Transfer Matrices and Partition-Function Zeros for Antiferromagnetic Potts Models

V. Further Results for the Square-Lattice Chromatic Polynomial

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Abstract

We derive some new structural results for the transfer matrix of square-lattice Potts models with free and cylindrical boundary conditions. In particular, we obtain explicit closed-form expressions for the dominant (at large $|q|$) diagonal entry in the transfer matrix, for arbitrary widths m, as the solution of a special one-dimensional polymer model. We also obtain the first 31 (free) or 15 (cylindrical) terms in the large-q expansion of the dominant eigenvalue for the zero-temperature antiferromagnet (= chromatic polynomial). Finally, we compute chromatic roots for strips of width $m = 9, 10, 11$ with free boundary conditions and locate roughly the limiting curves.

Key Words: Chromatic polynomial; chromatic root; antiferromagnetic Potts model; square lattice; transfer matrix; Fortuin–Kasteleyn representation; Beraha–Kahane–Weiss theorem; large-q expansion, one-dimensional polymer model.

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1 Introduction

The Potts model [1–3] on a regular lattice $\mathcal{L}$ is characterized by two parameters: the number q of Potts spin states, and the nearest-neighbor coupling $v = e^{\beta J} - 1$.[1] Initially q is a positive integer and v is a real number in the interval $[-1, +\infty)$, but the Fortuin–Kasteleyn representation (reviewed in Section 2.1 below) shows that the partition function $Z_G(q, v)$ of the q-state Potts model on any finite graph G is in fact a *polynomial* in q and v. This allows us to interpret q and v as taking arbitrary real or even complex values, and to study the phase diagram of the Potts model in the real (q, v)-plane or in complex (q, v)-space.

According to the Yang–Lee picture of phase transitions [4], information about the possible loci of phase transitions can be obtained by investigating the zeros of the partition function for finite subsets of the lattice $\mathcal{L}$ when one or more physical parameters (e.g. temperature or magnetic field) are allowed to take *complex* values; the accumulation points of these zeros in the infinite-volume limit constitute the (possible) phase boundaries. For the Potts model, therefore, by studying the zeros of $Z_G(q, v)$ in complex (q, v)-space for larger and larger pieces of the lattice $\mathcal{L}$, we can learn about the phase diagram of the Potts model in the real (q, v)-plane and more generally in complex (q, v)-space.

The partition function for $m \times n$ lattices can be efficiently computed using *transfer matrices*. Though the dimension of the transfer matrix (and thus the computational complexity) grows exponentially in the width m — thereby restricting us in practice to widths $m \lesssim 10$–30 — it is straightforward, by iterating the transfer matrix, to handle quite large lengths n. Indeed, by implementing the transfer-matrix method *symbolically* (i.e., as polynomials in q and/or v) and using the Beraha–Kahane–Weiss theorem (reviewed in Section 2.3), we can handle directly the limit $n \to \infty$ and compute the limiting curves $\mathcal{B}_m$ of partition-function zeros. At a second stage we attempt to extrapolate these curves to $m = \infty$.

Since the problem of computing the phase diagram in complex (q, v)-space is difficult, it has proven convenient to study first certain "slices" through (q, v)-space, in which one parameter is fixed (usually at a real value) while the remaining parameter is allowed to vary in the complex plane. One very interesting special case is the chromatic polynomial ($v = -1$), which corresponds to the zero-temperature limit of the Potts antiferromagnet ($\beta J = -\infty$). In previous papers [5–9] we have used symbolic transfer-matrix methods to study the square-lattice and triangular-lattice chromatic polynomials for free, cylindrical, cyclic and toroidal boundary conditions.[2,3] In this

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[1] Here we are considering only the *isotropic* model, in which each nearest-neighbor edge is assigned the same coupling v. In a more refined analysis, one could put (for example) different couplings v_1, v_2 on the horizontal and vertical edges of the square lattice, different couplings v_1, v_2, v_3 on the three orientations of edges of the triangular or hexagonal lattice, etc.

[2] See also the bibliographies of [5–9] for reference to the important related works of Shrock and collaborators.

