The Strength of First and Second Order Phase Transitions from Partition Function Zeroes

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Abstract

We present a numerical technique employing the density of partition function zeroes (i) to distinguish between phase transitions of first and higher order, (ii) to examine the crossover between such phase transitions and (iii) to measure the strength of first and second order phase transitions in the form of latent heat and critical exponents. These techniques are demonstrated in applications to a number of models for which zeroes are available.

1 Introduction

A long standing concern of statistical physics is how best to distinguish between phase transitions of first and second order (for recent reviews, see [1, 2, 3]). First order phase transitions involve the coexistence of two distinct phases and are characterised in the infinite-volume limit by the existence of a discontinuity in the first derivative of the free energy. For temperature (energy) driven first order phase transitions this discontinuity in the internal energy is the latent heat while for field (order parameter) driven first order phase transitions the discontinuity is the spontaneous magnetization. The specific heat and the magnetic susceptibility – the second derivatives of the free energy with respect to the temperature and external field respectively – then exhibit delta function singularities in these cases. This contrasts with the case of a phase transition of second order, where the appropriate second derivative of free energy diverges along with the correlation length. This divergence is characterised by critical exponents labelling the universality class of the system. The infinite volume system does not anticipate the onset of a phase transition of first order as the transition region is approached. There is therefore no critical region and no critical exponents in the usual sense of second and higher order phase transitions.

Finite volume systems do however anticipate the presence of the phase transition as the thermodynamic limit is approached for both of the above scenarios. Numerical methods of identifying the order of a phase transition exploit this anticipation by including finite size scaling (FSS) of extrema of thermodynamic quantities which are singular in the thermodynamic limit at the transition point. The counterparts of these singularities in finite systems are smooth peaks, the shapes of which depend on the order and the strength of the phase transition. The theory and use of FSS is by now well established for both first [4, 5, 6, 7, 8] and second order [9, 10, 11] scenarios.

An increasingly popular alternative to the analysis of these extrema is the use of the FSS behaviour of partition function zeroes [12, 13, 14, 15, 16]. For field driven phase transitions one is interested in the Lee–Yang zeroes in the plane of complex external magnetic field [12]. For temperature driven phase transitions the Fisher zeroes in the complex temperature plane are relevant [13]. In this case, FSS of the first Fisher zero yields the correlation length critical exponent ν. By formally identifying ν with $1/d$ in the first order case, FSS of this first zero can often be used to discriminate between the two types of phase transition. The strength of the transition, on the other hand, has to our knowledge heretofore not been determined from properties of the zeroes, but only by direct measurement of the latent heat or the interface tension. Analogous statements apply in the field driven case.

Here we wish to present an alternative method to investigate the strength of phase transitions. This method involves the *density* of zeroes – a quantity directly proportional to the latent heat in the first order case. The emphasis in this paper is on interpretation rather than new simulations and our motivation comes from recent experience with numerical studies of the density of zeroes [17, 18] coupled to the ongoing discussions regarding first order phase transitions [2]. The rest of the paper is organised as follows. The properties of partition function zeroes are discussed in Sec. 2. In Sec. 3 we present the results of our analysis applied to previously published data, and Sec. 4

contains our conclusions.

2 Partition Function Zeroes

The study of partition function zeroes was pioneered by Lee and Yang [12] in the complex external ordering variable for field driven phase transitions. Study of zeroes in the complex temperature plane was initiated by Fisher [13]. For convenience, one often refers to the zeroes in the complex external field strength plane as Lee-Yang zeroes and those in the complex temperature plane (in the absence of an external field) as Fisher zeroes. The emphasis in this paper is on Fisher zeroes, although the techniques can also be applied to Lee-Yang zeroes.

Itzykson, Pearson and Zuber [14] gave the FSS of partition function zeroes for d-dimensional systems below the upper critical dimension. They suggested a compact description of scaling which for the jth Lee-Yang and Fisher zero respectively reduces to (for large j)

$$h_j(L) \sim \left(\frac{j}{L^d}\right)^{\frac{d+2-\eta}{2d}} \quad , \qquad t_j(L) \sim \left(\frac{j}{L^d}\right)^{\frac{1}{\nu d}} \quad . \tag{2.1}$$

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. The FSS at and above the critical dimension was determined in [16] and [15] respectively. This behaviour of partition function zeroes offers a (generally very accurate) way to determine (i) the critical temperature and (ii) the critical exponents which describe the thermodynamic critical properties of the system.

Previous numerical studies of partition function zeroes mostly employed the following strategies:
(i) Determination of the distribution of zeroes to study the complex parameter phase diagram and to check (in a qualitative way) if the zeroes appear to cross the real axis – evidence for the existence of a phase transition [19, 20, 21, 22, 23, 24, 25].
(ii) Quantitative measurement of (finite size) scaling behaviour of those zeroes with the smallest imaginary parts to determine the critical exponents [16, 26, 27, 28, 29, 30, 31, 32, 33, 34] with possibly similar analyses applied separately to higher index zeroes [35] or determination of impact angle [36, 37, 38].
(iii) Fixed volume plots for Lee–Yang zeroes indicating onset of non–zero density of zeroes at first order phase transitions [24, 39].

