Complex-temperature-plane zeros: Scaling theory and multicritical mean-field models

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We formulate a finite-size scaling theory for the partition function. This leads to a scaling description of the complex-temperature-plane zeros. The asymptotic form of the scaling function for large complex arguments is conjectured and used to calculate *explicitly* the location of an unbounded number of zeros. Scaling predictions are checked against the exactly solvable generalized infinite-range models which exhibit multicritical mean-field behavior. New mathematical results are reported for the asymptotic behavior of integrals representing finite-size scaling functions of infinite-range models.

I. INTRODUCTION

The study of partition-function zeros in the complex-temperature-variable plane was initiated by Fisher.[1] He located the locus of zeros for the two-dimensional Ising model and, generally, emphasized the analogy with the complex magnetic field plane.[2] However, there is no strict Yang-Lee theorem[2] for complex-temperature zeros. For over a decade studies of the complex-temperature zeros have been mainly numerical (consult Refs. 3–5 for literature). Recently, however, some progress has been made along two lines. Firstly, there have been attempts to understand implications of duality and other symmetry properties on the distribution of zeros for two-dimensional models.[5] Secondly, Itzykson, Pearson, and Zuber[3] (see also Ref. 4) formulated a scaling theory assuming that the zeros accumulate at T_c along a complex conjugate pair of lines. These lines form an angle ϕ with the negative real axis, given by[3]

$$\tan[(2-\alpha)\phi]=[\cos(\pi\alpha)-A_-/A_+]/\sin(\pi\alpha) , \quad (1.1)$$

where α and $A_\pm$ are defined by the critical behavior of the singular part of the bulk free-energy density (measured here in units of k_BT)

$$f^{(s)}\approx A_\pm \mid t \mid^{2-\alpha} \text{ with } t\equiv(T-T_c)/T_c , \quad (1.2)$$

as $t\rightarrow 0\pm$. (Note that the ratio A_-/A_+ is universal.)

In the present work, we report several developments in the theory of the complex-temperature zeros. In Sec. II, we extend the scaling theory of Ref. 3 to higher dimensions and present a systematic formulation including identification of nonuniversal amplitudes and corrections to scaling. By considering the asymptotics of the finite-size scaling functions, extended into the complex plane, we establish the following asymptotic relation valid for an unbounded number of zeros (see Sec. III for details):

$$t_n \cong \left\{ \frac{2\pi}{[A_+^2+A_-^2-2A_+A_-\cos(\pi\alpha)]^{1/2}} \frac{n}{V} \right\}^{1/(2-\alpha)} \times\exp[i(\pi-\phi)] , \quad (1.3)$$

where V is the finite-system volume and n takes large positive integer values. Note that there is a conjugate zero at t_n^* and that the denominator in (1.3) is dimensionless (as is the product $A_\pm V$, provided free energies are measured in units of k_BT, as already mentioned). Relation (1.3) breaks down when pure power-law scaling behavior is complicated by logarithmic factors (see Secs. II and III for further discussion).

Since the scaling-theory predictions are rather phenomenological, it is of interest to check them against solvable model results. In Sec. IV, we review certain multicritical mean-field infinite-range models and discuss their scaling properties. Asymptotic behavior of the appropriately scaled partition function in the complex plane is analyzed in detail in Sec. V. This calculation involves deriving some new mathematical results. One of our conclusions is that for the tricritical mean-field models

$$\phi=60^\circ . \quad (1.4)$$

This ϕ value applies to three-dimensional tricritical lattice systems; although, as mentioned, the full relation (1.3) may break down due to logarithmic corrections at the upper critical dimension. The value (1.4) is very close to the three-dimensional Ising-model estimate of $\phi\cong 57^\circ$.[4]

