Singular Behaviour of the Potts Model in the Thermodynamic Limit

Ralph Kenna[a*]

[a]School of Mathematics,
Trinity College Dublin,
Ireland

The self–duality transformation is applied to the Fisher zeroes near the critical point in the thermodynamic limit in the $q > 4$ state Potts model in two dimensions. A requirement that the locus of the duals of the zeroes be identical to the dual of the locus of zeroes (i) recovers the ratio of specific heat to internal energy discontinuity at criticality and the relationships between the discontinuities of higher cumulants and (ii) identifies duality with complex conjugation. Conjecturing that all zeroes governing ferromagnetic critical behaviour satisfy the latter requirement, the full locus of Fisher zeroes is shown to be a circle. This locus, together with the density of zeroes is shown to be sufficient to recover the singular form of all thermodynamic functions in the thermodynamic limit.

1. INTRODUCTION

The question of the locus of Fisher zeroes in the $d = 2$ Potts model is one which has recently received an increased amount of attention [1–6]. In the two–state (Ising) case where the exact solution is available [7], the Fisher zeroes form two circles in the complex $u = \exp(-\beta)$ plane in the thermodynamic limit [8].

The partition function for the q–state Potts model is $Z_L(\beta) = \sum_{\{\sigma_i\}} \exp(\beta \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j})$ and in the thermodynamic limit is invariant under the duality transformation $u \rightarrow \mathcal{D}(u)$, where $\mathcal{D}(u) = (1-u)/(1+(q-1)u)$ [9]. The critical temperature at which the phase transition occurs is invariant under duality and is $u_c = 1/(1+\sqrt{q})$. Here the $d = 2$ $q > 4$ state model exhibits a first order phase transition [10].

Based on similarities with the Ising case, Martin and Maillard and Rammal [1] conjectured that the locus of Fisher zeroes in the $d = 2$, q–state Potts model be given by an extension of critical duality to the complex plane, namely $\mathcal{D}(u) = u^*$ where u^* is the complex conjugate of u. This identification yields a circle with centre $-1/(q-1)$ and radius $\sqrt{q}/(q-1)$. When $q = 2$ this recovers the ferromagnetic Fisher circle of the Ising model [8]. In the Ising case, the partition function is actually a function of u^2. There, the second (antiferromagnetic) Fisher circle comes from the map $\beta \rightarrow -\beta$. Numerical investigations for small lattices [1] provided evidence that the Fisher zeroes indeed lie on the circle given by the identification of duality with complex conjugation. However the numerics are highly sensitive to the boundary conditions used and the situation far from criticality remained unclear. Some progress was recently made in the non–critical region using low temperature expansions for $3 \leq q \leq 8$ [4].

Recently, and on the basis of numerical results on small lattices with $q \leq 10$, it has again been conjectured that for finite lattices with self–dual boundary conditions, and for other boundary conditions in the thermodynamic limit, the zeroes in the ferromagnetic regime are on the above circle [5]. The conjecture of [5] was, in fact, proven for infinite q in [6]. This circle–conjecture is similar to another recent conjecture [3], namely that the Fisher zeroes for the q–state Potts model on a triangular lattice with pure three–site interaction in the thermodynamic limit (which is also self–dual [10]) lie on a circle and a segment of the negative real axis.

All of the above conjectures regarding the locus of Fisher zeroes rely, at least in part, on numerical approaches. In this paper, the problem is addressed analytically and the origin of the circular locus is clarified.

*Supported bt EU TMR Project No. ERBFMBI-CT96-1757

2. Thermodynamic Functions

For finite L, the partition function is a polynomial in u and can be expressed in terms of its zeroes as $Z_L(\beta) \propto \prod_{j=1}^{dV}(u-u_j(L))$ [8]. The free energy is $\beta f(\beta) = -\ln Z(\beta)/V$. The internal energy is (up to a constant)

$$e(\beta) = \frac{u}{V}\sum_{j=1}^{dV}\frac{1}{u-u_j(L)} \quad . \tag{1}$$

The general $n^{\rm th}$ cumulant is defined as $\gamma_n(\beta) = (-)^{n+1}\partial^n(\beta f)/\partial\beta^n$. In conventional notation the specific heat is $c(\beta) = k_B\beta^2\gamma_2(\beta)$. With $\Delta\gamma_n \equiv \gamma_n(\beta^-) - \gamma_n(\beta^+)$, the discontinuity in the $n^{\rm th}$ cumulant at the critical temperature, the exact thermodynamic limit results include [10–13]

$$\Delta c = k_B\beta_c^2\frac{\Delta e}{\sqrt{q}} \quad . \tag{2}$$

3. Partition Function Zeroes

Recently, Lee [2] has derived a general theorem for first order phase transitions in which the zeroes can be expressed in terms of the discontinuities in the thermodynamic functions. For a system with a temperature–driven phase transition, Lee's result is (in terms of $t = 1-\beta/\beta_c$)

