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1999 J. Phys. A: Math. Gen. 32 5053

(http://iopscience.iop.org/0305-4470/32/27/306)

J. Phys. A: Math. Gen. **32** (1999) 5053–5070. Printed in the UK PII: S0305-4470(99)03190-X

Ground state entropy of Potts antiferromagnets on cyclic polygon chain graphs

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Received 6 April 1999

Abstract. We present exact calculations of chromatic polynomials for families of cyclic graphs consisting of linked polygons, where the polygons may be adjacent or separated by a given number of bonds. From these we calculate the (exponential of the) ground state entropy, W, for the q-state Potts model on these graphs in the limit of infinitely many vertices. A number of properties are proved concerning the continuous locus, $\mathcal{B}$, of nonanalyticities in W. Our results provide further evidence for a general rule concerning the maximal region in the complex q plane to which one can analytically continue from the physical interval where $S_0 > 0$.

1. Introduction

The q-state Potts antiferromagnet (AF) [1, 2] exhibits nonzero ground state entropy, $S_0 > 0$ (without frustration) for sufficiently large q on a given graph or lattice. This is equivalent to a ground state degeneracy per site $W > 1$, since $S_0 = k_B \ln W$. Such nonzero ground state entropy is important as an exception to the third law of thermodynamics [3]. The zero-temperature partition function of the above-mentioned q-state Potts antiferromagnet on a graph G satisfies $Z(G, q, T = 0)_{PAF} = P(G, q)$, where $P(G, q)$ is the chromatic polynomial expressing the number of ways of colouring the vertices of the graph G with q colours such that no two adjacent vertices have the same colour [4–6]. Thus

$$W(\{G\}, q) = \lim_{n\to\infty} P(G, q)^{1/n} \tag{1.1}$$

where $n = v(G)$ is the number of vertices of G and $\{G\} = \lim_{n\to\infty} G$. The minimum number of colours needed for this colouring of G is called its chromatic number, $\chi(G)$. At certain special points q_s (typically $q_s = 0, 1, \ldots, \chi(G)$), one has the noncommutativity of limits

$$\lim_{q\to q_s}\lim_{n\to\infty} P(G, q)^{1/n} \neq \lim_{n\to\infty}\lim_{q\to q_s} P(G, q)^{1/n} \tag{1.2}$$

and hence it is necessary to specify the order of the limits in the definition of $W(\{G\}, q_s)$ [7]. As in [7], we shall use the first order of limits here; this has the advantage of removing certain isolated discontinuities in W. In addition to [2–7], some other previous related works include [8–22]. Since $P(G, q)$ is a polynomial, one can generalize q from $\mathbb{Z}_+$ to $\mathbb{R}$ and indeed to $\mathbb{C}$. $W(\{G\}, q)$ is a real analytic function for real q down to a minimum value, $q_c(\{G\})$ [7, 14]. For a given $\{G\}$, we denote the continuous locus of non-analyticities of W as $\mathcal{B}$. This locus $\mathcal{B}$ forms as the accumulation set of the zeros of $P(G, q)$ (chromatic zeros of G) as $n \to \infty$ [7, 9, 10, 12]

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and satisfies $\mathcal{B}(q) = \mathcal{B}(q^*)$. A fundamental question concerning the Potts antiferromagnet is the form of this locus for a given graph family or lattice and, in particular, the maximal region in the complex q plane to which one can analytically continue the function $W(\{G\}, q)$ from physical values where there is nonzero ground state entropy, i.e., $W > 1$. We denote this region as R_1. Further, we denote as q_c the maximal point where $\mathcal{B}$ intersects the real axis, which can occur via $\mathcal{B}$ crossing this axis or via a line segment of $\mathcal{B}$ lying along this axis.

In this work we present exact calculations of $P(G, q)$ and $W(\{G\}, q)$ for families of cyclic graphs consisting of linked polygons, where the polygons may be adjacent or separated by a certain number of bonds. By the term cyclic we mean that these families of graphs contain a global circuit, defined as a route along the graph which has the topology of S^1 and a length $\ell_{g.c.}$ that goes to infinity as $n \to \infty$. The results provide new insight into W and $\mathcal{B}$ in an exactly solvable context where one can study their dependence on several parameters characterizing the families of polygon chain graphs. This work extends our recent studies of cyclic families of graphs [7, 22].

From our previous exact calculations of $P(G, q)$ and $W(\{G\}, q)$ on a number of families of graphs we have inferred several general results on $\mathcal{B}$: (i) for a graph G with well-defined lattice directions, a sufficient condition for $\mathcal{B}$ to separate the q plane into different regions is that G contains at least one global circuit [19]†, and (ii) the locus $\mathcal{B}$ for such a graph does not contain any endpoint singularities. Two other general features are that for graphs that (a) contain global circuits, (b) cannot be written in the form $G = K_p + H$ [15]‡ and (c) have compact $\mathcal{B}$, we have observed that $\mathcal{B}$ (iii) passes through $q = 0$ and (iv) crosses the positive real axis, thereby always defining a q_c. The families of polygon chain graphs studied in this paper do contain global circuits, and the exact results presented here are in accord with the above general properties.

The chromatic polynomial $P(G, q)$ has a general decomposition as

$$P(G, q) = c_0(q) + \sum_{j=1}^{N_a} c_j(q)(a_j(q))^{t_j n} \tag{1.3}$$

where the $a_j(q)$ and $c_{j\neq 0}(q)$ are independent of n, while $c_0(q)$ may contain n-dependent terms, such as $(-1)^n$, but does not grow with n like $(\mathrm{const.})^n$ with $|\mathrm{const.}| > 1$. The expression c_0 may be absent. A term $a_\ell(q)$ is 'leading' if it dominates the $n \to \infty$ limit of $P(G, q)$. The locus $\mathcal{B}$ occurs where there is an abrupt nonanalytic change in W as the leading terms a_ℓ changes; thus this locus $\mathcal{B}$ is the solution to the equation of degeneracy of magnitudes of leading terms. Hence, W is finite and continuous, although nonanalytic, across $\mathcal{B}$.

It is convenient to define the following polynomial:

$$D_k(q) = \frac{P(C_k, q)}{q(q-1)} = a^{k-2} \sum_{j=0}^{k-2} (-a)^{-j} = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s} \tag{1.4}$$

where

$$a = q - 1 \tag{1.5}$$

and $P(C_k, q)$ is the chromatic polynomial for the circuit (cyclic) graph C_k with k vertices,

$$P(C_k, q) = a^k + (-1)^k a. \tag{1.6}$$

† Some families of graphs that do not have regular lattice directions have noncompact loci $\mathcal{B}$ that separate the q plane into different regions [16, 18, 21]. The graphs in the present paper do not, in general, have regular lattice structure; however, they do have the equivalent of a lattice direction, i.e. that of the circuit.

‡ The complete graph on p vertices, denoted K_p, is the graph in which every vertex is adjacent to every other vertex. The 'join' of graphs G_1 and G_2, denoted $G_1 + G_2$, is defined by adding bonds linking each vertex of G_1 to each vertex in G_2.

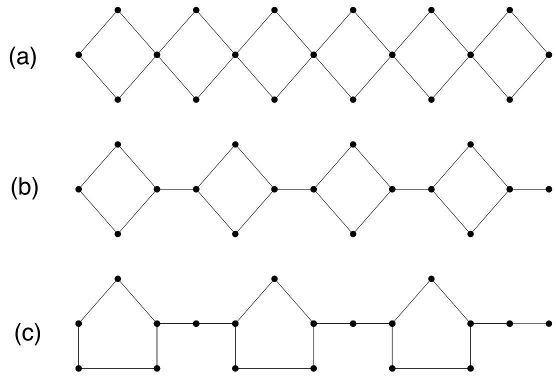


Figure 1. Illustrations of cyclic and open polygon chain graphs $G_{e_1,e_2,e_g,m}$ and $G_{e_1,e_2,e_g,m;o}$ with $(e_1, e_2, e_g, m) = (a)\ (2, 2, 0, 6)$, $(b)\ (2, 2, 1, 4)$, $(c)\ (2, 3, 2, 3)$. For the cyclic (open) graphs, the rightmost vertex on each graph is identified with (is distinct from) the leftmost vertex at the same level, respectively.

