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Chromatic polynomials and their zeros and asymptotic limits for families of graphs

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Abstract

Let $P(G, q)$ be the chromatic polynomial for coloring the n -vertex graph G with q colors, and define $W = \lim_{n \rightarrow \infty} P(G, q)^{1/n}$. Besides their mathematical interest, these functions are important in statistical physics. We give a comparative discussion of exact calculations of P and W for a variety of recursive families of graphs, including strips of regular lattices with various boundary conditions and homeomorphic expansions thereof. Generalizing to $q \in \mathbb{C}$, we determine the accumulation sets of the chromatic zeros, which constitute the continuous loci of points on which W is nonanalytic. Conditions for the chromatic zeros and their accumulation set to (i) include support for $\text{Re}(q) < 0$; (ii) to bound regions; and (iii) to be noncompact are discussed, and the role of boundary conditions is analyzed. Some corresponding results are presented for Potts model partition functions for nonzero temperature, equivalent to the full Tutte polynomials for various families of graphs. © 2001 Elsevier Science B.V. All rights reserved.

1. Introduction

We consider connected graphs G without loops or multiple bonds and denote the number of vertices as $n = v(G)$, the edges as $e(G)$, the girth as g , the number of circuits with this minimal length as k_g , and the chromatic number as $\chi(G)$. The chromatic polynomial $P(G, q)$ counts the number of ways that one can color the graph G with q colors such that no two adjacent vertices have the same color [10] (for reviews, see [18,42,21,5]). The minimum number of colors needed for this coloring, i.e., the smallest positive integer q for which $P(G, q)$ is nonzero, is the chromatic number, $\chi(G)$. Besides its intrinsic mathematical interest, the chromatic polynomial has an important connection with statistical mechanics since it is the zero-temperature partition function

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of the q -state Potts antiferromagnet (AF) [17,45] on G :

$$P(G, q) = Z(G, q, T = 0)_{\text{PAF}}. \quad (1.1)$$

We shall consider recursively defined families of graphs here, i.e., roughly speaking, those that can be formed by successive additions of a given subgraph. A precise definition of a recursive family G_m depending on a positive integer parameter m is a sequence of graphs for which the chromatic polynomials $P(G_m, q)$ are related by a linear homogeneous recurrence relation in which the coefficients are polynomials in q [5,7]. These include strips of regular lattices with various boundary conditions, chains of polygons linked in various ways, joins of such graphs with another graph such as a complete graph K_p , and families obtained from these by modifications such as removal of some edges or additions of degree-two vertices, i.e., homeomorphic expansions. These families of graphs may depend on several parameters (e.g. width, length, number of homeomorphic expansions, etc.), and there can be several ways in which one can obtain the limit $n \rightarrow \infty$. Let us concentrate on one such parameter, such as the length of a strip of a regular lattice of fixed width or polygon chain, m , so that n is a linear function of m .

Just as the chromatic polynomial counts the total number of ways of coloring the graph G with q colors subject to the above constraint, so also it is useful to define a quantity that measures the number of ways of performing this coloring per site, in the limit where the number of vertices goes to infinity. Denoting the formal limit $\{G\} = \lim_{n \rightarrow \infty} G$, we have²

$$W(\{G\}, q) = \lim_{n \rightarrow \infty} P(G, q)^{1/n}. \quad (1.2)$$

With the order of limits specified in the footnote, this limit exists for the recursive families of graphs considered here, as will be discussed further below. The function W is the ground state degeneracy per vertex in the $n \rightarrow \infty$ limit. The quantity $S_0 = k_B \ln W$, where k_B is the Boltzmann constant, is defined as the ground state entropy. The Potts antiferromagnet has the interesting feature that it exhibits nonzero ground state entropy $S_0 \neq 0$ (without frustration) for sufficiently large q on a given lattice or graph and is thus an exception to the third law of thermodynamics. This is equivalent to a ground state degeneracy per site $W > 1$. For example, for the square lattice, $W = (\frac{4}{3})^{3/2}$ [13]. We recall that, with $n = v(G)$, a general form for the chromatic polynomial of a connected graph G is

$$P(G, q) = \sum_{j=0}^{n-1} (-1)^j h_{n-j} q^{n-j}, \quad (1.3)$$

² At certain special points q_s (typically $q_s = 0, 1, \dots, \chi(G)$), one has the noncommutativity of limits $\lim_{q \rightarrow q_s} \lim_{n \rightarrow \infty} P(G, q)^{1/n} \neq \lim_{n \rightarrow \infty} \lim_{q \rightarrow q_s} P(G, q)^{1/n}$, and hence it is necessary to specify the order of the limits in the definition of $W(\{G\}, q_s)$ [28]. We use the first order of limits here; this has the advantage of removing certain isolated discontinuities in W .

where h_{n-j} are positive integers, with [15,21] $h_{n-j} = \binom{e}{j}$ for $0 \leq j < g - 1$ (whence $h_n = 1$ and $h_{n-1} = e$) and $h_{n-(g-1)} = \binom{e}{g-1} - k_g$.

Although in the Hamiltonian formulation of the q -state Potts model or the mathematical context of coloring a graph with q colors, q must be a non-negative integer, once one has the function $P(G, q)$, one can generalize the quantity q from \mathbb{Z}_+ to \mathbb{C} . A subset of the zeros of P in the q plane (chromatic zeros) may form a continuous accumulation set in the $n \rightarrow \infty$ limit, denoted \mathcal{B} , which is the continuous locus of points where $W(\{G\}, q)$ is nonanalytic [3,20,28] (\mathcal{B} may be null, and W may also be nonanalytic at certain discrete points). The maximal region in the complex q plane to which one can analytically continue the function $W(\{G\}, q)$ from the range of positive integer values where there is nonzero ground state entropy is denoted R_1 . The maximum value of q where \mathcal{B} intersects the (positive) real axis is labelled $q_c(\{G\})$. Thus, region R_1 includes the positive real axis for $q > q_c(\{G\})$. We have calculated \mathcal{B} for a variety of families of graphs and shall present rigorous results, some observations, and some conjectures here. Part of the interest in this area of research is that it combines, in a fruitful way, both theoretical physics and three areas of mathematics: graph theory, complex analysis, and algebraic geometry. In addition to the works already cited, some previous relevant papers are listed in the references.

As noted above, a recursive family of graphs may depend on several parameters, and there can be several ways in which one can obtain the limit $n \rightarrow \infty$. Concentrating on one such parameter, such as the length of a strip of a regular lattice or polygon chain, m , and denoting the graph as $(G_s)_m$, a general form for $P((G_s)_m, q)$ is

$$P((G_s)_m, q) = \sum_{j=1}^{N_a} c_j(q) a_j(q)^m, \tag{1.4}$$

where $c_j(q)$ and the N_a terms $a_j(q)$ (which we shall also denote equivalently as $\lambda_j(q)$) depend on the type of strip graph G_s but are independent of m . We define a term a_ℓ as ‘leading’ (ℓ) if it dominates the $n \rightarrow \infty$ limit of $P(G, q)$. The locus \mathcal{B} occurs where, as one changes q , there is an abrupt, nonanalytic change in W as the leading terms a_ℓ in eq. (1.4) changes. Hence, \mathcal{B} is the solution to the equation of degeneracy of magnitudes of leading terms, $|a_\ell| = |a_{\ell'}|$. It follows that $|W|$ is finite and continuous, although nonanalytic, across \mathcal{B} . In general, for the families of graphs considered here, \mathcal{B} is an algebraic curve, since it is the locus of solutions to the equation $|a_\ell| = |a_{\ell'}|$ and the terms $a_\ell, a_{\ell'}$ are algebraic functions of q . From (1.4), one can show constructively that limit (1.2) exists; it is given by $W(\{s\}, q) = (a_\ell)^t$ where $\lim_{m \rightarrow \infty} m/n = t$ and a_ℓ is the term among the $a_j, j = 1, \dots, N_a$ with maximum magnitude. Thus, a number of interesting questions can be asked and answered about its properties. Concerning the coefficients c_j , we note that

$$c_\ell(q) = 1 \quad \text{if } a_\ell(q) \text{ is dominant in } R_1. \tag{1.5}$$

