Finite-size scaling and corrections in the Ising model with Brascamp-Kunz boundary conditions

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(Received 22 March 2001; published 24 January 2002)

The Ising model in two dimensions with the special boundary conditions of Brascamp and Kunz is analyzed. Leading and subdominant scaling behavior of the Fisher zeros are determined exactly. The exact finite-size scaling, with corrections, of the specific heat is determined both at critical and effective critical (pseudocritical) points. The shift exponents associated with the scaling of these effective critical points are not the same as the inverse correlation length critical exponent. All corrections to scaling are analytic.

DOI: 10.1103/PhysRevB.65.064110 PACS number(s): 68.35.Rh, 64.60.Fr, 75.40.Cx, 05.70.Fh

I. INTRODUCTION

The Ising model is the simplest statistical physics system displaying critical behavior. In a classic paper, Ferdinand and Fisher[1] used the exactly known partition function of the two-dimensional Ising model on finite lattices with toroidal boundary conditions[2] to analytically determine the specific-heat finite-size scaling (FSS) to order L^{-1}. At the infinite volume critical point β_c, this was recently extended to order L^{-3} by Izmailian and Hu[3] and independently by Salas.[4] It was found that only integer powers of L^{-1} occur, with no logarithmic modifications (except of course for the leading logarithmic term). That is, if $C_L(\beta)$ is the specific heat at an inverse temperature β for a system of linear extent L,

$$C_L(\beta_c)=C_{00}\ln L+C_0+\sum_{k=1}^{\infty}\frac{C_k}{L^k}. \tag{1.1}$$

For the toroidal lattice, the coefficients C_{00}, C_0, C_1, C_2 and C_3 have been determined explicitly.[1,3,4]

The FSS of the specific heat is also characterized by the location of its peak β_L and its height $C_L(\beta_L)$. The peak position is known as an effective critical or pseudocritical point and approaches β_c as $L\to\infty$ in a manner dictated by the shift exponent λ with $|\beta_L-\beta_c|\sim L^{-\lambda}$. Ferdinand and Fisher also determined the behavior of the specific-heat pseudocritical point, finding $\lambda=1=1/\nu$ (except for special values of the ratio of the lengths of the lattice edges, in which case the scaling behavior was found to be of the form $L^{-2}\ln L$).[1] Here ν is the correlation length critical exponent. The coincidence of λ with $1/\nu$ is common to most models, but it is not a consequence of FSS and is not always true.[5]

The finite-size behavior of the specific heat is related to that of the complex temperature (Fisher) zeros of the partition function.[6] The leading FSS behavior of the imaginary part of a Fisher zero is[7]

$$\mathrm{Im}\, z_j(L)\sim L^{-1/\nu}, \tag{1.2}$$

where z is an appropriate function of temperature and the subscript j labels the zeros. The real part of the lowest zero may be viewed as another effective critical or pseudocritical point, scaling as

$$|\mathrm{Re}\, z_1(L)-z_c|\sim L^{-\lambda_{\mathrm{zero}}}, \tag{1.3}$$

where $z=z_c$ at $\beta=\beta_c$.

The specific heat (and Fisher zeros) of the Ising model was recently studied numerically on two-dimensional lattices with other boundary conditions in Refs. 8 and 9. For lattices with a spherical topology, the correlation length and shift exponents were found to be $\nu=1.00\pm0.06$ and $\lambda=1.745\pm0.015$, significantly away from $1/\nu$.[8] This is similar to an earlier study reporting $\lambda\approx1.8$.[10] Hoelbling and Lang used a variety of cumulants as well as Fisher zeros to study the universality of the Ising model on spherelike lattices.[9] The pseudocritical point (from the specific heat, the real part of the lowest zero, and from two other types of cumulants) is not of Ferdinand-Fisher type. While a shift exponent $\lambda=1.76(7)$ is consistent with their numerical results, this is not stringent, and pseudocritical FSS of the form $L^{-2}\ln L$ or even L^{-2} is possible.[9] Thus, while a possible leading L^{-1} term almost or completely vanishes and subleading terms are dominant, the precise nature of these corrections could not be unambiguously decided. In any case, in contrast to the situation with toroidal boundary conditions, the FSS of the specific-heat effective critical point does not match the correlation length scaling behavior.