This paper is organized as follows. In sections 2 and 3 we present our results for P, W, and $\mathcal{B}$ for the open and cyclic polygon chain graphs and some concluding remarks are included in section 4.

2. Open polygon chain graphs

Before giving our results for the cyclic polygon chain graphs, we discuss the simpler case of families of open polygon chain graphs comprised of m subunits, each subunit consisting of a p-sided polygon with one of its vertices attached to a line segment of length e_g edges (bonds). Thus, the members of each successive pair of polygons are separated from each other by a distance (gap) of e_g bonds along these line segments, with $e_g = 0$ representing the case of contiguous polygons. Since each polygon is connected to the rest of the chain at two vertices (taken to be at the same relative positions on the polygons in all cases), the family of graphs depends on two additional parameters, namely the number of edges of the polygons between these two connection vertices, moving in opposite directions along the polygon, e_1 and e_2. For $e_1 \neq e_2$ we denote the smaller (s) and larger (ℓ) edge lengths as

$$e_s \equiv \min(e_1, e_2) \qquad e_\ell \equiv \max(e_1, e_2). \tag{2.1}$$

Clearly,

$$e_1 + e_2 = p. \tag{2.2}$$

We denote this family of open (o) polygon chain graphs as $G_{e_1,e_2,e_g,m;o}$. Illustrations of these graphs are given in figure 1. Since it is immaterial whether one labels the upper and lower routes between the left and right-hand points on each polygon where it connects to the rest of the chain as e_1 and e_2 or in the opposite order, as e_2 and e_1,

$$G_{e_1,e_2,e_g,m;o} = G_{e_2,e_1,e_g,m;o}. \tag{2.3}$$

The number of vertices is

$$v(G_{e_1,e_2,e_g,m;o}) = (p + e_g - 1)m + 1 \tag{2.4}$$

and the number of edges or bonds is

$$e(G_{e_1,e_2,e_g,m;o}) = (p + e_g)m. \tag{2.5}$$

The chromatic number $\chi = 2$ if p is even and $\chi = 3$ if p is odd. The chromatic polynomial is easily calculated to be

$$P(G_{e_1,e_2,e_g,m;o}, q) = q(a_1)^m \tag{2.6}$$

where

$$a_1 = (q-1)^{e_g+1} D_p. \tag{2.7}$$

Evidently, the chromatic polynomial has the form of (1.3) with $c_0 = 0$, $N_a = 1$, $c_1 = q(a_1)^{-t_1}$ and $t_1 = t$, where

$$t = \frac{1}{p + e_g - 1}. \tag{2.8}$$

Note that this chromatic polynomial does not depend on e_1 or e_2 individually, but instead only on their sum p, i.e., the number of sides of each polygon†.

Let us next consider the limit of an infinitely long chain, i.e., $m \to \infty$. Formally, we denote this limit as

$$L_m : m \to \infty \qquad \text{with} \quad e_1, e_2, e_g \text{ fixed}. \tag{2.9}$$

We find

$$W\left(\left[\lim_{m\to\infty} G_{e_1,e_2,e_g,m;o}\right], q\right) = [(q-1)^{e_g+1} D_p]^{\frac{1}{p+e_g-1}}. \tag{2.10}$$

The nonanalyticities of this W function consist of discrete branch point singularities at its zeros, including the point $q = 1$ and the $p - 2$ zeros of D_p; there is no continuous locus of nonanalyticities of W; i.e., $\mathcal{B} = \emptyset$. If p is odd, then D_p contains a factor $(q - 2)$, so that one of the zeros of W is at $q = 2$.

Given the relation (2.4), there are also other ways to take the number of vertices to infinity:

$$L_{e_g} : e_g \to \infty \qquad \text{with} \quad e_1, e_2, m \text{ fixed} \tag{2.11}$$

$$L_{e_1} : e_1 \to \infty \qquad \text{with} \quad e_2, e_g, m \text{ fixed} \tag{2.12}$$

$$L_{e_2} : e_2 \to \infty \qquad \text{with} \quad e_1, e_g, m \text{ fixed} \tag{2.13}$$

and

$$L_p : p \to \infty \qquad \text{with} \quad e_2 - e_1, e_g, m \text{ fixed}. \tag{2.14}$$

For the L_{e_g} limit, we find

$$W\left(\left[\lim_{e_g\to\infty} G_{e_1,e_2,e_g,m;o}\right], q\right) = q - 1. \tag{2.15}$$

This is analytic for all q so that, in particular, $\mathcal{B} = \emptyset$. The W function in equation (2.15) is the same as the W function for linear and, more generally tree, graphs. This is understandable, since as $e_g \to \infty$, the vertices on the linear connecting segments occupy a fraction approaching unity of the total number of vertices of the graph.

Since the chromatic polynomial (2.6) only depends on e_1 and e_2 through the quantity p, it follows that for this family of open polygon chain graphs, the limits L_{e_1}, L_{e_2}, and L_p all yield the same result. Further, from equation (1.4), it follows that in these limits, W is the same as that for a circuit graph [7], namely,

$$W\left(\left[\lim_{p\to\infty} G_{e_1,e_2,e_g,m;o}\right], q\right) = q - 1 \qquad \text{for} \quad |q-1| \geqslant 1 \tag{2.16}$$

† One can consider a generalization of this family in which the order of the quantities e_1 and e_2 can be different for each polygon. The chromatic polynomial and W function for this much larger family of graphs are again given by (2.6) with (2.7) and by (2.10), respectively.

and†

$$\left|W\left(\left[\lim_{p\to\infty} G_{e_1,e_2,e_g,m;o}\right], q\right)\right| = 1 \qquad \text{for} \quad |q-1| < 1. \tag{2.17}$$

For this limit, $\mathcal{B}$ consists of the circle $|q-1| = 1$. Again, these results are easily understood, since as $p \to \infty$, the vertices on the polygonal circuit subgraphs occupy a fraction approaching unity of the total number of vertices.

3. Cyclic polygon chain graphs

We proceed to our main subject, families of graphs consisting of m p-sided polygons linked together to form closed circuits. The other parameters, e_g, e_1, and e_2, are the same as for the open polygonal chains discussed above. Thus, a given cyclic polygonal chain graph is specified by the four parameters (e_1, e_2, e_g, m), so we denote it as $G_{e_1,e_2,e_g,m}$, where the cyclic property is implicitly understood. For the same reason as given above for the open chain, we have

$$G_{e_1,e_2,e_g,m} = G_{e_2,e_1,e_g,m}. \tag{3.1}$$

The number of vertices in the graph $G_{e_1,e_2,e_g,m}$ is

$$n = v(G_{e_1,e_2,e_g,m}) = (p + e_g - 1)m \tag{3.2}$$

and the number of edges (bonds) is the same as for the open chain, $e(G_{e_1,e_2,e_g,m}) = (p + e_g)m$. If p is odd, then the chromatic number χ is 3. If p is even, then $\chi = 2$ or 3 depending on the values of e_1, e_2, e_g, and m. In figure 1 we show illustrative examples of families of cyclic polygon chain graphs. From (3.1), it follows that

$$P(G_{e_1,e_2,e_g,m}, q) = P(G_{e_2,e_1,e_g,m}, q). \tag{3.3}$$

Using the deletion–contraction theorem to get recursion relations which we then solve, we calculate the chromatic polynomial

$$P(G_{e_1,e_2,e_g,m}, q) = (a_1)^m + (q-1)(a_2)^m \tag{3.4}$$

where the term a_1 is the same as the term appearing in the chromatic polynomial for the open polygonal chain, (2.7), and

$$a_2 = (-1)^{p+e_g} q^{-1}[q - 2 + (1-q)^{e_1} + (1-q)^{e_2}] \tag{3.5}$$

$$= (-1)^{p+e_g}\left[1 - p - \sum_{s=2}^{e_1}\binom{e_1}{s}(-q)^{s-1} - \sum_{s=2}^{e_2}\binom{e_2}{s}(-q)^{s-1}\right]. \tag{3.6}$$

The chromatic polynomial (3.4) has the form of (1.3) with $c_0 = 0$, $N_a = 2$, $c_1 = 1$, $c_2 = (q-1)$, and $t_1 = t_2 = t$, where t was given in equation (2.8). Note that, owing to the second term, a_2, the chromatic polynomial (3.4) depends on the values of e_1 and e_2 individually, in contrast to the result (2.6) for the open polygon chain, which only depends on e_1 and e_2 through their sum, p.