This is proved by using the fact that region R_1 is defined to include the region of large real q , and then requiring expression (1.4) to match the general expression (1.3) and satisfy the property that the coefficient of the leading term, q^n , is unity. For

some families of graphs, the c_j and a_j are polynomials in q . However, there are also families of graphs, such as the $L_y=3$ cyclic and Möbius strips of the square and kagomé lattices [25,38] (see below for notation) which have nonpolynomial algebraic a_j 's with polynomial c_j 's, and families of graphs, such as certain strip graphs of regular lattices with free transverse and longitudinal boundary conditions [22,33], as well as the $L_y=2$ Möbius strips of the triangular lattice and asymmetric homeomorphic expansions of the $L_y=2$ Möbius square strip [25,38] for which some a_j 's and their respective c_j 's are both algebraic, nonpolynomial functions of q . When the a_j 's are algebraic nonpolynomial functions of q , this happens because these are roots of an algebraic equation of degree 2 or higher. There are then two possibilities: first, the roots may enter in a symmetric manner, and, because of a theorem on symmetric polynomial functions discussed below, their coefficients are all equal and are polynomial functions of q . In particular, if one of these a_j 's is leading in R_1 , then the coefficient functions for all of the roots are equal to unity, in accordance with (1.5). This happens, for example, for the $L_y=3$ cyclic and Möbius strips of the square lattice, where the leading term, $a_{sq,6} \equiv \lambda_{sq,6}$ in Eq. (4.1) is the root of a quadratic equation (see Eq. (4.2)) and enters the chromatic polynomial together with the other root of this equation, each with the same coefficient, which is unity. A second possibility is that the nonpolynomial algebraic roots enter in (1.4) in a manner that is not a symmetric function of these roots; in these cases, the corresponding coefficient functions are also nonpolynomial algebraic functions of q . For example, in many strips with free transverse and longitudinal boundary conditions [22,33] and in the the Möbius strip of the triangular lattice and the homeomorphic expansion of the Möbius strip of the square lattice, one finds [38] that two of the a_j 's are roots of a quadratic equation of the form $a_{\pm} = R \pm \sqrt{S}$, and they occur in the chromatic polynomial in the form $(a_+)^m - (a_-)^m$; for these families, this combination is multiplied by the factor $1/(a_+ - a_-)$, i.e., the coefficient functions contain the respective factors $\pm 1/\sqrt{S}$. In all cases, of course, these combine to yield a $P(G, q)$ that is a polynomial in q .

Two other general result that follow from Eqs. (1.2)–(1.4) are as follows. As $m, n \rightarrow \infty$, let $r = n/m$, which depends on G_s . Then

$$a_{\ell} \sim q^r \quad \text{for } q \in R_1, \quad |q| \rightarrow \infty, \quad (1.6)$$

$$W = (a_{\ell})^{1/r} \quad \text{for } q \in R_1, \quad (1.7)$$

so that $\lim_{|q| \rightarrow \infty; q \in R_1} q^{-1} W = 1$.

2. Calculation of chromatic polynomials

For a recursively defined family of graph G_s our calculational method is to use the deletion-contraction theorem iteratively. For some families of graphs we have directly solved for the chromatic polynomials from the recursion relations that follow from this

iterative procedure. A related method that we have found to be useful employs a generating function and is described below [22,33]. Let us consider strips of various lattices with arbitrary length $L_x = m$ vertices and fixed width L_y vertices (with the longitudinal and transverse directions taken to be \hat{x} and \hat{y}). The chromatic polynomials for the cyclic and Möbius strip graphs of the square lattice were calculated for $L_y = 2$ in [7] by means of iterative deletion-contraction operations, and subsequently via a transfer matrix method in [8] and a coloring matrix method in [4] (see also [6]). We have extended this to the corresponding cyclic [38] and Möbius [25] $L_y = 3$ strips. For each graph family, once one has calculated the chromatic polynomial for arbitrary length, one can take the limit of infinite length and determine the accumulation set \mathcal{B} . After studies of the chromatic zeros for $L_y = 2$ in [7,19,20], W and \mathcal{B} were determined for this case in [28] and for $L_y = 3$ in [25,38]. An interesting question concerns the effect of boundary conditions (BC's), and hence graph topology, on P , W , and \mathcal{B} . We use the symbols FBC_y and PBC_y for free and periodic transverse boundary conditions and FBC_x , PBC_x , and TPBC_x for free, periodic, and twisted periodic longitudinal boundary conditions. The term “twisted” means that the longitudinal ends of the strip are identified with reversed orientation. These strip graphs can be embedded on surfaces with the following topologies: (i) ($\text{FBC}_y, \text{FBC}_x$): strip; (ii) ($\text{PBC}_y, \text{FBC}_x$): cylindrical; (iii) ($\text{FBC}_y, \text{PBC}_x$): cylindrical (denoted cyclic here); (iv) ($\text{FBC}_y, \text{TPBC}_x$): Möbius; (v) ($\text{PBC}_y, \text{PBC}_x$): torus; and (vi) ($\text{PBC}_y, \text{TPBC}_x$): Klein bottle.³ We have calculated P , W , and \mathcal{B} for a variety of strip graphs having BC's of type (i) [22,23,27,33], (ii) [27], (iii) [34,36,38], (iv) [25,34]. Recently, strip graphs of the square lattice with BC's of torus (v) and Klein bottle (vi) type have also been studied [9]. In addition to strips of regular lattices, we have calculated P , W , and \mathcal{B} for cyclic graphs of polygons linked in various manners [36] and homeomorphic expansions of strip graphs [33,34,38].

We proceed to describe our generating function method for calculating chromatic polynomials. The generating function is denoted $\Gamma(G_s, q, x)$, and the chromatic polynomials for the strip of length $L_x = m$ are determined as the coefficients in a Taylor series expansion of this generating function in an auxiliary variable x about $x = 0$:

$$\Gamma(G_s, q, x) = \sum_{m=m_0}^{\infty} P((G_s)_m, q) x^{m-m_0}, \quad (2.1)$$

where m_0 depends on the type of strip graph G_s and is naturally chosen as the minimal value of m for which the graph is well defined. The generating functions $\Gamma(G_s, q, x)$ are rational functions of the form [22]

$$\Gamma(G_s, q, x) = \frac{\mathcal{N}(G_s, q, x)}{\mathcal{D}(G_s, q, x)} \quad (2.2)$$

³ These BC's can all be implemented in a manner that is uniform in the length L_x ; the case (vii) ($\text{TPBC}_y, \text{TPBC}_x$) with the topology of the projective plane requires different identifications as L_x varies and is not considered here.

with

$$\mathcal{N}(G_s, q, x) = \sum_{j=0}^{d_{\mathcal{N}}} A_{G_s, j}(q) x^j \tag{2.3}$$

and

$$\mathcal{D}(G_s, q, x) = 1 + \sum_{j=1}^{d_{\mathcal{D}}} b_{G_s, j}(q) x^j, \tag{2.4}$$

where the $A_{G_s, i}$ and $b_{G_s, i}$ are polynomials in q (with no common factors). Writing the denominator of $\Gamma(G_s, q, x)$ in factorized form, we have (with $d_D = \text{deg}_x D$)

$$\mathcal{D}(G_s, q, x) = \prod_{j=1}^{\text{deg}_x \mathcal{D}} (1 - \lambda_{G_s, j}(q) x). \tag{2.5}$$

One can then calculate c_j and a_j in (1.4) in terms of these quantities:

$$P(G_m, q) = \sum_{j=1}^{d_{\mathcal{D}}} \left[\sum_{s=0}^{d_{\mathcal{N}}} A_s \lambda_j^{d_{\mathcal{D}}-s-1} \right] \left[\prod_{1 \leq i \leq d_{\mathcal{D}}, i \neq j} \frac{1}{(\lambda_j - \lambda_i)} \right] \lambda_j^m. \tag{2.6}$$

In general,

$$a_j = \lambda_j. \tag{2.7}$$

We show here how the nonpolynomial algebraic roots in the various P 's yield polynomials in q . As is evident from (2.5), for a given strip, the λ_j 's arise as roots of the equation $\mathcal{D} = 0$. In general, \mathcal{D} contains some number of factors of linear, quadratic, cubic, etc. order in x . Consider a generic factor in \mathcal{D} of r th degree in x : $(1 + f_1 x + f_2 x^2 + \dots + f_r x^r)$, where the f_j 's are polynomials in x . This yields r λ_ℓ 's as roots of the equation $\zeta^r + f_1 \zeta^{r-1} + \dots + f_r = 0$. The expressions in P involving these roots are symmetric polynomial functions of the roots, namely terms of the form

$$s_m = \sum_{\ell=1}^r (\lambda_\ell)^m \tag{2.8}$$

and, for the Möbius strips of the $L_y = 2$ triangular lattice and asymmetric homeomorphic expansions of the $L_y = 2$ Möbius square strip, as well as strips with $(\text{FBC}_y, \text{FBC}_x)$, terms of the form

$$\frac{(\lambda_+)^m - (\lambda_-)^m}{\lambda_+ - \lambda_-} = \sum_{k=0}^{m-1} (\lambda_+)^{m-1-k} (\lambda_-)^k. \tag{2.9}$$

We can then apply a standard theorem (e.g. [43]) which states that a symmetric polynomial function of the roots of an algebraic equation is a polynomial in the coefficients, here f_ℓ , $\ell = 1, \dots, r$; hence, this function is a polynomial in q . For example, for s_r , one has the well-known formulas (due to Newton) $s_1 = -f_1$, $s_2 = f_1^2 - 2f_2$, $s_3 = -f_1^3 + 3f_1 f_2 - 3f_3$, etc.

