Finite-size scaling of the density of zeros of the partition function in first- and second-order phase transitions

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The finite-size scaling form for the density of zeros of the partition function in first- and second-order phase transitions is derived. Using the finite-size scaling of the density of zeros, the order of a phase transition can be easily determined and the order parameter calculated from finite-size data. We illustrate the scaling theory using exact values for the zeros of the partition function of the two-dimensional Ising model in the complex magnetic-field plane. [S1063-651X(97)03107-3]

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I. INTRODUCTION

In 1952 Yang and Lee [1] proposed a mathematical mechanism for the occurrence of phase transitions in the thermodynamic limit by introducing the concept of the zeros of the grand partition function. They also formulated the celebrated circle theorem stating that for the Ising ferromagnet, the zeros of the grand partition function in the complex magnetic field plane lie on the unit circle. Since then the zeros of the partition function have attracted continuous interest. In 1964 Fisher [2] initiated the study of the partition function zeros in the complex *temperature* plane for the square lattice Ising model. The study of the distribution of the partition function zeros in the complex *magnetic field* or *temperature* planes has been extended to the Ising model of arbitrarily high spin [3], the Ising model of multiple spin interactions [4], the three-dimensional Ising model [5,6], the quantum Heisenberg model [4], the classical XY and Heisenberg model [7], the continuous spin models [8], the six-vertex model [9], the eight-vertex model [4], the Potts model [10,11], the Blume-Capel model [12], the hierarchical model [13], etc. In particular, the circle theorem has been extended to general Ising models and other models [4,11,12,14].

Since its introduction in the early 1970s finite-size scaling theory [15] has been a very powerful tool in interpreting data obtained in finite-size systems, especially in numerical simulation. While finite-size scaling theory at second-order phase transitions has been well established [15,16], finite-size scaling theory at first-order phase transitions has a more recent history [17–21] and is a topic of considerable current interest. According to scaling arguments, it was shown [18] that all finite-size effects at a first-order phase transition depend on the volume of the system L^d. Binder *et al.* [19] proposed a phenomenological double Gaussian approximation for the probability distribution of finite-size systems at a first-order transition, built on the theory of thermodynamic fluctuations. Lee and Kosterlitz [20] discussed the finite-size effects at a first-order transition by a mimic partition function. Borgs *et al.* [21] studied the phenomenological theory of finite-size systems at a first-order transition from a rigorous point of view.

It is well known that in the thermodynamic limit first-order phase transitions are characterized by δ-function singularities in the second derivatives of the free energy at the transition point. However, in finite-size systems δ-function singularities are rounded and the *effective* transition point is shifted. These behaviors at first-order transitions in finite-size systems are qualitatively similar to the finite-size effects at second-order transitions. In the theory of Fisher and Berker [18], scaling at a first-order transition is treated identically to scaling at a second-order transition with the temperature or magnetic scaling exponents assuming the maximal values $y_t, y_h = d$. As a result, in a situation where the order of a phase transition is not known, ordinary finite-size scaling analysis may be ambiguous. The worst situation is a *weak* first-order transition, for example, the temperature-driven transition in the two-dimensional five-state Potts model [22–24]. This model suffers from severe crossover effects [23,24] and has a very small latent heat [25] and a very large (but finite) correlation length [23,26] at the critical point. Currently, the best calculations of the order parameter and latent heat in the Potts models, which for $Q>4$ exhibit a first-order transition in two dimensions, are low-temperature series expansions [27]. It is the purpose of this paper to present an alternative approach based on the finite-size scaling properties of the distribution of Yang-Lee zeros. In addition to condensed matter physics, the identification of the order of a phase transition and the study of first-order phase transitions are very important in particle physics, especially in quantum chromodynamics and lattice gauge theory [24,28] and in the theories of the very early Universe [29].

Until now the study of partition function zeros with finite-size scaling has been concentrated on the approach of the edge zeros to the real critical point [6,30,31]. However, the density of zeros of the partition function contains more information about a system. In this paper we introduce finite-size scaling of the density of zeros that enables us to extract this information from calculations on finite-size systems. By studying finite-size scaling of the density of zeros, we can determine the order of a phase transition from finite-size data and we can evaluate physical quantities such as the spontaneous magnetization and the latent heat. In this paper we give results for the Ising model in an external magnetic field, which exhibits a first-order phase transition below the critical temperature, but our method is very general and is extended to other models easily, especially to the Potts model [32].

Here we use an exact numerical technique for evaluation of partition functions, the microcanonical transfer matrix (μCTM), recently invented by one of us (R.J.C.) [31].

