Physica A 206 (1994) 441–453
North-Holland

SSDI 0378-4371(93)E0584-2

PHYSICA

Zeroes of the triangular Potts model partition function: a conjectured distribution

J.C. Anglès d'Auriac[a], J.M. Maillard[b], G. Rollet[b] and F.Y. Wu[c]

[a]*CRTBT, 25 Avenue des Martyrs, BP 166X, 38042 Grenoble Cedex, France*
[b]*Laboratoire de Physique Théorique et Hautes Energies, Tour 16, 1er étage, 4 place Jussieu, 75252 Paris Cedex, France*
[c]*Department of Physics, Northeastern University, Boston, MA 02115, USA*

Received 15 November 1993

We consider the q-state Potts model on the triangular lattice with two- and three-site interactions in alternate triangular faces, and determine zeroes of the partition function numerically in the case of pure three-site interactions. On the basis of a rigorous reciprocal symmetry and results on the zeroes for finite lattices, we conjecture that zeroes of the partition function of the triangular Potts model with pure three-site interactions in alternate triangular faces lie on a circle and a segment of the negative real axis. It is shown that the conjecture holds for $q = 2$, and that it reproduces the known critical point for general q, including the $q = 1$ site percolation.

1. Introduction

Generally speaking, there exist several different kinds of exact results on lattice models in statistical mechanics. Ideally, one would like to obtain the exact, closed-form, expressions of thermodynamic quantities such as the per-site free energy, the surface tension, spontaneous magnetization, and correlation functions. A knowledge of these exact expressions leads to a complete description of the system including the phase boundary (critical frontier) and the location of zeroes of the partition function. However, exact evaluations of physical quantities are not always possible. In such cases one can sometimes determine the critical frontier from properties such as the duality [1] and the inversion [2] relations, or analyzes analyticity properties of the free energy by locating the zeroes of the partition function [3,4]. But other than in the case of some special one-dimensional model [5], exact results on the zeros have been confined mostly to the Ising model [3,4]. In this paper we report results of a calculation of the zeroes of the partition function of a Potts model with pure three-spin interactions. On the basis of the numerical results as well as a rigorous reciprocal symmetry, we propose a conjecture on the exact location of zeroes of its partition function.

We consider first the q-state Potts model on the triangular lattice with nearest-neighbor and three-site interactions in alternate, say, the up-pointing, triangular faces of the lattice. This model was first studied by Baxter et al. [6] in the framework of the analysis of the star-triangle relation. They showed that the partition function possesses a duality relation. Recalling the importance of the Kagomé lattice for the resonating valence bond theory of high-T_c superconductivity [7], it is also worth noticing that this model is related to the standard Potts model on the Kagomé lattice [8]. The duality relation has since been rederived using a graphical analysis [9] and identified as the exact critical frontier in the ferromagnetic regime [10]. Here, we carry out a numerical determination of the zeroes of the partition function for the pure three-site interaction model on finite lattices. The results indicate that the zeroes lie on some loci which approach a circle and an interval of the negative real axis as the lattice size increases. In addition, we establish a rigorous reciprocal symmetry of the partition function in the thermodynamic limit. These results lead us to conjecture that, in the thermodynamic limit, the partition function zeroes for the pure three-spin model lie on a circle and a segment of the negative real axis. The conjecture is shown to hold for $q = 2$; it also reproduces the known critical point for general q including the $q = 1$ site percolation.

2. The triangular Potts model

Consider the q-state standard Potts model on a triangular lattice L of N sites with anisotropic two-site interactions K_1, K_2 and K_3 in respective directions, and three-site interaction K surrounding every up-pointing triangular face. The reduced Hamiltonian now reads

$$\mathcal{H} = \sum_{\triangle} E_{abc} , \tag{1}$$

where the summation is taken over all up-pointing triangular faces and

$$E_{abc} = -(K_1\delta_{bc} + K_2\delta_{ca} + K_3\delta_{ab} + K\delta_{abc}) . \tag{2}$$

Here a, b, c are the three sites surrounding a triangle, $\delta_{ab} = \delta_{\mathrm{Kr}}(\sigma_a, \sigma_b)$ is the Kronecker delta, $\delta_{abc} = \delta_{ab}\delta_{bc}$, and $\sigma_a = 1, 2, \ldots, q$ refers to the spin states at site a. The example of an $N = 12$ cluster with a twisted (helicoidal) periodic boundary condition preserving the rotational and translational symmetries is shown in fig. 1.