3. General results on \mathcal{B}

One can ask a number of questions about the properties of \mathcal{B} . We take the opportunity here to give a unified discussion of these which includes results from our various studies together with some new remarks.

1. Does \mathcal{B} have general symmetries? The answer is yes; a basic symmetry is that

$$\mathcal{B}(q) = \mathcal{B}(q^*), \quad (3.1)$$

i.e., \mathcal{B} is invariant under complex conjugation in the q plane. This follows from the fact that the chromatic zeros have this property, which, in turn, follows from the fact that the coefficients in the chromatic polynomial are real (cf. Eq. (1.3)).

2. What is the dimensionality of \mathcal{B} in the q plane? One proves from the definition of \mathcal{B} as the solution of the equality in magnitude of leading terms a_j in Eq. (1.4), that (in cases where it is not the empty set)

$$\dim(\mathcal{B}) = 1, \quad (3.2)$$

i.e. \mathcal{B} is comprised of curves (including possible line segments) on the real q -axis.

3. What is the topology of the curve \mathcal{B} and the associated ‘region diagram’ in the q plane? Does \mathcal{B} separate the q plane into two or more regions or not? Does \mathcal{B} cross the real q -axis, and, if so, at which points? From our studies [22,25,33,34,36,38], we arrive at the following inference, which we state as a conjecture:

Conjecture. For a family of graphs G_s with well-defined lattice structure,⁴ a sufficient condition for \mathcal{B} to separate the q plane into different regions is that G_s contains at least one global circuit, defined as a route following a lattice direction which has the topology of S^1 and a length $\ell_{\text{g.c.}}$ that goes to infinity as $n \rightarrow \infty$. In the context of strip graphs, this is equivalent to having PBC_x , i.e., periodic boundary conditions (or TPBC_x , twisted periodic boundary conditions) in the direction in which the strip length goes to infinity as $m \rightarrow \infty$.

That this is not a necessary condition was shown in [23]. A related conjecture is that, for a family of graphs G_s with well-defined lattice structure, a necessary and sufficient condition for \mathcal{B} to separate the q plane into regions and pass through $q=0$ is that G_s contains at least one global circuit. Indeed, all of the families of graphs that we have studied that contain global circuits also yield loci \mathcal{B} that pass through $q=2$ as well as $q=0$. In contrast, for the (homogeneous) strip graphs with $(\text{FBC}_y, \text{FBC}_x)$ studied in [22,23], \mathcal{B} consists of arcs that do not pass through $q=0$ and separate regions of the q plane. We find that as the width of the strip increases, these arcs tend to elongate and their ends tend to move toward each other, thereby suggesting that if one considered the sequence of strip graphs of this type with width L_y (having taken the limit $L_x \rightarrow \infty$ to obtain a locus \mathcal{B} for

⁴By well-defined lattice structure we mean that the vertices and edges of the graph can be put into a 1–1 correspondence with the vertices and edges of a section of a regular lattice.

- each member of this sequence), then in the limit $L_y \rightarrow \infty$, the arcs would close to form a \mathcal{B} that passes through $q=0$ and separates the q plane into two or more regions. The interesting feature of the cyclic and Möbius strips and cyclic polygon chain graphs [25,34,36,38] is that when the graphs contain a global circuit, this property of \mathcal{B} that it separates the q plane into regions and passes through $q=0$ already occurs for finite L_y . This means that the W functions of these graphs with cyclic and twisted cyclic longitudinal boundary conditions already exhibit a feature which is expected to occur for the \mathcal{B} for the W function of the full two-dimensional lattice. This expectation is supported by the calculation of W and \mathcal{B} for the 2D triangular lattice with cylindrical boundary conditions by Baxter [2]. Recently, in [9] with Biggs, we have found the same property for strips of the square lattice with $(\text{PBC}_y, \text{PBC}_x)$ (torus) and $(\text{PBC}_y, \text{TPBC}_x)$ (Klein bottle) boundary conditions.
4. Does \mathcal{B} have singular points in the technical terminology of algebraic geometry, such as (i) multiple points, where several branches of the curve intersect without crossing or cross each other, or (ii) endpoints? All of these possibilities are realized. There are cases where there are no multiple points, such as for the circuit and p -wheel graphs (defined in Eq. (3.3) below) and some polygon chain graphs. There are also cases where there are (a) multiple points associated with intersecting but non-crossing branches, such as the $L_y = 2$ and $L_y = 3$ cyclic and Möbius strips of the square lattice and the $L_y = 2$ strips of the kagomé ($3 \cdot 6 \cdot 3 \cdot 6$) lattice [25,28,38]; (b) multiple points associated with crossing curves, such as the $L_y = 2$ cyclic and Möbius strips of the triangular lattices and certain families of cyclic polygon graphs; and (c) multiple points associated with both branch intersections and crossings, such for as homeomorphic expansions of cyclic square strips [34]. We have also shown that homogeneous strips of regular lattices with free transverse and longitudinal boundary conditions have loci \mathcal{B} with endpoints [22] (see further below).
 5. Does \mathcal{B} consist of a single connected component, or several distinct components? In cases where \mathcal{B} does not contain any multiple points, the number of regions, N_{reg} , and the number of connected components on \mathcal{B} satisfy the relation $N_{\text{reg}} = N_{\text{comp}} + 1$. The Harnack theorem [24] gives the upper bound $N_{\text{comp}} \leq h + 1$, where h , the genus of the algebraic curve comprising \mathcal{B} , is $h = (d-1)(d-2)/2$. However, as we have discussed in [28,31], this is a very weak bound. For example, for the cyclic polygon chain family denoted $(e_1, e_2, e_g) = (2, 2, 1)$ in [36], we showed that $N_{\text{comp}} = 2$, while the Harnack theorem gives the upper bound $N_{\text{comp}} \leq 37$.
 6. Although \mathcal{B} is the continuous accumulation set of a subset of the chromatic zeros, these zeros do not, in general, lie precisely on this asymptotic locus \mathcal{B} for finite n . Are there families of graphs for which all or a subset of the zeros do lie exactly on \mathcal{B} for finite n ? We have answered this in the affirmative and have constructed a family of graphs, which we call p -wheels, and proved that except for a finite subset of chromatic zeros at certain nonnegative integer values (see below), all of the chromatic zeros lie exactly on \mathcal{B} [29]. Recall that the join of two graphs G and H is defined as the graph consisting of copies of G and H with additional edges added joining each vertex of G to each vertex of H [5]. A p -wheel is the

join

$$(Wh)_n^{(p)} = K_p + C_{n-p}, \quad (3.3)$$

so that $(Wh)_n^{(0)}$ is the circuit graph, C_n , $(Wh)_n^{(1)}$ is the usual wheel graph, etc. The locus \mathcal{B} is the circle

$$|q - p - 1| = 1 \quad (3.4)$$

and the real chromatic zeros occur at $q = 0, 1, \dots, p + 1$ for $n - p$ even and $q = 0, 1, \dots, p + 2$ for $n - p$ odd, while the complex zeros all lie on the above unit circle.

7. What is the density of the zeros on \mathcal{B} ? In special cases, in particular, the p -wheel graphs, it is a constant. In general, it varies as one moves along \mathcal{B} for a given family of graphs. Our calculations of chromatic zeros answer this question for specific families.
8. For many years, no examples of chromatic zeros were found with negative real parts, leading to the conjecture that $\text{Re}(q) \geq 0$ for any chromatic zero [11]. Although Read and Royle later showed that this conjecture is false [20], very few cases of graphs with chromatic zeros having $\text{Re}(q) < 0$ are known, and the investigation of such cases is thus valuable for the insight it yields into properties of chromatic zeros. Note that the condition that a graph has some chromatic zeros with $\text{Re}(q) < 0$ is a necessary but not sufficient condition that it has an accumulation set \mathcal{B} with support for $\text{Re}(q) < 0$. We have proved that certain homeomorphic expansions of square strip graphs with the boundary conditions $(\text{FBC}_y, \text{FBC}_x)$ [33] and $(\text{FBC}_y, \text{PBC}_x)$ [34], of length m units, have chromatic zeros with $\text{Re}(q) < 0$ for sufficiently large m and that they have loci \mathcal{B} with support for $\text{Re}(q) < 0$. We have also done the same for the $L_y = 3$ cyclic and Möbius strips of the square lattice and the $L_y = 2$ cyclic and Möbius strips of the kagomé $(3 \cdot 6 \cdot 3 \cdot 6)$ lattice [25,38]. A different example is families of graphs with noncompact \mathcal{B} [28,30,35,37]; with these, we constructed cases where the chromatic zeros have arbitrarily large negative $\text{Re}(q)$.
9. Is \mathcal{B} compact (which in our context is synonymous with the property of boundedness) in the q plane, or does it extend to complex infinity in some directions? This is related to the question of boundedness of the magnitudes of chromatic zeros. In [20] Read and Royle gave an example of a graph with a noncompact \mathcal{B} , namely the bipyramid graph. We have studied the question of the compactness of \mathcal{B} in a series of papers [28,30,35,37]. A necessary and sufficient condition such that \mathcal{B} is compact in the q plane is obtained as follows: one simply reexpresses the degeneracy equation for leading $a_j(q)$'s in terms of the variable $z = 1/q$ and determines if this has a solution for $z = 0$. By constructing and studying families of graphs with noncompact loci \mathcal{B} , we have elucidated the geometrical conditions leading to this noncompactness. Our studies show that a necessary condition is that some vertex has a degree Δ which goes to infinity as $n \rightarrow \infty$. However, this is obviously not a sufficient condition for noncompactness of \mathcal{B} , as is shown, for example, by the