II. SCALING THEORY

As a first step, let us formulate finite-size scaling relations for the partition function. It is crucial to restrict the consideration to finite systems of fixed shape (as $V\to\infty$) and with periodic boundary conditions.[6] Then the free energy can be represented in the form[6]

$$f(t,V)=f_b^{(a)}(t)+f^{(s)}(t,V)\ , \tag{2.1}$$

where $f_b^{(a)}$ is the bulk analytic background contribution. The singular part[7] scales according to[6]

$$f^{(s)}\cong V^{-1}W[t(AV)^{1/(2-\alpha)}]\ , \tag{2.2}$$

where the scaling function W can be made universal (up to possible system-shape dependence) by choosing, e.g.,

$$A=[A_+^2+A_-^2-2A_+A_-\cos(\pi\alpha)]^{1/2}\ . \tag{2.3}$$

This particular choice simplifies calculation of complex-t zeros [compare (1.3)]. In other applications, $A=|A_+|$ or $|A_-|$, or other choices can be used ($A>0$ is required). Corrections to scaling in (2.2) are, generally, additive and of order higher than V^{-1} (consult Ref. 8). Thus we explicitly exclude from consideration cases where logarithmic factors multiply power-law terms in (2.2) and/or (1.2), as happens at borderline dimensionalities and in some models with integer α.[9] By including (1.2) in the above restriction, we also require a power-law (no logarithms) asymptotic behavior of the scaling function W, in the bulk limit,

$$W(\tau)\approx(A_+/A)\tau^{2-\alpha}\quad \text{as } \tau\to+\infty\ , \tag{2.4}$$

$$W(\tau)\approx(A_-/A)(-\tau)^{2-\alpha}\quad \text{as } \tau\to-\infty\ . \tag{2.5}$$

We now turn to the partition function

$$Z\equiv\exp(-Vf)\ , \tag{2.6}$$

which according to (2.1) and (2.2) can be represented as

$$Z=\exp[-Vf_b^{(a)}(t)](e^{-W}+\cdots)\ . \tag{2.7}$$

The first factor is of no interest. In the scaling term, we expanded the corrections to scaling off the exponential [to where the ellipsis indicates them in relation (2.7)] because they are of the order of some negative power of V, which in many cases is $V^{-\Delta_1/(2-\alpha)}$ (consult Ref. 8 for notation and further details).

Suppose that we solve for the zeros of the scaling part,

$$G(\tau)\equiv\exp[-W(\tau)]=0\ , \tag{2.8}$$

continued analytically into the complex τ plane. Then each zero, τ_k, can be corrected by a perturbation expansion of the full relation

$$G(\tau)+\cdots=0\ . \tag{2.9}$$

The conclusion is that corrections to the scaling results for the zeros, τ_k, have a pattern similar to those for general real-axis thermodynamic quantities.

The scaling picture presented above applies provided $t\to0$, $V\to\infty$, while the scaling combination

$$\tau\equiv t(AV)^{1/(2-\alpha)}\ , \tag{2.10}$$

takes fixed values. Thus, only zeros which fall in the critical region can be described by

$$t_k\approx\tau_k(AV)^{-1/(2-\alpha)}\ , \tag{2.11}$$

where τ_k are universal [provided (2.3) is obeyed]. Without going into details[10] let us mention that a critical region is defined, to the required accuracy in the pure power-law bulk critical behavior, simply by $|t|\ll c$, where c is a very small system-dependent (and required accuracy-dependent) number. Thus, as $V\to\infty$, $O[c(AV)^{1/(2-\alpha)}]$ zeros are accurately represented by (2.11).

The scaling theory of this section extends the results of Ref. 3 into a systematic formulation in terms of the partition function, which accounts for the character of the corrections. It is valid both below and above the upper critical dimension (when hyperscaling is violated[6]). A nonuniversal factor in the complex-t zeros [see (2.11) and (2.3)] is identified in terms of the bulk amplitudes $A_\pm$. Extension to models with non-pure-power-law scaling behaviors will require analyzing each case separately, and is outside the scope of the present work, as is a study of nonperiodic boundary conditions.

III. COMPLEX-PLANE ASYMPTOTICS

In order to proceed with the scaling analysis, let us accept the conjecture[1,3,4] that at normal critical points the loci of partition-function zeros near T_c form two complex conjugate pairs of lines. In the critical region, for small $|t|$, these lines can be regarded as straight: The curvature is not seen in the scaling results, as can be surmised from (1.3). For the $d=2$ Ising model with unequal couplings, the zeros are known to fall into regions.[11] However, the boundaries become tangential near T_c so that the spread of the zeros away from T_c is perhaps a correction-to-scaling phenomenon.

