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Complex Temperature Plane Zeros in the Mean-Field Approximation

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We derive asymptotic expressions for the complex temperature plane zeros of the infinite-range Ising model in the scaling regime. The results also apply to high-dimensional, short-range Ising systems. For the nth zero in a system of N spins, the leading asymptotic result is $t_n \propto (n/N)^{1/2}(-1 \pm i)$.

KEY WORDS: Partition function zeros; infinite-range Ising models; phase transitions; mean-field theory.

1. INTRODUCTION

Recent successful attempts by several groups[1-3] to develop ε expansions for finite-size systems have renewed interest in the infinite-range Husimi–Temperley model (for review see Ref. 4). Indeed, the infinite-range model provides the zeroth-order[1,2] "mean-field approximation" appropriate for a finite system (of fixed shape). For definiteness, let us consider the nearest neighbor Ising model on the d-dimensional hypercubic lattice,

$$-\beta H = K \sum_{\text{n.n.}} s_i s_j, \qquad K > 0, \quad s_i = \pm 1 \tag{1.1}$$

It has been realized[1-3] that only the zero-momentum Fourier component of the order parameter need be kept for an asymptotic description of the critical behavior of a *finite* system in $d > 4$, provided *periodic* boundary

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conditions are imposed in all directions. In the lattice version (1.1), this amounts to the replacement

$$s_i s_j \to \left(\frac{1}{N}\sum_{i=1}^{N} s_i\right)^2 \tag{1.2}$$

where N is the total number of spins. Since the total number of the n.n. pairs is dN, the appropriate infinite-range interaction is

$$-\beta H_{\mathrm{MF}} = \frac{dK}{N}\left(\sum_{i=1}^{N} s_i\right)^2 \tag{1.3}$$

One can show[4] that the partition function of this model is proportional to

$$Z_N(K) = \int_{-\infty}^{\infty} d\mu \exp\{N[-dK\mu^2 + \ln\cosh(2dK\mu)]\} \tag{1.4}$$

and that the bulk phase transition occurs at $K_c = 1/2d$.

Our aim is to calculate the location of the complex temperature plane zeros of the partition function (1.4). Study of the complex-temperature zeros was initiated by Fisher,[5] who emphasized the analogy with the Yang–Lee zeros[6,7] in the complex magnetic field plane. Later studies of the complex temperature zeros are reviewed in Ref. 8. There is no strict Yang–Lee theorem in the temperature plane; however, Itzykson *et al.*[9] discovered an asymptotic property of equal importance. *Provided* that the zeros accumulate at T_c along a complex conjugate pair of lines, these lines form an angle ψ with the *negative* real axis that is an explicitly known universal function of the critical exponent α and the specific heat amplitude ratio. Here it suffices to quote[9]

$$\psi_{\mathrm{MF}} = 45^\circ \tag{1.5}$$

Note that the formation of a line of zeros is a likely but not general feature: at least one counterexample is rigorously known.[10,11]

In mean-field type models, the *locus* of zeros can be found[9] by considering the behavior of the bulk partition function for complex temperatures. Specifically, the prediction (1.5) has been confirmed for the Bethe lattice. Another obvious line of attack is to solve for zeros numerically for small N. Caliri and Mattis[12] reported calculations up to $N = 25$.

Our program is more ambitious. We will actually calculate the location of an unbounded number of zeros in the critical region, for large N. The underlying scaling analysis of the partition function of the infinite-range model, along with the results, are presented in Section 2. Related mathematical input, used to obtain the location of the zeros, is summarized in the Appendix.