p -wheel graphs $((Wh)^{(p)})_n$, in which the p vertices in the complete graph K_p have degree Δ that goes to infinity as $n \rightarrow \infty$ but for which \mathcal{B} is compact (Eq. (3.4)). From our studies we have found that in all cases of families with noncompact \mathcal{B} , the graphs have the common feature that, in the limit as $n \rightarrow \infty$, they contain an infinite number of different, non-overlapping non-self-intersecting circuits, each of which passes through two or more nonadjacent vertices. We are led to propose this as a conjecture for the condition on a graph family such that it has a noncompact \mathcal{B} [35,37].

10. The above conjecture also leads to the following corollary: A sufficient (not necessary) condition for a family of graphs to have a compact, bounded locus \mathcal{B} is that it is a regular lattice [30,35,37]. Clearly, if \mathcal{B} is noncompact, passing through the origin of the z plane, where $z = 1/q$, then the function $q^{-1}W$ has no large- q expansion, i.e., no Taylor series expansion in the variable z around the point $z = 0$. Our conjecture is in accord with the derivation of large- q expansions for regular lattices [16].
11. Another feature that we find is that for families of graphs that (a) contain global circuits, (b) cannot be written as the join $G = K_p + H$, where K_p is the complete graph on p vertices, and (c) have compact \mathcal{B} , this locus passes through $q = 0$ and crosses the positive real axis, thereby always defining a q_c . Note that $\mathcal{B}(\{K_p + H\}, q) = \mathcal{B}(\{H\}, q - p)$, i.e. the \mathcal{B} for $\{K_p + H\}$ is the same as that for $\{H\}$ shifted a distance p to the right in the q plane. Hence, examples of families of graphs with loci \mathcal{B} that do not pass through $q = 0$ include these joins, where H is a family whose \mathcal{B} does pass through zero. Other examples of graph families with \mathcal{B} not including $q = 0$ are those with noncompact \mathcal{B} [30,35,37].
12. What is the effect of the boundary conditions of the strip graph G_s on \mathcal{B} ? For homogeneous strip graphs with (FBC_y, FBC_x) boundary conditions, in the cases studied in [22] where \mathcal{B} is nontrivial, it consists of arcs and hence does contain endpoint singularities. In these cases, the λ_j 's are algebraic expressions and the arcs comprising \mathcal{B} run between branch point zeros of algebraic roots of polynomials in q . An arc can cross the real axis q axis if and only if it is self-conjugate, and it necessarily crosses vertically. \mathcal{B} contains a line segment on the positive real axis, say in the interval $q_1 < q < q_2$, if there are two λ_j 's, e.g. of the form $\lambda_{j,j'} = R(q) \pm \sqrt{S(q)}$ with R and S being polynomials in q such that $S < 0$ in the interval $q_1 < q < q_2$.
13. Again concerning the question of the role of boundary conditions: for the strip graph $(G_s)_m$ with a given type of transverse boundary conditions BC_y , the chromatic polynomial for PBC_x has a larger N_a than the chromatic polynomial for FBC_x , and the corresponding loci \mathcal{B} are different.
14. In the examples we have studied, we find that for a given type of strip graph G_s with FBC_y , the chromatic polynomials for PBC_x and $TPBC_x$ boundary conditions (i.e., cyclic and Möbius strips) have the same a_j , although in general different c_j . It follows that the loci \mathcal{B} are the same for these two different longitudinal boundary condition choices [25,34,38].

15. However, in the case of PBC_y , the reversal of orientation involved in going from PBC_x to TPBC_x longitudinal boundary conditions (i.e. from torus to Klein bottle topology) can lead to the removal of some of the a_j 's that were present; i.e., P for the $(\text{PBC}_y, \text{TPBC}_x)$ strip may involve only a subset of the a_j 's that are present for the $(\text{PBC}_y, \text{PBC}_x)$ strip. For example, for the $L_y = 3$ strips of the square lattice with $(\text{PBC}_y, \text{PBC}_x)$ boundary conditions, there are $N_a = 8$ a_j 's, but for the strip with $(\text{PBC}_y, \text{TPBC}_x)$ boundary conditions only a subset of $N_a = 5$ of these terms occurs in P [9]. None of the three a_j 's that are absent from P in the TPBC_x case is leading, so that \mathcal{B} is the same for both of these families.
16. How do W functions in region R_1 compare for different boundary conditions? We have shown that, for a given type of strip graph G_s , in the region R_1 defined for the PBC_x boundary conditions, the W function is the same for FBC_x , PBC_x , and TPBC_x .
17. For strips of regular lattices, as one increases L_y , how does W approach the limit for the 2D lattice? We have found that with $q > q_c$ for a given lattice type A , the approach of W to its 2D thermodynamic limit as L_y increases is quite rapid; for moderate values of q and $L_y \simeq 4$, $W(A, (L_x = \infty) \times L_y, q)$ is within about 5% and $\mathcal{O}(10^{-3})$ of the 2D value $W(A, (L_x = \infty) \times (L_y = \infty), q)$ for FBC_y and PBC_y , respectively, for a strip graph of the lattice A . We have proved that the approach of W to the 2D thermodynamic limit is monotonic for FBC_y and non-monotonic, although more rapid, for PBC_y [27]. (By the result noted in the previous item, the W function for these values of q , in region R_1 , is independent of the longitudinal boundary conditions.)
18. Concerning the analytic properties of W , one property is that W may have isolated branch point singularities (zeros) for strips with $(\text{FBC}_y, \text{FBC}_x)$ and $(\text{PBC}_y, \text{FBC}_x)$. For example, for the $(\text{FBC}_y, \text{FBC}_x)$ strips of the square lattice with $L_y = 2$, and $L_y = 3$, the respective W functions have square and cube root branch point singularities, while for the $(\text{PBC}_y, \text{FBC}_x)$ strips of the square lattice with $L_y = 3$, i.e. transverse cross sections forming triangles, the W functions have cube root branch point singularities where they vanish. Note that for these cases, R_1 is the full q plane, and the continuous locus $\mathcal{B} = \emptyset$. In contrast, for the corresponding lattice strips PBC_x , although the W functions have the same expressions in the respective R_1 regions, given below as Eqs. (4.9), (4.10), and (4.22), the zeros of the expressions do not occur in the R_1 regions where these expressions apply, and so the W functions in these R_1 regions do not have any isolated branch point singularities. We have also found this to be true of other strips.

4. Chromatic polynomials and loci \mathcal{B} for some specific families

To illustrate the general discussion of the previous section, we include here some loci that we have calculated for various specific families of graphs.

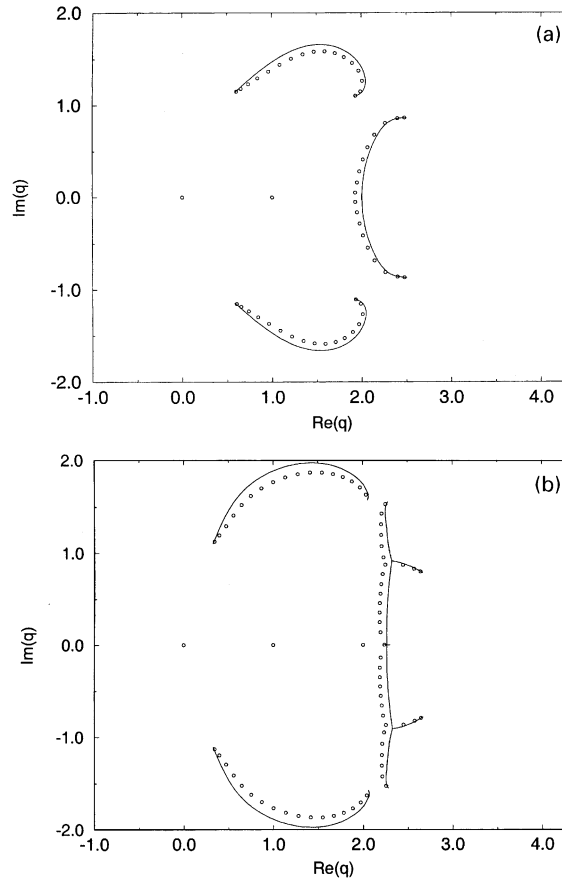


Fig. 1. \mathcal{B} for $W(\{G_{\text{sq}(L_y)}\}, q)$ with $L_y =$ (a) 3 (b) 4, where $\{G_{\text{sq}(L_y)}\}$ denotes the $(L_x = \infty) \times L_y$ strip of the square lattice. For comparison, the zeros of the chromatic polynomial $P((G_{\text{sq}(L_y)})_m, q)$ for (a) $L_y = 3$, $m = 16$ (hence $n = 54$ vertices) and (b) $L_y = 4$, $m = 16$ (hence $n = 72$) are shown.

