

Finite size scaling of branch-points in lattice models

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A finite size scaling method is proposed in which the branch-points of the largest transfer matrix eigen-value are used to calculate thermal and magnetic exponents. The effect of different boundary conditions is considered and the method is tested for the q -state Potts model.

Key words: finite size scaling, transfer matrix, eigen-value, branch-point, exponents, Potts model.

1 Introduction

According to the Lee-Yang circle theorem [1], the zeros of the partition function of the ferromagnetic Ising model, in the complex plane \mathbb{C}_H of the variable $z_H = \exp(-2\mathcal{H}/k_B T)$, lie on the circle $|z_H| = 1$. This result has been shown to apply to a larger class of models [2–5] but this does not include the $q > 2$ Potts model for which the circle theorem does not hold [6,7]. The distribution of zeros of the partition function in the complex pair-interaction plane \mathbb{C}_T of the variable $z_T = \exp(-2J/k_B T)$ has also been investigated [8,9]. For the zero-field square-lattice Ising model the asymptotic locus of zeros is given by the Fisher circles [8,10]

$$z_T = \sqrt{2} \exp(i\vartheta) \pm 1. \quad (1)$$

These circles are a result of the self-duality and spin-inversion symmetry of the Ising model. The duality (but not spin-inversion) generalizes to the q -state Potts model [11] which has a self-dual (Potts) circle

$$z_T = \sqrt{q} \exp(i\vartheta) + 1. \quad (2)$$

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A theory of finite size scaling of partition function zeros was developed by Itzykson *et al.* [12]. For a system of length M in each dimension they proposed the scaling forms

$$|z_T^\circ - z_T^c| \sim M^{-y_T}, \quad |z_H^\circ - z_H^c| \sim M^{-y_H}, \quad (3)$$

for the zero z_T° closest to the critical value z_T^c in \mathbb{C}_T and the zero z_H° closest to the critical value z_H^c in \mathbb{C}_H . This approach was extended by Glasser *et al.* [13], who obtained an explicit asymptotic form valid for an unbounded number of zeros. Monte Carlo calculations using (3) have been carried out by Marinari [14] and Kenna and Lang [15] and the method has been applied to a model with a wetting transition by Smith [16].

For the square-lattice Ising model on a semi-infinite lattice Wood [17] showed that the Fisher circles (1) could be computed as curves on which transfer matrix eigen-values were degenerate in modulus and thus that these latter yield the asymptotic locus of partition function zeros. Further investigations [18–22] have now established the salient elements of this relationship for different lattice systems (see section 2). In this letter we combine these ideas with the finite size scaling approach of Itzykson *et al.* to propose a scaling ansatz for semi-infinite systems, using the branch-points of the transfer matrix eigen-values. The method is tested by calculating the thermal and magnetic exponents y_T and y_H of the q -state two-dimensional Potts model.

2 Transfer matrix eigen-values

Let the lattice be a cylinder of N rings of M sites. If each site contains a q -state microsystem and interactions occur only between microsystems in the same or neighbouring rings, the partition function has the form

$$Z(N, M; z) = \sum_{i=1}^m a_i(M; z) \{\Lambda_i(M; z)\}^{N-1}, \quad (4)$$

where $m = q^M$ and Λ_i , $i = 1, 2, \dots, m$ are the eigen-values of the transfer matrix \mathbf{V} , labelled in order of decreasing magnitude at some arbitrarily chosen point of the positive real axis $\mathbb{R}^{(+)}$ of \mathbb{C} . Here $z \in \mathbb{C}$ represents either $z_T \in \mathbb{C}_T$ or $z_H \in \mathbb{C}_H$, with the other variable kept constant. The coefficients $a_i(M; z) = [\mathbf{x}_i \mathbf{B}] \cdot \mathbf{y}_i$ are given in terms of the left and right eigen-vectors $\{\mathbf{x}_i\}$ and $\{\mathbf{y}_i\}$ of \mathbf{V} with the matrix \mathbf{B} containing contributions from the ends of the cylinder. On $\mathbb{R}^{(+)}$ $\Lambda_1(M; z)$ is real, positive and non-degenerate with real, positive eigen-vectors [23]. Thus, on $\mathbb{R}^{(+)}$, $a_1(M, z) \neq 0$. Formula (4) has special cases corresponding to different boundary conditions. If $\mathbf{B} = \mathbf{V}$, then