[3] We adopt Shrock's [10] terminology for boundary conditions: free ($m_{\mathrm{F}} \times n_{\mathrm{F}}$), cylindrical ($m_{\mathrm{P}} \times n_{\mathrm{F}}$), cyclic ($m_{\mathrm{F}} \times n_{\mathrm{P}}$), toroidal ($m_{\mathrm{P}} \times n_{\mathrm{P}}$), Möbius ($m_{\mathrm{F}} \times n_{\mathrm{TP}}$) and Klein bottle ($m_{\mathrm{P}} \times n_{\mathrm{TP}}$). Here the

paper we provide some new structural results for the transfer matrices with free and cylindrical boundary conditions. (For simplicity we restrict attention to the square lattice, but the methods could easily be adapted to handle the triangular lattice.) In particular, we shall obtain explicit closed-form expressions for the dominant (at large $|q|$) diagonal entry in the transfer matrix, for arbitrary widths m, by solving a special one-dimensional polymer gas. We shall also obtain the first 31 (free) or 15 (cylindrical) terms in the large-q expansion of the dominant eigenvalue.

This paper is organized as follows: in Section 2 we review the Fortuin–Kasteleyn representation [11, 12] of the q-state Potts model, the basic facts about transfer matrices in this representation [5, 13], and the Beraha–Kahane–Weiss theorem [14–18]. In Section 3 we prove some new structural properties of the transfer matrix for a square-lattice strip of width m and free or cylindrical boundary conditions; in particular, we obtain closed-form expressions for the dominant entry of the transfer matrix, for arbitrary widths m. In Section 4 we study the large-q expansion of the leading eigenvalue of the transfer matrix; our results are similar to those obtained for the dominant entry, but less explicit. In Section 5 we study the limit $m \to \infty$ of the strip free energy and compare with a previous large-q expansion of the bulk free energy. In Section 6 we provide some additional information concerning the chromatic roots of strips of widths $m = 9, 10, 11$ with free boundary conditions. Finally, in Appendix A we discuss a conjecture concerning the upper zero-free interval for real chromatic roots of bipartite planar graphs.

2 Preliminaries

In this section we review briefly some needed background on chromatic and Tutte polynomials (Section 2.1), transfer matrices (Section 2.2) and the Beraha–Kahane–Weiss theorem (Section 2.3).

2.1 Chromatic polynomials, Potts models, and all that

Let $G = (V, E)$ be a finite undirected graph, let q be a positive integer, and let $\mathbf{v} = \{v_e\}_{e \in E}$ be real or complex edge weights. Then the ***q*-state Potts-model partition function** for the graph G is defined by the Hamiltonian

$$H_{\rm Potts}(\boldsymbol{\sigma}) \;=\; -\sum_{e=ij \in E} J_e \, \delta(\sigma_i, \sigma_j) \;, \tag{2.1}$$

where the spins $\boldsymbol{\sigma} = \{\sigma_i\}_{i \in V}$ take values in $\{1, 2, \ldots, q\}$, the J_e are coupling constants, and the δ is the Kronecker delta

$$\delta(a,b) \;=\; \begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases} \tag{2.2}$$

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first dimension (m) corresponds to the transverse ("short") direction, while the second dimension (n) corresponds to the longitudinal ("long") direction. The subscripts F, P and TP denote free, periodic and twisted-periodic boundary conditions, respectively.

The partition function can then be written as

$$Z_G^{\text{Potts}}(q,\mathbf{v}) \;=\; \sum_{\sigma\colon\; V\to\{1,2,\ldots,q\}} \; \prod_{e=ij\in E} \biggl[1+v_e\delta(\sigma_i,\sigma_j)\biggr] \;, \tag{2.3}$$

where $v_e = e^{\beta J_e}-1$. Please note, in particular, that if we set $v_e=-1$ for all edges e, then Z_G^{Potts} gives weight 1 to each proper coloring and weight 0 to each improper coloring, and so counts the proper colorings. Proper q-colorings ($v_e=-1$) thus correspond to the zero-temperature ($\beta\to+\infty$) limit of the antiferromagnetic ($J_e<0$) Potts model.