4.1. Strips with free transverse and longitudinal boundary conditions

We first show \mathcal{B} for the strip graphs of the square lattice with $(\text{FBC}_y, \text{FBC}_x)$ and $L_y = 2, 3$. The relevant generating functions are given in [22] (Fig. 1).

4.2. Strips with free transverse and periodic or Möbius longitudinal boundary conditions

For definiteness, we consider cyclic and Möbius strips of the square lattice. For $L_y = 1$, these reduce to the circuit graph, for which \mathcal{B} is the circle $|q - 1| = 1$. For the $L_y = 2$ strips of this type, from the P in [7] we obtain \mathcal{B} given in Fig. 2.

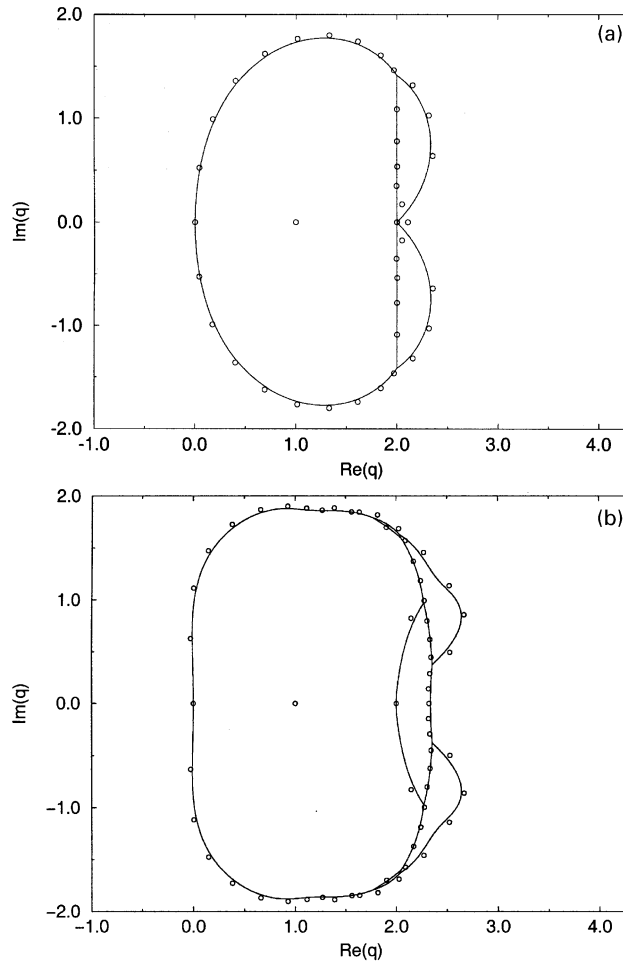


Fig. 2. \mathcal{B} for the infinite-length limit of strips of the square lattice with (FBC_y, PBC_x) (cyclic) boundary conditions and $L_y =$ (a) 2, (b) 3. For comparison, the zeros of the chromatic polynomial $P((G_{sq(L_y)})_m, q)$ for (a) $m = 19$ (hence $n = 38$) and (b) $m = 20$ (hence $n = 60$) are shown for comparison. The \mathcal{B} 's for the corresponding strips with $(FBC_y, TPBC_x)$ (Möbius) boundary conditions are identical.

For the cyclic $L_y = 3$ strip of the square lattice, we find [38]

$$\begin{aligned}
 &P(sq(L_y = 3, cyc.)_m, q) \\
 &= (q^3 - 5q^2 + 6q - 1)(-1)^m + (q^2 - 3q + 1) \\
 &\quad [(q - 1)^m + (q - 2)^m + (q - 4)^m] + (q - 1)[-(q - 2)^2]^m \\
 &\quad + [(\lambda_{sq,6})^m + (\lambda_{sq,7})^m] + (q - 1)[(\lambda_{sq,8})^m + (\lambda_{sq,9})^m + (\lambda_{sq,10})^m], \quad (4.1)
 \end{aligned}$$

where

$$\lambda_{\text{sq},(6,7)} = \frac{1}{2}[(q-2)(q^2-3q+5) \pm \{(q^2-5q+7)(q^4-5q^3+11q^2-12q+8)\}^{1/2}] \quad (4.2)$$

and $\lambda_{\text{sq},j}$, $j=8,9,10$, are the roots of the cubic equation

$$\xi^3 + b_{\text{sq},21}\xi^2 + b_{\text{sq},22}\xi + b_{\text{sq},23} = 0 \quad (4.3)$$

with

$$b_{\text{sq},21} = 2q^2 - 9q + 12, \quad (4.4)$$

$$b_{\text{sq},22} = q^4 - 10q^3 + 36q^2 - 56q + 31, \quad (4.5)$$

$$b_{\text{sq},23} = -(q-1)(q^4 - 9q^3 + 29q^2 - 40q + 22) \quad (4.6)$$

and for the corresponding Möbius strip [25]

$$\begin{aligned} P(\text{sq}(L_y=3, \text{Mb.})_m, q) &= (q^2 - 3q + 1)(-1)^m - (q-1)^m + (q-2)^m - (q-4)^m \\ &\quad - (q-1)[-(q-2)^2]^m + [(\lambda_{\text{sq},6})^m + (\lambda_{\text{sq},7})^m] \\ &\quad + (q-1)[(\lambda_{\text{sq},8})^m + (\lambda_{\text{sq},9})^m + (\lambda_{\text{sq},10})^m]. \end{aligned} \quad (4.7)$$

For the ($L_x \rightarrow \infty$ limits of the) $L_y=1$ and $L_y=2$ cyclic strips, $q_c=2$, while for the $L_y=3$ cyclic strip, $q_c=2.33654$. These values are obtained from exact solutions for the respective W and \mathcal{B} for these strips [25,28,38]. For these cyclic graphs this point q_c is a non-decreasing function of L_y . In the limit $L_y \rightarrow \infty$, continuity arguments imply that q_c approaches the value for the 2D square lattice, which is $q_c(sq)=3$ [13].

The W functions for the regions are given in [25,28,38]. In particular, note that in the respective region R_1 for each family,

$$W(\text{sq}(L_y=1), \text{cyc.}, q) = q - 1 \quad (4.8)$$

and, for both cyclic and Möbius strips,

$$W(\text{sq}(L_y=2), \text{cyc.}, q) = (q^2 - 3q + 3)^{1/2}, \quad (4.9)$$

$$\begin{aligned} W(\text{sq}(L_y=3, \text{cyc.}), q) &= 2^{-1/3}[(q-2)(q^2-3q+5) + [(q^2-5q+7) \\ &\quad (q^4-5q^3+11q^2-12q+8)]^{1/2}]^{1/3}. \end{aligned} \quad (4.10)$$

These W functions are the same as for the corresponding strips with $(\text{FBC}_y, \text{PBC}_x)$, which is a general result, as noted above.