If the smaller distance $e_s = 1$, then the chromatic polynomial (3.4) reduces to the factorized form

$$P(G_{e_s=1,e_\ell,e_g,m}, q) = (D_p)^m P(C_{n_c}, q) = q(q-1)(D_p)^m D_{n_c} \tag{3.7}$$

where

$$n_c = m(1 + e_g). \tag{3.8}$$

† For real $0 < q < q_c(\{G\})$, as well as other regions of the q plane that cannot be reached by analytic continuation from the real interval $q > q_c(\{G\})$, one can only determine the magnitude $|W(\{G\}, q)|$ unambiguously [7].

Having calculated the chromatic polynomial (3.4), we can next obtain the W function and its continuous locus of nonanalyticities $\mathcal{B}$ for the various limits (2.9) and (2.11)–(2.14). This locus is determined as the solution of the degeneracy equation of (nonzero) leading terms

$$|a_1| = |a_2|. \tag{3.9}$$

It will be useful to re-express this in the variable $a = q - 1$ of equation (1.5). Multiplying both sides of (3.9) by $|a + 1|$, we obtain

$$|a^{e_g}(a^p + (-1)^p a)| = |a - 1 + (-a)^{e_1} + (-a)^{e_2}|. \tag{3.10}$$

(Since the value $q = 0$, i.e., $a + 1 = 0$, is already a solution of (3.9), multiplying both sides of this equation by $|a + 1|$ to get (3.10) does not introduce a distinct spurious zero.)

We first discuss the limits that yield the simplest results. For the L_{e_g} limit, $\mathcal{B}$ consists of the unit circle $|q - 1| = 1$ and divides the q plane into two regions, the exterior and interior of this circle, which regions are denoted as R_1 and R_2, respectively. If $|q - 1| > 1$, then a_1 is the dominant term and

$$W\Big(\Big[\lim_{e_g\to\infty} G_{e_1,e_2,e_g,m}\Big], q\Big) = q - 1 \qquad \text{for} \quad |q - 1| > 1. \tag{3.11}$$

If $|q - 1| < 1$, then a_2 is dominant and

$$\Big|W\Big(\Big[\lim_{e_g\to\infty} G_{e_1,e_2,e_g,m}\Big], q\Big)\Big| = 1 \qquad \text{for} \quad |q - 1| < 1. \tag{3.12}$$

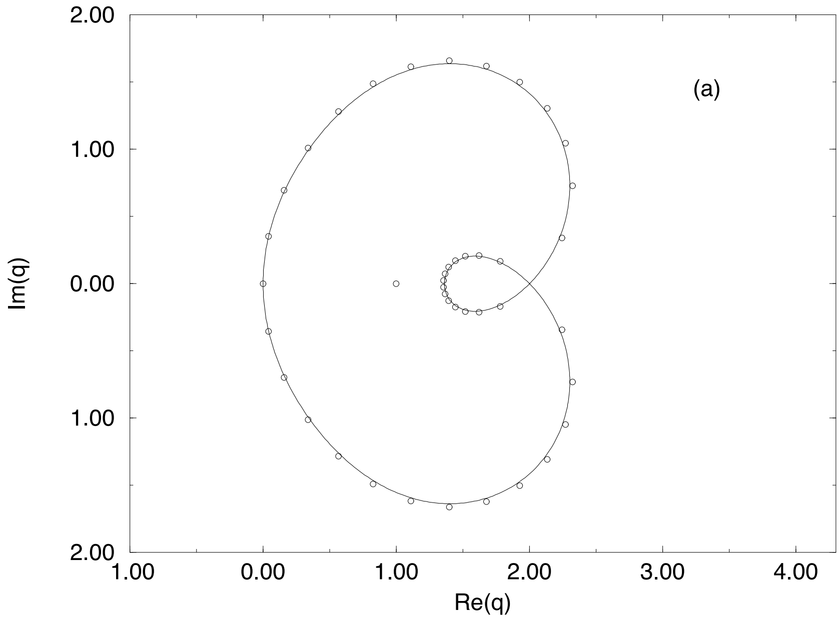
That is, in the L_g limit, the W function is the same as for the infinite-vertex limit of the circuit graph. This is expected, since as e_g increases, more and more of the vertices of the graph lie on a circuit graph where, e.g., the route of the circuit follows either the e_1 or e_2 bonds of a given polygon, then traverses the e_g connecting bonds to the next polygon, and so forth around the cyclic chain. As a result of the symmetry (3.3), the L_{e_1}, L_{e_2}, and L_p limits are equivalent; in this case, we find that for $|q - 1| > 1$, the a_1 term is dominant and W is again given by the right-hand side of (3.11) while for $|q - 1| < 1$, neither term dominates over the other, and $|W| = 1$. The results for W are thus the same as for the L_{e_g} limit, and the reason is similar: as $p \to \infty$, the vertices located on the polygons occupy a fraction approaching unity of all of the vertices.

The most interesting and complicated results are for the L_m limit. We have proved a number of general properties of $\mathcal{B}$. We show calculations of $\mathcal{B}$ and comparison with chromatic zeros in figures 2–9 for the families of cyclic polygon chain graphs. Because of the factorization (3.7), the families with $e_s = 1$ yield very simple results (see below) so that in the figures we concentrate on the cases with $e_s \geqslant 2$: $(e_1, e_2) = (2, 2)$, $(2, 3)$, $(2, 4)$, and $(3, 3)$ and, for each pair (e_1, e_2), the values $0 \leqslant e_g \leqslant 3$. The general properties of $\mathcal{B}$ are:

- (B1) $\mathcal{B}$ is compact.
- (B2) $\mathcal{B}$ passes through $q = 0$.
- (B3) $\mathcal{B}$ encloses regions in the q plane.
- (B4) if $e_s = 1$, then $\mathcal{B}$ is the unit circle $|q - 1| = 1$ independent of the values of e_ℓ and e_g; thus, in this case, $q_c = 2$. The chromatic zeros of $G_{e_1,e_2,e_g,m}$ lie exactly on this locus, independently of the values of e_ℓ, e_g, and m.
- (B5) if p is even, then $q_c = 2$.
- (B6) if p is odd and $e_s \geqslant 2$, then $q_c < 2$ and for fixed (e_1, e_2), q_c increases monotonically as e_g increases, approaching 2 from below as $e_g \to \infty$.

To prove (B1), we re-express equation (3.9) in terms of the variable

$$y = \frac{1}{a} = \frac{1}{q - 1}. \tag{3.13}$$



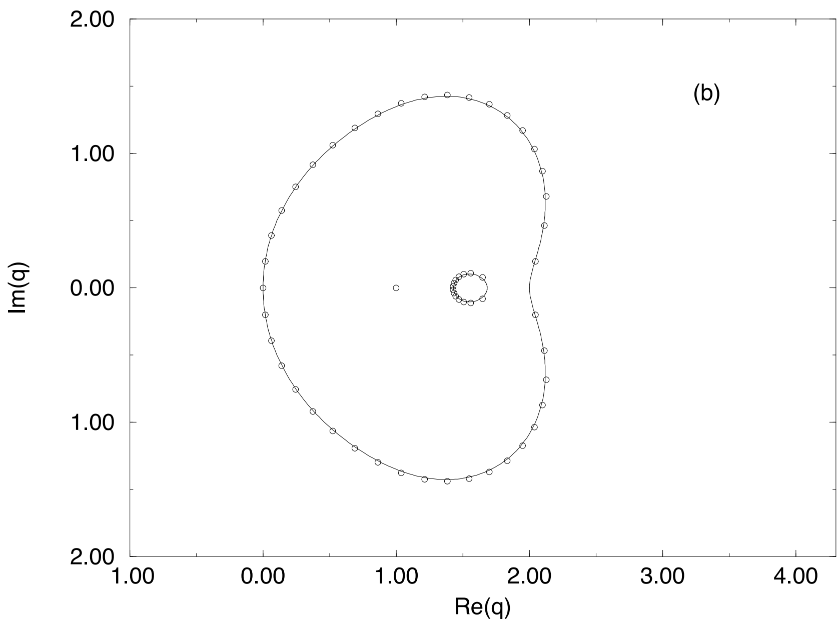


Figure 2. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 2, 0)$, (b) $(2, 2, 1)$. Chromatic zeros for $m = 14$ (i.e., $n = 42$ and $n = 56$ for (a) and (b)) are shown for comparison.

