Finite-size scaling in the complex temperature plane applied to the three-dimensional Ising model

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We extend the finite-size scaling theory into the complex temperature plane and present an alternative scenario for the second-order phase transition where the second-order derivatives of the partition function diverge at the transition point with the same exponent but different (discontinuous) amplitudes $A_\pm$. The complex scaling partition function Z_s for the $d = 3$ Ising model on a simple-cubic lattice is calculated using microcanonical Monte Carlo technique and is used to verify the scenario. The method of complex Z_s can be used as an alternative to the series method for the study of the second-order phase transition.

I. INTRODUCTION

It has been a central theme since the discovery of statistical mechanics to understand how the analytic partition function for the finite-size system acquires a singularity when we take the thermodynamic limit if the system undergoes a phase transition [1]. The Lee-Yang theory [2] has partly furnished the answer to this quest. In the case of the first-order transition, the zeros of the partition function in complex fugacity plane eventually form a cut that separate two phases in the thermodynamic limit.

In the case of the second-order or continuous phase transition no theory similar to the Lee-Yang theory exists. However, initiated by Fisher [3], there has been an extensive study of zeros of the partition function in complex temperature plane [4–6]. Recently the finite-size scaling theory has been incorporated in this endeavor and made some progress [7–9]. In these studies, attention has been focused only on the location of zeros of the partition function in the complex temperature plane in order to discover something similar to the Lee-Yang theory.

In this paper we present an alternative scenario for the second-order phase transition where the second-order derivatives of the partition function diverge at the transition point with the same exponent but different (discontinuous) amplitudes, $A_\pm$. Instead of studying the zeros of the partition function we study the whole of the singular part of the partition function (we will call it the scaling partition function and abbreviate as SPF) in the complex temperature plane. Unlike the case of the first-order phase transition, two phases are separated by a domain in the complex temperature plane where the SPF vanishes in the bulk limit. The SPF of the high- and low-temperature phases oscillates with different periods which are related to the amplitudes, $A_\pm$. These two domains are smoothly connected to the central domain of vanishing SPF. This scenario elucidates how a single analytic function, SPF, manifests the discontinuity in the amplitude, $A_\pm$, in the thermodynamic limit. We tested this theory by calculating the SPF for the $d = 3$ Ising model using the microcanonical Monte Carlo (MC) method [12] and found the calculated SPF confirm all the prediction of the theory. We also found that the complex SPF can be used as an alternative method (to the series method) to estimate the amplitudes, $A_\pm$ with comparable or better precision.

II. FINITE-SIZE SCALING IN THE COMPLEX TEMPERATURE PLANE

According to the two scaling factor universality hypothesis put forward by Privman and Fisher [10], the free energy density f consists of the analytic part f_a and the singular part f_s, i.e.,

$$f = f_a + f_s. \tag{1}$$

The singular part behaves as

$$f_s(t; L) \approx L^{-d} W(DtL^{1/\nu}), \tag{2}$$

where L is the side of d-dimensional cube (e.g., in the unit of lattice constant), t is the thermal scaling field, $1/\nu$ is the corresponding critical exponent, and D is the nonuniversal metric factor. The scaling function W can be made universal within a universality class by proper choice of nonuniversal metric factor together with normalization of W itself, as was done in [11].

The partition function now can be written as

$$Z = Z_a Z_s \ , \tag{3}$$

where $Z_a = \exp(L^d f_a)$ and $Z_s(t) = \exp(L^d f_s)$. Let us concentrate only on the SPF, Z_s, from now on. In terms of scaling variable $x = DtL^{1/\nu}$, Z_s can be written as

$$Z_s(x) = \exp[W(x)], \tag{4}$$

if L is sufficiently large so that corrections to scaling is negligible.

