

Analysis of the Density of Partition Function Zeroes - A Measure for Phase Transition Strength

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Abstract. We discuss a numerical analysis employing the density of partition function zeroes which permits effective distinction between phase transitions of first and second order, elucidates crossover between such phase transitions and gives a new way to measure their strengths in the form of latent heat and critical exponents. Application to a number of models demonstrates the efficacy of the technique.

A central theme of statistical physics is how best to distinguish between phase transitions of first and second order from simulational data for finite systems [1]. Numerical methods usually exploit the finite-size scaling (FSS) behaviour of thermodynamic quantities exhibiting rounded and shifted peaks whose shape depends on the order and the strength of the transition and which become singular in the thermodynamic limit at the transition point. An alternative strategy is the analysis of the FSS behaviour of partition function zeroes [2–4]. For field-driven phase transitions one is interested in the *Lee–Yang* zeroes in the plane of complex external magnetic field h [2], and for temperature-driven transitions the *Fisher* zeroes in the complex temperature plane are relevant [3]. For d -dimensional systems below the upper critical dimension, the FSS behaviour of the j^{th} partition function zero (for large j) is given by [4]

$$h_j(L) \sim (j/L^d)^{(d+2-\eta)/2d} \quad , \quad t_j(L) \sim (j/L^d)^{1/\nu d} \quad . \quad (1)$$

Here, L is the system size, η is the anomalous dimension, $t = T/T_c - 1$ is the reduced temperature which is zero in the first formula, and h denotes the external field which is zero in the second formula. The integer index j increases with distance from the critical point.

Despite early efforts [5], it has been considered prohibitively difficult if not impossible to extract the density of zeroes from finite lattice data [6]. This problem has resurfaced recently as zeroes-related techniques have become more widespread [7]. This provides the motivation for the present work in which we wish to suggest an approach suitable for density analyses.

For finite L , the partition function may always be factorized as $Z_L(z) = A(z) \prod_j (z - z_j(L))$, where z stands generically for an appropriate function of

field or temperature and $A(z)$ is a smooth non-vanishing function. Following Suzuki [8] and Abe [9], we assume the zeroes, $z_j(L)$, (or at least those close to the real axis and hence determining critical behaviour) are on a singular line for large enough L , impacting on to the real axis at an angle φ at the critical point $z = z_c$. The singular line is parameterised by $z = z_c + r \exp(i\varphi)$. If we define the density of zeroes as (with $z_j = z_c + r_j \exp(i\varphi)$)

$$g_L(r) = L^{-d} \sum_j \delta(r - r_j(L)) \quad , \quad (2)$$

then the cumulative distribution is a a step function,

$$G_L(r) = \int_0^r g_L(s) ds = j/L^d \quad \text{if } r \in (r_j, r_{j+1}) \quad . \quad (3)$$

It is natural to assume that at a zero, this distribution function is given by the average [2,10], $G_L(r_j) = (2j - 1)/2L^d$.

In the thermodynamic limit and for a phase transition of first order Lee and Yang [2] showed that the density of zeroes has to be non-zero crossing the real axis, $g_\infty(r) = g_\infty(0) + a|r|^w + \dots$. For the cumulative distribution this implies the functional form

$$G(r) = g_\infty(0)r + b|r|^{w+1} + \dots \quad , \quad (4)$$

with the slope at the origin being related to the latent heat (or magnetization) via [2] $g_\infty(0) \propto \Delta e$. At second-order phase transitions, Abe [9] and Suzuki [8] have shown that the necessary and sufficient condition for the specific heat to have the leading critical behaviour $C \sim t^{-\alpha}$, is $g_\infty(r) = Ar^{1-\alpha}$ or

$$G(r) \propto r^{2-\alpha} \quad . \quad (5)$$

For $\alpha = 0$, as is the case in the $d = 2$ Ising model, it has been demonstrated [9] that (5) leads to the correct *logarithmic* divergence in the specific heat.