Accepting a line locus, at least in the scaling regime, implies that thermodynamic functions, derived from the integral representation in terms of the density of zeros, have in the $V=\infty$ limit, two distinct analytic continuations into the complex t plane. Let us denote

$$t\equiv re^{i\theta}\ , \tag{3.1}$$

and restrict our consideration to the upper half plane $0\le\theta\le\pi$.[12] Then the bulk free-energy scaling behavior (1.2) can be formally extended away from the real t axis:

$$f_+^{(s)}\approx A_+r^{2-\alpha}e^{i\theta(2-\alpha)}\quad\text{for } 0\le\theta\lesssim\pi-\phi\ , \tag{3.2}$$

$$f_-^{(s)}\approx A_-r^{2-\alpha}e^{-i(\pi-\theta)(2-\alpha)}\quad\text{for } \pi-\phi\lesssim\theta\le\pi\ . \tag{3.3}$$

But what happens near $\theta=\pi-\phi$? As noted by Itzykson and Luck,[4] the continued scaling behavior satisfies conditions similar to those for the full integral-represented free energy.[3] The real parts of $f_\pm^{(s)}$ in (3.2) and (3.3) are equal exactly at $\theta=\pi-\phi$ [see (1.1)], while there is a discontinuity in the imaginary part.

We will propose an extension of the above observations to finite systems, following two lines of argument, both admittedly rather heuristic. Firstly, we can extend the asymptotics of the scaling function W, in (2.4)–(2.5), into the complex τ plane. Then in terms of

$$\zeta\equiv r(AV)^{1/(2-\alpha)}\ , \tag{3.4}$$

and θ [note $\tau\equiv\zeta\exp(i\theta)$], the partition-function scaling [see (2.7), (2.8)] has the following asymptotics for large $|\tau|\equiv\zeta$:

$$G(\tau)\cong g_+(\tau)\equiv\exp[-(A_+/A)\zeta^{2-\alpha}e^{i\theta(2-\alpha)}] , \quad (3.5)$$

$$G(\tau)\cong g_-(\tau)\equiv\exp[-(A_-/A)\zeta^{2-\alpha}e^{-i(\pi-\theta)(2-\alpha)}] , \quad (3.6)$$

for $0\lesssim\theta\lesssim\pi-\phi$ and $\pi-\phi\lesssim\theta\leq\pi$, respectively. At the Stokes line $\theta=\pi-\phi$, $g_\pm$ become equal in magnitude but not in phase. We conjecture that the leading-order behavior near this line is given by

$$G(\tau)\cong g_+(\tau)+g_-(\tau) . \quad (3.7)$$

In fact, this form may apply all over the upper half plane (for ζ large). Indeed, this is typically the case with asymptotic expansions near Stokes lines and can be checked explicitly for mean-field models: See Sec. V and Ref. 13. Corrections to (3.5) and (3.6) are terms additive in the exponentials, which (possibly) diverge more weakly than $\zeta^{2-\alpha}$ as $\zeta\to\infty$.

A different argument leading to (3.7) can be offered. Indeed, the balancing of the real parts of the bulk free energies continued into the complex plane, and the corresponding domination of the statistical sum by terms $\sim\exp(-Vf_\pm)$, are reminiscent of first-order transitions. Although analogy should probably not be taken too seriously, we may employ results on finite-size behavior at first-order transitions.[14] Thus, near $\theta=\pi-\phi$ and when critical fluctuations are not important (this eventually translates into having $|\tau|$ large), we have[14]

$$Z\cong e^{-Vf_+}+e^{-Vf_-} . \quad (3.8)$$

Here $f_\pm$ are the analytically continued bulk free-energy branches, which near T_c take forms

$$f_\pm=f_b^{(a)}+f_\pm^{(s)}+\cdots \quad (3.9)$$

[see (2.1), (3.2), and (3.3)]. Now we can employ the procedure of matching the scaling forms[15] to derive the asymptotics of the critical scaling function $G(\tau)$ for large $|\tau|$. By using (3.8), (3.9), and (2.7), we arrive[15] at the relation (3.7). [Note that (3.8) is more general.]