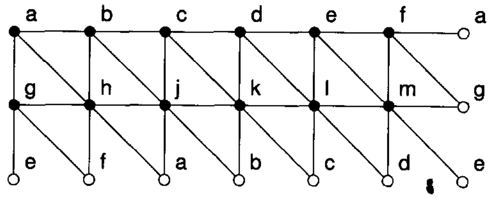

Fig. 1. A 12-site triangular lattice with twisted periodic boundary conditions. Open circles denote repeated lattice sites.

We first summarize relevant established results on this Potts model. The partition function Z of the model (1) satisfies a duality relation [6]

$$Z(x_1, x_2, x_3, y) \equiv \sum \prod_{\triangle} e^{-E_{abc}} \sim (y/q)^N Z(x_1', x_2', x_3', y') , \tag{3}$$

where

$$x_i' - 1 = q(x_i - 1)/y , \qquad y' = q^2/y , \qquad y = x x_1 x_2 x_3 - (x_1 + x_2 + x_3) + 2 ,$$
$$x = e^K , \qquad x_i = e^{K_i} , \tag{4}$$

and $\sim$ denotes the validity in the thermodynamic limit. The fixed point of this duality transformation is located at

$$y = q . \tag{5}$$

It is noteworthy to point out that, in terms of the variables

$$w = y/q = 1/w' , \qquad u_i = (x_i - 1)/\sqrt{w} = u_i' , \tag{6}$$

the duality relation (3) takes the more simple form

$$\tilde{Z}(u_1, u_2, u_3, w) \sim w^N \tilde{Z}(u_1, u_2, u_3, 1/w) \tag{7}$$

for $q \geqslant 2$, in which the variables u_i are invariant.

It can be readily seen that (5) admits physical solution only in the ferromagnetic regime[#1]

$$K + K_1 + K_2 + K_3 > \{0, K_i\} , \tag{8}$$

where the critical frontier is indeed (5) [10]. For pure two-site interactions and

[#1] The corresponding expressions in [10] contain misprints. The inequality signs in (11) of [10] should be reversed.

$q \geq 4$, the critical variety (5) can also be obtained by applying the Lee–Yang circle theorem [3] in a vertex model formulation of the model [11], or by applying an inversion relation type argument [2]. For pure three-site interactions, (5) reduces to the simple form

$$w = 1 \quad \text{or} \quad e^K - 1 = q \,. \tag{9}$$

3. Expansion of the partition function

The partition function of the Potts model (1) can be written as

$$\begin{aligned} Z(x, x_1, x_2, x_3) &= \sum \prod_{\triangle} (1 + v\delta_{abc})(1 + v_1\delta_{bc})(1 + v_2\delta_{ca})(1 + v_3\delta_{ab}) \\ &= \sum_G W(G) \,, \end{aligned} \tag{10}$$

where

$$v = e^K - 1 \,, \qquad v_i = e^{K_i} - 1 \,, \tag{11}$$

and the product is taken over the up-pointing triangles. It is convenient to represent terms in the expansion of the partition function by graphs G in which the up-pointing triangular faces are either occupied by a solid triangle with a fugacity v, or unoccupied. If the triangular face is unoccupied, then the three edges of the triangle can be independently occupied by bonds with fugacities v_i, $i = 1, 2, 3$. This is a weak-graph expansion (for definition of weak and strong graphs and embeddings, see [12]) in which G is a weak embedding of vertices, lines, and triangles, on L.

We next evaluate the weight $W(G)$ associated with the graph G. It is clear that each solid triangle contributes to $W(G)$ a factor v, and each bond a factor v_i. In addition, by combining with the associated bond factors, each solid triangle contributes an additional factor $(1 + v_1)(1 + v_2)(1 + v_3) = e^{K_1+K_2+K_3}$. Consider next the q dependence of $W(G)$. For a graph representing N isolated points we have simply $W(G) = q^N$. For other graphs, each triangle reduces the factor q^N by q^2, and each bond by q. But whenever the triangles and bonds close up to form a circuit[#2], the reduction must be restored by a factor q due to the overlapping of one lattice site summation. Thus we have

