intensively exact finite-size corrections for the Ising and dimer models on 2D lattices with various boundary conditions [18–22]. Ivashkevich, Izmailian, and Hu (IIH) [19] proposed a systematic method to compute finite-size corrections to the partition functions and their derivatives of free models on torus, including the Ising model, the dimer model, and the Gaussian model. Their approach is based on relations between the terms of the asymptotic expansion and the so-called Kronecker's double series [19] which are directly related to elliptic θ functions. Expressing the final result in terms of θ functions avoids messy sums (as in some earlier works) and greatly simplifies the task of verifying the behavior of different terms in the asymptotic expansion under duality transformation $M\leftrightarrow N$. Using this approach, Salas [23] computed the finite-size corrections to the free energy, the internal energy, and the specific heat of the critical Ising model on PT and HC lattices wrapped on a torus and Izmailian, Oganesyan, and Hu [20] obtained similar finite-size corrections of the Ising model on a SQ lattice with Brascamp-Kunz boundary conditions [24]. Based on exact partition functions of the Ising model on finite SQ, HC, and PT lattices with periodic and antiperiodic boundary conditions [25], Wu, Hu, and Izmailian obtained UFSSFs of the free energy, the internal energy, and the specific heat of the Ising model on these lattices from analytic equations [21]. Janke and Kenna [26] and Kong [27] also calculated exact finite-size corrections for the Ising and dimer models on 2D lattices with various boundary conditions.

Another interesting quantity related to the critical lattice model is the shift exponent λ. Finite-size properties of the

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specific heat $C(T)$ for the Ising model are characterized by the location of its peak, T_{max}, its height $C(T_{max})$, and its value at the infinite-volume critical point $C(T_c)$. The peak position T_{max} is a pseudocritical (or effective) point which typically approaches T_c as the characteristic size of the system L tends to infinity as

$$|T_{max} - T_c| \sim L^{-\lambda}, \tag{1}$$

where λ is the shift exponent. Let ν being the correlation length critical exponent. Usually the shift exponent λ coincides with $1/\nu$, but this is not always the case and it is not a consequence of the finite-size scaling (FSS) [1]. The actual value of the shift exponent depends on the lattice topology.

In a classic paper, Ferdinand and Fisher [5] used the exactly known partition function of the two-dimensional Ising model on finite lattices with toroidal boundary conditions to determine the behavior of the specific heat pseudocritical point. They found that the shift exponent for the specific heat is $\lambda = 1 = 1/\nu$, except for the special case of an infinitely long torus, in which case pseudocritical specific-heat scaling behavior was found to be of the form $L^{-2}\ln L$ [3].

The FSS of the specific heat of the Ising model was recently studied both analytically and numerically on two-dimensional lattices with other boundary conditions in Refs. [22,26,28–30]. For lattices with a spherical topology the shift exponent was found to be far away from $1/\nu=1$, with λ ranging from approximately 1.75 to 2 (with the possibility of logarithmic corrections) [29,30]. In another study of the FSS of the specific heat of the Ising model with Brascamp-Kunz boundary conditions, Janke and Kenna [26] found that the shift exponent for the specific heat is $\lambda = 2$.

In light of these and other recent analyses, we wish to present analytical results which may clarify the situation. To this end, we have selected the Ising model with helical boundary conditions [13,28]. These boundary conditions permit an analytical approach to the determination of a number of thermodynamic quantities.

In this paper, we take a complementary approach, exploiting FSS (i) to determine corrections to leading scaling and (ii) to determine the behavior of the specific heat near the critical point.

The rest of the paper is organized as follows. In Sec. II we relate the exact partition functions of the Ising model on the square lattice under helical boundary conditions obtained by Liaw *et al.* [28] to the partition functions $Z_{\alpha,\beta}$ with $(\alpha,\beta) = (1/2,0)$, $(0,1/2)$, and $(1/2,1/2)$. Based on such expressions, we then extend IIH's algorithm [19] to derive the exact asymptotic expansions of the logarithm of the partition functions and their derivatives and write down the expansion coefficients up to second order in Sec. III. In Sec. IV we provide a complete description for the finite-size effect of an Ising model subject to helical boundary conditions. Our main results are summarized in Sec. V. We have summarized the technical details in the Appendixes: in Appendix A we collect the definitions and properties of the Jacobi's θ functions and Kronecker's double series, and in Appendix B we recall the behavior of the θ functions, Dedekind's η function, and the Kronecker functions $K_{2p}^{\alpha,\beta}$ under the Jacobi transformation.

II. ISING MODEL UNDER HELICAL BOUNDARY CONDITIONS

For the Ising model on a lattice G of S sites, the ith site of the lattice for $1 \leqslant i \leqslant S$ is assigned a classical spin variable s_i, which has values ± 1. The spins interact according to the Hamiltonian

$$H = -J\sum_{\langle ij\rangle} s_i s_j, \tag{2}$$

where $J = J'/k_B T$ is exchange energy and the sum runs over the nearest-neighbor pairs of spins. The partition function of the Ising model is given by the sum over all spin configurations on the lattice:

$$Z_{Ising}(J) = \sum_s e^{-H(s)}. \tag{3}$$

As is mentioned in Introduction there are a few boundary conditions for which the Ising model has been solved exactly. Among them is the helical boundary conditions [13] studied by Liaw *et al.* [28]. For the Ising model on the $M \times N$ square lattice with the helicity factor $d \equiv D/M$, the system has periodic boundary conditions in the N direction and helical (tilted) boundary conditions in the M direction such that the ith site in the first column is connected with the mod $(i+D, M)$th site in the N column of the lattice [13].

An explicit expression for the partition function of the Ising model on $M \times N$ helical torus is given by [28]

$$Z_{M,N}(J) = \frac{1}{2}(\sqrt{2}\cosh J)^{2MN} \times \left\{ I_{1/2,1/2} + I_{1/2,0} + I_{0,1/2} - \mathrm{sgn}\left(\frac{T-T_c}{T_c}\right) I_{0,0} \right\}, \tag{4}$$

$$I_{\alpha,\beta}^2 = \prod_{m=1}^{M}\prod_{n=1}^{N} \left\{ a - b\cos\left[2\pi\left(\frac{m+\beta}{M} - d\frac{n+\alpha}{N}\right)\right] - b\cos\left[2\pi\frac{n+\alpha}{N}\right] \right\}, \tag{5}$$

where $a = (1+\tanh^2 J)^2$ and $b = 2\tanh J(1-\tanh^2 J)$. In addition, the function $\mathrm{sgn}(x)$ denotes the sign of the value x and T_c is the critical temperature of the bulk system ($\sinh 2J_c = 1$).

It is convenient to set up another parametrization of the interaction constant J in terms of the mass variable μ:

$$\mu = \ln\sqrt{\sinh 2J}. \tag{6}$$

The critical point corresponds to the massless case $\mu = \mu_c = 0$. Then an explicit expression for the partition function of the Ising model on an $M \times N$ helical torus can be rewritten as

$$Z_{M,N}(J) = \frac{1}{2}(\sqrt{2}e^{\mu})^{MN}\{Z_{1/2,1/2}(\mu,d) + Z_{0,1/2}(\mu,d) + Z_{1/2,0}(\mu,d) + \mathrm{sgn}(\mu)Z_{0,0}(\mu,d)\}, \tag{7}$$

where $Z_{\alpha,\beta}(\mu,d)$ is given by

$$Z^2_{\alpha,\beta}(\mu,d) = \prod_{n=0}^{N-1}\prod_{m=0}^{M-1} 4\left\{\sin^2\left(\frac{\pi}{N}(n+\alpha)\right) + \sin^2\left(\frac{\pi}{M}[m+\beta-d\rho(n+\alpha)]\right) + 2\sinh^2\mu\right\}, \tag{8}$$

where $\rho=M/N$ is the aspect ratio.

With the help of the identity [31]

$$4|\sinh(M\omega+i\pi\beta)|^2 = 4[\sinh^2 M\omega + \sin^2 \pi\beta] = \prod_{m=0}^{M-1} 4\left\{\sinh^2\omega + \sin^2\left(\frac{\pi}{M}(m+\beta)\right)\right\}, \tag{9}$$

the $Z_{\alpha,\beta}(\mu,d)$ can be transformed into a simpler form

$$Z_{\alpha,\beta}(\mu,d) = \prod_{n=0}^{N-1} 2\left|\sinh\left\{M\omega_\mu\left(\pi\frac{n+\alpha}{N}\right) + i\pi[\beta-d\rho(n+\alpha)]\right\}\right|, \tag{10}$$

where the lattice dispersion relation has appeared:

$$\omega_\mu(k) = \operatorname{arcsinh}\sqrt{\sin^2 k + 2\sinh^2\mu}. \tag{11}$$

Note that the general theory about the asymptotic expansion of $Z_{\alpha,\beta}(\mu,d)$, for the particular case $d=0$, has been given in [19]. In what follows we will show that the theory can be extended to the case with arbitrary rational number d.

First of all, let us mention the symmetry properties of the partition function $Z_{\alpha,\beta}(\mu,d)$. From its definition (10) one can easily verify that it is even and periodic with respect to its arguments α and β:

$$Z_{\alpha,\beta}(\mu,d) = Z_{\alpha,-\beta}(\mu,d) = Z_{-\alpha,\beta}(\mu,d),$$

$$Z_{\alpha,\beta}(\mu,d) = Z_{1+\alpha,\beta}(\mu,d) = Z_{\alpha,1+\beta}(\mu,d).$$

These imply that twist angles α and β can be taken from the interval $[0,1]$. Thus, for $(\alpha,\beta)\neq(0,0)$, the partition function $Z_{\alpha,\beta}(\mu,d)$ is even with respect to its mass argument μ. Hence, near the critical point $(\mu=0)$ we have

$$Z_{\alpha,\beta}(\mu,d) = Z_{\alpha,\beta}(0,d) + \frac{\mu^2}{2!}Z''_{\alpha,\beta}(0,d) + \cdots, \quad (\alpha,\beta)\neq(0,0). \tag{12}$$

The only exception is the point where both α and β are equal to zero. This case has to be treated separately since at this point the partition function turns to zero. As a result, we have

$$Z_{0,0}(\mu,d) = \mu Z'_{0,0}(0,d) + \frac{\mu^3}{3!}Z'''_{0,0}(0,d) + \cdots, \quad (\alpha,\beta)=(0,0). \tag{13}$$

From Eq. (10), one can easily verify that $Z_{\alpha,\beta}(\mu,d)$ is even and periodic with respect to its arguments d:

$$Z_{\alpha,\beta}(\mu,d) = Z_{\alpha,\beta}(\mu,-d), \tag{14}$$

$$Z_{\alpha,\beta}(\mu,d) = Z_{\alpha,\beta}(\mu,d+1/\rho). \tag{15}$$

Equations (14) and (15) imply that the partition function of the Ising model on an $M\times N$ helical torus is invariant under transformation:

$$d \to \frac{n}{\rho} \pm d, \tag{16}$$

where n is an integer number. In what follows the notation $Z_{\alpha,\beta}(\mu,d)$ will imply $(\alpha,\beta)\neq(0,0)$.