The preceding considerations show that a plot of $G_L(r_j) = (2j - 1)/2L^d$ against $r_j(L)$ should (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, parameterised generically as

$$G(r) = a_1 r^{a_2} + a_3 \quad . \quad (6)$$

In order to test the efficiency of the density method we have examined six different models [11] for which various sets of partition-function zeroes exist in the literature: 2D 10-state Potts, 3D 3-state Potts, 3D and 2D Ising, (3+1)D SU(3), 4D Abelian Surface Gauge. Here we shall summarize the results for the first three of these models.

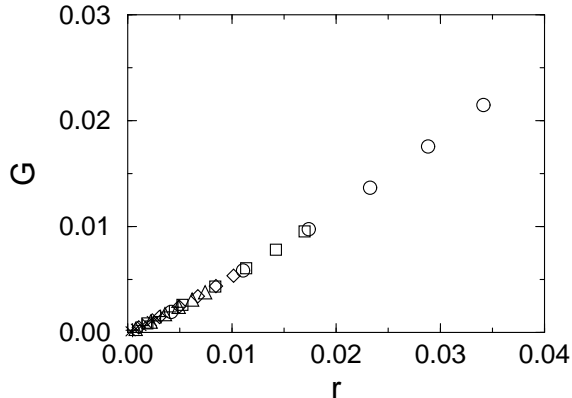


Fig. 1. Distribution of the $L = 16$ – 64 Fisher zeroes for the 2D 10-state Potts model. The symbols \times , $+$, Δ , \circ , \square , and \bigcirc correspond to $j = 1$ – 6 , respectively.

2D 10-state Potts model: The two-dimensional q -state Potts model is the classic testing ground for analytical and numerical studies of first-order ($q > 4$) and second-order ($q \leq 4$) phase transitions. Apart from the transition point, $\beta_0 = \ln(1 + \sqrt{q})$, also the critical exponents ($q \leq 4$), the latent heat ($q > 4$) and various other moments at β_0 are known exactly.

Our analysis of the density of zeroes as tabulated in Refs. [12,13] begins with Fig. 1 where the first six Fisher zeroes are plotted for $L = 16$ – 64 . We observe excellent L - and j -collapse indicating that $G_L(r_j) = (2j - 1)/2L^d$ is the correct functional form. Fitting (6) to the $j = 1$ – 4 points gives $a_2 = 1.10(1)$, $a_3 = 0.00004(1)$, strongly indicative of a first-order phase transition. Indeed, fixing $a_3 = 0$, and fitting the two remaining parameters to the lowest four data points gives $a_2 = 1.008(6)$. Assuming thus $a_2 = 1$, $a_3 = 0$, and applying a single-parameter fit to the full data set we obtain $g(0) = a_1 = 0.501(8)$. Further fits close to the origin yield the slopes and corresponding estimates for the latent heat $\Delta e = 2\pi g(0) \exp(-\beta_0)$ indicated in Table 1.

3D 3-state Potts model: It is generally accepted that this model exhibits a first-order phase transition, albeit a very weak one [14]. This is therefore a typical model used to test new methods to discriminate between first- and second-order transitions. A list of the first few Fisher zeroes (with $z = \exp(-3\beta/2)$) for $L = 10$ – 36 can be found in Refs. [12,13].

Table 1. Fits of the cumulative distribution $G(r)$ to the N lowest Fisher zeroes ($L = 16$ – 64 , $j = 1$ – 4) of the 2D 10-state Potts model.