Let us now analytically continue into the complex t plane by writing $t = re^{i\theta}$. Then

$$Z_s = \exp[W(\zeta)], \tag{5}$$

where $\zeta = DL^{1/\nu} re^{i\theta}$. By writing $\rho = DL^{1/\nu} r$, we now have complex scaling partition function

$$Z_s = \exp[W(\rho e^{i\theta})]. \quad (6)$$

Although the SPF in the real axes is a monotonous U-shaped function, it manifests rich complex features in the complex temperature plane. Since the discontinuity in the amplitude, $A_\pm$, appears in the asymptotic behavior of the SPF in the bulk limit, let us see what happens to the asymptotic behaviors:

$$W(x) \approx Q_\pm (\pm x)^{d\nu} \quad (7)$$

as $x \to \pm\infty$, when we analytically continue $\pm x$ into the complex plane. They will become

$$Z_s(\rho e^{i\theta}) \approx \exp(Q_\pm \rho^{d\nu} e^{id\nu\theta_\pm}), \quad (8)$$

where $\theta_+ = \theta$ and $\theta_- = \pi - \theta$. The real and imaginary part of the SPF in this limit can be written as

$$\mathrm{Re}(Z_s) \approx e^{Q_\pm \rho^{d\nu} \cos(d\nu\theta_\pm)} \cos[Q_\pm \rho^{d\nu} \sin(d\nu\theta_\pm)] \quad (9)$$

and

$$\mathrm{Im}(Z_s) \approx e^{Q_\pm \rho^{d\nu} \cos(d\nu\theta_\pm)} \sin[Q_\pm \rho^{d\nu} \sin(d\nu\theta_\pm)]. \quad (10)$$

The above relations show that there are three regions where the SPF manifests distinct behaviors. Clearly both real and imaginary parts are oscillating functions with the period and amplitude (the magnitude of the complex SPF) which has the same functional dependence on $\theta_\pm$ although they are different at low- and high-temperature sides due to different values, $Q_\pm$. The magnitude of the SPF in the bulk limit $\rho \to \pm\infty$ is very large near the real axes but decreases as the phase angle $\theta_\pm$ increase and eventually vanishes as $\theta_\pm$ become larger than $90°/d\nu$ since

$$\|Z_s(\rho \to \pm\infty)\| \approx e^{-Q_\pm \rho^{d\nu} |\cos(d\nu\theta_\pm)|}. \quad (11)$$

Therefore the asymptotic forms (9) and (10) break down beyond these phase angles. In any case if $\nu > d^{-1}$, there exists a finite domain where the magnitude of the SPF vanishes in the asymptotic limit so that two discontinuous regions can be joined smoothly to make the SPF continuous in the whole complex temperature plane. This picture is drastically different from that of the first-order phase transition where the line of zeros eventually forms a branch cut that separates two phases in the bulk limit.

We can exploit the oscillating behavior of the SPF near the real axes in order to study the discontinuity of the amplitudes $Q_\pm$ which is proportional to $A_\pm$. $Q_\pm$ dependence of the magnitude of the SPF does not differ much from that on the real axes. $Q_\pm$ dependence of the period, on the other hand, is a unique feature of the SPF in the complex temperature plane and worth further study. The period of the oscillation can be studied by looking at the zero-height contours of the SPF. Explicitly the equations for the zero-height contour of the real and imaginary part of the SPF,

$$\mathrm{Re}(Z_s) = 0 \quad (12)$$

and

$$\mathrm{Im}(Z_s) = 0\ , \quad (13)$$

become in the asymptotic limit

$$Q_\pm \rho^{d\nu} \sin(d\nu\theta_\pm) = \pi/2 + k\pi \quad (14)$$

and

$$Q_\pm \rho^{d\nu} \sin(d\nu\theta_\pm) = k\pi\ , \quad (15)$$

where $k = 0, \pm 1, \ldots$.

These equations can be used to estimate $Q_\pm$ if we can calculate contours by some numerical method. It should be noted that each set of above equations also represents the locus of the maxima or minima of the other part of the SPF due to the Cauchy-Riemann relation. It should be further noted that the zeros of the SPF can be found by locating the simultaneous root of the Eqs. (12) and (13). Obviously the asymptotic contour lines given by Eqs. (14) and (15) do not cross each other. This means that zeros of the partition function do not exist in the asymptotic region of the oscillating domain. Zeros may exist in the central domain of vanishing SPF. However, any zeros in the asymptotic region in this domain will be fused into the sea of the flat SPF.

III. APPLICATION TO THE $d = 3$ ISING MODEL

We have performed MC calculations on the Ising model on a simple cubic lattice with periodic boundary conditions, of sizes L^3 with even $L = 10, \ldots, 24$. The microcanonical Monte Carlo technique [12] lets us calculate the whole partition function and the recently developed technique [11] allows us to isolate the singular part of the partition function.