Then equation (3.10) becomes

$$|1 + (-1)^p y^{p-1}| = |y^{e_g+e_s}(y^{e_\ell-1} - y^{e_\ell} + (-1)^{e_\ell} + (-1)^{e_s} y^{e_\ell-e_s})| \tag{3.14}$$

where we have divided (3.9) by $|a^{e_g+p}|$, which factor is nonzero for $q \neq 1$ and thus, in particular, for the large-$|q|$ (small $|y|$) region of interest here. The necessary and sufficient condition that

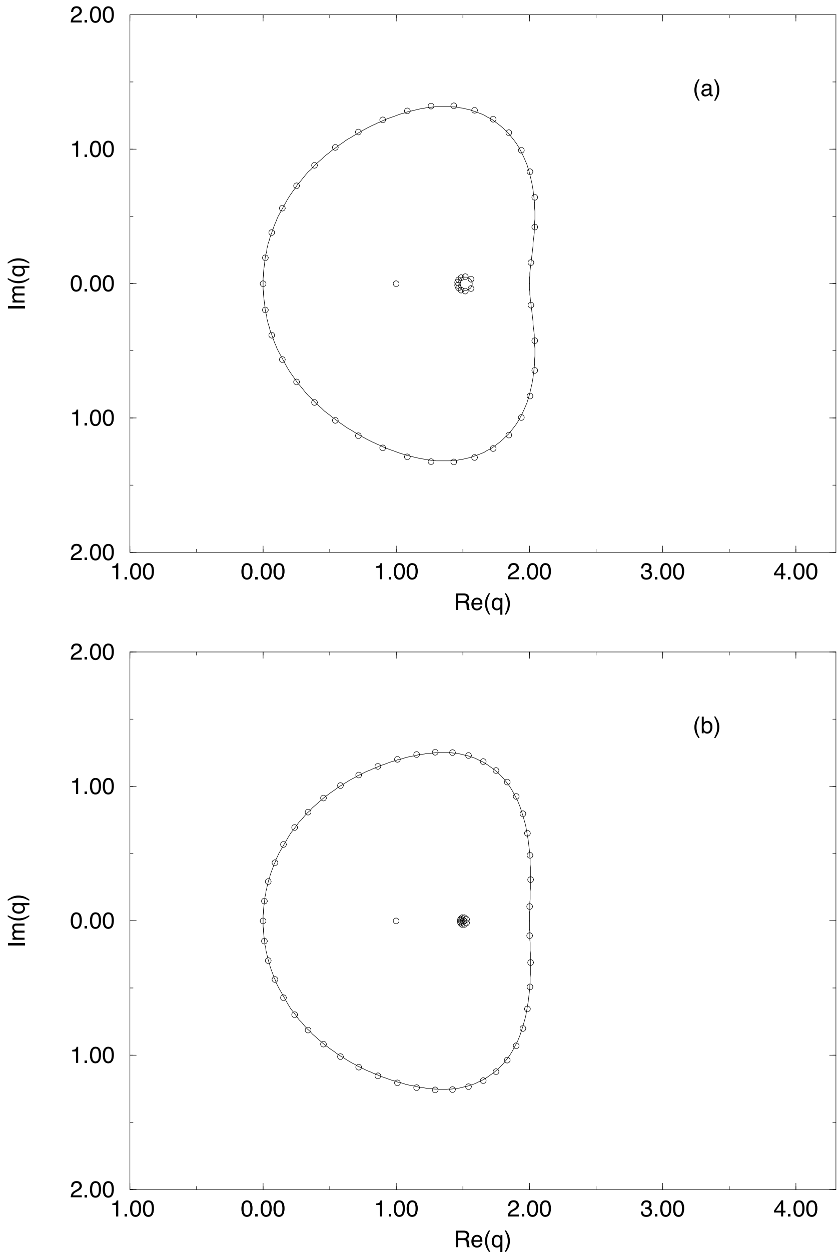


Figure 3. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 2, 2)$, (b) $(2, 2, 3)$. Chromatic zeros for $m = 10$ (i.e., $n = 50$ and $n = 60$ for (a) and (b)) are shown for comparison.

$\mathcal{B}$ is noncompact, i.e. unbounded, is that equation (3.14) has a solution for $y = 0$. Clearly, it does not have such a solution, which proves property (B1).

For (B2), we use the property that

$$D_p(q = 0) = (-1)^p(p - 1) \tag{3.15}$$

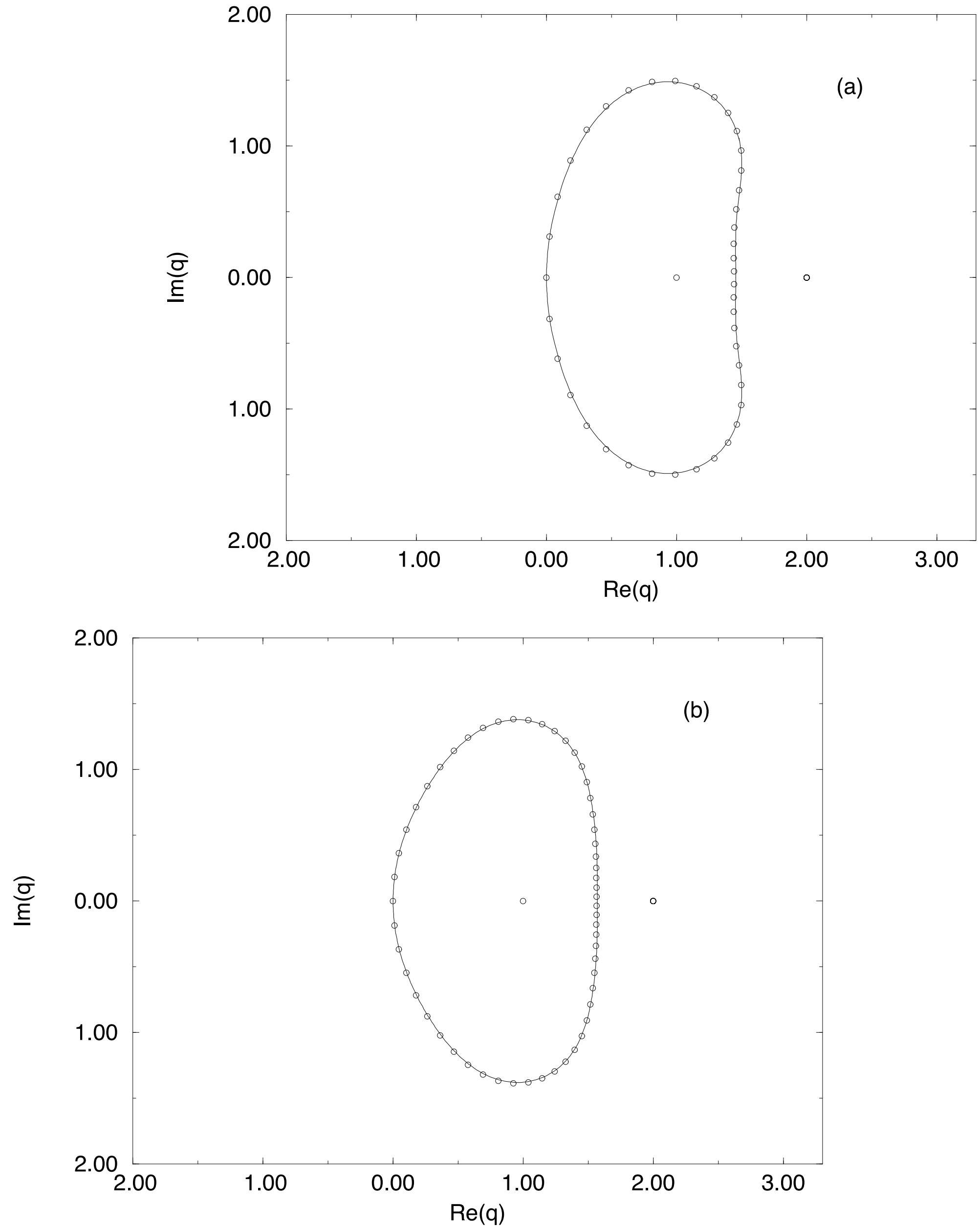


Figure 4. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 3, 0)$, (b) $(2, 3, 1)$. Chromatic zeros for $m = 14$ (i.e., $n = 56$ and $n = 70$ for (a) and (b)) are shown for comparison.

so that $|a_1| = |p - 1|$ at $q = 0$. From the second equivalent form of a_2 in equation (3.6), it follows that $|a_2| = |p - 1|$ at $q = 0$ also, so that the point $q = 0$ is a solution to equation (3.9) and hence is on the locus $\mathcal{B}$, which proves (B2).