$$\begin{aligned} \beta_c {\rm Re} t_j(L) &= A_1 I_j^2 + A_3 I_j^4 + A_5 I_j^6 + \dots \quad , \\ \pm\beta_c {\rm Im} t_j(L) &= I_j + A_2 I_j^3 + A_4 I_j^5 + \dots \quad , \end{aligned} \tag{3}$$

where $I_j = (2j-1)\pi/(V\Delta e)$ and $\dots$ includes terms which vanish in the infinite volume limit. The first few coefficients A_n are [2,14] $A_1 = \Delta c/2k_B\beta_c^2\Delta e$, $A_2 = -2A_1^2 + \Delta\gamma_3/3!\Delta e$.

3.1. The Locus of Zeroes

From (3) the real part of the zeroes (in the thermodynamic limit) can be expressed in terms of their imaginary parts as $\beta_c{\rm Re}t = \mathcal{L}(\beta_c{\rm Im}t)$ where $\mathcal{L}(\theta) = A_1\theta^2 + (-2A_1A_2+A_3)\theta^4 + \dots$. The zeroes are thus seen to lie on a curve. In the complex u upper half–plane the equation of this curve is $\gamma^{(+)}(\theta) = u_c\exp(\mathcal{L}(\theta)+i\theta)$.

3.2. The Dual of the Locus and the Locus of the Duals

Applying the duality transformation to $\gamma^{(+)}(\theta)$ and expanding in θ gives ${\rm Re}\mathcal{D}\left(\gamma^{(+)}(\theta)\right) = u_c[1 + (\theta^2/2q)(2\sqrt{q} - 2A_1q - q) + \dots]$ and ${\rm Im}\mathcal{D}\left(\gamma^{(+)}(\theta)\right) = -u_c[\theta - (\theta^3/6q)(6 - 6q^{1/2} + q - 12A_1q^{1/2} + 6A_1q) + \dots]$.

Alternatively, applying the duality transformation directly to the $j^{\rm th}$ zero in the finite–size system gives

$$\begin{aligned} \beta_c {\rm Re} t_j^D(L) &= A_1^D I_j^2 + A_3^D I_j^4 + A_5^D I_j^6 + \dots \\ \mp\beta_c {\rm Im} t_j^D(L) &= I_j + A_2^D I_j^3 + A_4^D I_j^5 + \dots \end{aligned} \tag{4}$$

where terms vanishing in the thermodynamic limit are included in $\dots$ and the first few A_n^D are

$$A_1^D = q^{-\frac{1}{2}} - A_1 \quad , \tag{5}$$

$$A_2^D = -q^{-1} + 2q^{-\frac{1}{2}}A_1 + A_2 \quad . \tag{6}$$

As in Sec.(3.1), (4) gives the locus of the dual of the upper half–plane zeroes in the thermodynamic limit to be ${\gamma^{(+)}}^D(\theta) = u_c\exp(\mathcal{L}^D(\theta) - i\theta)$, where $\mathcal{L}^D(\theta) = A_1^D\theta^2 + (-2A_1^DA_2^D + A_3^D)\theta^4 + \dots$. The expansion of this locus of duals is ${\rm Re}{\gamma^{(+)}}^D(\theta) = u_c[1+(\theta^2/2!)(-1+2A_1^D)+\dots]$ and ${\rm Im}{\gamma^{(+)}}^D(\theta) = -u_c[\theta + (\theta^3/3!)(-1+6A_1^D)+\dots]$.

Even when the finite–L system does not have duality–preserving boundary conditions, taking the thermodynamic limit restores self–duality. There the dual of the locus of zeroes and the locus of duals must be identical,

$$\mathcal{D}\left(\gamma^{(+)}\right) \equiv {\gamma^{(+)}}^D \quad . \tag{7}$$

Up to $\mathcal{O}(\theta^2)$ this is trivial. To $\mathcal{O}(\theta^3)$ and (separately at) $\mathcal{O}(\theta^4)$ they are identical if $A_1 = 1/(2\sqrt{q})$. This is the result (2). The identity (7) at $\mathcal{O}(\theta^5)$ and (separately at) $\mathcal{O}(\theta^6)$ gives $A_3 = A_2/\sqrt{q} - q^{-3/2}(q-3)/24$, or [11–13]

$$\Delta\gamma_4 = \frac{6}{\sqrt{q}}\Delta\gamma_3 + \frac{q-6}{q^{3/2}}\Delta e \quad . \tag{8}$$

Higher order results are obtainable using a computer algebra system such as Maple [14].

4. The Full Locus and the Singular Parts of the Thermodynamic Functions

Putting the above equations ((2) and (8)) into (5), (6) (and their higher order equivalents) yields $A_j^D = A_j$ (this has been verified up to $j = 8$).