II. SCALING THEORY FOR THE DENSITY OF ZEROS

The Hamiltonian for the Ising model in an external magnetic field H is

$$\mathcal{H}=-J\sum_{\langle i,j\rangle}\sigma_i\sigma_j-H\sum_i\sigma_i, \tag{1}$$

where J is the exchange constant, $\langle i,j\rangle$ means the sum over all nearest-neighbor pairs of lattice sites, and $\sigma_i=\pm 1$. In the thermodynamic limit, the free energy per site f is

$$-\beta f=\beta H+\int_{-\pi}^{\pi}g(\theta,t)\ln(x-e^{i\theta})d\theta, \tag{2}$$

where $t=(T-T_c)/T_c$, $x=e^{-h}$, $h=2H/k_BT=2\beta H$, and $g(\theta,t)$ is the density of zeros of the partition function, which satisfies the conditions

$$g(\theta,t)=g(-\theta,t) \tag{3}$$

and

$$\int_0^{\pi}g(\theta,t)d\theta=\frac{1}{2}. \tag{4}$$

The angle θ is the argument of the zeros in the complex-x plane, which, by the Yang-Lee theorem [1], lie on the unit circle. The spontaneous magnetization ($h=0$) is [1,33]

$$m_0(t)=2\pi g(0,t) \tag{5}$$

and the magnetization is given by [33]

$$m(t,h)\approx 4h\int_0^{\pi}\frac{g(\theta,t)}{\theta^2+h^2}d\theta. \tag{6}$$

It is well known that in the thermodynamic limit the properties of the density of zeros determine the critical behavior of the Ising model [1,33].

For a finite-size system of size L, the singular part of the magnetization has the scaling form

$$m(t,h,L)=L^{-d+y_h}m(tL^{y_t},hL^{y_h}), \tag{7}$$

where y_h is the magnetic scaling exponent and y_t the thermal scaling exponent. From Eq. (6) we see that if the magnetization is to be a homogeneous function of h, as in Eq. (7), then θ should scale in the same way as h. Therefore, we have

$$g(\theta,t,L)=L^{-d+y_h}g(\theta L^{y_h},tL^{y_t}). \tag{8}$$

At the critical temperature $t=0$, Eq. (8) reduces to

$$g_c(\theta,L)=L^{-d+y_h}g_c(\theta L^{y_h}), \tag{9}$$

which implies

$$g_c(\theta)\sim|\theta|^{(d-y_h/y_h)}=|\theta|^{1/\delta}. \tag{10}$$

For $t<0$ we expect the transition to be first order with a spontaneous magnetization given by Eq. (5). If we let $\theta\to 0$ and $L\to\infty$ keeping $\theta L^{y_h}=c$ fixed, then

$$g(0,t)=\lim_{\theta\to 0,L\to\infty}g(\theta,t,L)$$
$$=\left(\frac{\theta}{c}\right)^{(d-y_h/y_h)}g\left(c,t\left(\frac{\theta}{c}\right)^{-y_t/y_h}\right)\sim(-t)^{\beta}, \tag{11}$$

where we have assumed the asymptotic form for g,

$$g(c,y)\sim(-y)^{\beta}$$

for large negative values of y, and we have used $\beta=(d-y_h)/y_t$. Comparing Eqs. (5) and (11) we see that we recover the familiar result

$$\lim_{t\to 0^-}m_0(t)\sim|t|^{\beta}. \tag{12}$$

Well below the critical temperature, in the region of the strong first-order phase transition, according to the theory of Fisher and Berker [18], $y_t=y_h=d$, $\beta=0$, and we have the finite density of zeros on the positive real axis, which is a clear indicator of a first-order phase transition even in finite-size systems.

We can summarize these results as

$$\lim_{\theta\to 0}g(\theta,t)\sim\begin{cases}|\theta|^{1/\delta}, & t=0 \quad \text{(second order)}\\ m_0(t), & t<0 \quad \text{(first order)},\end{cases} \tag{13}$$

which is the magnetic analog of the result of Fisher [2] in the complex temperature plane,

$$\lim_{\theta\to 0}g(\theta)\sim\begin{cases}|\theta|^{1-\alpha}, & \text{second order}\\ \text{const (latent heat)}, & \text{first order.}\end{cases} \tag{14}$$

III. NUMERICAL RESULTS

The partition function $Z(x)$ for finite rectangular lattices as polynomials in the magnetic field parameter $x=e^{-2\beta H}$ can be calculated by the microcanonical transfer matrix [31]. These calculations were carried out for square lattices of sizes $4\leqslant L\leqslant 14$ with cylindrical boundary conditions and sizes $4\leqslant L\leqslant 10$ for square lattices with fully periodic boundary conditions. For the smaller lattices it is possible to obtain exact integer values for the restricted density of states $\Omega(M,E)$, which leads to the analytic form for Z,

$$Z(x,y)=\sum_M\sum_E\Omega(M,E)y^Ex^M, \tag{15}$$

where $y=e^{-2\beta J}$. For lattices $L>10$, memory limitations required us to use the restricted canonical transfer matrix, which yields, for a fixed value of y, the coefficients

$$\omega(M)=\sum_E\Omega(M,E)y^E \tag{16}$$

as real numbers of finite precision.