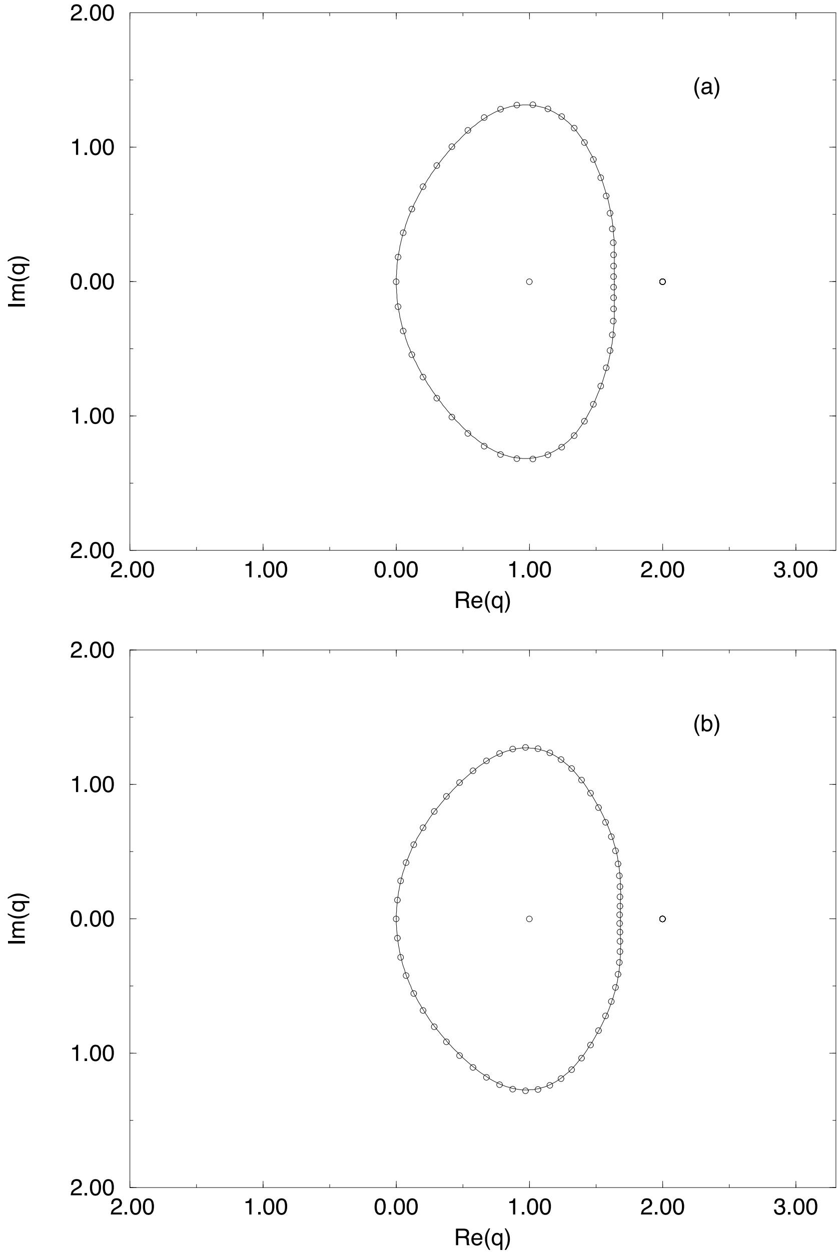


Figure 5. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (*a*) $(2, 3, 2)$, (*b*) $(2, 3, 3)$. Chromatic zeros for $m = 10$ (i.e., $n = 60$ and $n = 70$ for (*a*) and (*b*)) are shown for comparison.

Property (B3) can be proved by explicit solution of (3.9). One also observes from the results presented in figures 2–9 that in cases where $\mathcal{B}$ does not contain any multiple points†,

† In the technical terminology of algebraic geometry [23], a multiple point on an algebraic curve is a point where several branches of the curve intersect. If all n_i of the branches have different tangents, the multiple point is said to

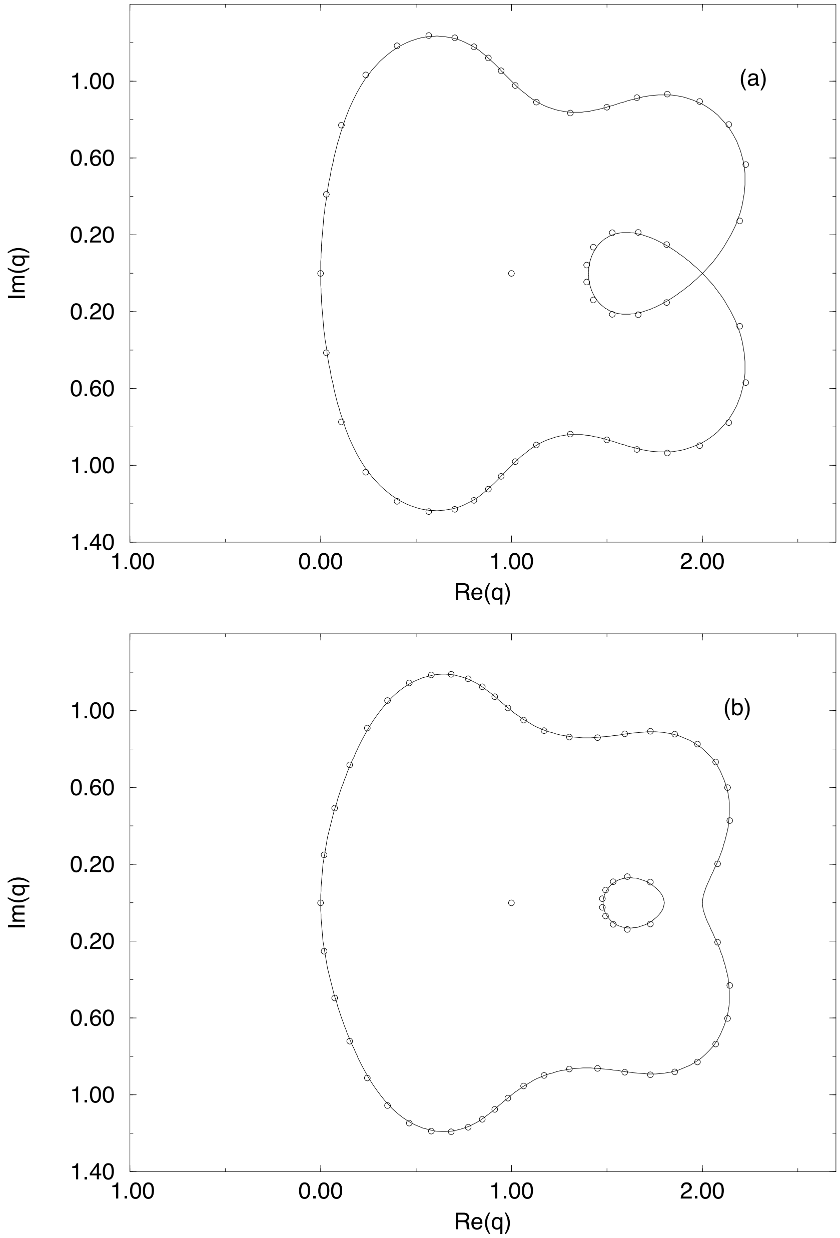


Figure 6. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 4, 0)$, (b) $(2, 4, 1)$. Chromatic zeros for $m = 10$ (i.e., $n = 50$ and $n = 60$ for (a) and (b)) are shown for comparison.

the number of regions, $N_{reg.}$ and the number of connected components on $\mathcal{B}$ satisfy the relation $N_{reg.} = N_{comp.} + 1$. As was the case in our earlier work [21], one can get a general upper bound on the number $N_{comp.}$ using the Harnack theorem [23] from algebraic geometry, but it is not very restrictive. To do this, we write the equation (3.9), whose solution set is $\mathcal{B}$, out in terms

have index n_i.