$a_i = \Lambda_i$, giving the usual formula for toroidal boundary conditions. When the lattice has lines of boundary sites at both ends $\mathbf{B} = [\mathbf{b}^{(R)}]^{(T)} \otimes \mathbf{b}^{(L)}$ and $a_i = [x_i \cdot \mathbf{b}^{(R)}][y_i \cdot \mathbf{b}^{(L)}]$. It is not difficult to show that, if either one or both of the boundary vectors $\mathbf{b}^{(R)}$ and $\mathbf{b}^{(L)}$ is invariant under the symmetry group of the transfer matrix, then $a_i \equiv 0$ unless Λ_i belongs to the one-dimensional symmetric representation A_1 of the group. Thus, under these conditions, the summation in (4) is confined to the set $i \in A_1$. The coefficients and eigen-values can then be obtained by solving the eigen problem for the one-dimensional symmetric block \mathbf{V}_1 of \mathbf{V} . Such a situation occurs in the case of free boundary conditions at the ends of the cylinder.

For any two eigen-values we define the spectral gap function by

$$g_{ij}(M; z) = \ln \{ \Lambda_i(M; z) / \Lambda_j(M; z) \}. \quad (5)$$

Since $\Lambda_1(M; z)$ is non-degenerate on $\mathbb{R}^{(+)}$, none of the functions $g_{1j}(M; z)$, $j = 2, 3, \dots, m$ has a zero on $\mathbb{R}^{(+)}$. In the case of the Ising model, however, the first-order transition, which exists in the limit $M \rightarrow \infty$, for $\mathcal{H} = 0$, $T < T_c$ is, for finite M , a line of closest approach ('avoided crossings') of the two largest eigen-values $\Lambda_1(M; z)$ and $\Lambda_2(M; z)$ along a path at constant T as \mathcal{H} passes through zero [24]. Thus $g_{12}(M; z)$ drops to a minimum at $\mathcal{H} = 0$ on that path. This property is not exhibited by the functions $g_{1j}(M; z)$, for $j > 2$. In a similar way on the zero-field axis, as T is decreased through T_c , $g_{12}(M; z)$ descends to a minimum and remains near that value in contrast to the behaviour of the functions $g_{1j}(M; z)$, for $j > 2$, which have minima along $\mathbb{R}^{(+)}$ near $T = T_c$, but do not exhibit the flattened effect for $T < T_c$. Since $\Lambda_2(M; z)$ is not in A_1 [25], the model with free boundary conditions will, for finite M , exhibit evidence of the critical point of the $M \rightarrow \infty$ model but not of the first-order transition. The importance of the role played by the second largest eigen value in the finite size scaling analysis of first-order transitions has been discussed in more detail by Privman and Fisher [24,26].

Let $\mathcal{C}_{ij}(M)$ be the curve in \mathbb{C} along which $g_{ij}(M; z)$ is purely imaginary. Those $\mathcal{C}_{ij}(M)$ defined by eigen-values in the same and different transfer matrix symmetry blocks will be termed *connection* and *cross-block* curves respectively [20]. In some cases the two eigen-values defining a connection curve are branches of a single (irreducible) algebraic function, although this is not always so. In the case of the square lattice Ising model it follows from Kaufman's work [25] that the eigen-values of the one-dimensional symmetric representation are branches of a number of different algebraic functions. Let $\mathfrak{M}(M)$ be that subset of $\{\mathcal{C}_{ij}(M)\}$ for which the eigen-values $\Lambda_i(M; z)$ and $\Lambda_j(M; z)$ are of maximum magnitude among those for which $a_i(M; z)$ and $a_j(M; z) \neq 0$. Then, for all $z \notin \mathfrak{M}(M)$, there is a unique eigen-value among those with coefficients not identically zero which has maximum magnitude. This eigen-value is denoted by $\Lambda_{\text{Max}}(M, z)$, with corresponding coefficient $a_{\text{Max}}(M; z)$. On the positive