2. COMPLEX TEMPERATURE PLANE ZEROS

In terms of the reduced temperature variable

$$t \equiv (K_c - K)/K_c = 1 - 2dK \tag{2.1}$$

the exponential in (1.4) can be written

$$-dK\mu^2 + \ln \cosh(2dK\mu) = -\tfrac{1}{2}t\mu^2(1-t) - \tfrac{1}{12}\mu^4(1-t)^4 + O(\mu^6) \tag{2.2}$$

For large N, and in the critical region of small $|t|$, the integral in (1.4) can be conveniently analyzed in terms of the new "scaled" variables

$$u = \mu(N/12)^{1/4} \tag{2.3}$$

$$z = t(3N)^{1/2} \tag{2.4}$$

With this rescaling,

$$N(-\tfrac{1}{2}t\mu^2 - \tfrac{1}{12}\mu^4) = -zu^2 - u^4 \tag{2.5}$$

while all the other terms in (2.2), when written in terms of z and u, acquire extra negative powers of N and can be treated in perturbation theory. The leading corrections to scaling for various quantities are of *relative* magnitude $N^{-1/2}$ (see Ref. 13). Thus, we have to solve for the complex-z zeros of the entire function

$$F(z) \equiv \int_0^\infty \exp(-zu^2 - u^4)\, du \tag{2.6}$$

For a complex zero z_j, the corresponding partition function zero in the t plane has N dependence given, for large N, by

$$t_j \sim z_j N^{-1/2} \tag{2.7}$$

provided the zero is in the critical region of small $|t_j|$. (We will work out the number of zeros that are correctly reproduced later in this section.)

If we subtract the ground-state, all + or all −, energy contribution $-\beta H_{gs} \equiv dNK$ from the original Ising model energy (1.1), then the partition function becomes a polynomial in some low-temperature variable, say e^{-K}, which has $O(N)$ zeros. Similar manipulation on the infinite-range partition function (1.3) can only produce a polynomial in an N-dependent variable, say $e^{-K/N}$. (A different, high-temperature, but still explicitly N-dependent variable was used in Ref. 12.) There are $O(N^2)$ zeros in the $e^{-K/N}$ plane. Thus, the analyticity and the zero structure in the e^{-K} plane is *globally* disrupted by the mean-field approximation (1.2). Specifically, the electrostatic analogy[5-8] may not apply *globally*. However, *locally* near T_c (or, say, e^{-K_c}) there should be no problem. In fact, the expansion leading to (2.6) does not depend on the details of the mean-field model away from T_c, because the square and the quartic contributions are nothing but the appropriately rescaled leading-power zero-momentum terms in the Ginzburg–Landau–Wilson expansion, as appropriate for $d>4$.[1-3] However, for general Ising models in higher dimensions, one must keep in mind that the gradient terms (nonzero-momentum order parameter components) induce additional corrections to scaling.[1] Thus, (2.7) must be interpreted as

$$t_j = Cz_j N^{-1/2}[1 + O(N^{-1/2}) + O(N^{-(d-4)/4})] \tag{2.8}$$

where C is a nonuniversal constant, while z_j are universal numbers given by

$$F(z) = 0 \tag{2.9}$$

For the particular model considered here, $C \equiv 3^{-1/2}$.

In the Appendix, we derive the following asymptotic formula for the nth zero of $F(z)$ in the upper half-plane ($\text{Im}\, z > 0$; there is always a conjugate zero at z_n^*):

$$z_n = 2(2\pi n)^{1/2} e^{3\pi i/4} \left[1 - \frac{\pi + i \ln 2}{8\pi n} - \frac{\pi^2 - 6 - (\ln 2)^2 + 2\pi i \ln 2}{128\pi^2 n^2} + O\left(\frac{1}{n^3}\right) \right] \tag{2.10}$$

The leading term in (2.10) is

$$z_n \approx (4\pi n)^{1/2}(-1 + i) \tag{2.11}$$

so that the zeros indeed accumulate asymptotically[9] near the 45° diagonal of the second complex-plane quadrant, approaching it from above. Relations (2.10)–(2.11) are valid for large $|z_n|$ and therefore describe quite accurately *all* the zeros of $F(z)$, since already $|z_1|$ is large. In Table I we compare the first five computer-located zeros with the asymptotic formula. Figure 1 displays the first 11 zeros.

Table I. Computer-Generated versus Asymptotic-Formula (2.10) Zeros for $n \leqslant 5$[a]

n	Calculated zero	Asymptotic formula
1	$-2.985 + i3.206$	$-2.982 + i3.202$
2	$-4.624 + i4.771$	$-4.623 + i4.770$
3	$-5.824 + i5.941$	$-5.824 + i5.941$
4	$-6.817 + i6.918$	$-6.817 + i6.917$
5	$-7.683 + i7.773$	$-7.683 + i7.772$

[a] Values rounded to the last digit shown. For $n > 3$, the asymptotic formula is more accurate than the computer routines we employed.