It is far from obvious that $Z_G^{\text{Potts}}(q,\mathbf{v})$, which is defined separately for each positive integer q, is in fact the restriction to $q\in\mathbb{Z}_+$ of a *polynomial* in q. But this is in fact the case, and indeed we have:

Theorem 2.1 (Fortuin–Kasteleyn [11, 12] representation of the Potts model)

For integer $q\geq 1$,

$$Z_G^{\text{Potts}}(q,\mathbf{v}) \;=\; \sum_{A\subseteq E} q^{k(A)} \prod_{e\in A} v_e \;, \tag{2.4}$$

where $k(A)$ denotes the number of connected components in the subgraph (V,A).

Proof. In (2.3), expand out the product over $e\in E$, and let $A\subseteq E$ be the set of edges for which the term $v_e\delta(\sigma_i,\sigma_j)$ is taken. Now perform the sum over maps $\sigma\colon V\to\{1,2,\ldots,q\}$: in each component of the subgraph (V,A) the color σ_i must be constant, and there are no other constraints. We immediately obtain (2.4). ■

Historical Remark. The subgraph expansion (2.4) was discovered by Birkhoff [19] and Whitney [20] for the special case $v_e=-1$ (see also Tutte [21, 22]); in its general form it is due to Fortuin and Kasteleyn [11, 12] (see also [23]).

The foregoing considerations motivate defining the **multivariate Tutte polynomial** of the graph G:

$$Z_G(q,\mathbf{v}) \;=\; \sum_{A\subseteq E} q^{k(A)} \prod_{e\in A} v_e \;, \tag{2.5}$$

where q and $\mathbf{v}=\{v_e\}_{e\in E}$ are commuting indeterminates. If we set all the edge weights v_e equal to the same value v, we obtain a two-variable polynomial that is equivalent to the standard Tutte polynomial $T_G(x,y)$ after a simple change of variables (see [24]). If we set all the edge weights v_e equal to -1, we obtain the **chromatic polynomial** $P_G(q)=Z_G(q,-1)$.

Further information on the multivariate Tutte polynomial $Z_G(q,\mathbf{v})$ can be found in a recent survey article [24].

2.2 Transfer matrices

For any family of graphs $G_n = (V_n, E_n)$ consisting of n identical "layers" with identical connections between adjacent layers, the multivariate Tutte polynomials of the G_n (with edge weights likewise repeated from layer to layer) can be written in terms of a transfer matrix [5,13]. Here we briefly summarize the needed formalism [5] specialized to the case of an $m \times n$ square lattice with free and cylindrical boundary conditions. As usual, free (resp. cylindrical) boundary conditions means free (resp. periodic) boundary conditions in the transverse ("short") direction and free boundary conditions in the longitudinal ("long") direction. These lattices are denoted by $m_{\rm F} \times n_{\rm F}$ and $m_{\rm P} \times n_{\rm F}$, respectively.

Consider the $m \times n$ square grid with edge weights $v_{i,i+1}$ on the horizontal edges $(1 \le i \le m)$ and v_i on the vertical edges $(1 \le i \le m)$. Site $m+1$ is always to be understood as a synonym for site 1. If the weight $v_{m,m+1} \equiv v_{m,1}$ is zero (resp. nonzero) we are considering free (resp. periodic) transverse boundary conditions.

We fix the "width" m and consider the family of graphs G_n obtained by varying the "length" n; our goal is to calculate the multivariate Tutte polynomials $Z_{G_n}(q, \mathbf{v})$ for this family by building up the graph G_n layer by layer. What makes this a bit tricky is the nonlocality of the factor $q^{k(A)}$ in (2.5). At the end we will need to know the number of connected components in the subgraph (V_n, A); in order to be able to compute this, we shall keep track, as we go along, of which sites in the current "top" layer are connected to which other sites in that layer by a path of occupied edges (i.e. edges of A) in lower layers. Thus, we shall work in the basis of connectivities of the top layer, whose basis elements $\mathbf{e}_{\mathcal{P}}$ are indexed by partitions $\mathcal{P}$ of the single-layer vertex set $\{1, \ldots, m\}$. The elementary operators we shall need are:

- The *join operators*
$$\mathsf{J}_{ij} \mathbf{e}_{\mathcal{P}} \;=\; \mathbf{e}_{\mathcal{P} \bullet ij} \;, \tag{2.6}$$
where $\mathcal{P} \bullet ij$ is the partition obtained from $\mathcal{P}$ by amalgamating the blocks containing i and j (if they were not already in the same block). Note that all these operators commute.