Finally, we solve for the zeros of the asymptotic expression (3.7),

$$g_+(\tau)+g_-(\tau)=0 . \quad (3.10)$$

It is a matter of straightforward algebra to show that $\theta=\pi-\phi$ and, provided A is defined exactly by (2.3),

$$\zeta_n=[2\pi(n-\tfrac{1}{2})]^{1/(2-\alpha)} . \quad (3.11)$$

Here the positive integer n labels different roots of (3.10). The $-\frac{1}{2}$ term appears when (3.10) is solved as is. However, corrections to (3.7) may change the relative phase of the two exponentials (changing the constant) and actually induce terms which are additive positive powers of n [subdominant to $n^{1/(2-\alpha)}$], in τ_n. Thus, we omitted the $-\frac{1}{2}$ in translating to (1.3) [by using (3.4)]. Regardless, the approximation (1.3) is valid for large n, but let us also recall the upper bound, growing with the system size $\propto O[(AV)^{1/(2-\alpha)}]$, described in Sec. II.

IV. OVERVIEW OF INFINITE-RANGE MODELS

There are several ways of defining multicritical infinite-range models. For example, one can have Ising spins ($\sigma=\pm1$) but allow for multiple spin couplings. We prefer, however, pair-interacting scalar spins, taking values in R with measure $d\mu(\sigma)$. We take

$$E=-(J/2N)\sum_{i=1}^{N}\sum_{j=1}^{N}\sigma_i\sigma_j,\ \ J>0 . \quad (4.1)$$

The partition function

$$Z=\int\cdots\int\prod_k d\mu(\sigma_k)\exp\left[(\beta J/2N)\sum_{i,j}\sigma_i\sigma_j\right] , \quad (4.2)$$

with $\beta\equiv(k_BT)^{-1}$, can be calculated as usual by "uncompleting the square" via a Gaussian integral,

$$Z=\int_{-\infty}^{\infty}dy\,e^{-y^2}\times\int\cdots\int\prod_k d\mu(\sigma_k)\times\exp\left[2y(\beta J/2N)^{1/2}\sum_i\sigma_i\right] , \quad (4.3)$$

where here (and below) we discard uninteresting prefactors in Z. This leads to

$$Z=\int_{-\infty}^{\infty}dy\,e^{-y^2}\left[\int d\mu(\sigma)\exp[2y\sigma(\beta J/2N)^{1/2}]\right]^N , \quad (4.4)$$

which is finally reduced by changing the integration variable to

$$x\equiv y(2\beta J/N)^{1/2} . \quad (4.5)$$

The result is

$$Z=\int_{-\infty}^{\infty}dx\exp\left[N\left[-\frac{x^2}{2\beta J}+Q(x)\right]\right] , \quad (4.6)$$

where

$$Q(x)\equiv\ln\left[\int d\mu(\sigma)e^{x\sigma}\right] . \quad (4.7)$$

The function $Q(x)$ is essentially arbitrary. The usual choice leading to multicritical mean-field theory is

$$Q(x)=q_2x^2-q_{2p}x^{2p}+o(x^{2p}) , \quad (4.8)$$

where q_2 and q_{2p} are both positive, while $p=2,3,\ldots$. For $p=2$ we have an ordinary (Ising) mean-field theory.[13] For $p=3$ a tricritical model is obtained. We keep both coefficients general in order to see how these nonuniversal quantities are absorbed in the amplitudes $A_\pm$. It is convenient to use free energies per spin (and in units of k_BT) here, so that $Z=\exp(-Nf)$. Then formulas of Secs. II and III can be used, with $V\to N$. We will also disregard completely the higher-order terms in (4.8) since they do not contribute to the scaling behavior.[13]