The leading-order relation (2.11) suggests, via (2.8),

$$t_n \propto (n/N)^{1/2}(-1+i) \tag{2.12}$$

for large N *and* n. The condition for t_n to remain in the critical region implies $n = o(N)$. Since there are $O(N)$ zeros for lattice Ising models, an unbounded number of zeros can be accurately represented.

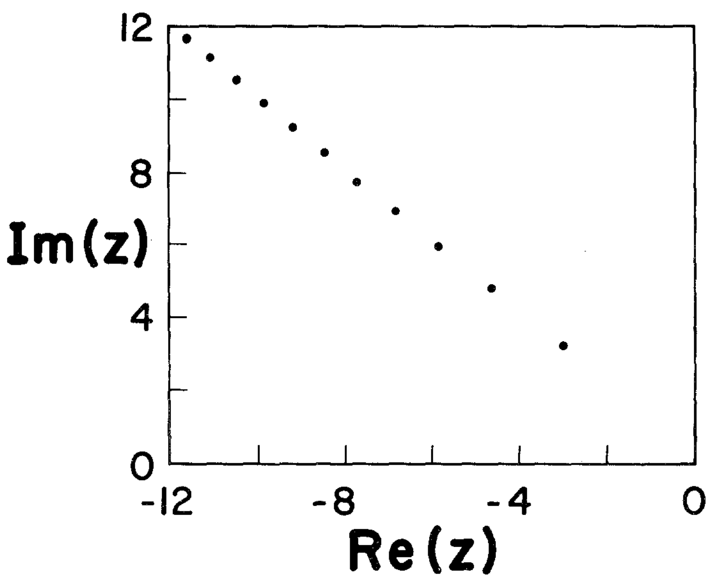

Fig. 1. The first 11 zeros in the upper half-plane. For $n \leqslant 5$, the computed and asymptotic formula values coincide to within about one-tenth of the size of the symbols. For $n \geqslant 6$, only asymptotic estimates are available.

APPENDIX

The function $F(z)$ in (2.6) can be related to standard mathematical functions,[14,15]

$$F(z) = \tfrac{1}{4} z^{1/2} \exp(z^2/8)\, K_{1/4}(z^2/8) \tag{A1}$$

$$F(z) = 2^{-5/4} \pi^{1/2} \exp(z^2/8)\, D_{-1/2}(z/\sqrt{2}) \tag{A2}$$

Here K and D denote the Bessel and the parabolic cylinder functions, respectively. Let us also introduce the complex-z plane notation

$$z = x + iy = re^{i\theta} \tag{A3}$$

By the general theory of the Bessel function zeros,[14] we learn that the zeros of $F(z)$ are all in $\pi/2 < \theta < 3\pi/4$ (with complex conjugates in $5\pi/4 < \theta < 3\pi/2$). The leading-order relation (2.11) can be established by using the last, unnumbered equation of Section 15.7 of Ref. 14. The more elaborate approximation (2.10) requires knowledge of the asymptotic expansion of $F(z)$ for large $|z|$ in the region of interest. This is most easily found from relation (A2), since the asymptotic behavior of $D_{-1/2}$ is well known.[15] Relation 9.246.2 from Ref. 15, when truncated to the order required here, reads, for $D_{-1/2}$ in the region $\pi/4 < \theta < 5\pi/4$,

$$\sqrt{z} D_{-1/2}(z/\sqrt{2}) \approx e^{-z^2/8} \left(1 - \frac{3}{4z^2} + \cdots\right) + i\sqrt{2} e^{z^2/8} \left(1 + \frac{3}{4z^2} + \cdots\right) \tag{A4}$$

where the omitted terms are of $O(z^{-4})$, $O(z^{-6})$, etc. By equating this to zero, we generate expansion (2.10).

It is interesting to note that the essence of the leading-order result (2.11) is the balancing of two exponentials in (A4), which become equal in magnitude when z^2 is purely imaginary.

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