4.3. Homeomorphic expansion of cyclic and Möbius strips

For comparison with the previous figure, we show homeomorphic expansions obtained by starting with cyclic and Möbius $L_y = 2$ square strips consisting of m squares, and inserting $k - 2$ additional vertices on each horizontal edge. We denote these graphs as $(\text{Ch})_{k,m,\text{cyc.}}$ and $(\text{Ch})_{k,m,\text{Mb.}}$. These graphs can be regarded as cyclic and Möbius strips of m p -sided polygons, where $p = 2k$, such that each p -gon intersects the previous one on one of its edges, and intersects the next one on its opposite edge. It is convenient to define

$$D_k(q) = \frac{P(C_k, q)}{q(q-1)} = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s}, \tag{4.11}$$

where $P(C_m, q)$ is the chromatic polynomial for the circuit (cyclic) graph C_m with m vertices, $P(C_m, q) = (q-1)^m + (q-1)(-1)^m$. We calculate [34]

$$\begin{aligned} P((\text{Ch})_{k,m,\text{cyc.}}, q) &= q^2 - 3q + 1 + (D_{2k})^m \\ &\quad + (q-1)[((-1)^{k+1}D_{k+1} + D_k)^m + ((-1)^{k+1}D_{k+1} - D_k)^m], \end{aligned} \tag{4.12}$$

$$\begin{aligned} P((\text{Ch})_{k,m,\text{cyc.},\text{Mb.}}, q) &= -1 + (D_{2k})^m + (-1)^k(q-1)[((-1)^{k+1}D_{k+1} + D_k)^m \\ &\quad - ((-1)^{k+1}D_{k+1} - D_k)^m]. \end{aligned} \tag{4.13}$$

In Fig. 3 we show \mathcal{B} and chromatic zeros for the cases $k = 3, 4$. In region R_1 , which includes the real axis for $q \geq 2$,

$$W = (D_{2k})^{1/2(k-1)}. \tag{4.14}$$

4.4. Cyclic chains of polygons

Consider a cyclic chain composed 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), this family of graphs depends on two additional parameters, namely the number of edges of the polygons between these two connection vertices, moving

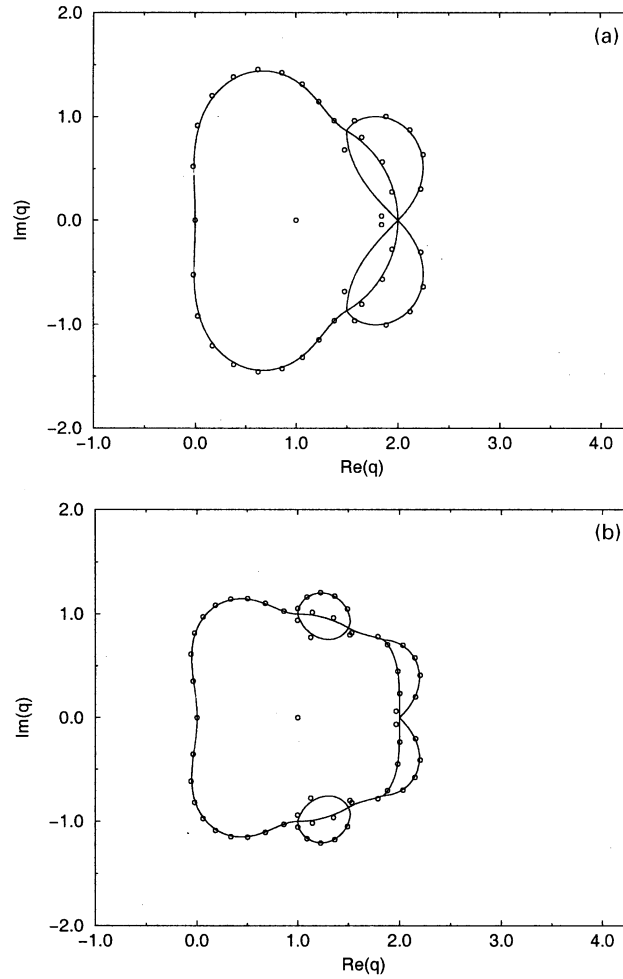


Fig. 3. \mathcal{B} for $\lim_{m \rightarrow \infty} (\text{Ch})_{k,m,\text{cyc}}$, with $k =$ (a) 3, (b) 4. Chromatic zeros are shown for the cyclic case with $m = 10$, i.e., $n =$ (a) 40, (b) 60.

in opposite directions along the polygon, e_1 and e_2 . We denote this family of cyclic polygon chain graphs as $G_{e_1, e_2, e_g, m; o}$ and define, in this context, $p = e_1 + e_2$. A symmetry property is

$$P(G_{e_1, e_2, e_g, m, q}) = P(G_{e_2, e_1, e_g, m, q}). \tag{4.15}$$

We calculate [36]

$$P(G_{e_1, e_2, e_g, m, q}) = (a_1)^m + (q - 1)(a_2)^m, \tag{4.16}$$

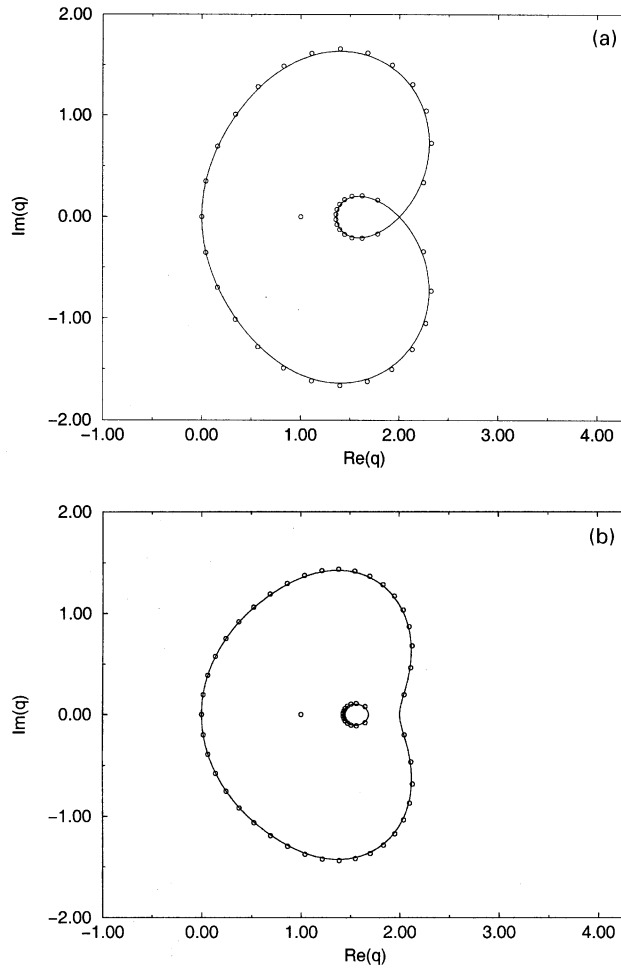


Fig. 4. Boundary \mathcal{B} in the q plane for W function for $\lim_{m \rightarrow \infty} G_{e_1, e_2, e_g, m}$ with $(e_1, e_2, e_g) =$ (a) $(2, 2, 0)$, (b) $(2, 2, 1)$. Chromatic zeros for $m = 14$ (i.e., $n = 42$ and $n = 56$ for (a) and (b)) are shown for comparison.

where

$$a_1 = (q - 1)^{e_g + 1} D_p, \tag{4.17}$$

$$a_2 = (-1)^{p + e_g} q^{-1} [q - 2 + (1 - q)^{e_1} + (1 - q)^{e_2}] \tag{4.18}$$

$$= (-1)^{p + e_g} \left[1 - p - \sum_{s=2}^{e_1} \binom{e_1}{s} (-q)^{s-1} - \sum_{s=2}^{e_2} \binom{e_2}{s} (-q)^{s-1} \right]. \tag{4.19}$$

The locus \mathcal{B} obtained by taking the limit $m \rightarrow \infty$ is shown in Fig. 4 for the cases $(e_1, e_2, e_g) =$ (a) $(2, 2, 0)$, (b) $(2, 2, 1)$. One sees the interesting phenomenon that as the

number of edges in the gap e_g increases from 0, the multiple point that was present on \mathcal{B} for $e_g = 0$ disappears and \mathcal{B} decomposes into two separate components. As e_g increases further, the inner boundary shrinks monotonically around the point at its center. This family also illustrates the fact that one can take the limit $n \rightarrow \infty$ in a different way, letting e_1 , e_2 , or e_g go to infinity with m held fixed. For the nontrivial case where $\min(e_1, e_2) > 1$, we find that, if p is even, then $q_c = 2$ while if p is odd, then $q_c < 2$ and, for fixed (e_1, e_2) , q_c increases monotonically as e_g increases, approaching 2 from below as $e_g \rightarrow \infty$. In region R_1 ,

$$W = [(q - 1)^{e_g+1} D_p]^{1/(p+e_g-1)}. \quad (4.20)$$

which is again the same W function as for the corresponding polygon chain graph with free (open) longitudinal boundary conditions.

4.5. Families with periodic transverse and free longitudinal boundary conditions

Here we consider strip graphs with $(\text{PBC}_y, \text{FBC}_x)$. For the strip graph of the square lattice with $L_y = 3$, i.e., cross sections forming triangles, and FBC_x , we find [22,27]

$$P(\text{sq}(L_y = 3)_m, \text{PBC}_y, \text{FBC}_x, q) = q(q - 1)(q - 2)(q^3 - 6q^2 + 14q - 13)^{m-1} \quad (4.21)$$

whence

$$W(\text{sq}(L_y = 3), \text{PBC}_y, \text{FBC}_x, q) = (q^3 - 6q^2 + 14q - 13)^{1/3} \quad (4.22)$$

with $\mathcal{B} = \emptyset$. Results for this lattice strip with larger $L_y = 4$, i.e. cross-sections forming squares, and for the triangular lattice, are given in [22].