real axis $\Lambda_{\text{Max}}(M, z)$ is $\Lambda_1(M; z)$. It is not difficult to show that the zeros of $Z(N, M; z)$, in the limit $N \rightarrow \infty$, converge onto the closed set $\mathfrak{M}(M)$ and onto the isolated zeros of $a_{\text{Max}}(M; z)$. Both $\mathfrak{M}(M)$ and these isolated zeros depend on the choice of boundary conditions. The part of $\mathfrak{M}(M)$ first encountered by any continuous path from $\mathbb{R}^{(+)}$ will be $\mathcal{C}_{1k}(M)$ for some k . This will be a connection curve or a cross-block curve according to whether $k \in A_1$ or not. For the Ising model [20,25] $\mathcal{C}_{12}(M)$ is a cross-block curve ($2 \notin A_1$) and our calculations indicate that this is also the case for the 3-state Potts model with M in the range of our results (see table 1). As we have indicated above cross-block curves can be eliminated from $\mathfrak{M}(M)$ by a choice of boundary conditions which make $a_k(M; z) \equiv 0$ if $k \notin A_1$.

3 The finite size scaling ansatz

Given that boundary conditions ensure that $\mathfrak{M}(M)$ involves only eigen-values in A_1 , the points of this set closest to $\mathbb{R}^{(+)}$ will be branch-points of $\Lambda_1(M; z)$, occurring in conjugate pairs. They correspond to bounds on the asymptotic distribution of partition function zeros. We denote the conjugate pair of branch-points closest to z_T^c in \mathbb{C}_T by z_T^* and \bar{z}_T^* , with similar notation in \mathbb{C}_H , and propose the modified forms

$$|z_T^* - z_T^c| \sim M^{-y_T}, \quad |z_H^* - z_H^c| \sim M^{-y_H}, \quad (6)$$

of the finite size scaling formulae of Itzykson *et al.* [12], for the calculation of y_T and y_H . Support for this method is given by the behaviour of the rounding exponent θ . The quantity $M^{-\theta}$ is of the order of the size of the neighbourhood in which the correlation length exceeds the lattice width [28]. This should be of the same order as the radius of convergence of a power series expansion of the free energy about the critical point, which will be given by the location of the nearest branch-point of $\Lambda_1(M; z_T)$. The equality $\theta = y_T$ is thought to be satisfied in a wide class of systems, particularly in the case of a cylinder with free boundary conditions at the ends [29].

4 Results

For the zero-field Ising model ($q = 2$) the location of the nearest branch-points have been obtained exactly [21]. In terms of the angle variable ϑ of the Fisher circles (1) they are located at $\vartheta = \pm\vartheta_b(M)$, where, in the limit of large M , $\vartheta_b(M) \sim 1/M$, giving, from the first of equations (6), the correct result $y_T = 1$.

Table 1

Estimates for y_T and y_H using the finite size scaling formulae (6). The exact values are given for y_T by den Nijs [31] and Black and Emery [32] and for y_H by Neinhuis *et al.* [33] and Pearson [34].

M	y_T			y_H		
	$q = 2$	$q = 3$	$q = 4$	$q = 2$	$q = 3$	$q = 4$
4	0.984382	1.186760	1.343198	1.96737	1.99611	2.06940
5	0.990986	1.190734	1.350089	1.93182	1.95150	2.00144
6	0.994105	1.192738	1.355016	1.91044	1.92423	1.96199
7	0.995834	1.194065	1.359108	1.89869	1.90877	1.93959
8	0.996897	1.195037	1.362600	1.89196	1.89954	1.92603
9	0.997597	1.195775	1.365598	1.88781	1.89357	
10	0.998084	1.196350	1.368194			
11	0.998436	1.196807	1.370464			
...						
17				1.87829		
Exact	1	1.2	1.5	1.875	1.86	1.875

In general, for the zero-field Potts model in \mathbb{C}_T , duality in the form

$$\Lambda_i(M; \sqrt{q}\zeta + 1) = \zeta^{2M} \Lambda_i(M; \sqrt{q}\zeta^{-1} + 1), \quad (7)$$

for all complex ζ , applies to all the eigen-values in Λ_1 [27]. Using this result, it can be shown [21] that on the Potts circle (2), given by $\zeta = \exp(i\vartheta)$, these eigen-values have the form

$$\Lambda_i(M; \sqrt{q} \exp(i\vartheta) + 1) = R(\vartheta) \exp\{i[M\vartheta \pm \omega(\vartheta)]\}. \quad (8)$$