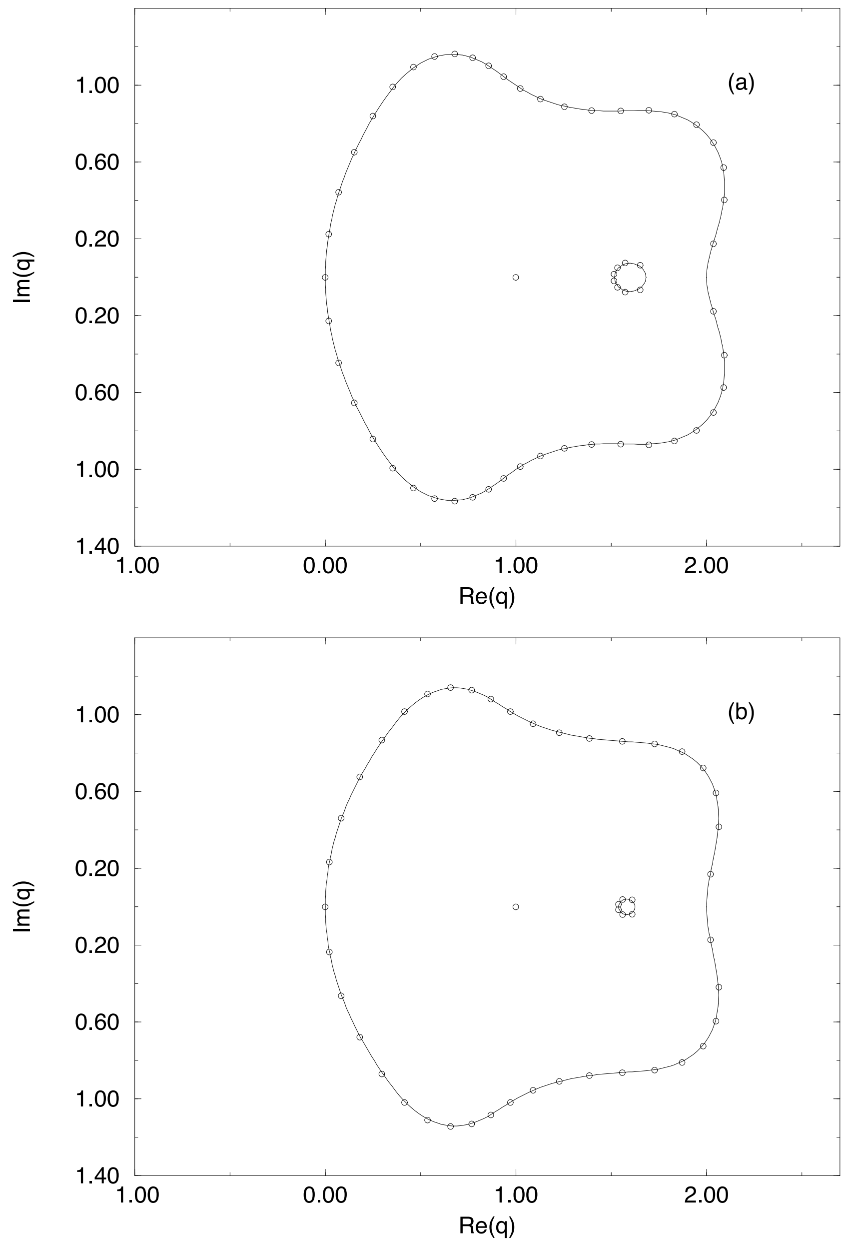


Figure 7. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 4, 2)$, (b) $(2, 4, 3)$. Chromatic zeros for (a) $m = 8$ (i.e., $n = 56$) and (b) $m = 6$ (i.e., $n = 48$) are shown for comparison.

of the real and imaginary components of q or, more conveniently, of $a = q - 1$. This yields a polynomial equation of general degree $d = 2(p+e_g)$ in these components. In the cases without singular (multiple) points on $\mathcal{B}$, the Harnack theorem then gives the upper bound $N_{comp.} \leqslant h+1$, where h, the genus of the algebraic curve comprising $\mathcal{B}$, is $h = (d-1)(d-2)/2$ [23]. Thus, for example, for the lowest case $(e_1, e_2, e_g) = (2, 2, 1)$, the Harnack theorem gives the upper

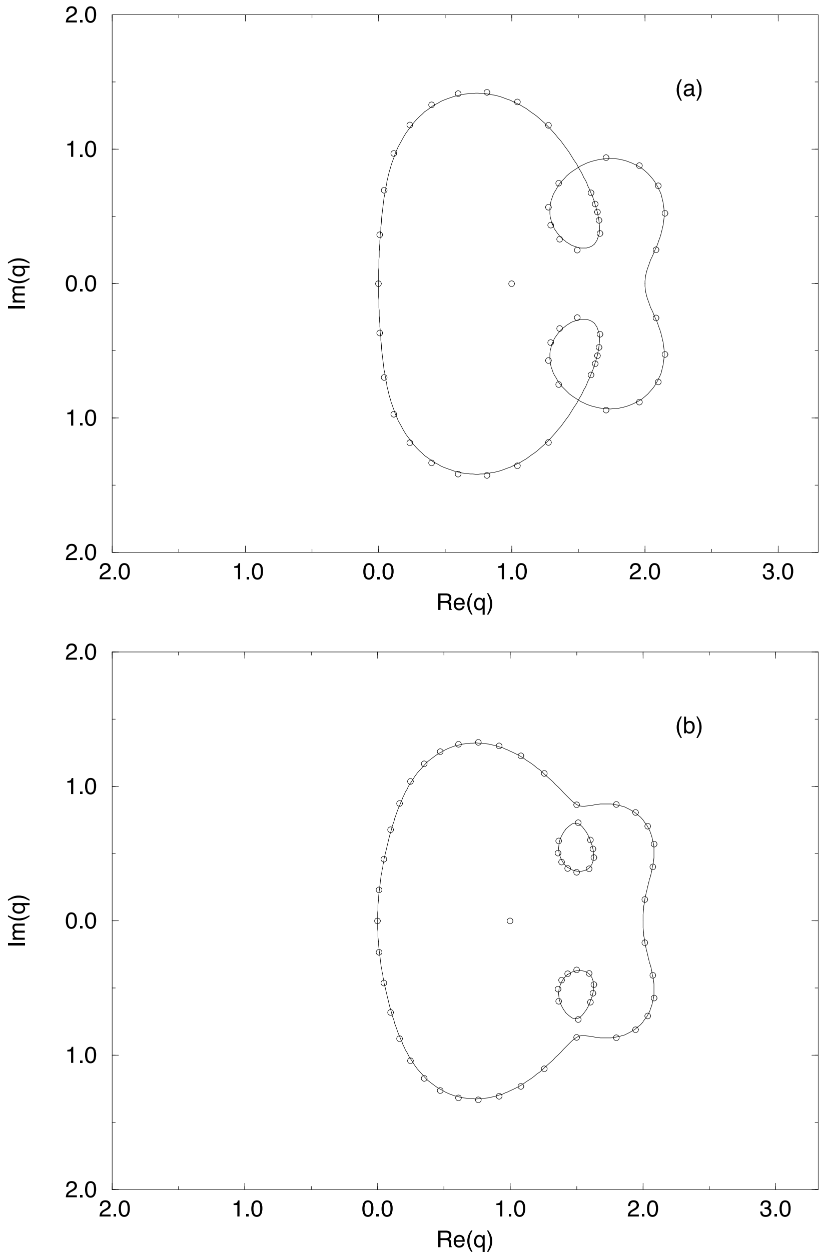


Figure 8. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (a) $(3, 3, 0)$, (b) $(3, 3, 1)$. Chromatic zeros for $m = 10$ (i.e., $n = 50$ and $n = 60$ for (a) and (b)) are shown for comparison.

bound $N_{comp.} \leqslant 37$. Clearly, this is a very weak upper bound compared with the actual result $N_{comp.} = 2$. The upper bound becomes even higher for larger values of e_g, and hence weaker, since the result remains $N_{comp.} = 2$ for all families of the form $(e_1, e_2, e_g) = (2, 2, e_g)$. Similar remarks apply for the Harnack bound applied to other cases (e_1, e_2, e_g).