[#2] Here, we use the term *circuit* in the topological sense that solid triangles can be regarded as stars having three branches, each of which can be connected to other triangles and bonds.

$$Z = q^N \sum_G \left(\frac{v}{q^2} e^{K_1+K_2+K_3}\right)^{m(G)} \left(\frac{v_1}{q}\right)^{b_1(G)} \left(\frac{v_2}{q}\right)^{b_2(G)} \left(\frac{v_3}{q}\right)^{b_3(G)} q^{c(G)}, \tag{12}$$

where the summation is over all graphs G in which lines and triangles do not overlap. $m(G)$ is the number of solid triangles, $b_i(G)$ the number of bonds with weight v_i, and $c(G)$ the number of independent circuits in G. A typical graph G occurring in (12) is shown in fig. 2. The expression (12) generates the high-temperature expansion of the partition function.

We have generated the exact partition function (12) for the 27-site lattice with twisted periodic boundary conditions for $q = 3$[#3]. In the case of pure three-site interactions, (12) reduces to

$$Z = Z(q, w) = q^N \sum_G (w/q)^{m(G)} q^{c(G)}, \tag{13}$$

where $w = (e^K - 1)/q$. The expression (13) suggests a more efficient bookkeeping for the expansion. This is to consider an associated lattice $\mathscr{L}$, which is also triangular, by shrinking the up-point triangular faces in L into points. Regard the presence of a solid triangle in L as denoting the corresponding site of $\mathscr{L}$ being occupied, and connect all pairs of occupied neighboring sites of $\mathscr{L}$ by bonds. A weak graph G on L is then mapped onto a strong graph $\mathscr{G}$ on $\mathscr{L}$, and vice versa [12]. An example of this mapping is shown in fig. 3. However, as seen in fig. 3, elementary down-pointing triangles in $\mathscr{G}$, which form circuits in $\mathscr{G}$, do not contribute to $c(G)$. Taking this correction into consideration, we can rewrite the summation (13) as

$$Z(q, w) = q^N \sum_{\mathscr{G}} W(\mathscr{G}, w), \qquad W(\mathscr{G}, w) = w^{m(\mathscr{G})} q^{c(\mathscr{G}) - d(\mathscr{G}) - m(\mathscr{G})}, \tag{14}$$

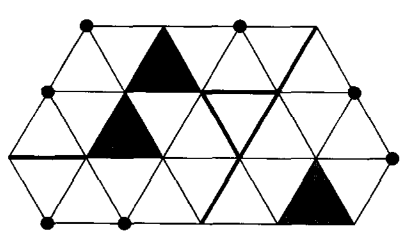

Fig. 2. A typical graph G on L showing $m(G) = 9$ components. Shaded triangles represent solid triangles mentioned in the text.

[#3] This series, which contains 27022 terms, can be obtained by sending a ftp request to anonymous@crtbt.polycnrs-gre.fr

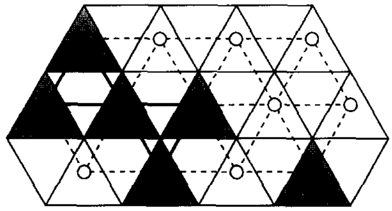

Fig. 3. A graph G on L with the associated graph $\mathscr{G}$ on $\mathscr{L}$. The lattice $\mathscr{L}$ is denoted by the heavy and broken lines with solid (open) circles denoting occupied (unoccupied) sites.

where the summation is taken over all strong graphs $\mathscr{G}$ on $\mathscr{L}$, $m(\mathscr{G})$ is the number of sites, $c(\mathscr{G})$ the number of independent circuits in the usual sense of graph theory, and $d(\mathscr{G})$ the number of down-pointing elementary triangles, in $\mathscr{G}$. Since the summation in (14) runs over $2^{m(\mathscr{L})}$ terms instead of $q^{m(\mathscr{L})}$ in (10), the expression (14) is easier to use in practice, and offers an efficient way of generating high temperature expansions. Also not that in general $\mathscr{L}$ contains fewer lattice points than L. This will be used in the numerical results presented in the last section of this paper.

4. A reciprocal symmetry

The duality relation (7) indicates that the partition function is invariant in the thermodynamic limit under the change of $w \to 1/w$. It is instructive to explicitly show that the high-temperature series (14) indeed possesses this symmetry, and to see how does the condition of thermodynamic limit enter into play. We present in the following a rigorous analysis of these facts.