We are interested in computing the asymptotic expansions for large N, M, and D with fixed aspect ratio ρ and helicity factor d,

$$\rho = \frac{M}{N}, \quad d = \frac{D}{M}, \tag{17}$$

of the free energy F, the internal energy U, and the specific heat C at the critical point $J=J_c$ $(\mu=\mu_c=0)$. These quantities are defined as follows:

$$F = -\frac{1}{MN}\ln Z_{M,N}(J), \tag{18}$$

$$U = \frac{\partial}{\partial J}F, \tag{19}$$

$$C = -\frac{\partial^2}{\partial J^2}F. \tag{20}$$

In Sec. III D we will also consider higher derivatives of the free energy at criticality:

$$F_c^{(k)} = -\left.\frac{\partial^k}{\partial J^k}F\right|_{J=J_c}, \tag{21}$$

with $k=3,4$.

III. ASYMPTOTIC EXPANSION OF THE FREE ENERGY AND HIS DERIVATIVES

A. Asymptotic expansion of the free energy

In what follows, we will show that the exact asymptotic expansion of the free energy can be written as

$$F = f_{bulk} + \sum_{p=0}^{\infty} f_p(\rho,d)S^{-p-1}, \tag{22}$$

where $S=MN$ and $\rho=M/N$ is the aspect ratio. We will show that all finite-size correction terms are invariant under transformation $\rho\to 1/(1+d^2)\rho$, which actually means that ξ,

$$\xi = \rho\sqrt{1+d^2}, \tag{23}$$

can be regarded as the effective aspect ratio.

In the previous section it was shown that the partition function of the $M\times N$ Ising model with helical boundary conditions can be expressed in terms of the partition function $Z_{\alpha,\beta}(\mu,d)$, which has been well studied in Ref. [19] for the particular case $d=0$. Further on we will use it and for simplicity we will recall some necessary parts from there. For the reader's convenience, all technical details of our calculations and definitions of the special functions are summarized in the Appendixes at the end of the paper.

Let us start with the basic quantity $Z_{\alpha,\beta}(0,d)$. Considering the logarithm of $Z_{\alpha,\beta}(0,d)$, we note that it can be transformed as

$$\ln Z_{\alpha,\beta}(0,d) = M\sum_{n=0}^{N-1} \omega_0\left(\frac{\pi(n+\alpha)}{N}\right) + \sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right|. \tag{24}$$

The second sum here vanishes in the formal limit $M\to\infty$ when the torus turns into an infinitely long cylinder of circumference N. Therefore, the first sum gives the logarithm of the partition function on that cylinder. Its asymptotic expansion can be found with the help of the Euler-Maclaurin summation formula (see Appendix A in [19])

$$M\sum_{n=0}^{N-1} \omega_0\left(\frac{\pi(n+\alpha)}{N}\right) = \frac{S}{\pi}\int_0^\pi \omega_0(x)dx - \pi\rho B_2^\alpha - 2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p \frac{\lambda_{2p}}{(2p)!}\frac{B_{2p+2}^\alpha}{2p+2}, \tag{25}$$

where $\int_0^\pi\omega_0(x)\mathrm{d}x=2G$, $G=0.915965\ldots$ is Catalan's constant, and B_p^α are so-called Bernoulli polynomials. We have also used the symmetry property $\omega_0(x)=\omega_0(\pi-x)$ of the lattice dispersion relation and its Taylor expansion

$$\omega_0(x) = x + \sum_{p=1}^{\infty}\frac{\lambda_{2p}}{(2p)!}x^{2p+1}, \tag{26}$$

where $\lambda_2=-2/3$, $\lambda_4=4$, etc.

The second term in Eq. (24) can be analyzed in the same way as in [19]: we first write $\ln|1-e^A|=\mathrm{Re}\ln(1-e^A)$, then expand $\ln(1-e^A)$ as a power series in e^A, and finally split the sum into two parts: $n\in[0,[N/2]-1]$ and $n\in[[N/2],N-1]$. Thus we obtain

$$\sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right| = -\mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{[N/2]-1}\frac{1}{m}e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} - \mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=[N/2]}^{N-1}\frac{1}{m}e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}. \tag{27}$$

By making the substitution $n\to N-1-n$ in the second sum, we obtain

$$\sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right| = -\mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{[N/2]-1}\frac{1}{m}e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} - \mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{N-[N/2]-1}\frac{1}{m}\times e^{-2m\{M\omega_0[\pi-\pi(n+1-\alpha)/N]+i\pi[\beta+d\rho(n+1-\alpha)]\}+2m\pi i d\rho N}. \tag{28}$$

Note that $e^{-2m\pi i d\rho N}=1$ due to the facts that $d\rho N=D$ and m and D are integer numbers. Now using the symmetry property $\omega_0(k)=\omega_0(\pi-k)$ of the lattice dispersion relation and noting that real part of the e^A does not depend on the sign of $\mathrm{Im}\,A$, we can finally obtain

$$\sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right| = -\mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{[N/2]-1}\frac{1}{m}e^{-2m\{M\omega_0[\pi(n+\alpha)/N]-i\pi d\rho(n+\alpha)+i\pi\beta\}} - \mathrm{Re}\sum_{m=1}^{\infty}\sum_{n=0}^{N-[N/2]-1}\frac{1}{m}e^{-2m\{M\omega_0[\pi(n+1-\alpha)/N]-i\pi d\rho(n+1-\alpha)-i\pi\beta\}}. \tag{29}$$

The argument of the first exponent can be expanded in powers of $1/S$ if we replace the lattice dispersion relation $\omega_0(x)$ with its Taylor expansion (26):

$$\exp\left\{-2\pi m[\tau_0\rho(n+\alpha)+i\beta] - 2\pi m\rho\sum_{p=1}^{\infty}\frac{\lambda_{2p}}{(2p)!}\left(\frac{\pi^2\rho}{S}\right)^p(n+\alpha)^{2p+1}\right\},$$

where $\tau_0\equiv 1-id$ is a complex number. The next step consists in expanding the exponentials in powers of $1/S$. Following the procedure introduced in Appendix B of [19], we obtain

$$e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} = e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]} - 2\pi m\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p\frac{\Lambda_{2p}}{(2p)!}\times(n+\alpha)^{2p+1}e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]}.$$

The differential operators Λ_{2p} that have appeared here can be expressed via the coefficients λ_{2p} of the expansion of the lattice dispersion relation. The first few terms are

$$\Lambda_2 = \lambda_2 = -\frac{2}{3}, \quad \Lambda_4 = \lambda_4 + 3\lambda_2^2\frac{\partial}{\partial\tau_0} = 4 + \frac{4}{3}\frac{\partial}{\partial\tau_0}.$$

The expansion for the second exponent in Eq. (29) can be obtained along the same lines by the substitution $\alpha\to 1-\alpha$.

Plugging the expansion of both of the exponents back into Eq. (29) we obtain

$$\sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right|$$
$$= -\text{Re} \sum_{m=1}^{\infty} \frac{1}{m}\left\{\sum_{n=0}^{[N/2]-1} e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]} + \sum_{n=0}^{N-[N/2]-1} e^{-2\pi m[\tau_0\rho(n+1-\alpha)-i\beta]}\right\}$$
$$+ 2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p \text{Re}\,\frac{\Lambda_{2p}}{(2p)!} \times\sum_{m=1}^{\infty}\left\{\sum_{n=0}^{[N/2]-1}(n+\alpha)^{2p+1}e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]} + \sum_{n=0}^{N-[N/2]-1}(n+1-\alpha)^{2p+1}e^{-2\pi m[\tau_0\rho(n+1-\alpha)-i\beta]}\right\}.$$

In all these series, the summation over n can be extended to infinity. The resulting errors are exponentially small and do not affect our asymptotic expansion in any finite power of $1/S$.

The key point of our analysis is the observation that all series that have appeared in such an expansion can be obtained by resummation of either the elliptic theta function $\theta_{\alpha,\beta}(\tau)$ [see Eq. (A9)] or Kronecker's double series $K_p^{\alpha,\beta}(\tau)$ [see Eq. (A14)]. As a result we obtain

$$\sum_{n=0}^{N-1} \ln\left|1 - e^{-2\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\right|$$
$$= \ln\left|\frac{\theta_{\alpha,\beta}(i\tau_0\rho)}{\eta(i\tau_0\rho)}\right| + \pi\rho B_2^{\alpha}\,\text{Re}\,\tau_0 - 2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p\frac{\text{Re}\,\Lambda_{2p}K_{2p+2}^{\alpha,\beta}(i\tau_0\rho) - \lambda_{2p}B_{2p+2}^{\alpha}}{(2p+2)(2p)!}. \tag{30}$$

Substituting Eqs. (25) and (30) into Eq. (24), we finally obtain exact asymptotic expansion of the $\ln Z_{\alpha,\beta}(0,d)$ in terms of the Kronecker's double series:

$$\ln Z_{\alpha,\beta}(0,d) = \frac{2G}{\pi}S + \ln\left|\frac{\theta_{\alpha,\beta}(i\tau_0\rho)}{\eta(i\tau_0\rho)}\right| - 2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p\frac{\text{Re}\,\Lambda_{2p}K_{2p+2}^{\alpha,\beta}(i\tau_0\rho)}{(2p+2)(2p)!}. \tag{31}$$

The free energy at the critical point can be compute directly from Eq. (7):

$$F_c = -\frac{S-2}{2S}\ln 2 - \frac{1}{S}\ln\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d), \tag{32}$$

where the sums go over $(\alpha,\beta)\neq(0,0)$.

Equations (31) and (32) imply that the free energy can be written in the form given by Eq. (22). Thus, finite-size corrections to the free energy are always integer powers of S^{-1}.

The first few coefficients in the exact asymptotic expansion of the free energy are given by

$$f_{\text{bulk}} = -\ln\sqrt{2} - \frac{2G}{\pi}, \tag{33}$$

$$f_0(\rho,d) = -\ln\frac{\theta_2+\theta_3+\theta_4}{2\eta}, \tag{34a}$$

$$f_1(\rho,d) = -\frac{\pi^3\rho^2}{180}\,\frac{\frac{7}{8}(\theta_2^9+\theta_3^9+\theta_4^9)+\theta_2\theta_3\theta_4[\theta_2^3\theta_4^3-\theta_3^3\theta_2^3-\theta_3^3\theta_4^3]}{\theta_2+\theta_3+\theta_4}. \tag{34b}$$

To simplify the notation we have use the short hand

$$\theta_k = |\theta_k(0,i\tau_0\rho)|, \quad k=2,3,4,$$
$$\eta = |\eta(i\tau_0\rho)|. \tag{35}$$

Let us now consider the behavior of the coefficients $f_k(\rho,d)$ in the asymptotic expansion of the free energy under the Jacobi transformation (see Appendix B). Using Eq. (B4) and Eq. (B8) we can easily check that $f_0(\rho,d)$ and $f_1(\rho,d)$ are invariant under transformation:

$$\rho \to \frac{1}{|\tau_0|^2\rho} = \frac{1}{(1+d^2)\rho}, \tag{36}$$

where $|\tau_0|$ is the absolute value of τ_0.