In another recent study[11] involving Fisher zeros, Beale's[12] exact distribution function for the energy of the two-dimensional Ising model was exploited to obtain the exact zeros for square periodic lattices up to size $L=64$. The FSS analysis in Ref. 11 yielded a value for the correlation length critical exponent ν, which appeared to approach the exact value (unity) as the thermodynamic limit is approached. Small lattices appeared to yield a correction-to-scaling exponent in broad agreement with early estimates [$\omega\approx1.8$ (Ref. 13)]. However, closer to the thermodynamic limit, these corrections appeared to be analytic with $\omega=1$.

In the light of these and other recent analyses,[14] we wish to present analytical results which may clarify the situation. To this end, we have selected the Ising model with special boundary conditions due to Brascamp and Kunz.[15] These boundary conditions permit an analytical approach to the determination of a number of thermodynamic quantities. Recently, Lu and Wu[16] exploited this fact to determine the density of Fisher zeros in the thermodynamic limit, a quantity of relevance to the determination of the strengths of phase transitions.[17] In this paper, we take a complementary approach, exploiting FSS (i) to determine critical exponents, (ii) to determine corrections to leading scaling, and (iii) to gain experience in the hope of eventual application to other, less transparent scenarios. The rest of this paper is organized as follows. In Sec. II the Brascamp-Kunz boundary conditions are introduced, and the exact FSS of the Fisher zeros is calculated. The specific heat and its pseudocritical point are analyzed in Sec. III. Our conclusions are contained in Sec. IV and the Appendix contains some calculations of relevance to the specific-heat analysis of Sec. III.

II. FISHER ZEROS FOR BRASCAMP-KUNZ BOUNDARY CONDITIONS

Brascamp and Kunz introduced special boundary conditions, for which the Fisher zeros are known for any finite-size lattice.[15] They considered a regular lattice with M sites in the x direction and $2N$ sites in the y direction. The special boundary conditions are periodic in the y direction and the $2N$ spins along the left and right borders of the resulting cylinder are fixed to $\cdots++++++++\cdots$ and $\cdots+-+-+-\cdots$, respectively. For such a lattice, the Ising partition function can be rewritten as

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

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

At this point it is convenient to introduce two shape parameters, in terms of which the FSS of zeros and thermodynamic functions is naturally expressed. These are σ and ρ, defined through

$$2N=\sigma M, \quad N=\rho(M+1). \tag{2.2}$$

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

$$z_{ij}=\exp(i\alpha_{ij}), \tag{2.3}$$

where

$$\alpha_{ij}=\cos^{-1}\left(\frac{\cos\theta_i+\cos\phi_j}{2}\right). \tag{2.4}$$

Using a computer algebra system such as Maple, one may expand Eq. (2.4) in M to determine the FSS of any zero to any desired order. Indeed, the first few terms in the expansion for the first zero, which is the one of primary interest, are

$$\alpha_{11}=M^{-1}\frac{\pi\sqrt{1+\sigma^2}}{\sqrt{2}\sigma}-M^{-2}\frac{\pi\sigma}{\sqrt{2}\sqrt{1+\sigma^2}}+O(M^{-3}). \tag{2.5}$$

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

$$\mathrm{Re}\, z_{11}=1-M^{-2}\frac{\pi^2}{4}\left(1+\frac{1}{\sigma^2}\right)+O(M^{-3}) \tag{2.6}$$

and

$$\mathrm{Im}\, z_{11}=\frac{\pi\sqrt{2}}{\sigma(1+\sigma^2)^{5/2}}\left\{M^{-1}\frac{(1+\sigma^2)^3}{2}-M^{-2}\frac{\sigma^2(1+\sigma^2)^2}{2}\right\}+O(M^{-3}), \tag{2.7}$$

respectively. Higher-order terms are straightforward to generate. From the leading term in Eq. (2.7), and from Eq. (1.2), one has, indeed, that the correlation length critical exponent is 1. Note, however, from Eq. (2.6) that the leading FSS behavior of the pseudocritical point in the form of the real part of the lowest zero is

$$z_c-\mathrm{Re}\, z_{11}=1-\mathrm{Re}\, z_{11}\sim M^{-2}, \tag{2.8}$$

giving a shift exponent $\lambda_{\text{zero}}=2$. This value is compatible with the numerical results of Ref. 9 for spherical lattices. One further notes that all corrections are powers of M^{-1} and in this sense entirely analytic.