Let $\mathscr{G}$ be an arbitrary strong graph on $\mathscr{L}$ with weight $W(\mathscr{G}; w)$ as in (14). Let $\mathscr{G}'$ be the "complement" of $\mathscr{G}$ obtained from $\mathscr{G}$ by interchanging the occupied and open sites, and rotating 180° to make it up-side-down. Let $W(\mathscr{L}, w) = w^{m(\mathscr{L})} q^{c(\mathscr{L})-d(\mathscr{L})-m(\mathscr{L})}$ as defined in (14) be the weight of the graph in which all sites of $\mathscr{L}$ are occupied. Expanding about this configuration we can write

$$Z(q, w) = W(\mathscr{L}, w) \sum_{\mathscr{G}'} W'(\mathscr{G}'; w) , \tag{15}$$

where $W'(\mathscr{G}', w)$ can be viewed as a correction to $W(\mathscr{L}, w)$ due to the deletion of the lattice sites in $\mathscr{G}$. We then have the following theorem relating $W'(\mathscr{G}', w)$ and $W(\mathscr{G}, w)$:

Theorem. For strong graphs $\mathscr{G}$ which do not extend to the boundary (in the sense that they are surrounded by unoccupied sites), we have the identity

$$W'(\mathcal{G}'; w) = W(\mathcal{G}; 1/w) . \tag{16}$$

Now, graphs extending to the boundary contribute to some "boundary effect" which can be neglected in the thermodynamic limit. Omitting such terms in (14) and (15) and using $u_i = 0$ and (16), one establishes the reciprocal symmetry

$$Z(q, w) \sim Z(q, 1/w) . \tag{17}$$

It follows that, if w is a root of the partition function in the thermodynamic limit, then $1/w$ is also a root. This reciprocal symmetry, which is certainly consistent if all zeroes are on the circle $|w| = 1$, also implies a $w \rightarrow 1/w$ invariance of the series in the limit of $N \rightarrow \infty$.

We now prove the theorem. First of all, we note that the weight $W(\mathcal{G}; w)$ in (14) can be written as a product of the weights of clusters (of connected sites). Now, the weight $W'(\mathcal{G}'; w)$ in (15), when viewed as a correction associated to $W(\mathcal{L}, w)$, can also be written as a product of those of the clusters. It then suffices to consider a single cluster and the corresponding correction.

For a single cluster represented by a graph g which does not extend to the boundary and for which a typical example is shown in fig. 4, the expression of $W(g, w)$ as defined in (14) is

$$W(g, w) = w^{m(g)} q^{c(g) - d(g) - m(g)} . \tag{18}$$

To find the corresponding correction factor for g', the complement of g, we need to compare g' with the configuration in which all sites are occupied. Let $t(g)$ be the number of elementary triangles in g excluding those bordered by (solid) lines. These triangles are those shaded in fig. 4. A simple inductive proof establishes that, if g is completely surrounded by unoccupied sites, we have

$$t(g) = 4m(g) + 2 - 2c(g) , \tag{19}$$

and half of these triangles are up (and down) pointing. Then, the total number of elementary triangles removed from a totally occupied configuration in order to create g' is

$$T(g') = t(g) + u(g) + d(g) , \tag{20}$$

where $u(g)$ and $d(g)$ are, respectively, the up-pointing and down-pointing elementary triangles in g bordered by (solid) lines. It is now clear that in the process of creating g', the number of circuits is reduced by $T(g') - 1$, since one circuit remains after the removal, and the number of down-pointing elementary

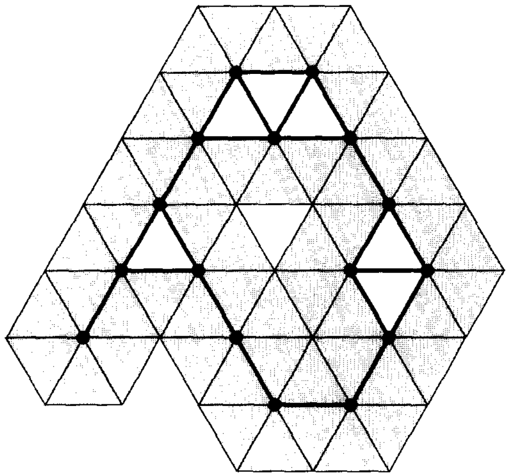

Fig. 4. A typical cluster of $m(g) = 16$ occupied sites with $t(g) = 52$ elementary triangles (those shaded), $c(g) = 7$, $d(g) = u(g') = 2$, and $u(g) = d(g') = 4$.