Using the properties of the θ functions and of the functions $K_{2p}^{\alpha,\beta}$ [see Eqs. (B4), (B5), and (B8)] we can easily check from Eq. (31) that the $\ln Z_{\alpha,\beta}(0,d)$ have the following behavior under the transformation $\rho\to 1/(1+d^2)\rho$:

$$\ln Z_{1/2,1/2}(0,d) \to \ln Z_{1/2,1/2}(0,d),$$
$$\ln Z_{0,1/2}(0,d) \to \ln Z_{1/2,0}(0,d),$$
$$\ln Z_{1/2,0}(0,d) \to \ln Z_{0,1/2}(0,d). \tag{37}$$

Equations (7) and (37) imply that the partition function of the Ising model at the critical point $Z_{M,N}(J_c)$ is invariant under transformation given by Eq. (36). This actually means that ξ given by Eq. (23) can be regarded as the effective aspect ratio.

In Fig. 1 we plot the aspect-ratio (ξ) dependence of the finite-size free-energy correction terms f_0 and f_1 for the Ising model with helical boundary conditions for several values of the helicity factor d. We use natural logarithmic scales for the horizontal axis. We can see that the finite-size correction terms f_0 and f_1 are invariant under the transformation $\xi\to 1/\xi$. In Fig. 2 we plot the conventional aspect-ratio (ρ) dependence of the finite-size free-energy correction terms f_0 and f_1 for the Ising model with helical boundary condition

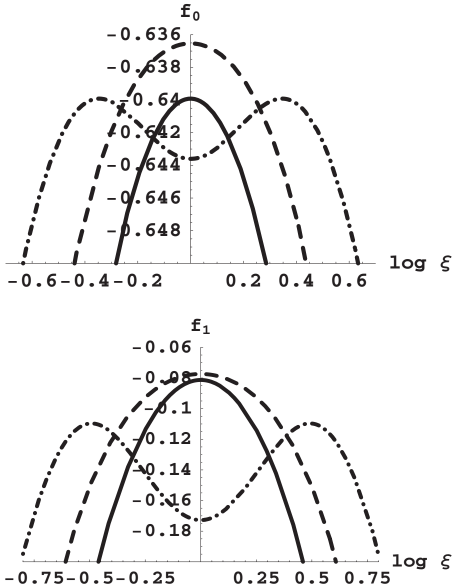

FIG. 1. Effective aspect-ratio (ξ) dependence of finite-size correction terms of the free energy (f_0 and f_1) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

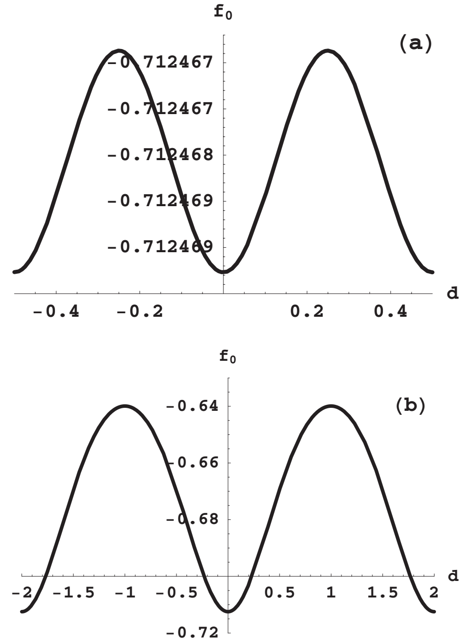

FIG. 3. Finite-size free-energy correction terms f_0 as a function of the helicity factor d for several values of the conventional aspect ratio ρ: (a) for $\rho=2$ and (b) for $\rho=1/2$.

for several values of the helicity factor d. For $\rho>1$, the finite-size properties of the Ising model with helical boundary conditions and those of the torus become the same, which means that the boundaries along the shorter direction determine the finite-size properties of the system; for both helical boundary conditions and the torus, the boundary condition along the y axis is a periodic one. Note that the case $d=0$ corresponds to the toroidal boundary condition. By increasing the helicity factor from 0 to 1, the behavior of the finite-size free energy correction terms f_0 and f_1 change from single-peak structure to a two-peak structure at $d=d_0$ with $d_0\simeq 0.8$ and $d_0\simeq 0.75$, respectively, for f_0 and f_1. We plot the helicity factor d dependence of the finite-size free-energy correction terms f_0 and f_1 for several values of the conventional aspect ratio (ρ) ($\rho=2$ and $1/2$) in Fig. 3.

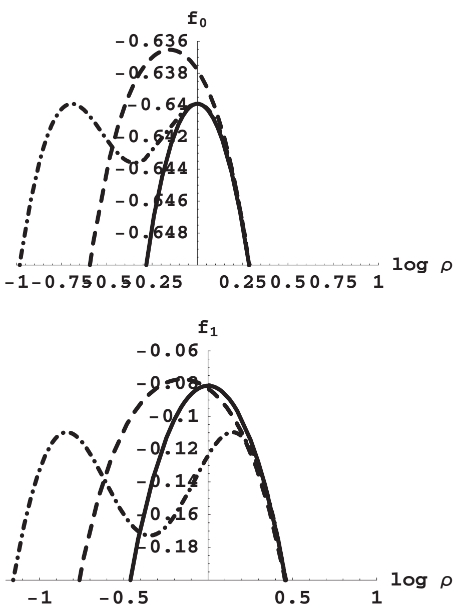

FIG. 2. Conventional aspect-ratio (ρ) dependence of finite-size correction terms of the free energy (f_0 and f_1) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

B. Asymptotic expansion of the internal energy

Now we will deal with the internal energy. The internal energy at the critical point can be computed directly from Eq. (19):

$$U_c=-\left(1+\frac{1}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right)\mu'$$

$$=-\sqrt{2}\left(1+\frac{1}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right), \tag{38}$$

where the sums go over $(\alpha,\beta)\neq(0,0)$.

Here $\mu'=\frac{d\mu}{dJ}|_{J=J_c}$ is the first derivative of $\mu(J)$ with respect to J at criticality. The derivatives $\mu^{(k)}=\frac{d^k\mu}{dJ^k}|_{J=J_c}$ can be easily computed from Eq. (6):

$$\mu'=\sqrt{2},\quad \mu''=-2,\quad \mu'''=8\sqrt{2},\quad \mu^{(4)}=-80,\ \dots\ . \tag{39}$$

Thus, the only unknown object is $Z'_{0,0}(0,d)$.

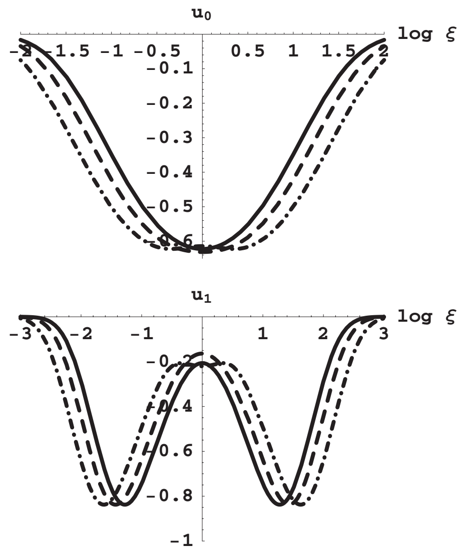

FIG. 4. Effective aspect-ratio (ξ) dependence of finite-size correction terms of the internal energy (u_0 and u_1) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

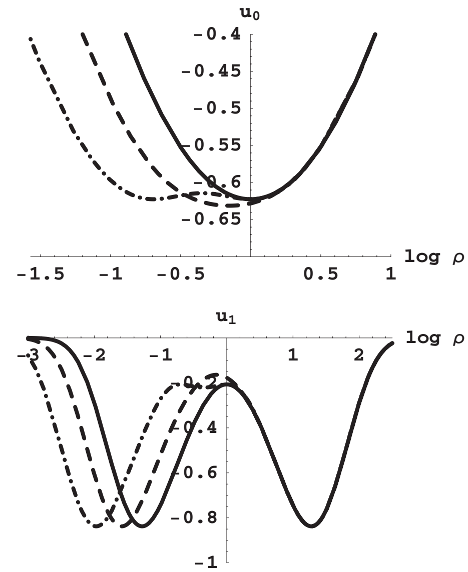

FIG. 5. Conventional aspect-ratio (ρ) dependence of finite-size correction terms of the internal energy (u_0 and u_1) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

As has already been mentioned, we have to treat the case $(\alpha,\beta)=(0,0)$ separately. Taking the derivative of Eq. (10) with respect to mass variable μ and then considering limit $\mu\to 0$ we obtain

$$Z'_{0,0}(0,d) = 2\sqrt{2}M\prod_{n=1}^{N-1} 2\left|\text{sh}\left[M\omega_0\left(\frac{\pi n}{N}\right) - i\pi d\rho n\right]\right|.$$

Asymptotic expansion of this expression can be found along the same lines as in above. In terms of the Kronecker's double series, the expansion can be written as

$$\ln Z'_{0,0}(0,d) = \frac{2G}{\pi}S + \frac{1}{2}\ln 8\rho S + 2\ln|\eta(i\tau_0\rho)| - 2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^p \frac{\text{Re}\,\Lambda_{2p}K_{2p+2}^{0,0}(i\tau_0\rho)}{(2p+2)(2p)!}. \quad (40)$$

This equation implies that the critical internal energy can be written as

$$U_c + \sqrt{2} = \sum_{p=0}^{\infty}\frac{u_p(\rho,d)}{S^{p+1/2}}. \quad (41)$$

Thus, the finite-size corrections to the critical internal energy are always half-integer powers of S^{-1}.

The first few coefficients in the exact asymptotic expansion of the critical internal energy are given by

$$u_0(\rho,d) = -2\sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4},$$

$$u_1(\rho,d) = \frac{\pi^3\rho^{5/2}}{48}\frac{\theta_2\theta_3\theta_4(\theta_2^9+\theta_3^9+\theta_4^9)}{(\theta_2+\theta_3+\theta_4)^2}.$$

Using the properties of the θ functions, Eq. (B4), and of the functions $K_{2p}^{\alpha,\beta}$, Eq. (B5), we can easily check that the coefficients u_k in the asymptotic expansion of the critical internal energy have the correct behavior under the transformation given by Eq. (36).