- The *detach operators*
$$\mathsf{D}_i \mathbf{e}_{\mathcal{P}} \;=\; \begin{cases} \mathbf{e}_{\mathcal{P} \setminus i} & \text{if } \{i\} \notin \mathcal{P} \\ q \mathbf{e}_{\mathcal{P}} & \text{if } \{i\} \in \mathcal{P} \end{cases} \tag{2.7}$$
where $\mathcal{P} \setminus i$ is the partition obtained from $\mathcal{P}$ by detaching i from its block (and thus making it a singleton). Note that these operators commute as well.

Note, finally, that D_k commutes with J_{ij} whenever $k \notin \{i, j\}$.

The horizontal transfer matrix, which adds a row of horizontal edges, depends on the boundary conditions, and is given by

$$\mathsf{H}_{\rm F} \;=\; \prod_{i=1}^{m-1} (1 + v_{i,i+1} \mathsf{J}_{i,i+1}) \tag{2.8a}$$

$$\mathsf{H}_{\rm P} \;=\; (1 + v_{m,1} \mathsf{J}_{m,1}) \mathsf{H}_{\rm F} \tag{2.8b}$$

(note that all the operators in both products commute). The vertical transfer matrix, which adds a new row of sites along with the corresponding vertical edges, is

$$\mathsf{V} \;=\; \prod_{i=1}^{m} (v_i I + \mathsf{D}_i) \tag{2.9}$$

(note once again that all the operators commute). The multivariate Tutte polynomial for G_n is then given [5] by the formula

$$Z_{G_n}(q, \mathbf{v}) \;=\; \boldsymbol{\omega}^{\mathrm{T}} \mathsf{H} (\mathsf{V}\mathsf{H})^{n-1} \mathbf{e}_{\mathrm{id}} \;, \tag{2.10}$$

where "id" denotes the partition in which each site $i \in \{1, \ldots, m\}$ is a singleton, and the "end vector" $\boldsymbol{\omega}^{\mathrm{T}}$ is defined by

$$\boldsymbol{\omega}^{\mathrm{T}} \mathbf{e}_{\mathcal{P}} \;=\; q^{|\mathcal{P}|} \;. \tag{2.11}$$

The transfer matrix is thus

$$\mathsf{T} \;=\; \mathsf{V}\mathsf{H} \;. \tag{2.12}$$

In principle we are working here in the space spanned by the basis vectors $\mathbf{e}_{\mathcal{P}}$ for all partitions $\mathcal{P}$ of $\{1, \ldots, m\}$; the dimension of this space is given by the Bell number B_m [25–28]. However, it is easy to see, on topological grounds (thanks to the planarity of the G_n), that only *non-crossing* partitions can arise. (A partition is said to be *non-crossing* if $a < b < c < d$ with a, c in the same block and b, d in the same block imply that a, b, c, d are all in the same block.) The number of non-crossing partitions of $\{1, \ldots, m\}$ is given by the Catalan number [26, 27]

$$C_m \;=\; \frac{(2m)!}{m!\,(m+1)!} \;=\; \frac{1}{m+1} \binom{2m}{m} \;. \tag{2.13}$$