Despite an early study [40], it was long considered difficult if not impossible to estimate the density of zeroes from their distribution for a finite lattice [21]. In recent years, however, there have been some attempts to extract the density of zeroes from numerical studies [17, 41]. In view of the increasing importance attached to this approach, we wish to suggest an appropriate way this should be done.

To this end, we present a novel and powerful technique with which (i) the order of the phase transition and (ii) the strength of the phase transition can be determined. This means determination of the latent heat in the first order case and measurement of the critical exponent α of the specific

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heat in the second order case. The method also elucidates crossover between second and first order transitions. We study the cumulative distribution of zeroes – curves involving L and j collapse – from which the density of zeroes and hence the order and strength of the phase transition can be determined.

2.1 Density of Zeroes

We start with the factorised representation of the partition function,

$$Z_L(z) = A(z) \prod_j (z - z_j(L)) \quad , \tag{2.2}$$

where z stands generically for an appropriate function of temperature (in the Fisher case) or field (in the Lee-Yang case), L is the linear extent of the lattice and $A(z)$ is a smooth function that never vanishes. The free energy density follows as

$$f_L(z) = \frac{1}{L^d} \ln Z_L(z) = \frac{1}{L^d} \ln A(z) + \frac{1}{L^d} \sum_j \ln (z - z_j(L)) \quad . \tag{2.3}$$

The first term on the right contributes only to the regular part of thermodynamic functions and we henceforth drop it. The remainder, which we refer to as $f_L^s(z)$, gives rise to singular behaviour.

Following Abe [42], we assume the zeroes, z_j, (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 $z = z_c + r \exp(i\varphi)$. Define the density of zeroes as (with $z_j = z_c + r_j \exp(i\varphi)$)

$$g_L(r) = L^{-d} \sum_j \delta(r - r_j(L)) \quad . \tag{2.4}$$

The free energy is

$$f_L^s(z) = \int_0^R g_L(r) \ln (z - z_c - re^{i\varphi}) dr + \text{c.c.} \quad , \tag{2.5}$$

where c.c. means complex conjugate and R is some appropriate cutoff. The cumulative distribution function of zeroes is defined as

$$G_L(r) = \int_0^r g_L(s) ds \quad . \tag{2.6}$$

For a finite size system, therefore, this is a step function with

$$G_L(r) = \frac{j}{L^d} \qquad \text{if} \quad r \in (r_j, r_{j+1}) \quad . \tag{2.7}$$

It is natural to assume that at a zero, this cumulative density is given by the average [12, 15, 43]

$$G_L(r_j) = \frac{2j - 1}{2L^d} \quad . \tag{2.8}$$

In the thermodynamic limit and for a phase transition of first order Lee and Yang [12] already showed that the density of zeroes has to be non–zero crossing the real axis,

$$g_\infty(r) = g_\infty(0) + ar^w + \dots \quad . \tag{2.9}$$

This corresponds to the cumulative distribution of zeroes

$$G_\infty(r) = g_\infty(0)r + br^{w+1} + \dots \quad , \tag{2.10}$$

where the slope at the origin is related to the latent heat (or magnetization) via [12]

$$\Delta e \propto g_\infty(0) \quad . \tag{2.11}$$

Abe [42] has shown that the necessary and sufficient condition for the specific heat at a second order phase transition to have the leading critical behaviour $C \sim t^{-\alpha}$, is (see also [44])

$$g_\infty(r) \propto r^{1-\alpha} \quad . \tag{2.12}$$

If $\alpha = 0$, as is the case in the $d = 2$ Ising model, (2.12) leads to a logarithmic divergence in the specific heat [42]. The corresponding expression for the cumulative distribution (integrated density) is

$$G_\infty(r) \propto r^{2-\alpha} \quad . \tag{2.13}$$

Thus while the scaling behaviour of the position of the first (few) zeroes in the complex temperature plane can be used to identify ν, the density of zeroes gives the strength of the transition. 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.

2.2   Finite Size Scaling

The above density approach yields new insights into traditional finite size scaling which emerges quite naturally from it for both first and second order phase transitions. Traditionally, FSS is based on a hypothesis whereby the only relevant length scale of the system is the correlation length. The FSS hypothesis can, in turn, be justified on renormalization group grounds.

Alternatively, and in the second order scenario, one may start from (2.8) and (2.13) with fixed j and identify G_L and G_∞ for large enough L. The distance of a zero from the critical point is

$$r_j(L) \sim \left(\frac{2j-1}{L^d}\right)^{1/(2-\alpha)} = \left(\frac{2j-1}{L^d}\right)^{1/\nu d} \sim L^{-\frac{1}{\nu}} \tag{2.14}$$

from hyperscaling. This is the standard formula for FSS of Fisher zeroes at a second order phase transition implied by [14]. It also recovers the compact expression (2.1) for high index zeroes. From this, FSS for all thermodynamic quantities can be found [16, 42, 44]. For the specific heat, for example, (2.3) yields

$$C_L(z) = \frac{1}{L^d} \sum_j \frac{1}{(z-z_j)^2} \quad . \tag{2.15}$$

At $z = z_c$, and assuming that pseudocritical behaviour is dominated by the lowest few zeroes [16], one finds the FSS of specific heat is

$$C_L(z_c) \sim L^{-d}(z_c - z_j)^{-2} \sim L^{-d}L^{2/\nu} = L^{\alpha/\nu} \quad . \tag{2.16}$$

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Thus the usual formulae for leading order FSS are recovered.