In Fig. 4 we plot the aspect-ratio (ξ) dependence of the finite-size internal energy correction terms u_0 and u_1 for the Ising model with helical boundary conditions for several values of the helicity factor d. We use the natural logarithmic scales for the horizontal axis. In Fig. 5 we plot conventional aspect-ratio (ρ) dependence of the finite-size internal energy correction terms u_0 and u_1 for the Ising model with helical boundary condition for several values of the helicity factor d. By increasing the helicity factor from 0 to 1, the behavior of the finite-size internal energy correction terms u_0 and u_1 changes from single-peak structure to a two-peak structure at $d=d_0$ with $d_0\simeq 0.8$ and $d_0\simeq 0.75$, respectively, for u_0 and u_1, as in the case of the finite-size free-energy correction terms.

C. Asymptotic expansion of the specific heat

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

$$C_c = -2\left(1+\frac{1}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right) + \frac{2}{S}\left[\frac{\sum_{\alpha,\beta}Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - \left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right)^2\right]. \quad (42)$$

The main goal of this section is to compute the ratio

$$\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}, \tag{43}$$

where the sums go over $(\alpha,\beta)\neq(0,0)$.

The analysis of the $Z''_{\alpha,\beta}(0,d)$ is a little more involved. Taking the second derivative of Eq. (10) with respect to mass variable μ and then considering limit $\mu\to 0$ we obtain

$$\begin{aligned}\frac{Z''_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)} &= \mathrm{Re}\, M\sum_{n=0}^{N-1}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right)\\ &\quad\times\coth\left[M\omega_0\left(\frac{\pi(n+\alpha)}{N}\right)+i\pi[\beta-d\rho(n+\alpha)]\right]\\ &= M\sum_{n=0}^{N-1}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right)\\ &\quad+2\,\mathrm{Re}\, M\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right)\\ &\quad\times e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}},\end{aligned} \tag{44}$$

where $\omega''_0(x)$ is the second derivative of $\omega_\mu(x)$ with respect to μ at criticality:

$$\omega''_0(x)=\frac{2}{\sin x\sqrt{1+\sin^2 x}}.$$

Using Taylor's theorem, the asymptotic expansion of the $\omega''_0(x)$ can be written in the following form:

$$\omega''_0(x)=\frac{2}{x}\left(1+\sum_{p=1}^{\infty}\frac{\kappa_{2p}}{(2p)!}x^{2p}\right),$$

where $\kappa_2=-2/3$, $\kappa_4=172/15$, etc.

By following the procedure introduced in [19] we obtain for the first sum in Eq. (44)

$$\begin{aligned}M\sum_{n=0}^{N-1}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right) &= \frac{4S}{\pi}\left[\frac{1}{4}\int_0^{\pi}f(x)dx+\ln N-\frac{\psi(\alpha)+\psi(1-\alpha)}{2}\right]\\ &\quad-2\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\frac{\kappa_{2p}B^{\alpha}_{2p}}{p(2p)!},\end{aligned} \tag{45}$$

where we have introduce the function $f(x)=\omega''_0(x)-2/x-2/(\pi-x)$, $\int_0^{\pi}f(x)dx=2\ln 2-4\ln\pi$, and $\psi(x)$ is the digamma function.

Let us now consider the second sum in Eq. (44). Note that the function $\omega''_0(x)$ can be represented as

$$\omega''_0(x)=\frac{2}{x}\exp\left\{\sum_{p=1}^{\infty}\frac{\bar{\kappa}_{2p}}{(2p)!}x^{2p}\right\}, \tag{46}$$

where the coefficients $\bar{\kappa}_{2p}$ and κ_{2p} are related to each other through the relation between moments and cumulants (see Appendix B in [19]). Following along the same lines as in Sec. III A, the second sum in Eq. (44) can be written as

$$\begin{aligned}&2\,\mathrm{Re}\, M\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right)e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\\ &= \frac{4S}{\pi}\mathrm{Re}\sum_{n=0}^{\infty}\sum_{m=1}^{\infty}\left\{\frac{1}{n+\alpha}e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]}\right.\\ &\quad\left.+\frac{1}{n+1-\alpha}e^{-2\pi m[\tau_0\rho(n+1-\alpha)-i\beta]}\right\}\\ &\quad-2\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\mathrm{Re}\,\Omega_{2p}K^{\alpha,\beta}_{2p}(i\tau_0\rho)\\ &\quad+2\pi\rho\sum_{p=1}^{\infty}\frac{\kappa_{2p}B^{\alpha}_{2p}}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}.\end{aligned} \tag{47}$$

The differential operators Ω_{2p} that have appeared here can be expressed via the coefficients $\omega_{2p}=\bar{\kappa}_{2p}+\lambda_{2p}\frac{\partial}{\partial\tau_0}$ as

$$\Omega_2=\omega_2=-\frac{2}{3}\left(1+\frac{\partial}{\partial\tau_0}\right),$$

$$\Omega_4=\omega_4+3\omega_2^2=\frac{172}{15}+\frac{20}{3}\frac{\partial}{\partial\tau_0}+\frac{4}{3}\frac{\partial^2}{\partial\tau_0^2},$$

$$\vdots$$

With the help of the identity (A18), Eq. (47) can be rewritten as

$$\begin{aligned}&2\,\mathrm{Re}\, M\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}\omega''_0\left(\frac{\pi(n+\alpha)}{N}\right)e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}\\ &= \frac{4S}{\pi}\left[-2\ln|\theta_{\alpha,\beta}(\tau_0\rho)|+C_E+2\ln 2+\frac{\psi(\alpha)+\psi(1-\alpha)}{2}\right]\\ &\quad-2\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\mathrm{Re}\,\Omega_{2p}K^{\alpha,\beta}_{2p}(i\tau_0\rho)\\ &\quad+2\pi\rho\sum_{p=1}^{\infty}\frac{\kappa_{2p}B^{\alpha}_{2p}}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}.\end{aligned} \tag{48}$$

Substituting Eqs. (45) and (48) into Eq. (44) we finally obtain an exact asymptotic expansion of the $Z''_{\alpha,\beta}(0,d)$:

$$\begin{aligned}\frac{Z''_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)} &= \frac{4S}{\pi}\left[\ln\sqrt{\frac{S}{\rho}}+C_E+\ln\frac{2^{5/2}}{\pi}-2\ln|\theta_{\alpha,\beta}(\tau_0\rho)|\right]\\ &\quad-2\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\mathrm{Re}\,\Omega_{2p}K^{\alpha,\beta}_{2p}(i\tau_0\rho).\end{aligned} \tag{49}$$

After reaching this point, one can easily write down all the terms of the exact asymptotic expansion of the specific heat at the critical point. We have found that the exact asymptotic expansion of the specific heat can be written in the following form:

$$C_c = \frac{4}{\pi}\ln S + \sum_{p=0}^{\infty}\frac{c_{2p}(\rho,d)}{S^p} + \sum_{p=0}^{\infty}\frac{c_{2p+1}(\rho,d)}{S^{p+1/2}} = \frac{4}{\pi}\ln S + c_0(\rho,d) + \frac{c_1(\rho,d)}{\sqrt{S}} + \frac{c_2(\rho,d)}{S} + \cdots . \quad (50)$$

Using Eq. (38) we can rewrite Eq. (42) in the following form:

$$C_c = \sqrt{2}(U_c+\sqrt{2}) - S(U_c+\sqrt{2})^2 - 2 + \frac{2}{S}\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0)}. \quad (51)$$

From Eqs. (41), (49), and (51) we conclude that all finite-size corrections to the specific heat with half-integer powers of S^{-1} are proportional to the corresponding coefficients of the internal energy expansion—namely,

$$c_{2p+1} = \sqrt{2}u_p \quad \text{for } p = 0,1,2,\ldots . \quad (52)$$

The first few coefficients in the exact asymptotic expansion of the specific heat given by Eq. (50) are

$$c_0(\rho,d) = \frac{4}{\pi}\left(5\ln 2 - 2\ln\pi + 2C_E - \frac{\pi}{2} - \ln\rho\right) - 4\rho\left(\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right)^2 - \frac{16}{\pi}\frac{\sum_{i=2}^{4}\theta_i\ln\theta_i}{\theta_2+\theta_3+\theta_4}, \quad (53)$$

$$c_1(\rho,d) = -2\sqrt{2}\sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}, \quad (54)$$

$$c_2(\rho,d) = \frac{\pi^2\rho^2}{6}\frac{(\theta_2^8-\theta_3^8)\theta_2\theta_3\ln\frac{\theta_3}{\theta_2} + (\theta_4^8-\theta_3^8)\theta_4\theta_3\ln\frac{\theta_3}{\theta_4} + (\theta_2^8-\theta_4^8)\theta_4\theta_2\ln\frac{\theta_4}{\theta_2}}{(\theta_2+\theta_3+\theta_4)^2} + \frac{\pi^2\rho^2}{9}\frac{\theta_3^4\theta_4^4(2\theta_2-\theta_3-\theta_4)}{\theta_2+\theta_3+\theta_4} + \frac{\pi^3\rho^3}{12}\frac{\theta_2^2\theta_3^2\theta_4^2(\theta_2^9+\theta_3^9+\theta_4^9)}{(\theta_2+\theta_3+\theta_4)^3} + \frac{\pi\rho}{9}\frac{\theta_2^5-\theta_4^5+\theta_3(\theta_2^4-\theta_4^4)-2\theta_2\theta_4(\theta_2^3-\theta_4^3)}{\theta_2+\theta_3+\theta_4}\left(1+4\,\mathrm{Re}\,\frac{\partial}{\partial\tau_0}\ln\theta_2\right), \quad (55)$$

$$c_3(\rho,d) = \frac{\pi^3\rho^{5/2}}{24\sqrt{2}}\frac{\theta_2\theta_3\theta_4(\theta_2^9+\theta_3^9+\theta_4^9)}{(\theta_2+\theta_3+\theta_4)^2}. \quad (56)$$

In Fig. 6(a) we plot the effective aspect-ratio ξ dependence of the finite-size specific heat correction term c_0 for several values of the helicity factor d (d=0, 0.6, and 1). In Fig. 6(b) we plot the conventional aspect-ratio ξ dependence of the finite-size specific heat correction term c_0 for several values of the helicity factor d (d=0, 0.6, and 1).