triangles reduced by $u(g) + t(g)/2$. Here, we have used the fact that, due to the 180° rotation of g in deducing g', up-pointing elementary triangles in g become down-pointing in g'. Consulting (18), the needed correction factor can now be readily written down as

$$\begin{aligned} W'(g'; w) &= w^{-m(g)} \times q^{-[T(g')-1]} \times q^{u(g)+t(g)/2} \times q^{m(g)} \\ &= w^{-m(g)} q^{c(g)-d(g)-m(g)} = W(g; 1/w) . \qquad \text{Q.E.D.} \end{aligned} \tag{21}$$

As a consequence, the ratio of the two coefficients of w^k and $w^{m(\mathcal{L})-k}$ is independent of k and is equal to $q^{c(\mathcal{L})-m(\mathcal{L})-d(\mathcal{L})}$. For finite lattices for which some clusters extend to the boundary, this independence holds only for k far from $m(\mathcal{L})/2$.

5. A conjecture on the zero distribution

On the basis of the reciprocal symmetry established in section 4, we now propose a conjecture on the distribution of zeroes for the pure three-site interaction model. A numerical check of the conjecture will be presented in the next section.

Conjecture. Zeroes of the partition function of the triangular q-state Potts model with pure three-site interactions K in alternate triangles lie, in the thermodynamic limit, on the unit circle

$$|w| = 1\,, \tag{22}$$

and a line segment on the real negative axis

$$-\alpha(q) \leqslant w \leqslant -1/\alpha(q)\,, \tag{23}$$

for some function $\alpha(q)$.

The conjecture certainly holds for $q = 1$ for which we have

$$Z = \mathrm{e}^{NK}\,, \tag{24}$$

whose N zeroes are degenerate at $\mathrm{e}^{K} = 0$. The conjecture also yields the exact critical point (9) for all q as the intersection, at $w = +1$, on the real axis.

The conjecture also holds for $q = 2$ with $\alpha(2) = 2$. To see that this is the case, we use the identity $\delta_{ab} = \frac{1}{2}(1 + \sigma_a\sigma_b)$, where σ_a, $\sigma_b = \pm 1$, to transform the partition function into that of a triangular Ising model with isotropic ferromagnetic interactions $J = K/4$. In the thermodynamic limit, the free energy of the triangular Ising model assumes the form [13]

$$f = \frac{-1}{8\pi^2}\int_0^{2\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, \ln[\cosh^3 2J + \sinh^3 2J - B(\theta, \phi)\sinh 2J]\,, \tag{25}$$

where

$$B(\theta, \phi) = \cos\theta + \cos\phi + \cos(\theta + \phi)\,. \tag{26}$$

The loci of the zeroes of the partition function in the thermodynamic limit can be traced, and identified, as those of the argument of the logarithm[#4]. This leads to the roots of the equation

$$w^2[1 - B(\theta, \phi)]w + 1 = 0\,, \tag{27}$$

where $w = (\mathrm{e}^{K} - 1)/2$. A little algebra shows that the two roots of (27) lie either on the unit circle $|w| = 1$ or in the interval $-2 \leqslant w \leqslant -1/2$ [15,16]. This verifies the conjecture for $q = 2$.

Finally, we note that the partition function in the $q = 1$ limit generates precisely the *site* percolation on $\mathscr{L}$ [17] with the occupation probability $p = 1 -$

[#4] For finite lattices with periodic boundary conditions, the partition function is a sum of four Pfaffians [14], and zeroes of the partition function will generally not be on a circle [3,10]. The zero distribution approaches a circle only in the thermodynamic limit.

e^{-K}. The conjecture then yields the critical probability $p_c = 1/2$, in agreement with the known exact result [18].