For a spin-$\frac{1}{2}$ Ising model of N spins in the absence of an external field, the energy of the system can be written as

$$\mathcal{E}(\{S_i\}) = -J \sum_{\langle i,j \rangle} S_i S_j, \quad (16)$$

where S_i is the spin variable assuming ± 1 values, J is the exchange energy, and $\langle i,j \rangle$ runs over interacting nearest neighbor pairs i, j.

The partition function Z is defined as

$$Z = \sum_{\{S_i\}}^{2^N} \exp[-\beta \mathcal{E}(\{S_i\})]. \quad (17)$$

As usual [11,12] we write

$$Z = \sum_{\mathcal{E}=\mathcal{E}_0}^{\mathcal{E}_m} \Omega(\mathcal{E}) \exp(-\beta \mathcal{E}) \quad (18)$$

using $\mathcal{E}$ and $\Omega(\mathcal{E})$, the number of configurations with given $\mathcal{E}$. This expression can be further rewritten using *the low-temperature variable* u defined as $e^{-4\beta J}$, as

$$Z = \sum_{n=0}^{n=qN/8} u^{n-qN/8}\Omega_n, \tag{19}$$

where $n = \mathcal{E}/4J + qN/8$. The summation is restricted only to the positive temperature side or ferromagnetic energies.

In measuring $\Omega(\mathcal{E})$, we have used the algorithm developed in [12]. For the size $L = 24$, the number of elements in $\{\Omega\}$ is $qN/8$ which is as large as 10 368. However, the algorithm is remarkably stable so that the sum rule

$$S \equiv \sum_{n=0}^{n=qN/8-1} \Omega_n + \Omega_{qN/8}/2 = 2^{N-1} \tag{20}$$

is satisfied with the relative error much less than 10^{-4}. In fact for the MC data used for $L = 24$, we have $\ln(S) = 9581.17$ which is only 0.002% off from the exact value, $\ln(2^{N-1}) = 9581.3735$.

In this analysis we used $u_c = 0.412\,050$ [13] and the exponent $\nu = 0.63$ [15], although we can determine these numbers from our MC data by methods such as used in the Refs. [13,9]. As usual we define $t = K_c - K$, with $K = J/k_BT$ and *free energy density*,

$$f = L^{-d}\ln(Z). \tag{21}$$

Both f_a and f_s are expanded in t and x variables as

$$f_a = \sum_{n=0} a_n t^n/n! \tag{22}$$

and

$$L^d f_s = \sum_{n=0} c_n x^n/n!. \tag{23}$$

Using the prescription given in [11] we determine the expansion coefficients and obtain 0.777 82(5), −0.9898(4), and −30.4(2) for a_n, 0.6243(1), −2.281(1), and 41.3(3) for $D^n c_n$, with $n = 0, 1$, and 2. We limited our Taylor series to the quadratic terms because we can calculate them without considering corrections to scaling (see Ref. [11]) and higher order terms in f_a can be negligible if L is sufficiently large unless they have unusually large coefficients. In the above a_0 is the critical free energy density which is estimated to be 0.777 88(15) by series method [14] and a_1 is the critical internal energy which is estimated to be 0.9901(1) by series method [15] and a previous estimation of c_0 by an MC method is 0.625(5) [16]. This shows that our data agree well with the most recent series estimates or other MC estimate with comparable or even better precision.

The construction of SPF is straightforward. Since we now have the whole partition function in a polynomial in u and the analytic partition function in a Taylor series in t, we can simply extend our variables into complex u or t. Using the complex u variable, we have now

$$Z_s(u) = Z(u)/Z_a[r(u)e^{\theta(u)}]. \tag{24}$$

In Fig. 1 we plot the log of the SPF with $L = 10, ..., 24$ on the real axis to show the existence of the scaling function. The range on which this plot and subsequent plots are made is $[u_c - 0.036(L_0/L)^{1/\nu}, u_c + 0.036(L_0/L)^{1/\nu}]$, with $L_0 = 10$ and $\nu = 0.63$. We believe that the region near the boundary of this range is good enough to study the asymptotic behavior of SPF for the system sizes we calculated.