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

III. SPECIFIC HEAT

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

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

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

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

It is straightforward to perform the i summation first in Eq. (3.2). Indeed, Eq. (A3) and its derivative yield the exact result, which is conveniently expressed as

$$C_{M,2N}^{\text{sing.}}(z)=\frac{1}{z^3}S_0+\frac{1}{2}\left(1-\frac{1}{z^2}\right)S_1-\frac{1}{2z^2}, \tag{3.3}$$

where

$$S_k=\frac{1}{M}\sum_{j=1}^{M}g_j^{(k)}(1), \tag{3.4}$$

in which $g_j^{(k)}(z)=d^kg_j(z)/dz^k$, and where

$$g_j(z)=\frac{\tanh[N\cosh^{-1}(1/z+z-\cos\phi_j)]}{\sqrt{(1/z+z-\cos\phi_j)^2-1}}. \quad (3.5)$$

One observes at this point that $g_j^{(1)}(1)=0$, and $g_j^{(3)}(1)=-3g_j^{(2)}(1)$.

Specific heat at the critical point

The sum S_0 is given in Eq. (A11) in terms of the ratio ρ defined in Eq. (2.2). From Eq. (3.3), this gives for the specific heat at the infinite volume critical temperature,

$$C_{M,2N}^{\text{sing.}}(1)=\frac{\ln M}{\pi}\left(1+\frac{1}{M}\right)+c_0+\frac{c_1}{M}+\frac{c_2}{M^2}+\frac{c_3}{M^3}+O\left(\frac{1}{M^4}\right), \quad (3.6)$$

where the coefficients c_k can be read off from the coefficients of M^{-k} in Eq. (A11). Typical values of c_0 are $-0.376\,67\ldots$, $-0.350\,88\ldots$, and $-0.349\,69\ldots$ for $\rho=1/2$, 1, and 2 respectively. Corresponding respective values for c_1 are $0.264\,86\ldots$, $0.290\,65\ldots$, and $0.291\,84\ldots$.

So for the critical specific heat, apart from a trivial $\ln M/M$ term, the FSS is qualitatively the same as (but quantitatively different from) that of the torus topology [see Eq. (1.1) and Refs. 1, 3, and 4]. This trivial qualitative difference could, in fact, be avoided by defining the volume V as the number of links rather than the number of sites which is what we do here (recall that, with fixed boundary spins, there are $M+1$ links in the x direction). We note that with Brascamp-Kunz boundary conditions, it is far easier to extract the FSS behavior because the partition function (2.1) involves only one such product, while that for the torus involves a sum of four such products. Indeed, a determination of $O(1/M^4)$ and higher terms proceeds in a similarly straightforward manner in the Brascamp-Kunz case.

Specific heat near the critical point

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

Expanding expression (3.3) about the critical point $z_c=1$ yields

$$C_{M,2N}(z)=S_0-\tfrac{1}{2}+(z-1)[-3S_0+1]+(z-1)^2[\tfrac{3}{2}S_2+6S_0-\tfrac{3}{2}]+(z-1)^3[-5S_2-10S_0+2]+O[(z-1)^4]. \quad (3.7)$$

The sums S_0 and S_2 are given in Eqs. (A11) and (A12), respectively.