When the horizontal couplings $v_{i,i+1}$ are all equal to 0 or -1 (which is the case for the chromatic polynomial with either free or periodic transverse boundary conditions), then the horizontal operator H is a *projection* (i.e., $\mathsf{H}^2 = \mathsf{H}$), so that our vector space $\mathcal{V}$ splits up as a direct sum $\mathcal{V} = \mathcal{V}_0 \oplus \mathcal{V}_1$, where $\mathsf{H}v = 0$ for $v \in \mathcal{V}_0$ and $\mathsf{H}v = v$ for $v \in \mathcal{V}_1$. Then every vector $v \in \mathcal{V}_0$ is an eigenvector of $\mathsf{T} = \mathsf{V}\mathsf{H}$ with eigenvalue 0; and for each eigenpair (λ, v) of $\mathsf{T} = \mathsf{V}\mathsf{H}$ with $v \notin \mathcal{V}_0$, the pair $(\lambda, \mathsf{H}v)$ is an eigenpair of $\mathsf{T}' = \mathsf{H}\mathsf{V}\mathsf{H}$. In this situation, therefore, we can work in the smaller vector space $\mathcal{V}_1$ by using the modified transfer matrix $\mathsf{T}' = \mathsf{H}\mathsf{V}\mathsf{H}$ in place of $\mathsf{T} = \mathsf{V}\mathsf{H}$, and using the basis vectors

$$\mathbf{f}_{\mathcal{P}} \;=\; \mathsf{H}\mathbf{e}_{\mathcal{P}} \tag{2.14}$$

in place of $\mathbf{e}_{\mathcal{P}}$. Indeed, if $\mathsf{T}\mathbf{e}_{\mathcal{P}} = \sum_{\mathcal{P}'} t_{\mathcal{P}\mathcal{P}'} \mathbf{e}_{\mathcal{P}'}$, then $\mathsf{T}'\mathbf{f}_{\mathcal{P}} = \sum_{\mathcal{P}'} t_{\mathcal{P}\mathcal{P}'} \mathbf{f}_{\mathcal{P}'}$, as is easily seen by applying H to both sides and using $\mathsf{H}^2 = \mathsf{H}$. Please note that $\mathbf{f}_{\mathcal{P}} = 0$ if $\mathcal{P}$ has any pair of nearest neighbors in the same block. We thus work in the space spanned by the basis vectors $\mathbf{f}_{\mathcal{P}}$ where $\mathcal{P}$ is a non-crossing non-nearest-neighbor partition of $\{1, \ldots, m\}$. The dimensionality of this space depends on the transverse boundary conditions:

- *Free transverse boundary conditions*: The number of non-crossing non-nearest-neighbor partitions of $\{1,\ldots,m\}$ is given [29, Proposition 3.6] [30] by the Motzkin number M_{m-1}, where [26,27,31–34][4]

$$M_n \;=\; \sum_{j=0}^{\lfloor n/2 \rfloor} \binom{n}{2j} C_j \;. \tag{2.15}$$

- *Periodic transverse boundary conditions*: The number of non-crossing non-nearest-neighbor partitions of $\{1,\ldots,m\}$ when it is considered periodically (i.e. when 1 and m also are considered to be nearest neighbors) is given by [34, Section 3.2, family R2]

$$d_m \;=\; \begin{cases} 1 & \text{for } m=1 \\ R_m & \text{for } m \geq 2 \end{cases} \tag{2.16}$$

  where the *Riordan numbers* (or Motzkin alternating sums) R_m [31,32,34][5] are defined by $R_0 = 1$, $R_1 = 0$ and

$$R_m \;=\; \sum_{k=0}^{m-1} (-1)^{m-k-1} M_k \qquad \text{for } m \geq 2 \tag{2.17}$$

Finally, spatial symmetries further restrict the subspace whenever the couplings $v_{i,i+1}$ and v_i are invariant under the symmetry. Again the symmetries depend on the transverse boundary conditions:

- *Free transverse boundary conditions*: Here the relevant symmetry is reflection in the center line of the strip. For reflection-invariant couplings, we can work in the space of equivalence classes of non-crossing non-nearest-neighbor partitions modulo reflection. The dimension SqFree(m) of the transfer matrix is then given by the number of these equivalence classes. The exact expression for SqFree(m) was obtained in [35, Theorem 2]:

$$\mathrm{SqFree}(m) \;=\; \frac{1}{2} M_{m-1} + \frac{(m'-1)!}{2} \sum_{j=0}^{\lfloor m'/2 \rfloor} \frac{m'-j}{(j!)^2 (m'-2j)!} \tag{2.18}$$

  where

$$m' \;=\; \left\lfloor \frac{m+1}{2} \right\rfloor \tag{2.19}$$

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[4] *Warning:* Several references use the notation m_n to denote what we call M_n; and one reference [31] writes M_n to denote a *different* sequence.