D. Asymptotic expansion of the higher derivatives of the free energy

The third derivative of the logarithm of the partition function at the criticality $F_c^{(3)}$ is given by the following formula:

$$F_c^{(3)} = 8\sqrt{2} + \frac{8\sqrt{2}}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - \frac{6\sqrt{2}}{S}\left[\frac{\sum_{\alpha,\beta}Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - \left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right)^2\right] + \frac{2\sqrt{2}}{S}\left[\frac{Z'''_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - 3\frac{Z'_{0,0}(0,d)\sum_{\alpha,\beta}Z''_{\alpha,\beta}(0,d)}{\left(\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)\right)^2} + 2\left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right)^3\right]. \quad (57)$$

Thus, the only unknown object is $Z'''_{0,0}(0,d)$. Taking the third derivative of Eq. (10) with respect to mass variable μ and then considering limit $\mu \to 0$ we obtain

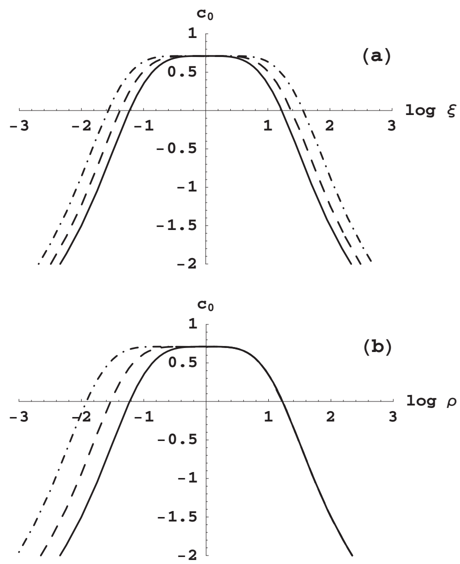

FIG. 6. Finite-size specific-heat correction term c_0 as a function of the effective aspect ratio ξ (a) and conventional aspect ratio ρ (b) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

$$\frac{Z'''_{0,0}(0,d)}{Z'_{0,0}(0,d)} = 2M^2 - 1 + 3M\sum_{n=1}^{N-1}\omega_0''\left(\frac{\pi n}{N}\right) \times\coth\left[M\omega_0\left(\frac{\pi n}{N}\right) - i\pi d\rho n\right]. \tag{58}$$

Asymptotic expansion of the $Z'''_{0,0}(0,d)$ can be found along the same lines as above. In terms of the Kronecker's double series, the expansion can be written as

$$\frac{Z'''_{0,0}(0,d)}{Z'_{0,0}(0,d)} = \frac{12S}{\pi}\left[\ln\sqrt{\frac{S}{\rho}} + C_E + \ln\frac{2^{1/2}}{\pi} - 2\ln|\eta(i\tau_0\rho)|\right] - 1 - 6\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\mathrm{Re}\,\Omega_{2p}K_{2p}^{0,0}(i\tau_0\rho). \tag{59}$$

Using Eqs. (38) and (51) we can rewrite Eq. (57) in the following form

$$F_c^{(3)} = 2\sqrt{2} - 3\sqrt{2}[C_c - \sqrt{2}(U_c+\sqrt{2})] + (U_c+\sqrt{2})\left[-2\frac{Z'''_{0,0}(0,d)}{Z'_{0,0}(0,d)} + S^2(U_c+\sqrt{2})^2 + 3S[C_c - \sqrt{2}(U_c+\sqrt{2})] + 6S - 8\right]. \tag{60}$$

From Eqs. (41), (50), (59), and (60), we conclude that all finite-size corrections to the $F^{(3)}$ with integer powers of S^{-1} are proportional to the corresponding coefficients of the specific heat expansion—namely,

$$d_0(\rho,d) = -3\sqrt{2}c_0(\rho,d) + 2\sqrt{2},$$

$$d_{2p}(\rho,d) = -3\sqrt{2}c_{2p}(\rho,d) \quad \text{for } p=1,2,\ldots\,. \tag{61}$$

After reaching this point, one can easily write down all the terms of the exact asymptotic expansion of the third derivative of the free energy at the critical point. We have found that the exact asymptotic expansion can be written in the following form:

$$F_c^{(3)} = -\frac{12\sqrt{2}}{\pi}\ln S + \sum_{p=0}^{\infty}\frac{d_{2p-1}(\rho,d)}{S^{p-1/2}} + \sum_{p=0}^{\infty}\frac{d_{2p}(\rho,d)}{S^p} = d_{-1}(\rho,d)\sqrt{S} - \frac{12\sqrt{2}}{\pi}\ln S + d_0(\rho,d) + \frac{d_1(\rho,d)}{\sqrt{S}} + \frac{d_2(\rho,d)}{S} + \cdots\,. \tag{62}$$

The first few coefficients in the expansion are

$$d_{-1}(\rho,d) = 16\sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4} \times\left[\rho\left(\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right)^2 + \frac{6}{\pi}\left(\frac{\sum_{i=2}^{4}\theta_i\ln\theta_i}{\theta_2+\theta_3+\theta_4} - \ln 2\eta\right)\right], \tag{63}$$

$$d_0(\rho,d) = -3\sqrt{2}c_0(\rho,d) + 2\sqrt{2}, \tag{64}$$

$$d_1(\rho,d) = \sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\left[12 - 6c_1(\rho,d) - 16\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0} + \frac{\partial^2}{\partial\tau_0^2}\right)\ln\eta(\tau_0\rho)\right] - \pi^2\rho^{5/2}\frac{\theta_2\theta_3\theta_4(\theta_2^9+\theta_3^9+\theta_4^9)}{(\theta_2+\theta_3+\theta_4)^2} \times\left(\frac{\sum_{i=2}^{4}\theta_i\ln\theta_i}{\theta_2+\theta_3+\theta_4} - \ln 2\eta\right), \tag{65}$$

$$d_2(\rho,d) = -3\sqrt{2}c_2(\rho,d), \tag{66}$$

where $c_0(\rho,d)$ and $c_2(\rho,d)$ are given in Eqs. (53) and (55).

Let us now consider the fourth derivative of the logarithm of the partition function at the criticality $F_c^{(4)}$ which can be written as follows:

$$F_c^{(4)} = -80\left(1+\frac{1}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right) + \frac{76}{S}\left[\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)} - \left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right)^2\right] - \frac{24}{S}\left[\frac{Z'''_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)} - 3\frac{Z'_{0,0}(0,d)\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0,d)}{\left(\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)\right)^2} + 2\left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right)^3\right] + \frac{4}{S}\left[\frac{\sum_{\alpha,\beta} Z^{(4)}_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)} - 4\frac{Z'_{0,0}(0,d)Z'''_{0,0}(0,d)}{\left(\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)\right)^2} - 3\left(\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right)^2 + 12\frac{\sum_{\alpha,\beta} Z''_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)} \times\left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right)^2 - 6\left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}\right)^4\right]. \quad (67)$$

The main goal of this section is to compute the ratio

$$\frac{\sum_{\alpha,\beta} Z^{(4)}_{\alpha,\beta}(0,d)}{\sum_{\alpha,\beta} Z_{\alpha,\beta}(0,d)}, \quad (68)$$

where the sums go over $(\alpha,\beta)\neq(0,0)$.

The analysis of the $Z^{(4)}_{\alpha,\beta}(0,d)$ is a more involved. Taking the fourth derivative of Eq. (10) with respect to mass variable μ and then considering limit $\mu\to 0$ we obtain

$$\frac{Z^{(4)}_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)} - 3\left(\frac{Z''_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)}\right)^2 = -\,\mathrm{Re}\,3M^2\sum_{n=0}^{N-1}\omega_0''^2\left(\frac{\pi(n+\alpha)}{N}\right) \times \mathrm{csch}^2\left[M\omega_0\left(\frac{\pi(n+\alpha)}{N}\right)+i\pi[\beta-d\rho(n+\alpha)]\right] + \mathrm{Re}\,M\sum_{n=0}^{N-1}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right) \times \coth\left[M\omega_0\left(\frac{\pi(n+\alpha)}{N}\right)+i\pi[\beta-d\rho(n+\alpha)]\right], \quad (69)$$

where $\omega_0^{(4)}(x)$ is the fourth derivative of $\omega_\mu(x)$ with respect to μ at criticality:

$$\omega_0^{(4)}(x) = 4\frac{2\sin x^4 - 4\sin x^2 - 3}{\sin x^3(1+\sin^2 x)^{3/2}}.$$

Using expansions of $\mathrm{csch}^2\, x = 4\sum_{m=1}^{\infty} m e^{-2mx}$ and $\coth x = 1 + 2\sum_{m=1}^{\infty} e^{-2mx}$ we can rewrite Eq. (69) in the following form:

$$\frac{Z^{(4)}_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)} - 3\left(\frac{Z''_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)}\right)^2 = M\sum_{n=0}^{N-1}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right) - 12M^2\,\mathrm{Re}\sum_{n=0}^{N-1}\sum_{m=1}^{\infty} m\omega_0''^2\left(\frac{\pi(n+\alpha)}{N}\right) \times e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} + 2M\,\mathrm{Re}\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right) \times e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}}. \quad (70)$$

The first sum in Eq. (70) we may transform as

$$M\sum_{n=0}^{N-1}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right) = M\sum_{n=0}^{N-1} f_1\left(\frac{\pi(n+\alpha)}{N}\right) - \frac{4S}{\pi}\sum_{n=0}^{N-1}\left(\frac{1}{n+\alpha}+\frac{1}{n+1-\alpha}\right) - \frac{12SN^2}{\pi^3}\sum_{n=0}^{N-1}\left(\frac{1}{(n+\alpha)^3}+\frac{1}{(n+1-\alpha)^3}\right), \quad (71)$$

where we have introduce the function $f_1(x)=\omega_0^{(4)}(x)+4/x+12/x^3+4/(\pi-x)+12/(\pi-x)^3$. This function and all its derivatives are integrable over the interval $(0,\pi)$. Thus, for the first term in Eq. (71) we may use again the Euler-Maclaurin summation formula, and after a little algebra we obtain

$$M\sum_{n=0}^{N-1} f_1\left(\frac{\pi(n+\alpha)}{N}\right) = \frac{S}{\pi}\int_0^{\pi} f_1(x) + 12\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\frac{a_{2p+2}B^{\alpha}_{2p}}{p(2p+2)!} - \frac{4S}{\pi}\sum_{p=1}^{\infty}\frac{B^{\alpha}_{2p}}{p}\frac{1}{N^{2p}} - \frac{12S}{\pi^3}\sum_{p=1}^{\infty}(2p+1)B^{\alpha}_{2p}\frac{1}{N^{2p}}, \quad (72)$$

where

$$\int_0^{\pi} f_1(x)dx = 8 - \frac{12}{\pi^2} - 4\ln 2 + 8\ln\pi. \quad (73)$$

We have also used the symmetry properties $\omega_0^{(4)}(x)=\omega_0^{(4)}(\pi-x)$ and the Taylor expansion of the $\omega_0^{(4)}(x)$:

$$\omega_0^{(4)}(x) = -\frac{12}{x^3}\left(1+\sum_{p=1}^{\infty}\frac{a_{2p}}{(2p)!}x^{2p}\right), \quad (74)$$

where $a_2=2/3$, $a_4=-244/15$, etc.