From Eq. (3.7), the first derivative of the specific heat on a finite lattice near the infinite volume critical point can be found, and is seen to vanish when

$$z-1=\frac{3S_0-1}{3[S_2+4S_0-1]}+\frac{[5S_2+10S_0-2][3S_0-1]^2}{9[S_2+4S_0-1]^3}+O[(z-1)^3]. \quad (3.8)$$

Expansion of Eq. (3.8) now gives the FSS of the pseudocritical point to be

$$z_{M,2N}^{\text{pseudo}}=1+a_2\frac{\ln M}{M^2}+\frac{b_2}{M^2}+a_3\frac{\ln M}{M^3}+\frac{b_3}{M^3}+O\left(\frac{(\ln M)^2}{M^4}\right), \quad (3.9)$$

higher terms being of the form $\ln M/M^4$ and $1/M^4$. Here

$$a_2=-\frac{\pi^2}{2[\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)]}, \quad (3.10)$$

$$b_2=-\frac{\pi^2}{12}\frac{6\gamma_E+9\ln 2-6\ln\pi-2\pi-12W_{1,1}^0(\rho)}{\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)}, \quad (3.11)$$

$$a_3=\frac{\pi^2}{\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)}, \quad (3.12)$$

$$b_3=-\frac{\pi^2}{2}\times\frac{1-2\gamma_E-3\ln 2+2\ln\pi+\pi-\pi/(4\sqrt{2})+4W_{1,1}^0(\rho)}{\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)}, \quad (3.13)$$

where γ_E is the Euler-Mascheroni constant and $\zeta(3)$ is the Riemann zeta function. The functions $W_{j,k}^l(\rho)$ are given in Eq. (A10). Typical values of the coefficient a_2 are $-5.696\,64\ldots$, $-4.200\,05\ldots$, and $-4.105\,62\ldots$ for $\rho=1/2$, 1, and 2, respectively. The corresponding values for b_2 are $3.758\,41\ldots$, $2.430\,67\ldots$, and $2.360\,72\ldots$. Thus there is no leading $1/M$ or $\ln M/M$ term in the FSS of the specific-heat pseudocritical point and the specific-heat shift exponent does not coincide with $1/\nu=1$. This is consistent with result (2.8) for the finite-size scaling of the real part of the Fisher zeros. One notes, however, that, in contrast to Eq. (2.8), logarithmic corrections are present to all orders in the FSS of the specific-heat pseudocritical point.

Inserting Eq. (3.9) for the pseudocritical point into Eq. (3.7) gives the FSS behavior of the peak of the specific heat. This is

$$C_{M,2N}^{\text{sing.}}(z_{M,2N}^{\text{pseudo}})=\frac{\ln M}{\pi}\left(1+\frac{1}{M}\right)+c_0'+\frac{c_1'}{M}+d_2'\frac{(\ln M)^2}{M^2}+\mathcal{O}\left(\frac{\ln M}{M^2}\right), \quad (3.14)$$

Higher-order terms are of the form $1/M^2$, $(\ln M)^2/M^3$, $\ln M/M^3$, and $1/M^3$. Here $c_0'=c_0$, $c_1'=c_1$, and

$$d_2' = \frac{3\pi}{4} \frac{1}{\zeta(3) - 2W^0_{3,1}(\rho) - 4\pi\rho W^1_{2,2}(\rho)}. \qquad (3.15)$$

One remarks that, up to $O(1/M)$, Eq. (3.14) is quantitatively the same as the critical specific-heat scaling of Eq. (3.6). The higher-order terms of Eq. (3.14) differ from those in Eq. (3.6) in that there are logarithmic modifications of the form $(\ln M)^k/M^l$ (with integer k and l).

IV. CONCLUSIONS

We have derived exact expressions for the finite-size scaling of the Fisher zeros, the critical specific heat, the effective critical points, and the specific-heat peak for the Ising model with Brascamp-Kunz boundary conditions. The FSS of the specific heat at criticality is qualitatively similar to that on a torus.[1,3,4] All corrections to scaling are analytic.

The shift exponents, characterizing the scaling of the effective critical (pseudocritical) point is $\lambda = 2$ and is not the same as the inverse of the correlation length critical exponent $1/\nu = 1$. That λ does not match $1/\nu$ was observed numerically in Refs. 8–10. Our exact approach, however, yields the integral nature (up to logarithms) of the critical exponents and correction exponents. Such precision is not attainable through the numerical means of Refs. 8–10.

The first few terms for the FSS of the specific-heat peak are also derived. Again all corrections are analytic, but in contrast to the specific heat at the critical point, they include logarithms.