In Fig. 2 we plot the real and imaginary part of the SPF for $L = 24$. Since both real and imaginary parts can take negative values, it is not possible to plot the log of the SPF on the complex u plane. Therefore we had to clip the SPF surfaces both above and below a certain height. These surfaces confirm the new scenario of the second-order phase transition; namely there are two oscillating domains separated by the domain of vanishing magnitude in the asymptotic region. The phase angle $\theta_\pm$ at which the flat SPF begins is roughly equal to 47.62°, which is $90.0°/(d\nu)$.

In Fig. 3 we plot contours given by Eqs. (12) and (13). The curves start at circled points (open circles are real part and solid circles are imaginary part contours). The right hand side of the curves goes uphill (compare with Fig. 2). In the upper semicircle, eight contours with $L = 10, 12, ..., 24$ are drawn while in the lower semicircle contours of three largest L, i.e., $L = 20, 22$, and 24 are drawn. It seems that for the system sizes larger than $L = 20$, the calculated SPF's in the outmost circular band are in the asymptotic region. In this region the asymptotic behaviors of the calculated contours follow the predicted contours given by Eqs. (14) and (15). There seem to be two zeros closest to real axes in the circular plotting region (apart from the complex conjugates). Both zeros are in the domain of flat SPF. The first zero is located well short of the asymptotic region where the SPF still has finite values. This is the reason that it can be located rather easily. On the other hand the second zero is in

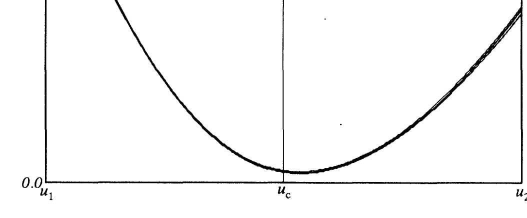

FIG. 1. $\ln[Z_s(u; L)] = L^d f_s(u)$ vs real u with $L = 10, ..., 24$, where $u_1 = u_c - 0.036(L_0/L)^{1/\nu}$ and $u_2 = u_c + 0.036(L_0/L)^{1/\nu}$.

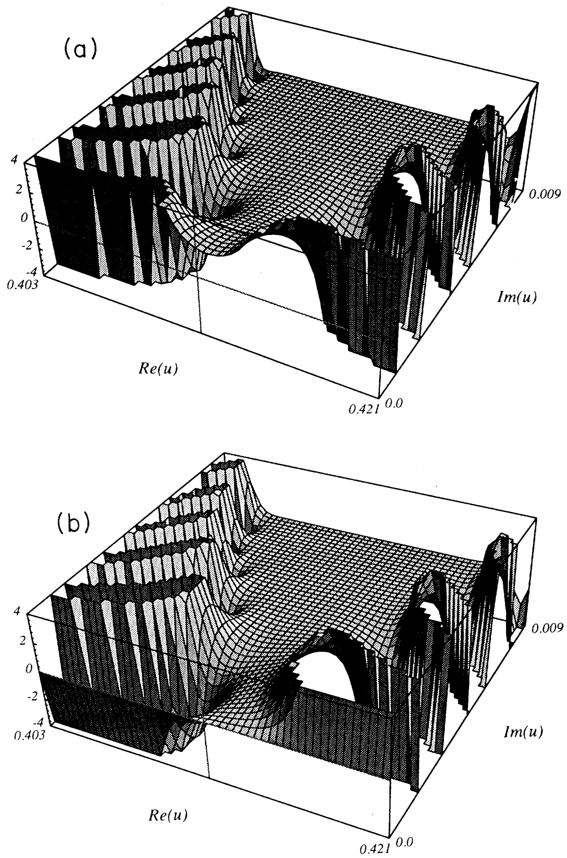

FIG. 2. (a) $\text{Re}[Z_s(u;L)]$ vs complex u with $L = 24$. (b) $\text{Im}[Z_s(u;L)]$ vs complex u with $L = 24$.

the truly flat region and the statistical errors bar the determination of the precise location of the zero as we see in Fig. 3.