The second sum in Eq. (71) can be written in terms of the digamma function $\psi(x)$:

$$\sum_{n=0}^{N-1}\left(\frac{1}{n+\alpha}+\frac{1}{n+1-\alpha}\right) = [\psi(N+\alpha)+\psi(N+1-\alpha)-\psi(\alpha)-\psi(1-\alpha)]. \tag{75}$$

Using the asymptotic expansion of the digamma function $\psi(x)$ Eq. (75) can be rewritten as

$$\sum_{n=0}^{N-1}\left(\frac{1}{n+\alpha}+\frac{1}{n+1-\alpha}\right) = 2\ln N-\sum_{p=1}^{\infty}\frac{B_{2p}^{\alpha}}{p}\frac{1}{N^{2p}}-\psi(\alpha)-\psi(1-\alpha). \tag{76}$$

The third sum in Eq. (71) can be obtained by taking second derivative of Eq. (76) with respect to α

$$\sum_{n=0}^{N-1}\left(\frac{1}{(n+\alpha)^3}+\frac{1}{(n+1-\alpha)^3}\right) = -\sum_{p=1}^{\infty}(2p-1)B_{2p-2}^{\alpha}\frac{1}{N^{2p}}-\frac{\psi''(\alpha)+\psi''(1-\alpha)}{2}. \tag{77}$$

Plugging Eqs. (72), (73), (76), and (77) back into Eq. (71) we finally obtain

$$\begin{aligned} M\sum_{n=0}^{N-1}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right) &= \frac{4S}{\pi}[-\ln N+2-\ln 4+2\ln\pi+\psi(\alpha)+\psi(1-\alpha)] \\ &+\frac{6S^2}{\rho\pi^3}[\psi''(\alpha)+\psi''(1-\alpha)] \\ &+12\pi\rho\sum_{p=1}^{\infty}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\frac{a_{2p+2}B_{2p}^{\alpha}}{p(2p+2)!}. \end{aligned} \tag{78}$$

Let us now consider the second sum in Eq. (70). Note that the functions $\omega_0^{(4)}(x)$ and $\omega_0''(x)$ can be represented as

$$\omega_0^{(4)}(x) = -\frac{12}{x^3}\exp\left\{\sum_{p=1}^{\infty}\frac{\bar{a}_{2p}}{(2p)!}x^{2p}\right\},$$

$$\omega_0''^2(x) = \frac{4}{x^2}\exp\left\{\sum_{p=1}^{\infty}\frac{\bar{b}_{2p}}{(2p)!}x^{2p}\right\}, \tag{79}$$

where the coefficients a_{2p} and $\bar{a}_{2p}$ are related to each other through the relation between moments and cumulants (see Appendix B in [19]):

$$\bar{a}_2=\frac{2}{3}, \quad \bar{a}_4=-88/5, \ldots,$$

$$\bar{b}_2=-\frac{4}{3}, \quad \bar{b}_4=\frac{304}{15}, \ldots .$$

Following along the same lines as in [19], the second sum in Eq. (70) can be written as

$$\begin{aligned} &-12M^2\,\mathrm{Re}\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}m\omega_0''^2\left(\frac{\pi(n+\alpha)}{N}\right) \times e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} \\ &= \frac{6S^2}{\pi^3\rho}\,\mathrm{Re}\,\frac{\partial}{\partial\tau_0}R_4^{\alpha,\beta}(\tau_0\rho)+\frac{6S}{\pi}\,\mathrm{Re}\,\Sigma_2\frac{\partial}{\partial\tau_0}R_2^{\alpha,\beta}(\tau_0\rho) \\ &-12\pi\rho\,\mathrm{Re}\sum_{p=1}^{\infty}\frac{\Sigma_{2p+2}}{p(2p+2)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\frac{\partial}{\partial\tau_0}K_{2p}^{\alpha,\beta}(\tau_0\rho). \end{aligned} \tag{80}$$

For the third sum in Eq. (70) we obtain

$$\begin{aligned} &2M\,\mathrm{Re}\sum_{n=0}^{N-1}\sum_{m=1}^{\infty}\omega_0^{(4)}\left(\frac{\pi(n+\alpha)}{N}\right)e^{-2m\{M\omega_0[\pi(n+\alpha)/N]+i\pi[\beta-d\rho(n+\alpha)]\}} \\ &= -\frac{6S^2}{\pi^3\rho}\,\mathrm{Re}\,R_4^{\alpha,\beta}(\tau_0\rho)-\frac{6S}{\pi}\,\mathrm{Re}\,\Upsilon_2R_2^{\alpha,\beta}(\tau_0\rho) \\ &-\frac{6S^2}{\rho\pi^3}[\psi''(\alpha)+\psi''(1-\alpha)]-\frac{4S}{\pi}[\psi(\alpha)+\psi(1-\alpha)] \\ &+12\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p+2)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}\mathrm{Re}\,\Upsilon_{2p+2}K_{2p}^{\alpha,\beta}(i\tau_0\rho) \\ &-12\pi\rho\sum_{p=1}^{\infty}\frac{a_{2p+2}B_{2p}^{\alpha}}{p(2p+2)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1}. \end{aligned} \tag{81}$$

The differential operators Σ_{2p} (Υ_{2p}) that have appeared here can be expressed via the coefficients $\sigma_{2p}=\bar{b}_{2p}+\lambda_{2p}\frac{\partial}{\partial\tau_0}$ ($\upsilon_{2p}=\bar{a}_{2p}+\lambda_{2p}\frac{\partial}{\partial\tau_0}$), respectively, as

$$\Sigma_2=\sigma_2=-\frac{2}{3}\left(2+\frac{\partial}{\partial\tau_0}\right), \quad \Upsilon_2=\upsilon_2=\frac{2}{3}\left(1-\frac{\partial}{\partial\tau_0}\right),$$

$$\Sigma_4=\sigma_4+3\upsilon_2^2=\frac{128}{5}+\frac{28}{3}\frac{\partial}{\partial\tau_0}+\frac{4}{3}\frac{\partial^2}{\partial\tau_0^2},$$

$$\Upsilon_4=\upsilon_4+3\upsilon_2^2=-\frac{244}{15}+\frac{4}{3}\frac{\partial}{\partial\tau_0}+\frac{4}{3}\frac{\partial^2}{\partial\tau_0^2},$$

$$\vdots$$

The key point of our analysis is the observation that all the series that have appeared in such an expansion can be obtained by resummation of either the elliptic theta function $\theta_{\alpha,\beta}(\tau)$ [see Eq. (A9)] or Kronecker's double series $K_p^{\alpha,\beta}(\tau)$

[see Eq. (A14)] or double series $R_p^{\alpha,\beta}(\tau)$ [see Eq. (A17)]. As a result we obtain

$$\frac{Z_{\alpha,\beta}^{(4)}(0,d)}{Z_{\alpha,\beta}(0,d)} - 3\left(\frac{Z''_{\alpha,\beta}(0,d)}{Z_{\alpha,\beta}(0,d)}\right)^2 = \frac{6S^2}{\pi^3\rho}\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}-1\right)R_4^{\alpha,\beta}(\tau_0\rho) - \frac{2S}{\pi}\ln S + \frac{8S}{\pi}\left[\frac{1}{4}\ln\rho + 1 + \ln\frac{\pi}{2} + \frac{3}{4}\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}\Sigma_2 - \Upsilon_2\right)R_2^{\alpha,\beta}(\tau_0\rho)\right] - 12\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p+2)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1} \times \mathrm{Re}\left[\frac{\partial}{\partial\tau_0}\Sigma_{2p+2} - \Upsilon_{2p+2}\right]K_{2p}^{\alpha,\beta}(\tau_0\rho) \tag{82}$$

$$= -\frac{2S}{\pi}\ln S + \frac{6S^2}{\pi^3\rho}\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}-1\right)R_4^{\alpha,\beta}(\tau_0\rho) + \frac{8S}{\pi}\left[\frac{1}{4}\ln\rho + 1 - \ln\frac{8}{\pi} - C_E + 2\ln|\theta_{\alpha,\beta}(i\tau_0\rho)|\right] + \frac{16S}{\pi}\left[\mathrm{Re}\left(1+\frac{\partial}{\partial\tau_0}\right)\frac{\partial}{\partial\tau_0}\ln\theta_{\alpha,\beta}(i\tau_0\rho)\right] - 12\pi\rho\sum_{p=1}^{\infty}\frac{1}{p(2p+2)!}\left(\frac{\pi^2\rho}{S}\right)^{p-1} \times \mathrm{Re}\left[\frac{\partial}{\partial\tau_0}\Sigma_{2p+2} - \Upsilon_{2p+2}\right]K_{2p}^{\alpha,\beta}(\tau_0\rho). \tag{83}$$

From Eqs. (31), (40), (49), (59), (83), and (67) we conclude that all finite-size corrections to $F_c^{(4)}$ with half-integer powers of S^{-1} come from

$$-\frac{80}{S}\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - \frac{24}{S}\left[\frac{Z'''_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)} - 3\frac{Z'_{0,0}(0,d)\sum_{\alpha,\beta}Z''_{\alpha,\beta}(0,d)}{\left(\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)\right)^2} + 2\left(\frac{Z'_{0,0}(0,d)}{\sum_{\alpha,\beta}Z_{\alpha,\beta}(0,d)}\right)^3\right]. \tag{84}$$

Using Eqs. (38), (51), and (57) we can rewrite Eq. (84) in the following form:

$$-8\sqrt{2}(U_c+\sqrt{2}) - 6\sqrt{2}\{F_3 - 2\sqrt{2} + 3\sqrt{2}[C_c - \sqrt{2}(U_c+\sqrt{2})]\}. \tag{85}$$

From Eq. (85) we conclude that all finite-size corrections to the $F^{(4)}$ with half-integer powers of S^{-1} are given by

$$g_{2p-1} = -8\sqrt{2}u_p - 6\sqrt{2}d_{2p-1} \quad \text{for } p = 0,1,2,\ldots\,. \tag{86}$$

After reaching this point, one can easily write down all the terms of the exact asymptotic expansion of the fourth derivative of the free energy at the critical point. We have found that the exact asymptotic expansion can be written in the following form:

$$F_c^{(4)} = \frac{144}{\pi}\ln S + \sum_{p=0}^{\infty}\frac{g_{2p-2}(\rho,d)}{S^{p-1}} + \sum_{p=0}^{\infty}\frac{g_{2p-1}(\rho,d)}{S^{p-1/2}} = g_{-2}(\rho,d)S + g_{-1}(\rho,d)\sqrt{S} + \frac{144}{\pi}\ln S + g_0(\rho,d) + \frac{g_1(\rho,d)}{\sqrt{S}} + \frac{g_2(\rho,d)}{S} + \cdots\,. \tag{87}$$

The first few coefficients in the expansion are

$$g_{-2}(\rho,d) = \frac{768}{\pi^2}\frac{\theta_3\theta_4\left(\ln\frac{\theta_4}{\theta_3}\right)^2 + \theta_2\theta_4\left(\ln\frac{\theta_2}{\theta_4}\right)^2 + \theta_2\theta_3\left(\ln\frac{\theta_2}{\theta_3}\right)^2}{(\theta_2+\theta_3+\theta_4)^2} - 96\rho\left(\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right)^2\left[\rho\left(\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right)^2 + \frac{8}{\pi}\left(\frac{\sum_{i=2}^{4}\theta_i\ln\theta_i}{\theta_2+\theta_3+\theta_4} - \ln 2\eta\right)\right] + \frac{24}{\pi^3\rho}\,\frac{\theta_2\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}-1\right)R_4^{0,1/2}(\tau_0\rho) + \theta_3\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}-1\right)R_4^{1/2,1/2}(\tau_0\rho) + \theta_4\,\mathrm{Re}\left(\frac{\partial}{\partial\tau_0}-1\right)R_4^{1/2,0}(\tau_0\rho)}{\theta_2+\theta_3+\theta_4}, \tag{88}$$

$$g_{-1}(\rho,d) = 16\sqrt{2}\sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4} - 96\sqrt{2}\sqrt{\rho}\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4} \times\left[\rho\left(\frac{\theta_2\theta_3\theta_4}{\theta_2+\theta_3+\theta_4}\right)^2 + \frac{6}{\pi}\left(\frac{\sum_{i=2}^{4}\theta_i\ln\theta_i}{\theta_2+\theta_3+\theta_4} - \ln 2\eta\right)\right]. \tag{89}$$