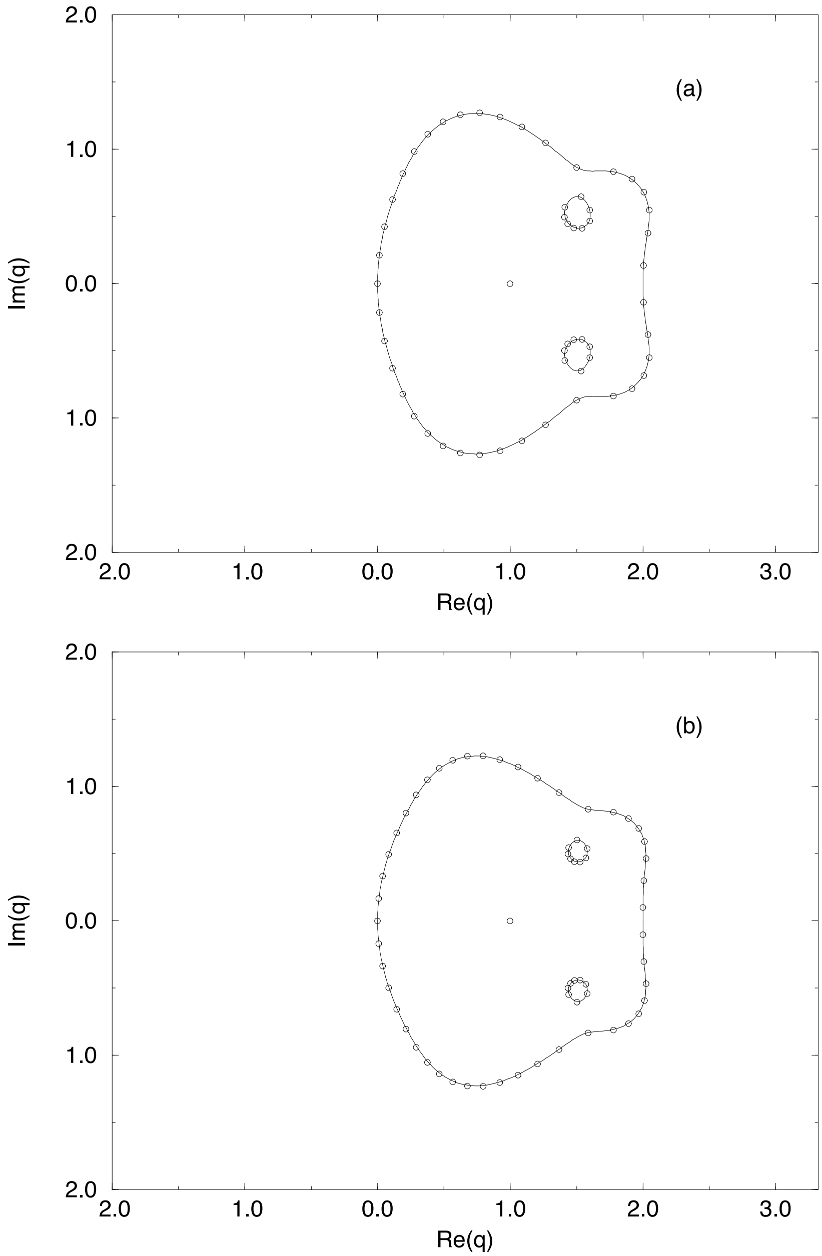


Figure 9. Boundary $\mathcal{B}$ in the q plane for W function for $\lim_{m\to\infty} G_{e_1,e_2,e_g,m}$ with $(e_1, e_2, e_g) =$ (*a*) $(3, 3, 2)$, (*b*) $(3, 3, 3)$. Chromatic zeros for $m = 8$ (i.e., $n = 56$ and $n = 64$ for (*a*) and (*b*)) are shown for comparison.

To prove (B4), we observe that for families where $e_s = 1$, because of the factorization (3.7), for any values of e_ℓ and e_g, the locus $\mathcal{B}$ is the unit circle $|q-1| = 1$. The result on chromatic zeros follows immediately from (3.7) and the fact that the zeros of the chromatic polynomial of the circuit graph lie exactly on the circle $|q-1| = 1$ [15].

To prove property (B5), we first observe that since p is even, the left-hand side of equation (3.10) has the value 2 for $q = 2$, i.e., for $a = 1$. The condition that p is even means that either both e_1 and e_2 are even or both e_1 and e_2 are odd. In both of these cases, the right-hand side of equation (3.10) is also equal to 2 for $q = 2$, so that $q = 2$ is a solution of this equation. Furthermore, one easily checks that (3.10) has no solution for larger real q. This yields (B5).

For property (B6) pertaining to odd p, we recall that the case $e_s = 1$ is already covered by (B4); for $e_s \geqslant 2$, we first note that since p is odd, one of (e_1, e_2) is odd and the other is even; these are denoted e_{even} and e_{odd}. We next observe that for odd $p = 2k + 1$, D_p contains a factor $(q - 2)$ times a polynomial:

$$D_{2k+1} = (q-2)F_{2k+1} \tag{3.16}$$

where

$$F_{2k+1} = k \qquad \text{at} \quad q = 2. \tag{3.17}$$

Now let us consider the limit $q \to 2$. From equations (3.16) and (3.17), we have

$$a_1 \to \frac{(q-2)(p-1)}{2} \qquad \text{as} \quad q \to 2. \tag{3.18}$$

Furthermore,

$$a_2 \to \tfrac{1}{2}(-1)^{e_g+1}(q-2)(1 + e_{even} - e_{odd}) \qquad \text{as} \quad q \to 2. \tag{3.19}$$

Hence for the chromatic polynomial (3.4),

$$P(G_{e_{even},e_{odd},e_g,m}, q \to 2) \to \left[\frac{(q-2)(p-1)}{2}\right]^m \left[1 + \left(\frac{(-1)^{e_g+1}(1 + e_{even} - e_{odd}}{p-1}\right)^m\right]. \tag{3.20}$$

Since

$$\frac{|1 + e_{even} - e_{odd}|}{p-1} < 1 \tag{3.21}$$

for the relevant case $e_s \geqslant 2$ considered here, it follows that, taking the $m \to \infty$ limit first, before the $q \to 2$ limit, the contribution of the second term in the square brackets, i.e., the a_2 term, in equation (3.20), relative to that of the first, i.e., the a_1 term, goes to zero. Recalling our order of limits (1.2), it follows that at $q = 2$, the function W is determined completely by the a_1 term. Hence, although a_1 and a_2 both vanish at $q = 2$, this point is not on the locus $\mathcal{B}$ since W is determined only by a_1 at this point. This shows that the condition of the degeneracy of terms $|a_1(q)| = |a_2(q)|$ is necessary in order that the point q lie on the locus $\mathcal{B}$, but, as noted in connection with equation (3.9), a further necessary (and sufficient) condition is that this equality in magnitudes, holds, where a_1 and a_2 are both nonzero leading terms. Since W is determined by a_1 at $q = 2$, the same as in region R_1 (see below), this shows that $q_c < 2$, which was to be proved.

The other property in (B6) follows in a similar manner from the solution to equation (3.10). The fact that $q_c \to 2$, i.e., $a_c \to 1$, where $a_c = q_c - 1$, is clear from (3.10) since if $a > 1$ ($a < 1$), the left-hand side diverges (vanishes) as $e_g \to \infty$, precluding equality with the right-hand side.