The existence of the domain of the flat SPF can also be explained by looking at the mathematical structure of the complex SPF. Since the analytic partition function Z_a is slowly varying in this tiny scaling regime the gross features of SPF is more or less same as that of the total partition function Z. Let us now substitute complex $u = \varrho e^{i\vartheta}$ into Eq. (19) and write the real and imaginary part of the Z separately as

$$\text{Re}(Z) = \sum_{n=0}^{n=qN/8} \varrho^{n-qN/8}\Omega_n \cos[(n - qN/8)\vartheta], \quad (25)$$

and

$$\text{Im}(Z) = \sum_{n=0}^{n=qN/8} \varrho^{n-qN/8}\Omega_n \sin[(n - qN/8)\vartheta]. \quad (26)$$

In the above, the summands are the canonical weight factor $\varrho^{n-qN/8}\Omega_n$ which is a bell-shaped function (primarily characteristic Gaussian; see Ref. [12]) multiplied by the sinusoidal function of period $2\pi/\vartheta$. As we move away from the real axis, ϑ increases shortening the period while the width of the bell which is a measure of the thermal fluctuation grows large near the critical temperature. When the period of sinusoidal function becomes much smaller than the width of the bell, most of contributions to the sum will be washed away by the oscillating sinusoidal factor making the magnitude of the SPF diminish. The zeros may be formed when both sums vanish exactly by a delicate balancing of summands. Thus any zeros farther away from the real axes will eventually be fused into the sea of vanishing partition function.

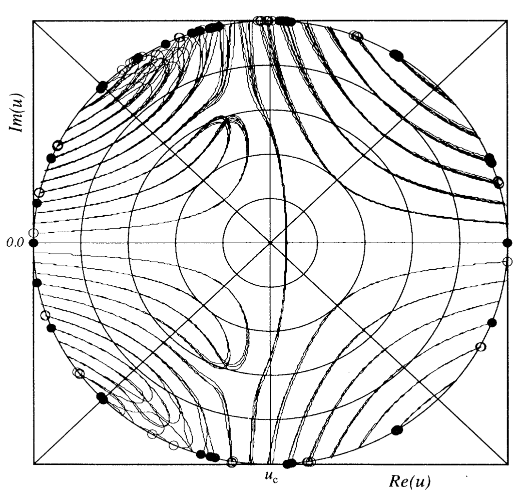

FIG. 3. Contours $\text{Re}[Z_s(u;L)] = 0$ and $\text{Im}[Z_s(u;L)] = 0$. The plotting region is a circle with radius $0.036(L_0/L)^{1/\nu}$ centered at u_c.

There are several ways to determine the specific heat amplitudes $A_\pm$ defined by

$$C(T)/k_B \cong A_\pm|\tilde{t}|^{-\alpha}, \quad (27)$$

where $C(T)/k_B$ is the specific heat per spin, $\alpha = 2 - d\nu$ and $\tilde{t} = T/T_c - 1$, using the Eqs. (14) and (15). In this analysis we used end points of the asymptotic contour lines of the real part of the SPF closest to the real axes [Eq. (14) with $k = 0$]. In Fig. 3 these points correspond to two open circles closest to the real axes on both sides. If we designate the phase angles of these points by $\theta^a_\pm$, we obtain

$$A_\pm = \pi[-u_c \ln(u_c)]^{d\nu} d\nu(d\nu - 1)/2L_0^d(0.036)^{d\nu} \sin(d\nu\theta^a_\pm). \quad (28)$$

For our best estimate, we have 1.335(5) for A_+ and 2.474(5) for A_- with $A_+/A_- = 0.539(8)$. Only $A_\pm$ differ some 10% from the series estimates of 1.464(7) and 2.79(3) [15] although the ratio is relatively close to 0.523(9) of the series estimate which is within the error bounds.

IV. CONCLUSION

In conclusion we have presented an alternative scenario for the second-order phase transition similar to the Lee-Yang scenario of the first-order phase transition. Unlike the case of the first-order phase transition, the two phases are not separated by a single line but are joined continuously by a finite domain of vanishing SPF in the bulk limit if $\nu > d^{-1}$. Zeros of the partition function appear to play no significant role in this case. Applying the microcanonical MC method for the thermodynamic functions and recently developed numerical technique of separating the singular part of the partition function, a complex SPF is calculated. The SPF so calculated are found to confirm the proposed scenario in every detail. Furthermore the example presented in this paper now convinces us that the method of the complex SPF is certainly as good as the series method in solving statistical models numerically and can be used for the study of the second-order phase transition.

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