The asymptotic expansions for the free energy, the internal energy, the specific heat, and $F_c^{(3)}$ and $F_c^{(4)}$ of the critical Ising model on the square lattice wrapped on a helical torus given by Eqs. (22), (41), (50), (62), and (87) are the main results of this paper. The first important observation is that all corrections are integer or half-integer powers of S^{-1}. The only exceptions are the logarithmic terms in the specific heat, $F^{(3)}$ and $F^{(4)}$. In the first case, this term is the leading one, while in the other ones it is subleading. In the expansions of $Z_{0,1/2}(0,d)$, $Z_{1/2,0}(0,d)$, and $Z_{1/2,1/2}(0,d)$ and their derivatives only integer powers of S^{-1} can occur, while in the expansions of $Z'_{0,0}(0,d)$ and $Z'''_{0,0}(0,d)$ only half-integer of S^{-1} appear. Note that in the case of the Ising model with Brascamp-Kunz boundary conditions only integer powers of S^{-1} can occur in the asymptotic expansion of the free energy and its derivatives, since the partition function of the Ising model with Brascamp-Kunz boundary conditions can be expressed only in the terms of the $Z_{1/2,0}(\mu,0)$ [20]. In the case of the Ising model with helical boundary conditions only integer powers of S^{-1} can occur in the free-energy expansion, while in the internal energy expansion only half-integers of S^{-1} appear. In the specific heat, $F^{(3)}$ and $F^{(4)}$ expansions both integer and half-integer powers of S^{-1} can occur.

IV. SPECIFIC HEAT NEAR THE CRITICAL POINT

The pseudocritical point μ_{pseudo} is the value of the temperature at which the specific heat has its maximum for finite $M\times N$ lattice. One can determine this quantity as the point where the derivative of $C_{M,N}(\mu)$ vanishes.

Expanding expression (20) about the critical point $\mu_c=0$ yields

$$C_{M,N}(\mu) = C_c + \frac{\mu}{\sqrt{2}}F_c^{(3)} + \frac{\mu^2}{4}(F_c^{(4)} + \sqrt{2}F_c^{(3)}) + O(\mu^3), \tag{90}$$

where C_c, $F_c^{(3)}$, and $F_c^{(4)}$ are given in Eqs. (50), (62), and (87), respectively.

From Eq. (90), the first derivative of the specific heat on a finite lattice near the infinite-volume critical point can be found, and it seen to vanish when

$$\mu = -\frac{\sqrt{2}F_c^{(3)}}{F_c^{(4)} + \sqrt{2}F_c^{(3)}}. \tag{91}$$

Expansion of Eq. (91) now gives the FSS of the pseudocritical point as

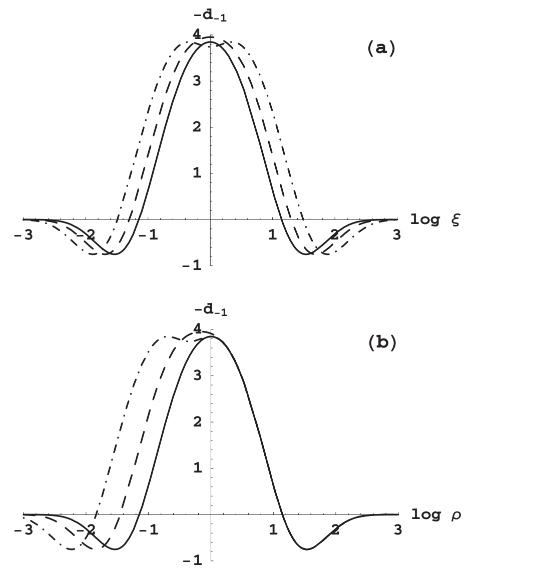

FIG. 7. Finite-size correction term d_{-1} as a function of the effective aspect ratio ξ (a) and conventional aspect ratio ρ (b) for several values of the helicity factor d. Solid curve is for $d=0$, dashed curve for $d=0.6$, and dot-dashed curve for $d=1$. We use the natural logarithmic scales for the horizontal axis.

$$\mu_{pseudo} = -\sqrt{2}\frac{d_{-1}(\rho,d)}{g_{-2}(\rho,d)}L^{-1} + O(L^{-2}), \tag{92}$$

where $L=\sqrt{S}$ is the characteristic size of the system and $d_{-1}(\rho,d)$ and $g_{-2}(\rho,d)$ are given in Eqs. (63) and (88). Thus we find that the shift exponent is $\lambda=1$ for all values of the helicity factor d and is the same as the inverse of the correlation length critical exponent $1/\nu=1$.

In Fig. 7(a) we plot the effective aspect-ratio ξ dependence of the finite-size correction term d_{-1} for several values of the helicity factor d ($d=0$, 0.6, and 1). In Fig. 7(b) we plot the conventional aspect-ratio ξ dependence of the finite-size correction term d_{-1} for several values of the helicity factor d ($d=0$, 0.6, and 1). The pseudocritical point μ_{pseudo} displays some unusual and intriguing behavior. For $d=0$ the pseudocritical point at first decrease, passing through $\mu_{pseudo}=0$ for $\rho=3$ and continuing to decrease until $\rho=7$. With further increase of ρ it reverses directions, increasing monotonically to an asymptotic value $\mu_{pseudo}=0$ as $\rho\to\infty$. By increasing the helicity factor from 0 to 1, the behavior of the finite-size correction term d_{-1} changes from single-peak structure to a two-peak structure at $d=d_0$ with $d_0\simeq 0.82$.

V. CONCLUSIONS

We have obtained exact asymptotic expansions for the free energy, the internal energy, the specific heat, and the third and fourth derivatives of the free energy of a critical Ising model on the square lattice wrapped on a helical torus. These expansions are given in Eqs. (22), (41), (50), (62), and (87). We have also derived exact expressions for the effective critical point for the Ising model with helical boundary conditions. The FSS of the specific heat is qualitatively similar to that on a torus [5,19]. All corrections to scaling are analytic. The shift exponent, characterizing the scaling of the effective critical (pseudocritical) point, is $\lambda=1$ for all values of the helicity factor d and is the same as the inverse of the correlation length critical exponent $1/\nu=1$. We find that finite-size corrections for the free energy, the internal energy, the specific heat, and the third and fourth derivatives of the free energy of the model in crucial way depend on the helicity factor of the lattice. Equations (90)–(92) show that calculations of the third and fourth derivatives of the free energy are necessary in order to obtain the shift exponent of the specific heat.

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APPENDIX A: THETA FUNCTIONS AND KRONECKER'S DOUBLE SERIES

In this appendix we gather all the definitions and properties of the Jacobi's θ functions and Kronecker's double series needed in this paper. We adopt the following definition of the elliptic θ functions:

$$\theta_{\alpha,\beta}(z,\tau)=\sum_{n\in Z}\exp\left\{\pi i\tau\left(n+\frac{1}{2}-\alpha\right)^2+2\pi i\left(n+\frac{1}{2}-\alpha\right)\left(z-\frac{1}{2}+\beta\right)\right\}$$
$$=\eta(\tau)\exp\left\{\pi i\tau B_2^\alpha+2\pi i\left(\frac{1}{2}-\alpha\right)\left(z-\frac{1}{2}+\beta\right)\right\}\times\prod_{n=0}^{\infty}[1-e^{2\pi i\tau(n+\alpha)-2\pi i(z+\beta)}]\times[1-e^{2\pi i\tau(n+1-\alpha)+2\pi i(z+\beta)}], \quad \text{(A1)}$$

where B_2^α is the Bernoulli polynomial, $B_2^\alpha=\alpha^2-\alpha+\frac{1}{6}$, and $\eta(\tau)$ is Dedekind η function:

$$\eta(\tau)=e^{\pi i\tau/12}\prod_{n=1}^{\infty}[1-e^{2\pi i\tau n}],$$

$$\ln Q(\tau)=\ln\eta(\tau)-\frac{\pi i\tau}{12}=\sum_{n=1}^{\infty}[1-q^{2n}], \quad \text{(A2)}$$

with $q=e^{\pi i\tau}$.

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

$$\theta_{0,0}(z,\tau)=\theta_1(z,\tau)=-i\sum_{n\in\mathbb{Z}}(-1)^n e^{2\pi iz(n+1/2)+\pi i\tau(n+1/2)^2}, \quad \text{(A3)}$$

$$\theta_{0,1/2}(z,\tau)=\theta_2(z,\tau)=\sum_{n\in\mathbb{Z}}e^{2\pi iz(n+1/2)+\pi i\tau(n+1/2)^2}, \quad \text{(A4)}$$

$$\theta_{1/2,0}(z,\tau)=\theta_4(z,\tau)=\sum_{n\in\mathbb{Z}}(-1)^n e^{2\pi izn+\pi i\tau n^2}, \quad \text{(A5)}$$

$$\theta_{1/2,1/2}(z,\tau)=\theta_3(z,\tau)=\sum_{n\in\mathbb{Z}}e^{2\pi izn+\pi i\tau n^2}. \quad \text{(A6)}$$

Dedekind's η function satisfies the following identity:

$$\eta(\tau)^3=\frac{1}{2}\theta_2(0,\tau)\theta_3(0,\tau)\theta_4(0,\tau). \quad \text{(A7)}$$

In this paper we will only need these functions evaluated at $z=0$ and $\tau=i\tau_0\rho$ where $\tau_0=1-id$.