4.6. Families with periodic transverse and (twisted) periodic longitudinal boundary conditions

With N. Biggs, we have recently studied the case of the strip of the square lattice with $(\text{PBC}_y, \text{PBC}_x)$ (torus) and $(\text{PBC}_y, \text{TPBC}_x)$ (Klein bottle) boundary conditions; see Ref. [9] for the chromatic polynomials and W functions. We find $q_c = 3$, which, interestingly, is the same as for the full 2D square lattice.

4.7. Families with noncompact \mathcal{B}

As an example of a family of graphs with a noncompact \mathcal{B} is obtained as follows [22]. We start with the join $(K_p) + G_r$ and remove some bonds from K_p . The simplest case is to let $G = \bar{K}_r$, $K_p = K_2$, and remove the edge connecting the two vertices of the K_2 . We can homeomorphically expand this by adding degree-2 vertices to the r edges connecting each of the two vertices of the original K_2 to the r vertices of the

\bar{K}_r . We denote this family as $H_{k,r}$ [37,35]. We find [37,35]

$$\begin{aligned} P(H_{k,r}, q) &= q(q-1)[D_{2k-2}(D_k)^{r-2} - (q-1)(D_{k-1})^2 \\ &\quad \times [(D_k)^{r-2} - \{(q-1)D_{k-1}\}^{r-2}]] \\ &= q(q-1)[(q-1)^{r-1}(D_{k-1})^r + (D_k)^r]. \end{aligned} \tag{4.23}$$

Because of the noncompactness of \mathcal{B} in the q plane, it is more convenient to plot it in the $z=1/q$ plane. In Fig. 5 we show two typical plots. For further details, see Refs. [30,35,37]. General bounds on chromatic zeros of graph have been discussed in a number of papers, e.g. [7] and recently [39].

5. Zeros and their accumulation sets for Potts partition functions at finite temperature or Tutte dichromatic polynomials

We have recently generalized our studies to the case of the q -state Potts model at arbitrary temperatures. At temperature T on a graph G or lattice Λ this model is defined by the partition function

$$Z = \sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}} \tag{5.1}$$

with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}, \tag{5.2}$$

where $\sigma_i = 1, \dots, q$ are the spin variables on each vertex $i \in G$; $\beta = (k_B T)^{-1}$; and $\langle ij \rangle$ denotes pairs of adjacent vertices. (Our terminology for this partition function is standard in physics; obviously Z should not be confused with the partition function $p(n)$ in number theory and combinatorics.) We use the notation $K = \beta J$,

$$a = u^{-1} = e^K \tag{5.3}$$

and

$$v = a - 1 \tag{5.4}$$

and denote the (reduced) free energy per vertex (site) as $f = -\beta F = \lim_{n \rightarrow \infty} n^{-1} \ln Z$. The partition function can be written as

$$Z(G, q, a) = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} (1 + v \delta_{\sigma_i, \sigma_j}) \tag{5.5}$$

which shows that it is a polynomial in q and v or a . From (5.5), it follows that [44,40,12,45]

$$Z(G, q, a) = \sum_{G' \subseteq G} q^{k(G')} v^{e(G')}, \tag{5.6}$$

where G' is a spanning subgraph of G and $e(G')$ and $k(G')$ denote the edges (bonds) and connected components, including single vertices, of G' , respectively.

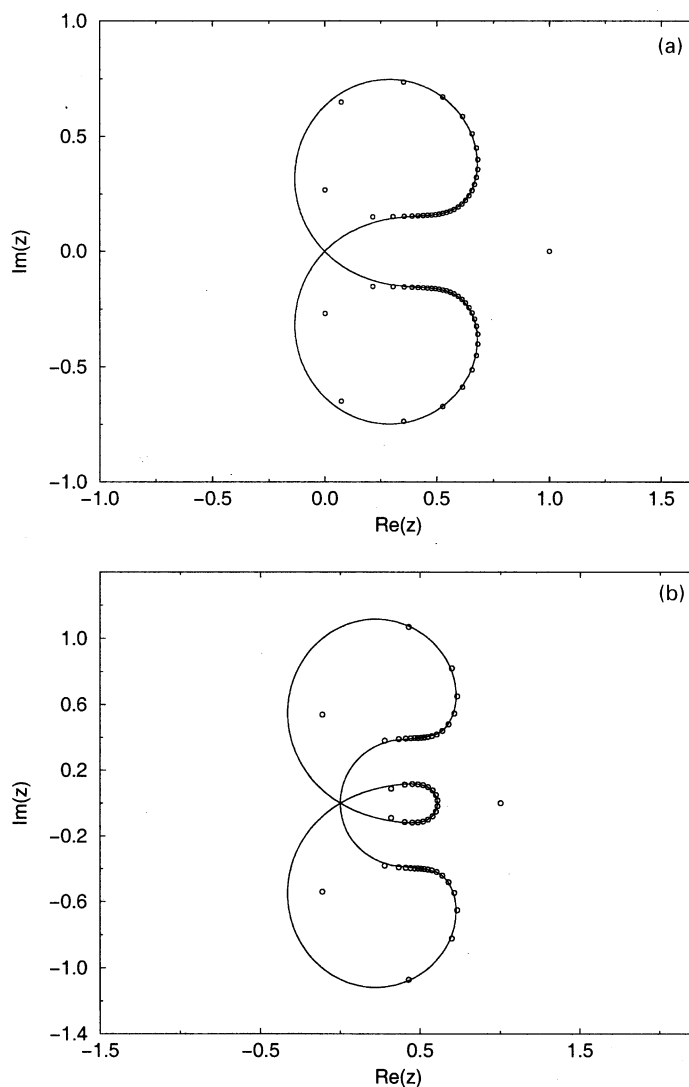


Fig. 5. Boundary \mathcal{B} in the $z = 1/q$ plane for $\lim_{r \rightarrow \infty} H_{k,r}$ with $k =$ (a) 4, (b) 5. Chromatic zeros for $H_{k,r}$ with $(k,r) =$ (a) (4,30), (b) (5,18) are shown for comparison.

The ferromagnetic and antiferromagnetic signs of the spin–spin exchange coupling are $J > 0$ and $J < 0$, respectively, and hence as the temperature varies from 0 to ∞ , the variable a varies from 0 to 1 for the Potts antiferromagnet and from ∞ to 1 for the Potts ferromagnet. At $T = \infty$, i.e., $\beta = 0$ or $a = 1$, the Potts ferromagnet and antiferromagnet are identical, since J does not enter in Z , which reduces simply to

$$Z(G, q, a = 1) = q^{n(G)}. \quad (5.7)$$

As indicated in Eq. (1.1), the $T = 0$ ($a = 0$) case yields the chromatic polynomial. For other special cases one has the elementary results $Z(G, q = 0, a) = 0$ and

$$Z(G, q = 1, a) = a^{e(G)}. \tag{5.8}$$

The zeros of Z are now functions of both complex q and a . In the limit $n \rightarrow \infty$, these zeros have an accumulation set which is a singular submanifold \mathcal{B} in the \mathbb{C}^2 space defined by q and a (or equivalently, u). Just as, in the one-variable situation, the $W(\{G\}, q)$ function was singular across the locus \mathcal{B} in the q plane as it switched its analytic form due to a change in the dominant term $a_j(q)$ in (1.4), so in the two-variable situation, the reduced free energy is singular across the locus \mathcal{B} in the (q, a) space as it switches its analytic form due to a change in the dominant term λ_j in (5.13). We denote the slices of this submanifold \mathcal{B} in the q plane, and in the a or u variable as \mathcal{B}_q , \mathcal{B}_a , and \mathcal{B}_u .