Also, in the first order case, (2.8) and (2.10), with fixed j give

$$r_j(L) \sim L^{-d} \quad , \tag{2.17}$$

and hence $C_L(z_c) \sim L^d$, explaining the formal identification of ν with $1/d$ alluded to in the introduction.

3   Analysis of Various Models

In the following examples we perform fits to the cumulative density of zeroes allowing for first or second order behaviour,

$$G(r) = a_1 r^{a_2} + a_3 \quad . \tag{3.1}$$

where we also allow for an additional parameter a_3. The criterion for a good fit, apart from good data collapse (in L and j), is that a_3 be compatible with zero. In fact, a value of a_3 inconsistent with zero indicates the absence of a phase transition, for, if $a_3 > 0$, the zeroes have already crossed the real axis corresponding to the broken phase and if $a_3 < 0$ the zeroes remain away from the real axis which is the situation in the symmetric phase. A first order phase transition is then hinted at if $a_2 \sim 1$ for small r (constant slope near the origin). Then the latent heat is proportional to the measured slope a_1. A value of a_2 larger than (and not compatible with) 1 is indicative of a second order phase transition. In this case, the strength of the transition is given by $\alpha = 2 - a_2$. The cumulative distribution of zeroes is given by (2.8) and the parameter r may be taken to be the imaginary part of the position of the jth zero. That is, in practice, we fit to

$$\frac{2j-1}{2L^d} = G_L(r_j) = a_1 (\text{Im} z_j(L))^{a_2} + a_3 \quad . \tag{3.2}$$

A straightforward error analysis is not possible because of the semi-discrete nature of this equation. We employ a proceedure adapted from [45] and which requires some explanation.

We observe that (2.8) arose from the natural assumption that the density associated with a zero in the finite volume case is obtained from averaging the exact formula (2.7). If one relaxes this assumption, and, since the cumulative density is monotone, its actual value cannot deviate from the mean position (2.8) by more than $\pm 1/2L^d$. Denote the data point corresponding to the jth zero of the size L lattice by $G_j^{\text{obs}}(L)$. Inspired by [45], initially, assign an error $\sigma_j(L) = \sigma_{\text{arb}}/L^d$ to this data point, where σ_{arb} is a fixed arbitrary number. Set

$$\chi_1^2 = \sum_{L,j} \frac{(G_j^{\text{obs}}(L) - G_j^{\text{exp}}(L))^2}{\sigma_j(L)^2} = \sum_{L,j} \frac{L^{2d}}{\sigma_{\text{arb}}^2}(G_j^{\text{obs}}(L) - G_j^{\text{exp}}(L))^2 \quad , \tag{3.3}$$

where $G_j^{\text{exp}}(L)$ is the expected density value coming from the model (3.1) and the sum runs over the lattice sizes and indices used in the fit. One proceeds in the usual way to fit the parameters a_i in (3.1) by minimizing χ_1^2. The errors associated with a_i resulting from this fit are denoted da_i^{arb}.

Assume, now, each data point has, in fact, an error σ/L^d. The corresponding chi-squared is

$$\chi_2^2 = \sum_{L,j} \frac{L^{2d}}{\sigma^2}(G_j^{\text{obs}}(L) - G_j^{\text{exp}}(L))^2 = \frac{\sigma_{\text{arb}}^2}{\sigma^2}\chi_1^2 \quad . \tag{3.4}$$

Assuming, the model fits well, this should be close to the number of degrees of freedom N_{dof}. In this case, the error assigned to each point becomes

$$\sigma^2 = \sigma_{\text{arb}}^2 \chi_1^2/N_{\text{dof}} = \chi_1^2/N_{\text{dof}} \quad , \tag{3.5}$$

if σ_{arb} is chosen to be unity. Furthermore, the true errors associates with the fit parameters are

$$da_i = \frac{\sigma}{\sigma_{\text{arb}}}da_i^{\text{arb}} = \sigma da_i^{\text{arb}} \tag{3.6}$$

if $\sigma_{\text{arb}} = 1$. One notes, however, that as in [45], this approach prohibits an independent goodness-of-fit test.

3.1   The Potts Model

The q–state Potts model is the classic testing ground for the analytical and numerical study of first and second order phase transitions. Despite the lack of a complete solution for general q, some exact results are known. In two dimensions, the model has a second order phase transition for $q \leq 4$ and a first order phase transition for $q > 4$. In terms of the Boltzmann factor, $\beta = 1/k_B T$, the critical temperature is given by $\beta_c = \ln(1 + \sqrt{q})$ and the exact values of the latent heat and a number of other thermodynamic quantities are known [46]. In the three dimensional Potts model, it is numerically established that there is a second order phase transition in the Ising case ($q = 2$) and a first order phase transition for $q \geq 3$. For a review on the Potts model, see [47].

In the following examples we use the zeroes published in a number of papers. If, for the Fisher zeroes, the parameter z used is $\exp(-\kappa\beta)$ where κ is a trivial scale parameter depending on the model under consideration, then the latent heat (for a first order phase transition) is [12]

$$\Delta e = \kappa z_c 2\pi g(0) \quad , \tag{3.7}$$

where $z_c = \exp(-\kappa\beta_c)$ is the coupling at the phase transition point and $g(0)$ is the slope of the cumulative density plots.