Equation (A1) can be rewritten as

$$\ln\frac{\theta_{\alpha,\beta}(0,i\tau)}{\eta(i\tau)}=-\pi\tau B_2^\alpha+2\pi i\left(\frac{1}{2}-\alpha\right)\left(\beta-\frac{1}{2}\right)+\sum_{n=0}^{\infty}\{\ln(1-e^{-2\pi[\tau(n+\alpha)+i\beta]})+\ln(1-e^{-2\pi[\tau(n+1-\alpha)-i\beta]})\}, \quad \text{(A8)}$$

from which we arrive at the following identity valid when $(\alpha,\beta)\neq(0,0)$:

$$\ln\left|\frac{\theta_{\alpha,\beta}(0,i\tau_0\rho)}{\eta(i\tau_0\rho)}\right|=-\pi\rho B_2^\alpha\,\mathrm{Re}\,\tau_0+\sum_{n=0}^{\infty}\{\ln|1-e^{-2\pi[\tau_0\rho(n+\alpha)+i\beta]}|+\ln|1-e^{-2\pi[\tau_0\rho(n+1-\alpha)-i\beta]}|\}. \quad \text{(A9)}$$

For the case $(\alpha,\beta)=(0,0)$ the analog of the identity (A9) can be obtained from Eq. (A2):

$$\ln|\eta(i\tau_0\rho)|=-\frac{1}{2}\pi\rho B_2\,\mathrm{Re}\,\tau_0+\sum_{n=1}^{\infty}\ln|1-e^{-2\pi\tau_0\rho n}|. \quad \text{(A10)}$$

Taking the derivative of Eq. (A8) with respect to τ we can obtain the following useful identity:

$$\mathrm{Re}\sum_{n=0}^{\infty}\sum_{m=1}^{\infty}[(n+\alpha)e^{2\pi im[\tau(n+\alpha)-\beta]}+(n+1-\alpha)e^{2\pi im[\tau(n+1-\alpha)+\beta]}]=\frac{B_2^\alpha}{2}+\frac{1}{2\pi}\mathrm{Re}\frac{\partial}{\partial\tau}\ln\frac{\theta_{\alpha,\beta}(0,i\tau)}{\eta(i\tau)}. \quad \text{(A11)}$$

Taking the derivative of $\ln\eta(i\tau)$ with respect to τ we can obtain the analog of identity Eq. (A11) for the case $(\alpha,\beta)=(0,0)$:

$$\mathrm{Re}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}ne^{2\pi imn\tau}=\frac{B_2}{4}+\frac{1}{2\pi}\mathrm{Re}\frac{\partial}{\partial\tau}\ln\eta(i\tau). \quad \text{(A12)}$$

Kronecker's double series can be defined as [32]

$$K_p^{\alpha,\beta}(\tau) = -\frac{p!}{(-2\pi i)^p}\sum_{m,n\in Z}{}' \frac{e^{-2\pi i(n\alpha+m\beta)}}{(n+\tau m)^p}, \qquad \text{(A13)}$$

where the prime over the sum denotes the restriction $(m,n) \neq (0,0)$. In this form, however, they cannot be directly applied to our analysis. The basic property we need is the following:

$$B_{2p}^{\alpha} - K_{2p}^{\alpha,\beta}(i\tau_0\rho) = 2p\Bigg\{\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}(n+\alpha)^{2p-1}e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]} + \sum_{m=1}^{\infty}\sum_{n=0}^{\infty}(n+1-\alpha)^{2p-1} \times e^{-2\pi m[\tau_0\rho(n+1-\alpha)-i\beta]}\Bigg\}. \qquad \text{(A14)}$$

From Eqs. (A11), (A12), and (A14) we can obtain

$$\mathrm{Re}\, K_2^{\alpha,\beta}(i\tau_0\rho) = -\frac{1}{\pi\rho}\,\mathrm{Re}\,\frac{\partial}{\partial\tau_0}\ln\frac{\theta_{\alpha,\beta}(0,i\tau_0\rho)}{\eta(i\tau_0\rho)}, \qquad \text{(A15)}$$

$$\mathrm{Re}\, K_2^{0,0}(i\tau_0\rho) = -\frac{2}{\pi\rho}\,\mathrm{Re}\,\frac{\partial}{\partial\tau_0}\ln\eta(i\tau_0\rho). \qquad \text{(A16)}$$

Equations for $K_{2p}^{\alpha,\beta}(\tau)$ with $p=2,3,4,5$ and other useful relations for elliptic θ functions and Kronecker's double series can be found in Refs. [19,22,23].

Let us also introduce the function $R_{2p}^{\alpha,\beta}(\tau_0\rho)$, which can be considered as extension of the Kronecker's double series $K_{2p}^{\alpha,\beta}(\tau)$ for negative value of p:

$$R_{2p}^{\alpha,\beta}(\tau_0\rho) + \psi^{(2p-2)}(\alpha) + \psi^{(2p-2)}(1-\alpha) = 2p\sum_{n=0}^{\infty}\sum_{m=1}^{\infty}\Bigg\{\frac{1}{(n+\alpha)^{2p-1}}e^{-2\pi m[\tau_0\rho(n+\alpha)+i\beta]} + \frac{1}{(n+1-\alpha)^{2p-1}}e^{-2\pi m[\tau_0\rho(n+1-\alpha)-i\beta]}\Bigg\}, \qquad \text{(A17)}$$

where $\psi^{(p)}(\alpha)$ is the pth derivative of the digamma function $\psi(\alpha)=d/d\alpha \ln\Gamma(\alpha)=\psi(\alpha+1)-1/\alpha$, with $\psi(1)=-C_E$, $\psi(1/2)=-2\ln 2 - C_E$, and C_E is Euler's constant.

The Kronecker functions $K_{2p}^{\alpha,\beta}(\tau)$ with α and β taking values 0 or 1/2 can be related to the function $K_{2p}^{0,0}(\tau)$ by means of simple resummation of double series

$$K_{2p}^{0,1/2}(\tau) = 2K_{2p}^{0,0}(2\tau) - K_{2p}^{0,0}(\tau),$$

$$K_{2p}^{1/2,0}(\tau) = 2^{1-2p}K_{2p}^{0,0}(\tau/2) - K_{2p}^{0,0}(\tau),$$

$$K_{2p}^{1/2,1/2}(\tau) = (1+2^{2-2p})K_{2p}^{0,0}(\tau) - 2^{1-2p}K_{2p}^{0,0}(\tau/2) - 2K_{2p}^{0,0}(2\tau).$$

For the cases $(\alpha,\beta)=(0,1/2),(1/2,0),(1/2,1/2)$ equations for $R_2^{\alpha,\beta}(\tau)$ have been obtained in [19] and given by

$$R_2^{\alpha,\beta}(\tau) = -4\ln|\theta_{\alpha,\beta}(\tau)| + 2C_E + 4\ln 2. \qquad \text{(A18)}$$

For practical calculations the following identities are also helpful:

$$2\theta_2^2(2\tau) = \theta_3^2(\tau) - \theta_4^2(\tau), \quad \theta_2^2(\tau/2) = 2\theta_2(\tau)\theta_3(\tau),$$

$$2\theta_3^2(2\tau) = \theta_3^2(\tau) + \theta_4^2(\tau), \quad \theta_3^2(\tau/2) = \theta_2^2(\tau) + \theta_3^2(\tau),$$

$$2\theta_4^2(2\tau) = 2\theta_3(\tau)\theta_4(\tau), \quad \theta_4^2(\tau/2) = \theta_3^2(\tau) - \theta_2^2(\tau),$$

$$2\eta^2(2\tau) = \theta_2(\tau)\eta(\tau), \quad \eta^2(\tau/2) = \theta_4(\tau)\eta(\tau).$$

APPENDIX B: JACOBI TRANSFORMATION

We also need the behavior of the θ functions, Dedekind's η function, and the Kronecker functions $K_{2p}^{\alpha,\beta}$ under the Jacobi transformation

$$\tau \to \tau' = -1/\tau. \qquad \text{(B1)}$$

The result for the θ functions and Dedekind's η function when $z=0$ is given in Ref. [33]:

$$\theta_3(0,\tau') = (-i\tau)^{1/2}\theta_3(0,\tau),$$

$$\theta_2(0,\tau') = (-i\tau)^{1/2}\theta_4(0,\tau),$$

$$\theta_4(0,\tau') = (-i\tau)^{1/2}\theta_2(0,\tau),$$

$$\eta(0,\tau') = (-i\tau)^{1/2}\eta(0,\tau). \qquad \text{(B2)}$$

The result for the Kronecker functions $K_{2p}^{\alpha,\beta}$ for $(\alpha,\beta)=(0,0)$, $(0,1/2)$, $(1/2,0)$, and $(1/2,1/2)$ can be obtain from the relation between the coefficients in the Laurent expansion of the Weierstrass function and Kronecker functions (see Appendix F in [19]) and is given by

$$K_{2p}^{0,1/2}(\tau') = \tau^{2p}K_{2p}^{1/2,0}(\tau), \quad K_{2p}^{1/2,0}(\tau') = \tau^{2p}K_{2p}^{0,1/2}(\tau),$$

$$K_{2p}^{1/2,1/2}(\tau') = \tau^{2p}K_{2p}^{1/2,1/2}(\tau), \quad K_{2p}^{0,0}(\tau') = \tau^{2p}K_{2p}^{0,0}(\tau). \qquad \text{(B3)}$$

In particular, if $\tau=i\tau_0\rho$, the θ functions and $K_{2p}^{\alpha,\beta}$ functions transform under Eq. (B1) as follows:

$$\theta_3\left(0,\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (\tau_0\rho)^{1/2}\theta_3(0,i\tau_0\rho),$$

$$\theta_2\left(0,\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (\tau_0\rho)^{1/2}\theta_4(0,i\tau_0\rho),$$

$$\theta_4\left(0,\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (\tau_0\rho)^{1/2}\theta_2(0,i\tau_0\rho),$$

$$\eta\left(0,\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (\tau_0\rho)^{1/2}\eta(0,i\tau_0\rho), \qquad \text{(B4)}$$

$$K_{2p}^{0,1/2}\left(\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (i\tau_0\rho)^{2p}K_{2p}^{1/2,0}(i\tau_0\rho),$$

$$K_{2p}^{1/2,0}\left(\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right) = (i\tau_0\rho)^{2p}K_{2p}^{0,1/2}(i\tau_0\rho),$$

$$K_{2p}^{1/2,1/2}\left(\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right)=(i\tau_0\rho)^{2p}K_{2p}^{1/2,1/2}(i\tau_0\rho),$$

$$K_{2p}^{0,0}\left(\frac{i\tau_0^\star}{|\tau_0|^2\rho}\right)=(i\tau_0\rho)^{2p}K_{2p}^{0,0}(i\tau_0\rho), \qquad (B5)$$

where

$$\tau_0^\star = 1 + id = \frac{|\tau_0|^2}{\tau_0} \qquad (B6)$$

is the complex conjugate of τ_0 and

$$|\tau_0| = \sqrt{1+d^2} \qquad (B7)$$

is the absolute value of τ_0.

Finally, we should mention that the absolute value of the above θ functions and the real part of the above function $R_{2p}^{\alpha,\beta}$ and Kronecker functions $K_{2p}^{\alpha,\beta}$ do not depend on the sign of Im τ_0. Thus,

$$|\theta_i(0,i\tau_0)| = |\theta_i(0,i\tau_0^\star)|, \quad \mathrm{Re}\, R_{2p}^{\alpha,\beta}(i\tau_0) = \mathrm{Re}\, R_{2p}^{\alpha,\beta}(i\tau_0^\star),$$

$$\mathrm{Re}\, K_{2p}^{\alpha,\beta}(i\tau_0) = \mathrm{Re}\, K_{2p}^{\alpha,\beta}(i\tau_0^\star). \qquad (B8)$$

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