Phase transition strengths from the density of partition function zeroes

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We report on a new method to extract thermodynamic properties from the density of partition function zeroes on finite lattices. This allows direct determination of the order and strength of phase transitions numerically. Furthermore, it enables efficient distinguishing between first- and second-order transitions, elucidates crossover between them and illuminates the origins of finite-size scaling. The power of the method is illustrated in typical applications for both Fisher and Lee-Yang zeroes.

1. INTRODUCTION

The characterisation of phase transitions, in particular of their order and strength, is among the hard numerical problems that are common to lattice field theory and spin model physics. Frequently applied techniques focus either on the finite-size scaling (FSS) behaviour of thermodynamic functions such as the specific heat, susceptibility or Binder parameter, or somewhat more "microscopically" on the limiting shape of the underlying probability densities of energy and magnetization as the thermodynamic limit is approached. A related and increasingly popular alternative approach are FSS analyses of zeroes of the partition function [1].

If $t = T/T_c - 1$ denotes the reduced temperature and h the external field, then the FSS of the $j^{\rm th}$ complex partition function zero for a d-dimensional system of linear extent L is given by

$$t_j(L) \sim \left(j/L^d\right)^{1/\nu d} \quad , \qquad (1)$$

$$h_j(L) \sim \left(j/L^d\right)^{(d+2-\eta)/2d} \quad , \qquad (2)$$

where ν and η are the standard critical exponents. In (1) we assume $h = 0$ and $t_j(L)$ are called Fisher zeroes. Conversely, in (2), $t = 0$ is assumed and $h_j(L)$ are the Lee-Yang zeroes. The standard approach to FSS of zeroes is to fix the index to $j = 1$ and extract an estimate for the critical exponents from a range of lattice sizes.

In recent years, however, there have also been some attempts [2] to extract the density of zeroes

(a continuous function) from their (discrete) distribution for a finite and numerically accessible lattice. In view of the increasing importance attached to this approach, we recently suggested an appropriate way this should be done [3].

2. DENSITY OF ZEROES

The partition function for finite L is $Z_L(z) \propto \prod_j (z - z_j(L))$, where z is an appropriate function of temperature or field. We assume the zeroes, z_j, are on a line impacting on to the real axis at the critical point, z_c. Parameterising zeroes on this line by $z_j = z_c + r_j \exp(i\varphi)$ we may define the density of zeroes as $g_L(r) = L^{-d} \sum_j \delta(r - r_j(L))$. The cumulative distribution function of zeroes is then $G_L(r) = \int_0^r g_L(s)ds$ which is j/L^d if $r \in (r_j, r_{j+1})$. At a zero one may assume the cumulative density is given by the average $G_L(r_j) = (2j - 1)/2L^d$.

For a first-order phase transition this integrated density of zeroes is, in the thermodynamic limit, given by

$$G_\infty(r) = g_\infty(0)r \quad , \qquad (3)$$

so that the density is non-vanishing at the real axis [4]. The slope at the origin in (3) is related to the latent heat (magnetization) in the Fisher (Lee-Yang) case via [4] $g_\infty(0) \propto \Delta e$.

For a second-order transition the corresponding expressions for Fisher and Lee-Yang zeroes are [5]

$$G_\infty(r) \propto r^{2-\alpha} \quad \text{and} \quad G_\infty(r) \propto r^{2d/(d+2-\eta)} \quad . \qquad (4)$$

Traditional FSS emerges quite naturally from this density approach. Equating $G_L(r_j)$ to (4) in the second-order Fisher case, gives the usual FSS formula for fixed index zeroes, $r_j(L) \sim L^{-1/\nu}$, where r_j may be taken to be the imaginary part of the jth zero. Similarly, in the Lee-Yang case, one recovers the fixed index FSS formula $h_j(L) \sim L^{-(d+2-\eta)/2}$. Moreover, considering (3) gives $r_j(L) \sim L^{-d}$, explaining also the usual identification of ν with $1/d$ for a first-order temperature driven phase transition.

A plot of $G_L(r_j)$ against $r_j(L)$ should thus (*i*) go through the origin, (*ii*) display L- and j- collapse and (*iii*) reveal the order and strength of the phase transition by its slope near the origin.

3. APPLICATIONS

Superimposing the behaviour (3) and (4) at first- and second-order transitions, the ansatz for the cumulative density can be written as

$$G(r) = a_1 r^{a_2} + a_3 \quad , \tag{5}$$

where we also introduced an additional parameter a_3 signalising the absence of a phase transition: if $a_3 > 0$ the zeroes have already crossed the real axis (broken phase scenario) while for $a_3 < 0$ the zeroes have not yet reached the real axis (symmetric phase). For Fisher zeroes, a first-order transition is indicated if $a_2 \sim 1$ for small r, in which case the latent heat is proportional to the slope a_1. A value of a_2 larger than 1 signals a second-order transition whose strength is given by $\alpha = 2 - a_2$.