The $d = 2, q = 10$ Potts Model: Villanova [30] has listed the first six Fisher zeroes in the $z = \exp(-\beta)$ plane (i.e., $\kappa = 1$) for the two-dimensional 10–state Potts model for lattice sizes $L = 4, 8, 16, 24, 32, 38, 48,$ and 64 (see also [31]). In [30, 31] a conventional FSS analysis was applied to the first index zeroes *only*. The leading scaling behaviour using the three largest lattices yielded an acceptable fit and $\nu^{-1} = 2.0026(11)$. Including the leading additive correction term gives an acceptable fit for $L = 24, 32, 38, 48$ and 64 with the result $\nu^{-1} = 2.0028(17)$. This is good evidence for $\nu = 1/d$ and hence a first order phase transition. However, the determination of the lattice size above which FSS (or FSS with corrections) sets in is, by necessity, somewhat arbitrary. Indeed,
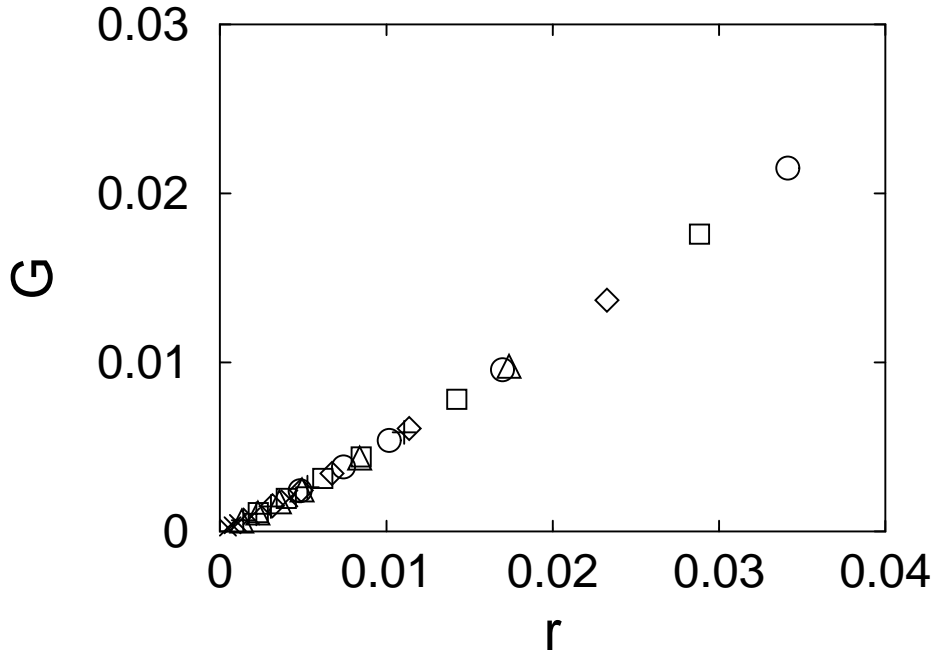
Figure 1: Distribution of Fisher zeroes for the $d = 2$, $q = 10$ Potts model which has a strong first order phase transition. The symbols $\times$, $+, \triangle, \diamond, \square$, and $\circ$, correspond to $j = 1, 2, 3, 4, 5$, and 6, respectively, obtained on lattices of size $L = 16$-64.

Table 1: Fits of the $d = 2$, $q = 10$ Fisher zeroes to the cumulative distribution $G = g(0) \times \text{Im}z$. Here, the N lowest zeroes from the $L = 16$-64, $j = 1$-4 data are used. As the origin is approached, the resulting estimates of the latent heat approach the exact value 0.6961.

N	24	20	16	12	08	04
$g(0)$	0.501(8)	0.486(4)	0.479(3)	0.471(2)	0.469(2)	0.463(1)
Δe	0.756(11)	0.734(6)	0.723(4)	0.711(3)	0.708(2)	0.698(2)

when one extends the analysis to higher index zeroes (FSS applied to each index separately), one finds that when corrections are ignored, no two-parameter fit gives an acceptable result. Allowing for corrections however (fitting to four parameters) may yield acceptance indicative of a first order phase transition. These higher index zeroes were not however analysed in [30, 31].