We observe several other interesting features of the locus $\mathcal{B}$. For $e_g = 0$ and $e_s \geqslant 2$ and for certain values of (e_1, e_2), this locus, as an algebraic curve, may contain one or more multiple point(s), which are of index 2, i.e., they involve a crossing of four curves forming two branches of $\mathcal{B}$. A particularly simple set of families for which this occurs is the set where $e_1 = e_2 = p/2 \equiv e_{12}$. By an analysis of equation (3.10), we find that for this set there are

$$N_{m.p.} = e_{12} - 1 \tag{3.22}$$

multiple points, which occur at

$$q_j = 1 + \mathrm{e}^{\mathrm{i}\theta_j} \tag{3.23}$$

where

$$\theta_j = \pm\frac{2j\pi}{e_{12}} \qquad j = 0, 1, \ldots, \frac{e_{12}-2}{2} \qquad \text{for} \quad e_{12} \text{ even} \tag{3.24}$$

$$\theta_j = \pm\frac{(2j+1)\pi}{e_{12}} \qquad j = 0, 1, \ldots, \frac{e_{12}-3}{2} \qquad \text{for} \quad e_{12} \text{ odd.} \tag{3.25}$$

For example, in figure 2(a) for $(e_1, e_2, e_g) = (2, 2, 0)$ one sees that there is one such multiple point, located at $q = q_c = 2$, while in figure 8(a) for $(e_1, e_2, e_g) = (3, 3, 0)$ there are two complex-conjugate multiple points, located at $q = 1 + \mathrm{e}^{\pm\mathrm{i}\pi/3}$. Figure 6 illustrates another case with a multiple point, namely $(e_1, e_2, e_g) = (2, 4, 0)$, for which the multiple point is at $q = q_c = 2$. In figures 2–9 one sees that the multiple points that are present for $e_g = 0$ disappear when $e_g \geqslant 1$. Figures 4 and 5 illustrate a family with p odd, namely, $(e_1, e_2) = (2, 3)$ for which $\mathcal{B}$ has no multiple points.

In the cases where $\mathcal{B}$ contains multiple point(s) for $e_g = 0$, which disappear when $e_g \geqslant 1$, each such disappearance is accompanied by the appearance of a new disconnected component of $\mathcal{B}$. As e_g increases, the sizes of the regions bounded by these components of $\mathcal{B}$ decrease, and as $e_g \to \infty$, the regions shrink to points. For example, in figures 2 and 3 one sees that for the case $(2, 2, e_g)$, as e_g increases from $e_g = 0$ to $e_g \geqslant 1$, the multiple point at $q = q_c = 2$ that was present for $e_g = 0$ disappears and there appears a disconnected component of $\mathcal{B}$ defining a new region, so that the number $N_{comp.}$ of (separate, disconnected) components of $\mathcal{B}$ increases from 1 to 2. As $e_g \to \infty$, this region shrinks to a point at $q = \frac{3}{2}$. Similarly, in figures 8 and 9 one sees that for the case $(e_1, e_2) = (3, 3)$, as e_g increases from 0 to $e_g \geqslant 1$, the complex-conjugate multiple points that were present for $e_g = 0$ at $q = 1 + e^{\pm\mathrm{i}\pi/3}$ disappear and $N_{comp.}$ increases from 1 to 3. As $e_g \to \infty$, the inner regions shrink to points at $q \simeq \frac{3}{2} \pm \mathrm{i}/2$.

Another feature that one observes in the results shown in the figures is that these loci $\mathcal{B}$ do not have any support for $\mathrm{Re}\,(q) < 0$. Since the present families of graphs do not, in general, have a regular lattice structure, this result is independent of our conjecture [19, 22] that for families of graphs with regular lattice structure, global circuits are a necessary, but not sufficient, condition for $\mathcal{B}$ to have support for $\mathrm{Re}\,(q) < 0$. (Recall that in [20] we exhibited families of graphs that do not have lattice structure or global circuits but do have $\mathcal{B}$ having support for $\mathrm{Re}\,(q) < 0$.)

For $W([\lim_{m\to\infty} G_{e_1,e_2,e_g,m}], q)$, which henceforth will be abbreviated simply as W, we have the following general results. In region R_1,

$$W = (a_1)^{\frac{1}{p+e_g-1}} = [(q-1)^{e_g+1} D_p]^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad q \in R_1. \tag{3.26}$$

We note that the function on the right-hand side of equation (3.26) is the same as that for the open chain, (2.10), although in the latter case, the result holds throughout the full q plane whereas for the cyclic chain, the result holds only in region R_1. One can approach the origin, $q = 0$ from the left staying within the region R_1, and in this limit, using the property (3.15), we have

$$W = (p-1)^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad q \to 0, \quad q \in R_1. \tag{3.27}$$

Let us denote region R_2 as the one containing the point $q = 1$; this region is contiguous to R_1 at the origin, $q = 0$. In region R_2, a_2 is the dominant term, so that

$$|W| = |a_2|^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad q \in R_2. \tag{3.28}$$

In particular, for families of graphs with $e_s = 1$, where the factorization (3.7) holds,

$$|W| = |D_p|^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad e_s = 1 \quad \text{and} \quad q \in R_2. \tag{3.29}$$

For cases where there are additional regions R_j enclosed within R_2,

$$|W| = |a_1|^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad q \in R_j \text{ enclosed within } R_2. \tag{3.30}$$

For $e_g = 0$ these additional regions are contiguous with R_1 at multiple points on $\mathcal{B}$.

Concerning values of W at special points, we observe that since $q_c \leqslant 2$, the expression (3.26) always holds at $q = 2$, so that, as a consequence of the property (3.16),

$$W(q = 2) = 0 \qquad \text{for odd } p. \tag{3.31}$$

Note that this does not follow just from the property that the chromatic polynomial P vanishes at $q = 2$ for odd p, but requires the stronger property that P contains the factor $(q-2)^{\nu}$ with $\nu \propto n$ as $n \to \infty$. In contrast, for even $p = 2k$, using the property

$$D_{2k} = 1 \qquad \text{for} \quad q = 2 \tag{3.32}$$

we have

$$W(q = 2) = 1 \qquad \text{for even } p. \tag{3.33}$$

As one approaches $q = 0$ from within region R_2, using (3.15), it follows that

$$|W| = |p-1|^{\frac{1}{p+e_g-1}} \qquad \text{for} \quad q \to 0, \quad q \in R_2 \tag{3.34}$$

in accord with (3.27) and the equality of the magnitude of $|W|$ across any point on $\mathcal{B}$.

In figures 2–9 we have also shown the chromatic zeros of $G_{e_1,e_2,e_g,m}$ for large finite values of m to compare with the $m \to \infty$ accumulation set $\mathcal{B}$. We first observe that the chromatic zeros lie quite close to the asymptotic locus $\mathcal{B}$. Second, the density of chromatic zeros appears to vanish at multiple points, just as was the case for multiple points on complex-temperature phase boundaries for which we carried out exact calculations previously [24]. As one increases e_g above 0, so that new components of $\mathcal{B}$ pinch off, one still sees a remnant of the reduction of density on the sides facing the location of the multiple point that had existed for $e_g = 0$.

4. Conclusions

In this paper we have given exact expressions for the chromatic polynomial $P(G, q)$ and the resultant exponent of the ground state entropy for the Potts antiferromagnet in the $n \to \infty$ limit, $W(\{G\}, q)$ for families of cyclic polygon chain graphs $G = G_{e_1,e_2,e_g,m}$. We have studied several types of limits yielding $n \to \infty$, namely, L_{e_g}, L_p, and L_m, the last of which yielded the most interesting results. From these calculations we have derived the continuous locus, $\mathcal{B}$, of nonanalyticities of W, which is also the accumulation set of the zeros of the chromatic polynomial in the $n \to \infty$ limit. Various properties of this locus were proved. A comparison with the results for the open polygon chain graph shows the important effect of global circuits. The results of this study agree with and extend our earlier inferences concerning the locus $\mathcal{B}$, in particular, that a sufficient condition that in the $n \to \infty$ limit the locus $\mathcal{B}$ separates the q plane into two or more regions is that the graph has a global circuit with $\lim_{n\to\infty} \ell_{g.c.} = \infty$.

Acknowledgment

This research was supported in part by the NSF grant PHY-97-22101.

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