The calculation of the bulk free energy is straightforward, the results are as follows:

$$\beta_c=(2q_2J)^{-1} , \tag{4.9}$$

$$t=\frac{T-T_c}{T_c}=\frac{1}{2q_2J\beta}-1 , \tag{4.10}$$

$$A_+=0 , \tag{4.11}$$

$$\alpha=(p-2)/(p-1) , \tag{4.12}$$

$$A_-=\frac{1-p}{p}q_2\left[\frac{q_2}{pq_{2p}}\right]^{1/(p-1)} . \tag{4.13}$$

Following (2.10), with $A=|A_-|$ here, we introduce a scaled variable

$$\tau=t(AN)^{1/(2-\alpha)}$$
$$=\left[\frac{1}{2q_2J\beta}-1\right]\left[\frac{p-1}{p}q_2\right]^{(p-1)/p}\left[\frac{q_2}{pq_{2p}}\right]^{1/p}N^{(p-1)/p} . \tag{4.14}$$

The finite system partition function then reduces to

$$Z=\int_{-\infty}^{\infty} du\exp[-p(p-1)^{(1-p)/p}\tau u^2-u^{2p}]$$
$$\equiv G(\tau) , \tag{4.15}$$

where the new integration variable is

$$u=x(q_{2p}N)^{1/(2p)} \tag{4.16}$$

[compare (4.6)]. Relation (4.15) is the anticipated universal scaling representation of the partition function: It does not contain βJ, q_2, q_{2p}. Note that some discarded prefactors (contributing to the background in the free energy) were system dependent. The correction terms in (4.8), which we did not consider (but see Ref. 13), acquire extra negative powers of N [provided they were powers in (4.8)] in the process of rescaling (4.16) and contribute corrections to scaling (see Sec. II).

According to the scaling theory presented in Secs. II and III, the partition-function zeros are given by (2.11) in terms of the zeros of $G(\tau)$ defined in (4.15). For large $|\tau|$, these zeros must approach

$$\tau_n\cong(2\pi n)^{(p-1)/p}\exp\left[i\left[\frac{\pi}{2}+\frac{\pi}{2p}\right]\right] , \tag{4.17}$$

by (3.11) and (1.1). For $p=2$ this checks against the results of Ref. 13, where a variable

$$z\equiv p(p-1)^{(1-p)/p}\tau \tag{4.18}$$

was used. Exact asymptotic analysis of the function

$$G(z)\equiv\int_{-\infty}^{\infty} du\exp(-zu^2-u^{2p}) \tag{4.19}$$

will be presented in Sec. V.

V. ASYMPTOTIC BEHAVIOR OF THE MEAN-FIELD SCALING FUNCTION

The behavior of $G(z)$ in the lower half complex z plane is simply the complex conjugate of its behavior in the upper half plane, so we restrict our attention to this region.[12] Consider z in the first quadrant. Since the integrals are absolutely convergent, Watson's lemma[16] immediately gives the following for large $|z|$:

$$G(z)\cong 2\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^{\infty}e^{-zu^2}u^{2pn}du$$
$$=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Gamma(np+\tfrac{1}{2})z^{-np-1/2} . \tag{5.1}$$

Careful examination of arguments involved[16] shows that this algebraic expansion is dominant arbitrarily close to, and to the right of, the ray

$$\arg(z)=\frac{\pi}{2}+\frac{\pi}{2p} , \tag{5.2}$$

which is a Stokes line for $G(z)$. Next, consider z in the second quadrant to the left of the Stokes line (5.2). In particular, for negative z, if we make the substitutions

$$z=p\xi^{2p-2}e^{i\pi},\quad u\rightarrow\xi u , \tag{5.3}$$

then

$$G(z)=\xi\exp[(p-1)\xi^{2p}]$$
$$\times\int_{-\infty}^{\infty}\exp\{\xi^{2p}[u^{2p}-pu^2+(p-1)]\}du . \tag{5.4}$$