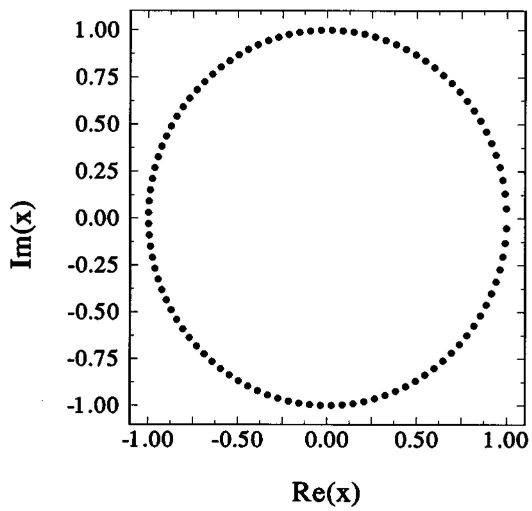

FIG. 1. Zeros of the partition function for a 10×10 Ising model in the complex-x plane at $y = y_c = 0.4142\ldots$.

The calculations of the zeros of such large polynomials require arbitrary precision arithmetic; our calculations were carried out using MATHEMATICA. The zeros for $L = 10$, $y = y_c = 0.4142\ldots$ are shown in Fig. 1 for illustrative purposes, and as expected they lie on the unit circle.

Below y_c the zeros approach the real axis and in the limit $y \to 0$ the zeros are uniformly distributed on the unit circle. As y is increased above y_c a gap opens up and the edge zero, or the Yang-Lee edge singularity [34,35], moves away from the real axis. By using the BST algorithm [36], we extrapolated our results for finite lattices to infinite size, and these results are shown in Fig. 2. Note that below y_c the edge zero lies on the real axis, while as y increases beyond y_c, the angle for the edge zero θ_0 increases. Using Eq. (8), the angle for the edge zero for finite-size systems scales as

$$\theta_0(t,L) = L^{-y_h}\theta_0(tL^{y_t}), \tag{17}$$

so that in the limit $L \to \infty$ we have, for $t > 0$,

$$\theta_0 \sim t^{\nu y_h} = t^{15/8}. \tag{18}$$

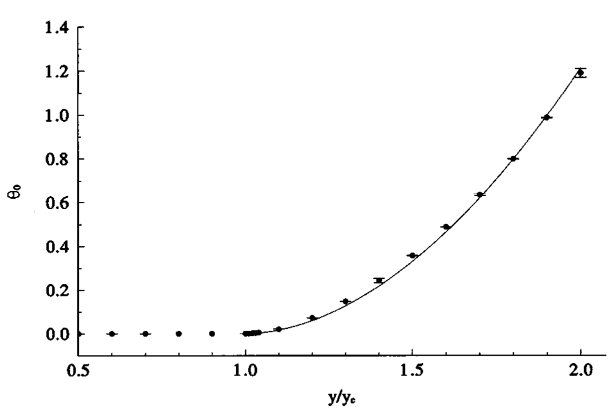

FIG. 2. Edge zero in the complex-x plane as a function of y. The solid curve is a fit to the scaling form $\theta_0(y) \propto (y - y_c)^{15/8}$.

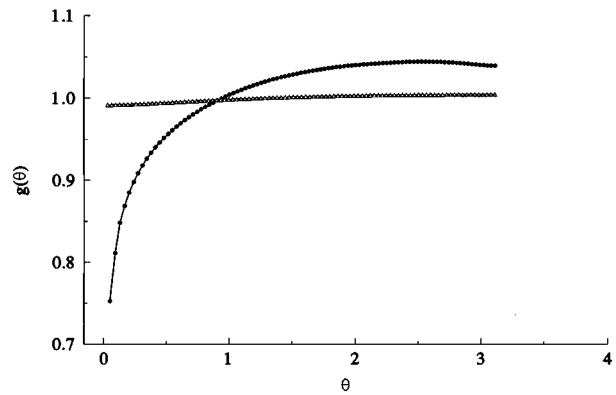

FIG. 3. Density of zeros for $L = 14$, cylindrical boundary conditions, for $y = y_c$ (filled circles) and $y = 0.5y_c$ (open triangles).

Equation (18) agrees with the result of Abe [33], Suzuki [33], Kortman and Griffiths [34], and Itzykson *et al.* [6]. The solid curve in Fig. 2 is a one-parameter fit to Eq. (18).