Therefore (at least up to θ^{10}) the dual of the locus of zeroes is the complex conjugate of the original locus of zeroes. We now assume that this is the case for all θ. Then, the full feromagnetic locus of zeroes (that part of the full locus which intersects the real temperature axis at the physical ferromagnetic critical point) is found by identifying [1] $\mathcal{D}\left(\gamma^{(+)}(\theta)\right) = {\gamma^{(+)}}^*(\theta)$, where ${\gamma^{(+)}}^*$ represents the complex conjugate of $\gamma^{(+)}$. The full ferromagnetic locus is then [1]

$$\gamma(\theta) = \frac{1}{q-1}\left(-1+\sqrt{q}e^{i\theta}\right) \quad . \tag{9}$$

The density of zeroes is given by [2]

$$2\pi g(\theta) = \left(1+\frac{1}{(q-1)\gamma(\theta)}\right)\Big[1+ \\ \sum_{n=2}^{\infty}\frac{\Delta\gamma_n}{(n-1)!}\left(\ln\left((\sqrt{q}+1)\gamma(\theta)\right)\right)^{(n-1)}\Big]. \tag{10}$$

The internal energy is (from (1) or [15])

$$e = \text{cnst.} + u\int_0^{2\pi}\frac{g(\theta)}{u-\gamma(\theta)}d\theta \quad . \tag{11}$$

Therefore, from (9), (10) and (11), the internal energy is $e(\beta<\beta_c) = e_0$ and

$$e(\beta>\beta_c) = e_0 - \Delta e + \sum_{n=2}^{\infty}\frac{\Delta\gamma_n(\beta_c-\beta)^{(n-1)}}{(n-1)!}, \tag{12}$$

with e_0 a constant (one expects that when separate Fisher loci which don't cross the positive real temperature axis are accounted for, e_0 becomes temperature dependent). At β_c the internal energy discontinuity $e(\beta=\beta_c^-) - e(\beta=\beta_c^+) = \Delta e$ is recovered. Appropriate differentiation recovers the discontinuities in specific heat and higher cumulants.

5. Conclusions

The requirement that the dual of the locus of zeroes be identical to the locus of the duals of zeroes (i) recovers the ratio of specific heat to internal energy discontinuity at criticality and relations between the discontinuities of higher cumulants and (ii) identifies duality with complex conjugation.

Conjecturing that all zeroes governing ferromagnetic critical behaviour satisfy (ii) gives that this locus is the circle (9). This puts the conjecturs of [1,3,5] on an analytic footing. The locus (9), together with the density of zeroes (10) is sufficient to recover the *singular* parts of all thermodynamic functions in the thermodynamic limit. It is to be expected that the *regular* parts come from separate loci of zeroes which don't cross the positive real temperature axis.

The author thanks A. Irving, W. Janke and J. Sexton.

REFERENCES

1. P.P. Martin, Nucl. Phys. B 225 (1983) 497; J.M. Maillard and R. Rammal, J. Phys. A 16 (1983) 353; P.P. Martin and J.M. Maillard, J. Phys. A 19 (1986) L547; ibid. 20 (1987) L601.
2. K.-C. Lee Phys. Rev. Lett. 73 (1994) 2801.
3. J.C. Anglès d'Auriac, J. M. Maillard, G. Rollet and F.Y. Wu Physica A 206 (1994) 441.
4. V. Matveev and R. Shrock, Phys. Rev. E 54 (1996) 6174.
5. C.-N. Chen, C.-K. Hu and F.Y. Wu, Phys. Rev. Lett., 76 (1996) 169.
6. F.Y. Wu, G. Rollet, H.Y. Huang, J.M. Maillard, C.-K. Hu and C.-N. Chen, Phys. Rev. Lett., 76 (1996) 173.
7. B. Kaufman, Phys. Rev. 76 (1949) 1232.
8. M.E. Fisher, in *Lectures in Theoretical Physics, Vol. VIIC*, ed. W.E. Brittin, (Gordon and Breach, New York: 1968) 1.
9. R.B. Potts, Proc. Camb. Phil. Soc. 48 (1952) 106.
10. R.J. Baxter, J. Phys. C 6 (1973) L445; J. Stat. Phys. 28 (1982) 1; R.J. Baxter, H.N.V. Temperley and S. Ashley Proc. Roy. Soc. London, Ser. A 358 (1978) 535.
11. F.Y. Wu, Rev. Mod. Phys. 54 (1982) 235.
12. T. Bhattacharya, R. Lacaze and A. Morel, Nucl. Phys. B **435** (1995) 526; J. Phys. I France **7** (1997) 81.
13. W. Janke and S. Kappler, Phys. Lett. A **197** (1995) 227; J. Phys. I France **7** (1997) 663.
14. R. Kenna cond-mat/9707039.
15. R. Abe, Prog. Theor. Phys. 37, (1967) 1070; ibid. 38 322.