When $\omega(\vartheta)$ is real (8) gives a pair of eigen-values defining a connection curve on the Potts circle, with branch-points located at the solutions of $\omega(\vartheta) = 0$. For $\Lambda_1(M; z_T)$ it must be the case that $\omega(0) = 0$ and the nearest branch-points z_T^* and \bar{z}_T^* to z_T^c can be determined by following the Potts circle from the real axis until the imaginary part of $\ln\{\Lambda_1(M; \sqrt{q} \exp(i\vartheta) + 1)\}$ differs from $M\vartheta$. Numerical computations are simplified by using the transfer matrix $\mathbf{V}^{(\text{WP})}$ of the simple Whitney polynomial representation of the Potts model [30]. For a given lattice width, $\mathbf{V}^{(\text{WP})}$ has elements continuously parameterized by q , but a size independent of q . On the real axis $\mathbf{V}^{(\text{WP})}$ has the same largest eigenvalue $\Lambda_1(M; z_T)$ as \mathbf{V} . So the characteristic equation of $\mathbf{V}^{(\text{WP})}$ con-

tains the whole of the algebraic function of which $\Lambda_1(M; z_T)$ is a branch. This means that $\mathbf{V}^{(\text{WP})}$ gives the correct branch-points for $\Lambda_1(M; z_T)$. The dominant eigenvalues were calculated using a variant of the power method with initial vector $(1, 1, \dots, 1)$. This restricts the iteration to eigen-values in the A_1 block of $\mathbf{V}^{(\text{WP})}$. The branch-points of $\Lambda_1(M; z_T)$ on the Potts circle were located by finding the point where $\omega(\vartheta)$ of formula (8) becomes non-zero. The amplitude of the leading asymptotic term in $|z_T^* - z_T^c|$ was eliminated between the expressions for M and $M - 1$. Results for y_T are given in table 1.

The calculations for y_T , were carried out with $z_H = z_H^c = 1$. The corresponding computations for y_H were performed with $z_T = z_T^c = \sqrt{q} + 1$. In the \mathbb{C}_H plane, for general q , the only exact information is the location $z_H^c = 1$ of the critical point. For $q = 2$ the branch-points are on the circle $|z_H| = 1$ and, above the critical temperature, in the limit $M \rightarrow \infty$ they give the Yang-Lee edge singularities [35]. As may be expected, for general q , the structure of the connection curve for $\Lambda_1(M; z_H)$ is affected by whether the field is coupled with one or more states. Results for $M = 1$ [36] show that, with a field coupled to one state, the zeros lie on a circle whose radius depends on q and z_T . For $M > 1$ the connection curve is a single smooth arc which, according to our calculations, approaches the unit circle for increasing M . The eigen-values in this case were obtained for $q = 2$ and $q = 3$ using \mathbf{V} and for $q = 4$ using the extended Whitney polynomial method [30]. The method is similar to that for y_T . The estimates for y_H are given in table 1.

5 Conclusions

The results of this method show convincing convergence towards the exact values for $q = 2$ and $q = 3$. Using both finite and $M \times \infty$ lattices Blöte and Nightingale [30] obtained finite size scaling estimates for y_T from three-point fits to the critical heat capacity. These gave ‘best estimates’ of $y_T = 1, 1.1955, 1.3934$ for $q = 2, 3, 4$ respectively. While our results and those of Blöte and Nightingale are comparably close to the exact results for $q = 2$ and 3, they show a similar difference for $q = 4$. In their method this is due to an additional term in the leading singular behaviour of the heat capacity at $q = 4$. For $q > 4$ the transition is first-order. Blöte and Nightingale obtain the power law behaviour described by discontinuity fixed point exponents for completely finite systems, but for semi-infinite systems exponential divergence occurs. We have obtained similar results.

In the case of y_H the quality of our results are again similar to those of Blöte and Nightingale. However, the main aim of our work is not to produce more accurate values for critical exponents. In the case of the Potts model the exact values are already known. Our motive is to explore the hypotheses that eigen-

value branch-points have a finite size scaling relationship to the temperature and field exponents. These branch-points are those of the eigen-value of the one-dimensional symmetric block which is largest on the positive real axis. We have, therefore, a particularly simple procedure for obtaining approximations to critical exponents. The method has also been applied to the quasi-Potts model of Young and Lavis [37] with encouraging results. In that case no exact information is available and comparison with other approximation methods is necessary. This work will be reported in a later communication.

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