N	24	16	12	8	4	exact
$g(0)$	0.501(8)	0.479(3)	0.471(2)	0.469(2)	0.463(1)	0.4611
Δe	0.756(11)	0.723(4)	0.711(3)	0.708(2)	0.698(2)	0.6961

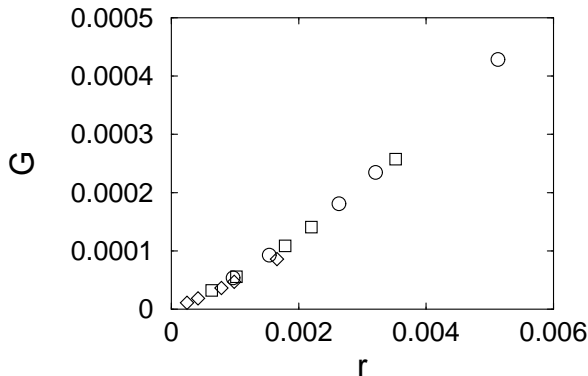


Fig. 2. Distribution of the $L = 18$ – 36 Fisher zeroes for the 3D 3-state Potts model. The symbols \diamond , \square , and \circ correspond to $j = 1, 2$, and 3 , respectively.

Our density analysis is presented in Fig. 2. A 3-parameter fit to all data yields $a_3 = 0.000005(2)$ and becomes even closer to zero as the fit is restricted closer to the origin. Clearly the slope is non-zero near the origin – the signal of a first-order phase transition. In fact, a 2-parameter fit to the data corresponding to $L = 22, 24, 30, 36$, $j = 1$ yields $a_2 = 1.06(2)$. Accepting that the plot is in fact linear near the origin, and fitting for the slope only gives $g(0) = a_1 = 0.0454(9)$. Using $\beta_0 = 0.3670$ [12–14] and $\Delta e = 2\pi g(0)(3/2) \exp(-3\beta_0/2)$, we find that the corresponding latent heat is $\Delta e = 0.247(5)$, comparing well with $0.2409(8)$ from [12,13] and with $0.2421(5)$ from the more sophisticated analysis of [14].

3D Ising model: The first seven exact Fisher zeroes in the $z = \exp(-4\beta)$ plane for $L = 4$ are given in [15], together with numerically determined zeroes for $L = 5$, $j = 1 - 4$. We also use the zeroes in Refs. [12,16] for $L = 7$, $j = 1, 2$; $L = 6, 8, 10, 14$, $j = 1 - 3$; $L = 32$, $j = 1$.

Fitting the ansatz (6) to the full set of $L = 4 - 32$, $j = 1 - 3$ data shown in Fig. 3 indicates a second-order phase transition with $a_2 = 1.81(3)$, $a_3 = -0.00001(1)$. Accepting $a_3 = 0$ and applying a 2-parameter fit to the six data points corresponding to $L = 10 - 32$, $j = 1$, gives $a_2 = 1.879(2)$ or $\alpha = 0.121(2)$, roughly compatible with the weighted “world average” [17] of $\alpha = 0.10985(54)$.

To summarize, we have shown that from the qualitative behaviour of the cumulative density of partition function zeroes we can distinguish between first- and second-order transitions while from the quantitative details we can extract the latent heat and the specific-heat exponent α , respectively. Our method meets with a high degree of success even in the borderline case of the 3D 3-state Potts model where with traditional methods the distinction between a first- and second-order phase transition is quite difficult.

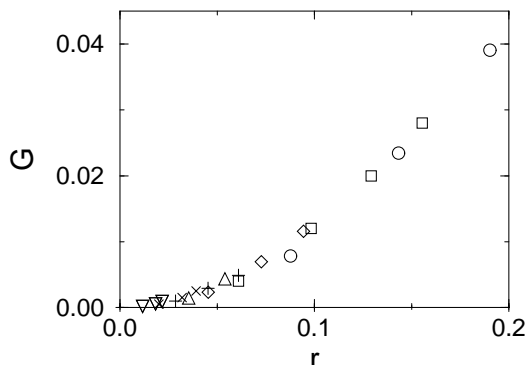


Fig. 3. Distribution of the $L = 4$ – 32 Fisher zeroes for the 3D Ising model. The symbols \times , $+$, \square , and \circ correspond to $j = 1, 2, 3$, and 4 , respectively.

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