However, the integral in (5.4) is analytic in the sector

$$|\arg(\xi)|<\pi/4p , \tag{5.5}$$

so that this representation is valid throughout the second quadrant to the left of the Stokes line. Since p is an integer, the integrand in (5.4) has equivalent saddle points $u=1$ and $u=-1$. Consider the former, and let

$$b(\omega)=(1+\omega)^{2p}-p(1+\omega)^2+(p-1)$$
$$=2p(p-1)\omega^2+\left[\begin{matrix}2p\\3\end{matrix}\right]\omega^3+\cdots+\omega^{2p} , \tag{5.6}$$

where $\omega\equiv u-1$. By expanding

$$\exp[-\xi^{2p}b(\omega)]=\exp[-2p(p-1)\xi^{2p}\omega^2]$$
$$\times\sum_{n=0}^{\infty}\sum_{m=3n}^{2pn}\frac{(-1)^n}{n!}D(n,m)\omega^m\xi^{2pn} , \tag{5.7}$$

where the $D(n,m)$ are easily calculable combinatorial coefficients, we have again by Watson's lemma,

$$G(z)\cong 2\exp[(p-1)\xi^{2p}]\sum_{n=0}^{\infty}\sum_{m=3n}^{2pn}\frac{(-1)^n}{n!}D(n,m)\xi^{2pn}\int_{-\infty}^{\infty}\exp[-2p(p-1)\xi^{2p}\omega^2]\omega^m d\omega$$
$$=\exp[(p-1)(z/p)^{p/(p-1)}e^{-ip\pi/(p-1)}]\sum_{n=0}^{\infty}\sum_{m=3n}^{2pn}\frac{(-1)^n}{n!}D(n,m)\Gamma[\tfrac{1}{2}(m+1)]$$
$$\times[p(p-1)]^{-(m+1)/2}2^{-(m-1)/2}(ze^{-i\pi})^{[1+2pn-p(m+1)]/2(p-1)} \tag{5.8}$$

(a factor of 2 is due to the equal contribution from the saddle point $u=-1$).

Finally, near the Stokes line the algebraic expansion (5.1) and the exponential expansion (5.8), each of which are subdominant in the domain of the other, are of comparable order of magnitude and must be combined.[16] Consequently, the complete asymptotic expansion in the upper half z plane is

$$G(z)\cong \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Gamma(pn+\tfrac{1}{2})z^{-np-1/2}+\exp[(p-1)(z/p)^{p/(p-1)}e^{-p\pi i/(p-1)}]$$
$$\times\sum_{n=0}^{\infty}\sum_{m=3n}^{2pn}\frac{(-1)^n}{n!}D(n,m)2^{-(m-1)/2}[p(p-1)]^{-(m+1)/2}(ze^{-i\pi}/p)^{[1+p(2n-m-1)]/2(p-1)}\,, \tag{5.9}$$

as $|z|\to\infty$, with $0\le\arg(z)\le\pi$. The form of (5.9) supports the observations concerning the scaling functions made in conjunction with (3.7).

Next, we investigate the large modulus zeros of $G(z)$. Because neither the exponential nor algebraic portions of the expansion (5.9) have zeros in their regions of dominance, the desired zeros must cluster about the Stokes line. We calculate explicitly the leading-order result, and the first correction term, for which only the leading terms in (5.9) must be retained. Thus, asymptotically the zeros of $G(z)$ are given by the equation

$$1+i\left[\frac{2}{p-1}\right]^{1/2}\exp[(p-1)(z/p)^{p/(p-1)}e^{-p\pi i/(p-1)}]=0\,. \tag{5.10}$$

The large modulus roots to this equation are[17]

$$z_n\cong p\left[\frac{2\pi n}{(p-1)}\right]^{(p-1)/p}\exp\left[i\left[\frac{\pi}{2}+\frac{\pi}{2p}\right]\right]\left[1-\frac{p-1}{4p\pi n}\left[\pi+i\ln\frac{2}{p-1}\right]\right]\,, \tag{5.11}$$

where n is a large positive integer. This completely substantiates the proposals made concerning these roots in Sec. IV.

In summary, our present work achieves asymptotic scaling description of an unbounded number of complex-temperature-plane zeros clustering near a line forming an angle ϕ with the negative temperature axis. The closed form (1.3) is proposed for zeros outside the immediate vicinity of the critical point, which expresses these zeros in terms of the bulk parameters $A_\pm$ and α. Exact results for mean-field models support the phenomenological scaling theory.

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