We recall that the partition function $Z(G, q, a)$ is related to the Tutte (dichromatic) polynomial $T(G, x, y)$ [40,41] and the rank function $R(G, \xi, \eta)$ [44]. Defining

$$x = 1 + \frac{q}{v} \tag{5.9}$$

and

$$y = a = v + 1, \tag{5.10}$$

so that $q = (x - 1)(y - 1)$, one has

$$T(G, x, y) = (x - 1)^{-k(G)}(y - 1)^{-n(G)}Z(G, q, v). \tag{5.11}$$

This is equivalent to the usual expression of the Tutte polynomial in terms of spanning trees [40]. The connection with the rank function follows from the relation $T(G, x + 1, y + 1) = x^{n-1}R(G, x^{-1}, y)$, viz.,

$$Z(G, q, v) = q^{n(G)}R\left(G, \xi = \frac{v}{q}, \eta = v\right). \tag{5.12}$$

The partition function or Tutte polynomial can be calculated either by the iterative use of the deletion-contraction theorem or by a generalization of the usual transfer matrix method from statistical mechanics. For recursive families, from the transfer matrix method, it follows that Z has the structure

$$Z(G, q, a) = \sum_{j=1}^{N_\lambda} c_j(\lambda_j)^m, \tag{5.13}$$

where the c_j and the λ_j depend on G but are independent of m . This is a generalization of Eq. (1.4) (with the equivalent notation $N_\lambda \equiv N_a$ and $\lambda_j \equiv a_j$). Given formula (5.6), the zero-temperature limit of the Potts antiferromagnet is studied by taking $a \rightarrow 0$. For the Potts ferromagnet, since $a \rightarrow \infty$ as $T \rightarrow 0$ and Z diverges like $a^{e(G)}$ in this limit, it is convenient to use the low-temperature variable $u = 1/a = e^{-K}$ and the reduced partition function Z_r defined by

$$Z_r = a^{-e(G)}Z = u^{e(G)}Z, \tag{5.14}$$

which has the finite limit $Z_r \rightarrow 1$ as $T \rightarrow 0$. For a general strip graph $(G_s)_m$ of type G_s and length $L_x = m$, we can write

$$Z_r((G_s)_m, q, a) = u^{e((G_s)_m)} \sum_{j=1}^{N_i} c_j(\lambda_j)^m \equiv \sum_{j=1}^{N_i} c_j(\lambda_{j,r})^m \tag{5.15}$$

with

$$\lambda_{j,r} = u^{e((G_s)_m)/m} \lambda_j. \tag{5.16}$$

An elementary calculation for the circuit graph C_n (e.g., [14]) yields $Z(G = C_n, q, v) = (q + v)^n + (q - 1)v^n$. The locus \mathcal{B} is the solution of the degeneracy equation $|a + q - 1| = |a - 1|$. The slice in the q plane, \mathcal{B}_q , thus consists of the circle centered at $q = 1 - a$ with radius $|1 - a|$:

$$q = (1 - a)(1 + e^{i\theta}), \quad \theta \in [0, 2\pi). \tag{5.17}$$

For the Potts antiferromagnet, as a increases from 0 to 1, this circle contracts monotonically toward the origin, and at $a = 1$ it degenerates into a point at $q = 0$. For the Potts ferromagnet, as a increases from 1 to ∞ , the circle expands into the $\text{Re}(q) < 0$ half-plane. One can also consider other values of a that do not correspond to physical temperature in the Potts ferromagnet or antiferromagnet. In all cases, from Eq. (5.17) it is evident that \mathcal{B}_q passes through the origin, $q = 0$. For real $a \neq 1$, \mathcal{B} intersects the real q axis at $q = 0$ and at

$$q_c(\{C\}) = 2(1 - a). \tag{5.18}$$

If, as is customary in physics, one restricts to $q \in \mathbb{Z}_+$, then the Potts antiferromagnet on $\{C\}$ has a zero-temperature phase transition if and only if $q = 2$ (Ising case). In the ferromagnetic case, \mathcal{B}_q does not cross the positive real q -axis. For $q \neq 0, 2$, the slice of this submanifold in the u plane forms the circle

$$\mathcal{B}_u: u = (q - 2)^{-1}(-1 + e^{i\omega}), \quad \omega \in [0, 2\pi), \quad q \neq 0, 2, \tag{5.19}$$

while for $q = 2$, \mathcal{B}_u is the imaginary u -axis. For $q = 0$, $Z = 0$ and no \mathcal{B}_u is defined. We have obtained similar results for other graphs, including cyclic ladder graphs L_m [26]. The corresponding Tutte polynomial obeys a recursion relation given in [9]. Some zeros in the q plane are shown in Figs. 6 and 7:

The locus \mathcal{B} always passes through the origin, $q = 0$. For $0 \leq a < 1$, \mathcal{B} crosses the positive real q -axis at q_c , where

$$q_c(\{L\}) = (1 - a)(a + 2) \quad \text{for } 0 \leq a \leq 1 \tag{5.20}$$

and separates the q plane into several regions. As a increases from 0 to 1, the locus \mathcal{B} contracts monotonically toward the origin, $q = 0$ and in the limit as $a \rightarrow 1$, it degenerates to a point at $q = 0$. This also describes the general behavior of the partition function (dichromatic) zeros themselves. That is, for finite graphs, there are no isolated partition function zeros whose moduli remains large as $a \rightarrow 1$. This is clear from continuity arguments in this limit, given Eq. (5.7).

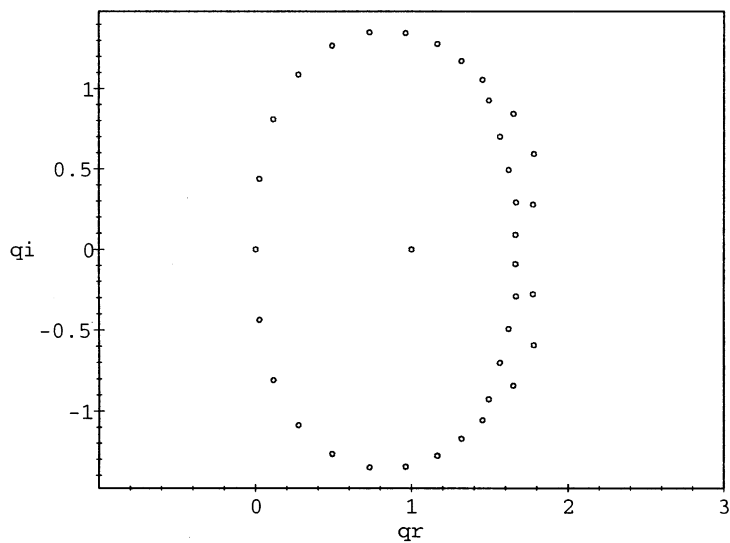


Fig. 6. Zeros of $Z(L_m, q, a)$ in q for $m = 18$ and $a = 0.25$. The axis labels $qr \equiv \text{Re}(q)$ and $qi \equiv \text{Im}(q)$.

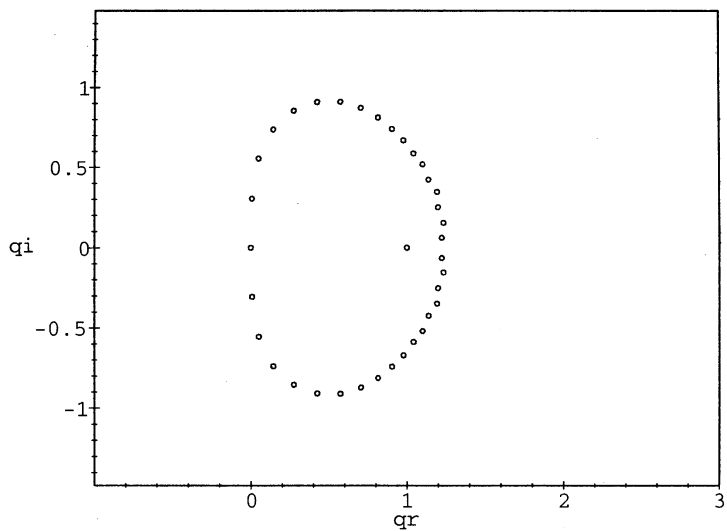


Fig. 7. Zeros of $Z(L_m, q, a)$ in q for $m = 18$ and $a = 0.5$.

6. Rigorous bounds on W

Using a coloring matrix method, Biggs [4] proved upper and lower bounds for W for the square lattice. We applied this method to prove such bounds for the triangular and honeycomb lattices [32]. These bounds are very restrictive even for moderate q .

Although a bound on a given function need not, a priori, coincide with a series expansion of that function, the lower bound for the honeycomb lattice coincides with the first eleven terms of the large- q expansion for $W(hc, q)$. We have proved a general lower bound, which is applicable for any Archimedean lattice [31]. Here an Archimedean lattice is defined as a uniform tiling of the plane with one or more regular polygons such that all vertices are equivalent to each other. It can be specified by the ordered sequence of polygons p_i traversed by a circuit around any vertex: $A = \prod_i p_i^{a_i}$. Let $\sum a_i = a_{i,s}$ and $v_i = a_{i,s}/p_i$. Then our general lower bound is [31]

$$W \geq \frac{\prod_i D_{p_i}(q)^{v_{p_i}}}{q-1}. \quad (6.1)$$

For the function

$$\bar{W}(A, y) = \frac{W(A, q)}{q(1-q^{-1})^{A/2}} \quad (6.2)$$

this bound reads

$$\bar{W} \geq \prod_i [1 + (-1)^{p_i} y^{p_i-1}]^{v_{p_i}}. \quad (6.3)$$

Note added. Since BCC99, we have, with S.-C. Chang, also calculated (i) $T(G, x, y)$ and \mathcal{B} for the $L_y=2$ cyclic strip of the triangular lattice; (ii) $P(G, q)$, $W(q)$, and \mathcal{B} for the $L_y=4$ cyclic strips of the square and triangular lattices and $L_y=3$ strip of the triangular lattice with torus and Klein bottle boundary conditions; and (iii) a general formula for the c_j coefficients for cyclic square and triangular strips.

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