ACKNOWLEDGMENTS

R.K. would like to thank Wolfgang Grill for his hospitality during an extended stay at Leipzig University in the framework of the *International Physics Studies Program*, where this work was initiated.

APPENDIX

Consider, first, the sum

$$\frac{1}{N} \sum_{i=1}^{N} \frac{1}{(Z - \cos\theta_i)^k}, \qquad (A1)$$

where $\theta_i = (2i-1)\pi/2N$, k is a positive integer and $Z > 1$ is independent of i. We first treat the case $k=1$. We follow a similar calculation in Ref. 18 and construct

$$\mathcal{F}(z) = \frac{\cot \pi z}{Z - \cos\frac{(2z-1)\pi}{2N}}. \qquad (A2)$$

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

$$\frac{1}{N} \sum_{i=1}^{N} \frac{1}{Z - \cos\theta_i} = \frac{1}{\sqrt{Z^2-1}} \tanh(N \cosh^{-1} Z). \qquad (A3)$$

This result is also implicitly contained in Ref. 19. Differentiation of Eq. (A3) with respect to Z gives the sum (A1), with larger values of k.

The purpose of the remainder of this appendix is to calculate the two sums S_0 and S_2 where S_k is defined in Eqs. (3.4) and (3.5). It is convenient to rewrite $g_j(z)$ as

$$g_j(z) = \frac{1}{\sqrt{(2+m^2-\cos\phi_j)^2-1}} - 2h_j(m), \qquad (A4)$$

where

$$h_j(m) = \frac{1}{\sqrt{(2+m^2-\cos\phi_j)^2-1}} \{\exp[2N \cosh^{-1}(2+m^2 - \cos\phi_j)]+1\}^{-1}, \qquad (A5)$$

and where $m^2 = 1/z + z - 2$. We first consider the sum of the first terms in Eq. (A4), and we are interested in the limit $m \to 0$. This may be calculated by a direct application of the Euler-Maclaurin formula. In fact, the more general summation with $m = \eta/(M+1)$, has been calculated in Ref. 18 [see Eq. (B52) therein]. That sum is given by

$$\begin{aligned}
\frac{1}{M+1} \sum_{j=1}^{M} & \frac{1}{\sqrt{\left(2+\left(\frac{\eta}{M+1}\right)^2 - \cos\phi_j\right)^2 - 1}} \\
&= \frac{\ln(M+1)}{\pi} + \frac{1}{\pi}\left[\gamma_E - \ln\pi + \frac{3\ln 2}{2} + G_0\left(\frac{\sqrt{2}\eta}{\pi}\right)\right] \\
&\quad - \frac{1}{M+1}\frac{1}{4\sqrt{2}} - \frac{\ln(M+1)}{(M+1)^2}\frac{\eta^2}{4\pi} + \frac{1}{2}\frac{1}{(M+1)^2} \\
&\quad \times \left\{\frac{\pi}{6}\left[\frac{1}{12} - G_1\left(\frac{\sqrt{2}\eta}{\pi}\right)\right] + \frac{\eta^4}{3\pi^3} H_1\left(\frac{\sqrt{2}\eta}{\pi}\right)\right. \\
&\quad \left. - \frac{\eta^2}{2\pi}\left[\gamma_E - \ln\pi + \frac{3\ln 2}{2} + \frac{2}{3}G_0\left(\frac{\sqrt{2}\eta}{\pi}\right) - \frac{1}{3}\right]\right\} \\
&\quad + \frac{1}{(M+1)^3}\frac{3\sqrt{2}}{64}\eta^2 + O\left(\frac{\ln M}{(M+1)^4}\right) \\
&\quad + O\left(\frac{1}{(M+1)^4}\right), \qquad (A6)
\end{aligned}$$

where γ_E is the Euler-Mascheroni constant, and $G_0(\alpha)$, $G_1(\alpha)$ and $H_1(\alpha)$ are remnant functions and are given in Ref. 18. Setting $\eta=0$, one has the first component of the sum appearing in S_0:

$$\frac{1}{M+1}\sum_{j=1}^{M}\frac{1}{\sqrt{(2-\cos\phi_j)^2-1}} =\frac{\ln(M+1)}{\pi}+\frac{1}{\pi}\left[\gamma_E-\ln\pi+\frac{3\ln 2}{2}\right] -\frac{1}{M+1}\frac{1}{4\sqrt{2}}+\frac{1}{(M+1)^2}\frac{\pi}{144}+O\left(\frac{1}{(M+1)^4}\right). \quad \text{(A7)}$$