2D 10-State Potts Model: This is the paradigm for models exhibiting a strong first-order transition. Using the first six Fisher zeroes for $L = 4$–64 as listed in [6] we find the distribution of zeroes depicted in Fig. 1(a). The excellent data collapse for various L and j indicates that the interpolated $G_L(r_j)$ is the proper choice. Fitting (5) to the $L = 16$–64, $j = 1$–4 data points gives $a_2 = 1.10(1)$ and $a_3 = 0.00004(1)$, a strong indication of a first-order transition. Fixing $a_3 = 0$, $a_2 = 1$, a single-parameter fit close to the origin yields a slope corresponding to latent heat $\Delta e = 0.698(2)$ which compares well with the exact value of 0.6961.
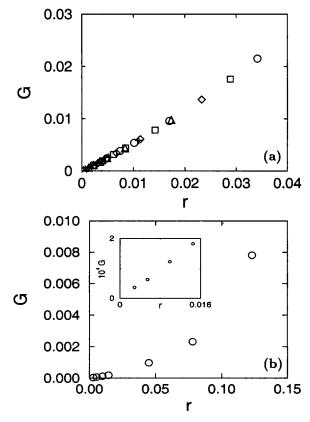

Figure 1. Distribution of partition function zeroes. (a) 2D 10-state Potts model and (b) 3D $L_t = 4$ SU(3) lattice gauge theory.

3D SU(3) Lattice Gauge Theory: Here we consider the deconfinement transition for $L_t L^3$ lattices. The lowest Fisher zeroes for $L_t = 4$ and spatial extent $L = 4$–24 are given in [7]. Applying standard FSS analysis to the $L \geq 14$ data only yields $\nu = 0.35(2)$, compatible with $1/d = 0.33$ and thus indicative of a first-order transition, while fits for $L \leq 8$ suggest a continuous transition. Figure 1(b) shows the distribution of zeroes for all lattices, and the insert highlights $L \geq 14$. The figure, clearly supportive of a non-zero slope through the origin, justifies restricting the analysis to the largest lattices and thereby elucidating the procedure of deciding where FSS sets in. This slope is 0.0121(3), implying a latent heat of 0.0760(19) in agreement with the estimate 0.0758(14) using standard methods [7].
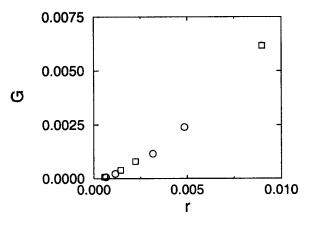
Figure 2. 4D Abelian surface gauge model.

Figure 3. 2D XY model (Lee-Yang case).

4D Abelian Surface Gauge Model: Being the dual of the 4D Ising model one expects for this model, up to logarithmic corrections, mean-field critical exponents $\alpha = 0$, $\nu = 1/2$. The first two Fisher zeroes for lattices of size $L = 3$–12 are listed in [8] where a conventional analysis applied to the first index zero yields the best estimate of $\nu = 0.469(17)$ from the two largest lattices. A fit of (5) to the distribution in Fig. 2 yields a_2 incompatible with unity. Using the data near the origin gives $a_2 = 1.90(9)$ or $\alpha = 0.10(9)$, compatible with zero.

2D XY Model: Here we demonstrate that the density technique is also applicable in the Lee-Yang case. Figure 3 depicts the distribution of these zeroes for the 2D XY model at the critical point, $\beta_c = 1.113$, obtained for lattice sizes $L = 32$–256 [9]. From (4), and with $\eta = 1/4$, one expects $G(r) \sim r^{16/15}$. A three-parameter fit (5) gives $a_3 = 0$, indicating that criticality has indeed been reached. A two-parameter fit now yields $a_2 = 1.063(3)$, compatible with expectation (taking logarithmic corrections into account).

4. CONCLUSIONS

We have discussed a new method to extract the (continuous) density of zeroes from (discrete) finite-size data and demonstrated how this can be used to distinguish between phase transitions of first and second order as well as to measure their streng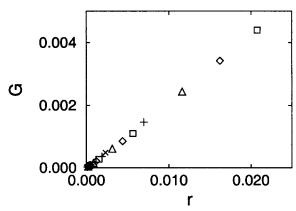ths. The method meets with a high degree of success in lattice field theory and statistical physics and lends new insights into the origins of finite-size scaling.

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