Our analysis of the density of zeroes begins with Figure 1 where all six zeroes are plotted for $L = 16$–64. We do not plot the results from smaller lattices simply for clarity – including them will only give some more data points to the right of the figure and will not affect the slope in the region of interest, namely near the origin. Figure 1 displays excellent L– and j– collapse indicating that (2.8) is the correct functional form of the density of zeroes. Fitting (3.1) to the $L = 16$–64, $j = 1$–4 points gives $a_1 = 0.84(2)$, $a_2 = 1.10(1)$ and $a_3 = 0.00004(1)$ strongly indicative of a first order phase transition. Fixing $a_3 = 0$, and fitting for the two remaining parameters again gives a_2 close to 1. Indeed, such a fit to the lowest four data points gives $a_2 = 1.008(6)$. Fixing $a_2 = 1$
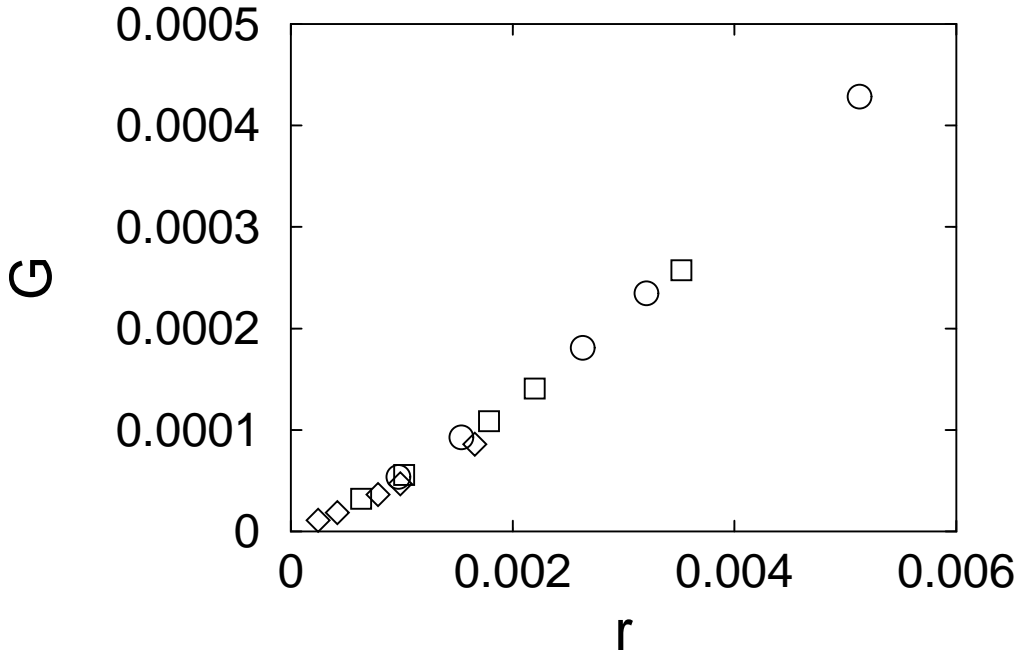
Figure 2: Distribution of the $L = 18 - 36$ Fisher zeroes for the $d = 3$, $q = 3$ Potts model which has a weak first order phase transition. The symbols $\diamond, \square$ and $\bigcirc$ correspond to $j = 1, 2$ and 3, respectively.

(and $a_3 = 0$) and applying a single parameter fit to the full data set yields $g(0) = a_1 = 0.501(8)$. Further fits close to the origin yield the slopes indicated in table 1. From (3.7), the latent heat is $\Delta e = 2\pi g(0)/(1 + \sqrt{10})$ and these corresponding values are also listed in the table and appear to converge to the exact value 0.6961.

The $d = 3$, $q = 3$ Potts Model: It is generally accepted that the three dimensional three state Potts model has a first order phase transition, albeit a very weak one [48]. This is therefore a typical model used to test new methods to discriminate between phase transitions of first and second order. A list of the first few Fisher zeroes (in the $z = \exp(-3\beta/2)$ plane) for the $d = 3$, $q = 3$ Potts model for $L = 10$–36 can be found in [30, 31]. In fact there is some ambiguity regarding the labelling of the higher zeroes in [30, 31] as can be seen by comparing their distributions for different L. To be cautious, therefore, our analysis only employs the zeroes with index $j = 1$–3. Again in [30, 31], ν is determined by applying FSS to the first index zeroes only. However, even with the first index zeroes, one finds rather bad fits for any combination of more than two lattice sizes and these are not much improved upon by allowing for corrections. The way out taken by [30, 31] is to measure ν using the first index zeroes for pairs of consecutive lattice sizes in order to convince oneself that ν approaches $1/d$ as L increases. Their result using only the two largest lattices is $\nu^{-1} = 2.955(26)$. Thus the evidence presented points towards a first order phase transition, with, however, the caution that "with the presented trend from other lattices, one does not feel confident to exclude accidental agreement".

Our density analysis is presented in Figure 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 $a_1 = 0.070(8)$, $a_2 = 1.06(2)$. 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 $\beta_c = 0.3670$ [30, 31, 48] and $\Delta e = (3/2) \exp\left[-(3/2)\beta_c\right] 2\pi g(0)$, from (3.7) with $\kappa = 3/2$, we find that the corresponding latent heat is $0.247(5)$ comparing well with $0.2409(8)$ from [30, 31] and with $0.2421(5)$ from the more sophisticated analysis of [48].