6. Zeroes of the partition function

To test the correctness of the conjectured circle theorem, we have carried out an exact calculation of the partition function and its zeroes for the pure three-site interaction model, for arbitrary q and finite lattices using the relation (14). Keeping in mind the importance of the rotational invariance [9] in this model we have used the twisted boundary conditions of fig. 1 but now with 27 sites. This partition function is regarded as a polynomial in the complex variable w.

For the twisted 27-site lattice, we obtain the polynomial

$$Z(q, w) = q^{27} + 27q^{26}w + 351q^{25}w^2 + (2898q^{24} + 27q^{25})w^3 + \cdots \\ + (2898q^{25} + 27q^{26})w^{24} + 351q^{26}w^{25} + 27q^{27}w^{26} + q^{28}w^{27} . \quad (28)$$

Here the reciprocal symmetry (17) holds for the first and last six coefficients of this polynomial as shown. Coefficients of the remaining terms not shown are not symmetric due to the occurrence of graphs 'percolating' to the boundary. The 27 zeroes of the partition function (28) are shown in fig. 5 for $q = 3, 4, 50$.

A similar polynomial in w and q has been calculated for a 36-sites lattice with standard periodic boundary conditions (instead of the twisted boundary conditions because 36 is not of the form $3 \times L^2$). In this case, there are 2^{36} graphs $\mathcal{G}$ which were generated in an order such that two consecutive graphs differ by the addition or deletion of only one site. This ordering makes it easier to update the numbers of connected components, sites, bonds and down-pointing triangles. The CPU time needed to complete this enumeration to ten days on a cluster of twelve I 860 processors[#5]. The 36 zeroes of the partition function thus obtained are shown in fig. 6 for $q = 3, 4, 50$.

From figs. 5 and 6, it is seen that the zeroes approach the unit circle as the number of lattice sites increases. This is in agreement with our conjecture that it holds in the thermodynamic limit. Furthermore, better agreement with the conjecture is also obtained for smaller q. In fact, loci of zeroes in the large q limit can be determined by keeping only the leading terms. For the partition function (28) with *periodic* boundary conditions, for example, this leads to

[#5] Again the complete series for both cases, namely the 27-site and 36-site lattice models, can be obtained by sending a ftp request to anonymous@crtbt.polycnrs-gre.fr

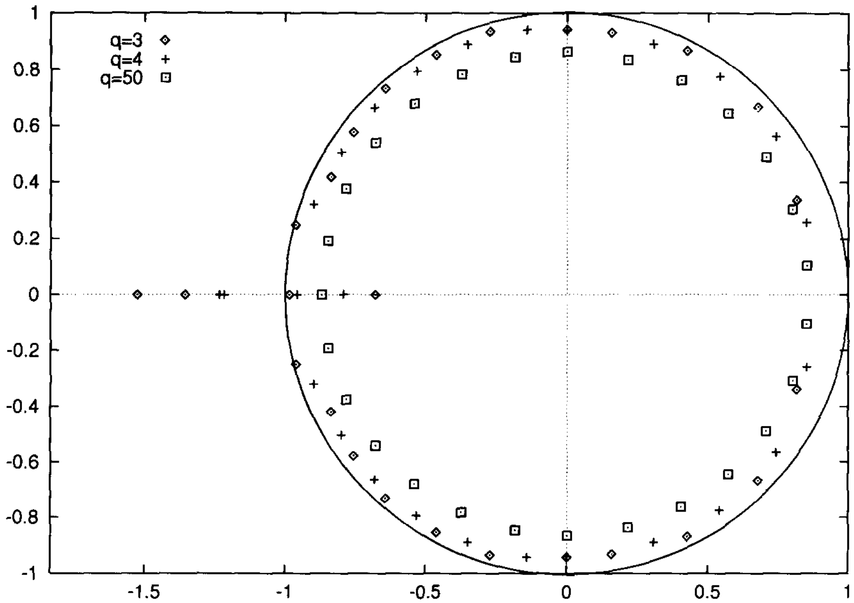

Fig. 5. Zeroes in the w plane for the pure three-site interaction model for a 27-site lattice with twisted periodic boundary conditions.