Next we consider the contribution of the second term in Eq. (A4) to the sum S_0. To calculate this we firstly expand $h_j(m)$ viz.

$$h_j(m)=\frac{M+1}{X_jY_j}+\frac{1}{M+1}\left\{\frac{1}{24}\frac{\pi^4j^4}{X_j^3Y_j}-\frac{X_j}{8Y_j} +\frac{\rho}{12}\frac{Y_j-1}{Y_j^2}\left(\frac{\pi^4j^4}{X_j^2}+X_j^2\right)\right\}+O\left(\frac{1}{(M+1)^3}\right), \quad \text{(A8)}$$

where $X_j=\sqrt{2\eta^2+\pi^2j^2}$ and $Y_j=\exp(2\rho X_j)+1$. Dominant contributions to the sum come from the small j terms. The sum may thus be replaced by $\Sigma_{j=1}^{\infty}h_j(\eta)$.[18] Taking the limit as $\eta\rightarrow 0$ gives the second component of the sum appearing in S_0:

$$\frac{1}{M+1}\sum_{j=1}^{M}h_j(0)=\frac{1}{\pi}W_{1,1}^0(\rho)+\frac{1}{(M+1)^2}\left[-\frac{\pi}{12}W_{-1,1}^0(\rho) +\frac{\rho\pi^2}{6}W_{-2,2}^1(\rho)\right]+O\left(\frac{1}{(M+1)^4}\right), \quad \text{(A9)}$$

where

$$W_{j,k}^l(\rho)=\sum_{n=1}^{\infty}\frac{e^{2\rho\pi l n}}{n^j(e^{2\rho\pi n}+1)^k} \quad \text{(A10)}$$

are rapidly converging sums which may be computed numerically. For example, at $\rho=1$, $W_{1,1}^0\approx 0.001\,865\ldots$, $W_{-1,1}^0\approx 0.001\,870\ldots$, and $W_{-2,2}^1\approx 0.001\,874\ldots$. Finally, from Eqs. (3.4), (A4), (A7), and (A9), the desired result is

$$S_0=\frac{\ln M}{\pi}+\frac{1}{\pi}\left(\gamma_E+\frac{3\ln 2}{2}-\ln\pi-2W_{1,1}^0(\rho)\right)+\frac{\ln M}{M}\frac{1}{\pi} +\frac{1}{M}\frac{1}{\pi}\left(\gamma_E+\frac{3\ln2}{2}-\ln\pi+1-\frac{\pi}{4\sqrt{2}}-2W_{1,1}^0(\rho)\right) +\frac{1}{M^2}\left(\frac{1}{2\pi}+\frac{\pi}{144}+\frac{\pi}{6}W_{-1,1}^0(\rho)-\frac{\rho\pi^2}{3}W_{-2,2}^1(\rho)\right) -\frac{1}{M^3}\left(\frac{1}{6\pi}+\frac{\pi}{144}+\frac{\pi}{6}W_{-1,1}^0(\rho)-\frac{\rho\pi^2}{3}W_{-2,2}^1(\rho)\right) +O\left(\frac{1}{M^4}\right). \quad \text{(A11)}$$

The sum S_2 is calculated by taking appropriate derivatives of Eqs. (A6) and (A8). The result for S_2 is

$$S_2=-M^2\frac{2}{\pi^3}[\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)] -M\frac{6}{\pi^3}[\zeta(3)-2W_{3,1}^0(\rho)-4\pi\rho W_{2,2}^1(\rho)]-\frac{\ln M}{2\pi} +O(1), \quad \text{(A12)}$$

where $\zeta(3)$ is the Riemann zeta function. Typical values of these rapidly converging sums appearing here are $W_{3,1}^0\approx 0.001\,864\ldots$ and $W_{2,2}^1\approx 0.001\,861\ldots$ at $\rho=1$.

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