The $d = 3$ Ising Model: The Fisher zeroes in the $u = \exp(-4\beta)$ plane for the three dimensional Ising model with $L = 4$, $j = 1 - 7$ have been determined exactly in [20] and are listed in [37] where the zeroes for $L = 5$, $j = 1 - 4$ are also determined. We also use the zeroes for $L = 7$, $j = 1, 2$ from [35], those for $L = 6, 8, 10, 14$, $j = 1, 2, 3$ which are listed in [30, 32] and $j = 1$ zeroes up to $L = 32$ recently obtained in [49]. The cumulative density of zeroes (using all of the above data)
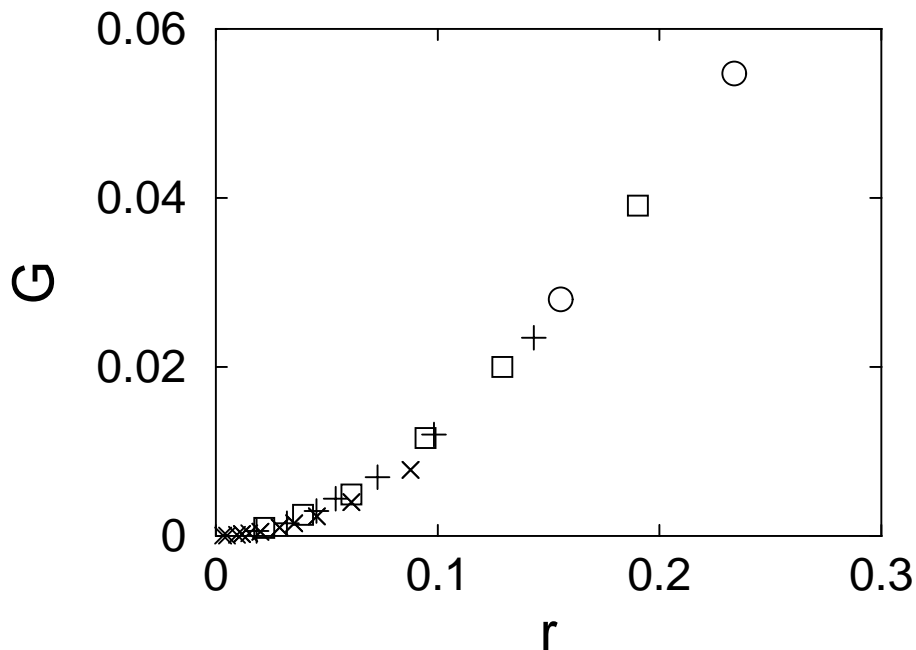

Figure 3: Distribution of Fisher zeroes for the $d = 3$ Ising model which has a second order phase transition. The symbols $\times, +, \square$ and $\bigcirc$ correspond to $j = 1, 2, 3$ and 4, respectively and the lattice size ranges from 4 to 32.

is plotted in Figure 3. Fitting the full set of $L = 4 - 32, j = 1 - 3$ data to (3.1) indicates a second order phase transition with $a_2 = 1.81(3)$, $a_3 = -0.00001(1)$. Accepting the plot goes through the origin and applying a 2-parameter fit to the $L \geq 6$ data gives $a_2 = 1.874(42)$ which corresponds to $\alpha = 0.126(42)$. Fitting closer to the origin (using the six data points corresponding to $L = 10$–32, $j = 1$ gives $a_2 = 1.879(2)$ or $\alpha = 0.121(2)$, close to the expected value $\approx 1/8$. Note that the value of ν was measured to be $0.612(22)$, $0.6295(10)$, and $0.6285(19)$ in references [35],[37], and [30, 32]. The corresponding α values from hyperscaling are $\alpha = 2 - \nu d = 0.164(66)$, $0.1115(30)$,
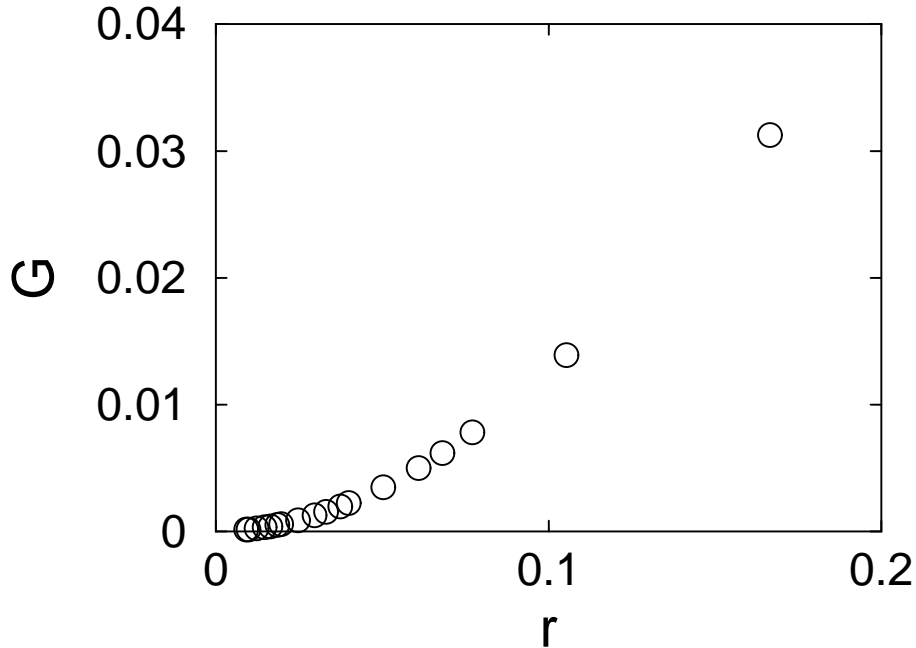
Figure 4: Distribution of $j = 1$ Fisher zeroes for the Ising model in two dimensions which has a second order phase transition. The lattice sizes range from $L = 4$ to $L = 64$.