The density of zeros (per site) at $\overline{\theta_k} = (\theta_{k+1} + \theta_k)/2$ is defined as

$$g(\overline{\theta_k}) = \frac{1}{N}\,\frac{1}{\theta_{k+1} - \theta_k}, \tag{19}$$

where $N = L^d$ and $\{\theta_k, k = 1, \ldots, N\}$ are the arguments of the zeros of $Z(x)$. In Fig. 3 we show the density of zeros for $L = 14$, $y = y_c$, and $y = 0.5y_c$. Note that well below the critical temperature the density is nearly constant, while close to the critical point it decreases sharply as θ tends to zero. Similar results for much smaller lattices have been reported by Suzuki *et al.* [37].

To extract the behavior of the density of zeros in the infinite size limit, we again applied the BST algorithm. In Fig. 4 we show the density at $\theta = 0$ (normalized to unity at zero temperature) and compare it with Onsager and Yang's exact solution for the spontaneous magnetization [38]. Well below the critical temperature our extrapolated values, which scale as L^{-2}, agree very well with the exact spontaneous magnetization. Close to the critical temperature, the domi-

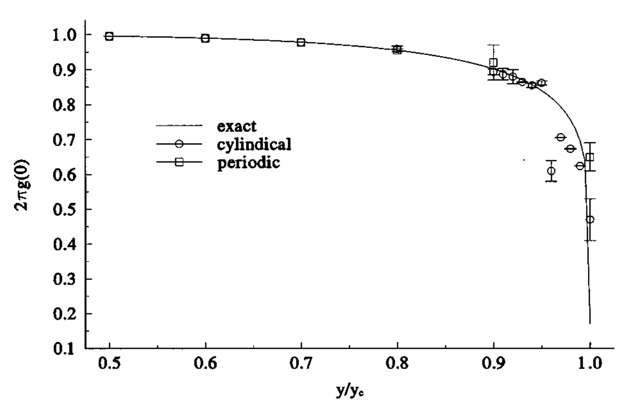

FIG. 4. Extrapolated density of zeros as a function of y. The solid curve is Onsager and Yang's exact result for the spontaneous magnetization. Open circles are our results for cylindrical boundary conditions and open squares are for periodic boundary conditions.

nant scaling exponent crosses over to the magnetic exponent, $y_h = 15/8$. The error bars on our data are estimates from the penultimate BST extrapolants, as described by Henkel and Schütz [36]. It is well known [36] that the BST algorithm does not work well for functions of the form

$$g(x) = g_0 + x^p(a_0 + a_1 x + \cdots), \tag{20}$$

which is what one expects near the critical point. This is clearly shown in our calculations close to y_c, where the agreement is not as good. Also, we expect finite-size scaling to work well when $\xi \sim L$, and for L of the order 14 this limits us to $y/y_c \lesssim 0.97$.

IV. CONCLUSION

The development of techniques [30,31] for calculating the partition function of finite systems has led to the possibility of studying in detail the zeros of the partition function. In order to extrapolate the behavior of the zeros for finite lattices to the thermodynamic limit, we have introduced the finite-size scaling form for the density of zeros of the partition function $g(\theta)$.

We find that the behavior at both first- and second-order transitions can be understood from the finite-size scaling form of the density of zeros $g(\theta,t,L)$. Figures 2–4 show the clear difference between a first-order phase transition and a second-order phase transition. Furthermore, quantities such as the order parameter, which are difficult to calculate by other numerical methods, can be found directly from the density of zeros. The power of this approach is illustrated by our calculation of the spontaneous magnetization of the Ising model, which reproduces the exact result of Onsager and Yang [38] except very close to the critical point. However, we should emphasize that this approach is not limited to problems whose solution is known exactly [39]; the microcanonical transfer matrix can be used to calculate the partition function for any two-dimensional system and some (small) three-dimensional lattices. We are currently carrying out calculations for the Q-state Potts models for $Q = 3 \sim 8$ on relatively small two-dimensional lattices using the μCTM [32]. Larger lattices (and bigger values of Q) require the use of *umbrella sampling* techniques. Calculations for the three-dimensional Ising model in the magnetic-field variable [40] have been completed. Calculations for the Q-state Potts models for $Q \geqslant 3$ on large two- and three-dimensional lattices [41] are currently in progress.

In addition to the density of zeros at and below the critical temperature, which is the main interest of this paper, the density of zeros above the critical temperature can be studied using our method. Kortman and Griffiths [34] showed that above the critical temperature the density of zeros at the Yang-Lee edge is singular for the two-dimensional Ising model. This behavior of the zeros above the critical temperature has also been studied for the hierarchical model [42] and other models [35,43] and by conformal field theory [44]. The details on zeros above the critical temperature are planned to be addressed in another paper [45].

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