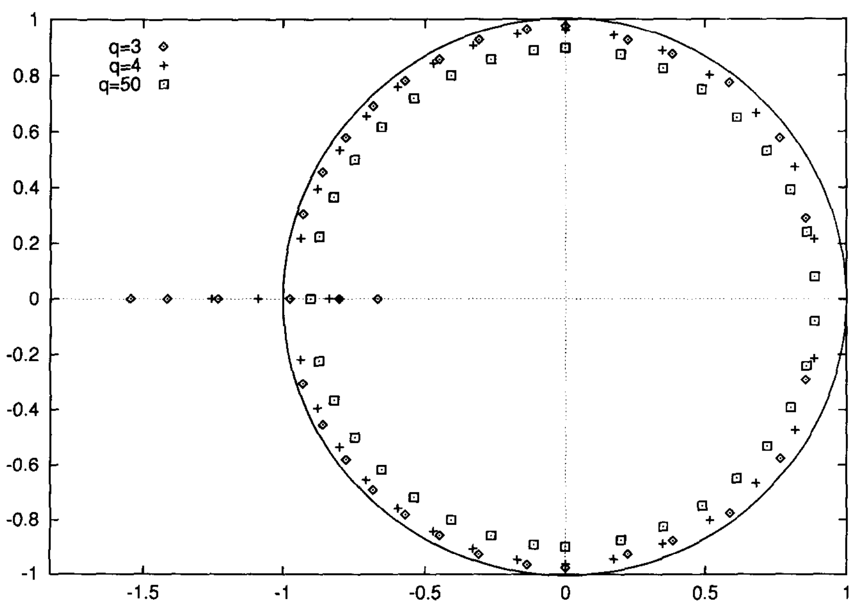

Fig. 6. Zeroes in the w plane for the pure three-site interaction model for a 36-site lattice with standard periodic boundary conditions.

$qw^{27} + 27w^{26} + 1 = 0$ which yields the location of zeroes close to a circle of radius $q^{-1/27}$. This demonstrates that the distribution of zeroes approaches a circle in the large q limit, albeit with a smaller radius. However, our data are insufficient to determine the function $\alpha(q)$.

7. Summary

We have numerically evaluated the zeroes of the partition function of the triangular Potts model in the complex temperature plane. Based on our numerical evidence and a rigorous reciprocal symmetry, we conjecture that zeroes of the partition function of the Potts model with pure three-site interaction in alternate triangles lie on the circle (22) and the segment (23) on the negative axis. The conjecture is verified for $q = 2$, the Ising model, and shown to yield the known critical point for general q.

Acknowledgements

Work has been supported by CNRS (JCAd'A, JMM and GR) and by NSF grants INT-9113701 and DMR-9015489 (FYW).

References

[1] F.Y. Wu and Y.K. Wang, J. Math. Phys. 17 (1976) 439.
[2] J.M. Maillard and R. Rammal, J. Phys. A 16 (1983) 353.
[3] T.D. Lee and C.Y. Yang, Phys. Rev. 87 (1952) 410.
[4] M.E. Fisher, Lecture in Theoretical Physics, Vol. 7c (University of Colorado Press, Boulder, CO, 1964).
[5] L. Mittag and M.J. Stephen, J. Stat. Phys. 35 (1984) 303.
[6] R.J. Baxter, H.N.V. Temperley, and S. Ashley, Proc. R. Soc. A 358 (1978) 535.
[7] P.W. Anderson, Science 235 (1987) 1196.
[8] J.M. Maillard, G. Rollet and F.Y. Wu, J. Phys. A 26 (1993) L495.
[9] F.Y. Wu and K.Y. Lin, J. Phys. A 13 (1980) 629.
[10] F.Y. Wu and R.K.P. Zia, J. Phys. A 14, (1981) 721.
[11] A. Hintermann, H. Kunz and F.Y. Wu, J. Stat. Phys. 19 (1978) 623.
[12] C. Domb, in: Phase Transitions and Critical Phenomena, Vol. 3 (Academic Press, London, 1974) p. 1.
[13] C. Domb, Adv. Phys. 9 (1960) 149.
[14] B.M. McCoy and T.T. Wu, Two-Dimensional Ising Model (Harvard Univ. Press, Cambridge, MA, 1973).

[15] J. Stephenson and R. Couzens, Physica A 129 (1984) 201.
[16] P. Martin and J.M. Maillard, J. Phys. A 19 (1986) L547.
[17] H. Kunz and F.Y. Wu, J. Phys. C 11 (1978) L1.
[18] M.F. Sykes and J.W. Essam, J. Math. Phys. 5 (1964) 1117.