Table 2: Fits of the $d = 2$, $q = 2$ Fisher zeroes to the cumulative distribution $G = a_1 \times (\mathrm{Im}z)^{a_2}$. As the origin is approached, the parameter a_2 approaches 2.

L	4-64	10-64	16-64	20-64	24-64	32-64	36-64	40-64	48-64
a_2	1.924(9)	1.958(4)	1.968(3)	1.972(2)	1.975(2)	1.978(1)	1.980(1)	1.981(1)	1.982(1)

and 0.1145(54), respectively. A weighted mean value of ν from various literature estimates for the $d = 3$ Ising model is given in [50] as 0.63005(18) and corresponds to $\alpha = 0.10985(54)$.

The $d = 2$ Ising Model: The (numerically) exact Fisher zeroes for the Ising model in two dimensions for large lattices with periodic boundary conditions (up to $L = 64$) have only recently been determined in [51]. These are plotted in the $z = \exp(-4\beta)$ plane in Figure 4.

The results from two parameter fits to the L–ranges available are given in table 2. Fitting near the origin gives $a_2 = 1.982(1)$, close to 2 which corresponds to $\alpha = 0$. This value for α is both sufficient and necessary to attain the logarithmic singularity of the specific heat in the $d = 2$ Ising model [42].

Although only the first index zeroes are available in this case, the cumulative density method is still useful. The conventional FSS technique can only yield the ratio α/ν from the analysis of specific heat. Furthermore, here the specific heat leading scaling behaviour is complicated by logarithms while the density and cumulative density are free from such terms [42]. Also, FSS applied to the
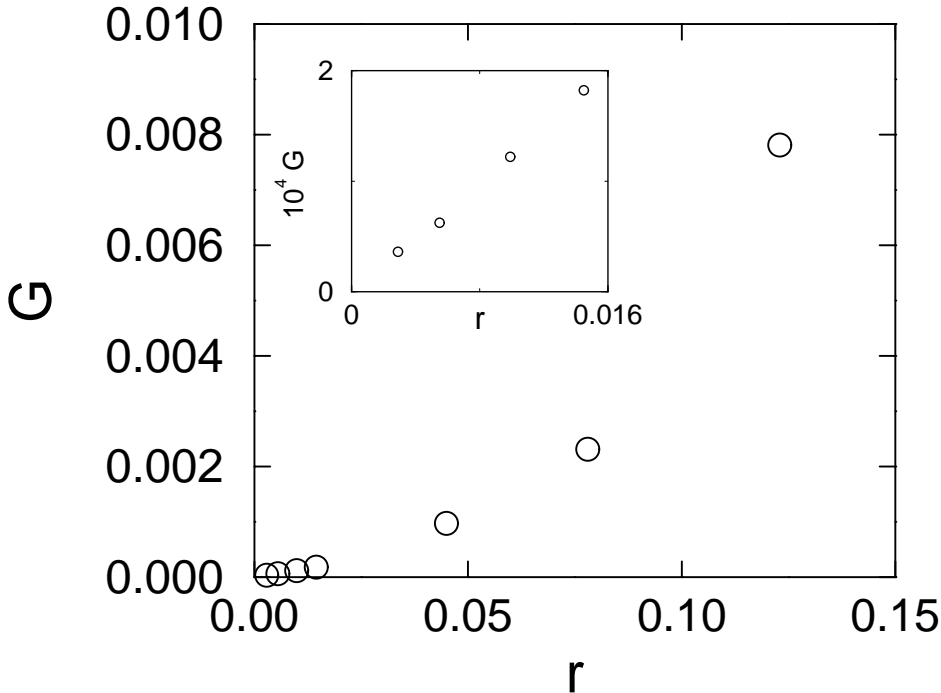
Figure 5: Distribution of Fisher zeroes for the $d = 3$, $SU(3)$ pure gauge model which has a first order phase transition. The insert is a blow-up of the region near the origin.

zeroes themselves (in the conventional manner) yields the correlation length critical exponent ν, which is related to α in cases where hyperscaling holds. The cumulative density method is thus the only method by which α can be measured *directly* from finite size data.

3.2 Lattice Gauge Theories

Since lattice gauge theories may be viewed as statistical systems (see, e.g., [52] for a review), we complete this section by presenting some applications of our method to published zeroes of such theories.

The $d = 3$, $SU(3)$ Model: Alves, Berg and Sanielevici [33] have analysed the $SU(3)$ finite temperature deconfining phase transition using the FSS of the lowest Fisher zeroes for $L_t L^3$ lattices (see also [38]). They determined the zeroes in β for $L_t = 4$ on lattices of size $L = 4, 6, 8, 14, 16, 20$, and 24. Their conventional FSS analysis gives the "illusion of a second order phase transition" when lattice sizes $L = 4$, 6 and 8 are involved in the fits. Claiming FSS only sets in for larger lattices, their best result is $\nu = 0.35(2)$ for $L = 14$–24. This value is compatible with $\nu = 1/d = 0.33$ and thus indicative of a first order phase transition. Figure 5 is a plot of the cumulative density of zeroes for all lattice sizes. The insert is the same plot using only $L = 14$–24. The figure, clearly supportive of a non-zero slope through the origin, justifies restriction of the analysis to these largest lattices and thereby elucidating the procedure of deciding where FSS sets in. This slope is 0.0121(3), which gives a latent heat of 0.0760(19). This is fully consistent with the result for the latent heat coming from conventional methods [33] which is 0.0758(14).
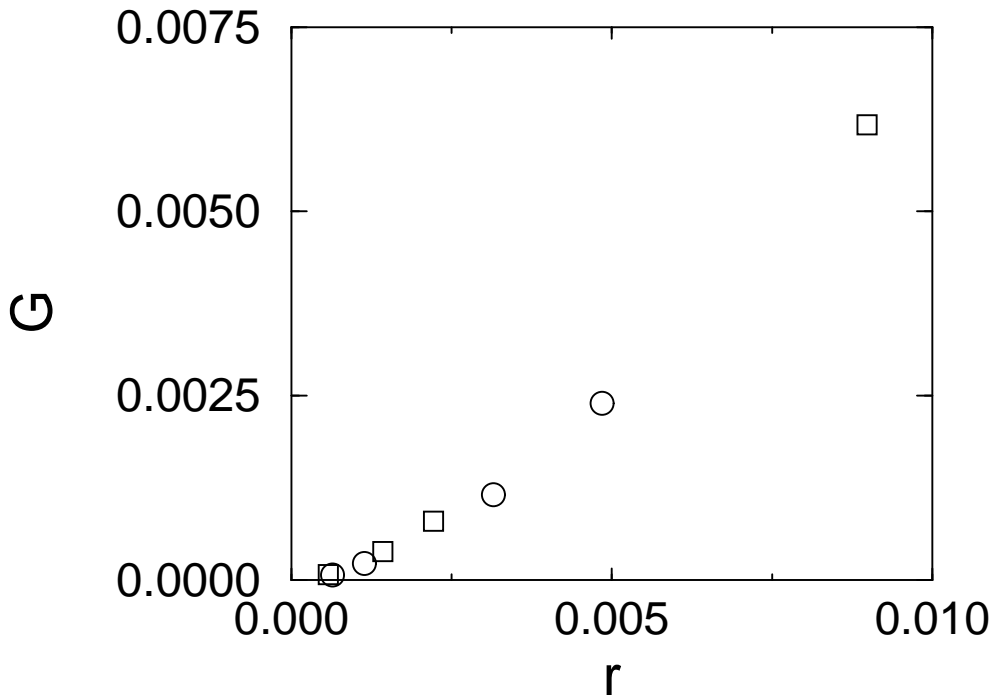
Figure 6: Distribution of Fisher zeroes for the four dimensional abelian surface gauge model which has a second order (mean-field like) phase transition equivalent by duality to the four dimensional Ising model. The $\square$ and $\bigcirc$ correspond to the $j = 1$ and $j = 2$ index zeroes respectively.

The $d = 4$, Abelian Surface Gauge Model: In the abelian surface gauge model, abelian gauge variables are assigned to plaquettes of the lattice. Models such as this are of relevance to supergravity theories amongst others. It is known that the $d = 4$ version is dual to the $d = 4$ Ising model, which, up to logarithmic corrections has mean field critical exponents [16]. One therefore expects the $d = 4$ abelian surface gauge model also to be characterised by mean field exponents (up to corrections) with $\alpha = 0, \nu = 1/2$.

This model was analysed in [53] where the first and second Fisher zeroes for lattices of size $L = 3$ to $L = 12$ are listed. A conventional FSS analysis applied to the first index zero yields the best estimate of $\nu = 0.469(17)$ from the two largest lattices ($L = 9$ and $L = 12$). It is remarked that inclusion of the smaller lattices worsens the fit and drives ν away from $1/2$. The appearance of a bimodal structure in the energy histograms was discussed in [53] as a spurious indication of a first order transition, at odds with the critical exponents which clearly favour second order.

A fit of the data of [53] to (3.1) yields a_2 incompatible with unity (see Figure 6). In fact, a two parameter fit near the origin (using the lowest 6 zeroes) yields $a_2 = 1.90(9)$ corresponding to $\alpha = 0.10(9)$, compatible with zero. Note, again, that only the region near the origin in Figure 6 is of interest. The slope at the origin is not compatible with a first order transition and the bimodal structure of the energy histograms observed in [53] can only be a (so far unexplained) finite size effect which merits further investigation.

4 Conclusions

The two basic questions to be addressed in the numerical study of phase transitions are (i) identification of the order of the transition and (ii) determination of physical quantities such as the transition point and critical exponents or the latent heat.

We have presented a method to determine the order and strength of phase transitions based on an analysis of the cumulative density of partition function zeroes. From the qualitative behaviour of this cumulative density we can distinguish between first and second order while from the quantitative details we can extract the latent heat in the case of first order transitions and the specific heat exponent α in the second order case. This should be compared with traditional finite size analyses where only the combination α/ν can be extracted directly.

Our method meets with a high degree of success even in the borderline cases of the $d = 3$, $q = 3$ Potts model and $SU(3)$ finite temperature lattice gauge theory where the distinction between first and second order phase transitions is quite difficult. There, the conclusions based on the conventional FSS analysis are tenuous or ambiguous. Furthermore, the method leads to alternative insights into statistical physics methods in general and especially illuminates the origin of finite size scaling.

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