[5] In most of the literature (e.g. [31,32]) these numbers are called γ_m. We have adopted the recent proposal of Bernhart [34] to name them after Riordan [32] and denote them R_m.

and $\lfloor p \rfloor$ stands for the largest integer $\leq p$.[6] The asymptotic behavior of SqFree(m) is given by [35, Corollary 1]

$$\mathrm{SqFree}(m) \;\sim\; \frac{\sqrt{3}}{4\sqrt{\pi}}\, 3^m\, m^{-3/2} \left[1 + O\left(\frac{1}{m}\right)\right] \qquad \text{as } m \to \infty \tag{2.20}$$

- *Periodic transverse boundary conditions*: For the square lattice with periodic transverse boundary conditions, both reflections and translations are symmetries. We therefore define equivalence classes of non-crossing non-nearest-neighbor partitions modulo reflections and translations and the corresponding number SqCyl(m) of equivalence classes. To our knowledge there is no known closed form for these numbers; but there is a conjectured formula [37, Conjecture 2.2]

$$\mathrm{SqCyl}(m) \;=\; \begin{cases} \frac{1}{2}\left[\mathrm{TriCyl}(m) + \frac{1}{2} N_{\mathrm{FP}}\left(\frac{m}{2}\right)\right] & \text{for even } m \\[2ex] \frac{1}{2}\left[\mathrm{TriCyl}(m) + \frac{1}{4} N_{\mathrm{FP}}\left(\frac{m+1}{2}\right) - \frac{1}{2} R_{\frac{m-1}{2}}\right] & \text{for odd } m \geq 3 \end{cases} \tag{2.21}$$

  where $N_{\mathrm{FP}}(m)$ is the number of different eigenvalues for a strip of either square or triangular lattice with cyclic boundary conditions (i.e., free transverse and periodic longitudinal boundary conditions), and TriCyl(m) is the number of equivalence classes of non-crossing non-nearest-neighbor partitions modulo translations. It is known [38] that

$$N_{\mathrm{FP}}(m) \;=\; 2(m-1)! \sum_{j=0}^{\lfloor m/2 \rfloor} \frac{(m-j)}{(j!)^2 (m-2j)!}\,. \tag{2.22}$$

  It is conjectured [37, Conjecture 2.1] that

$$\mathrm{TriCyl}(m) \;=\; \frac{1}{m}\left[d_m + \sum_{d|m;\; 1 \leq d < m} \phi(m/d)\, t_d\right] \tag{2.23}$$

  where t_d is the coefficient of z^d in the expansion of $(1+z+z^2)^d$, i.e., the central trinomial coefficient (given as sequence A002426 in [27]), and $\phi(x)$ is Euler's totient function.

The values of all these dimensions for $m \leq 16$ are displayed in Table 2 of Ref. [5].

2.3 Beraha–Kahane–Weiss theorem

A central role in our work is played by a theorem on analytic functions due to Beraha, Kahane and Weiss [14–17] and generalized slightly by one of us [18]. The situation is as follows: Let D be a domain (connected open set) in the complex plane,

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[6] We have recently rederived this formula using a different method [36].

and let $\alpha_1, \ldots, \alpha_M, \lambda_1, \ldots, \lambda_M$ ($M \geq 2$) be analytic functions on D, none of which is identically zero. For each integer $n \geq 0$, define

$$f_n(z) \;=\; \sum_{k=1}^{M} \alpha_k(z)\, \lambda_k(z)^n \;. \tag{2.24}$$

We are interested in the zero sets

$$\mathcal{Z}(f_n) \;=\; \{z \in D\colon\; f_n(z) = 0\} \tag{2.25}$$

and in particular in their limit sets as $n \to \infty$:

$$\liminf \mathcal{Z}(f_n) \;=\; \{z \in D\colon\; \text{every neighborhood } U \ni z \text{ has a nonempty intersection with all but finitely many of the sets } \mathcal{Z}(f_n)\} \tag{2.26}$$

$$\limsup \mathcal{Z}(f_n) \;=\; \{z \in D\colon\; \text{every neighborhood } U \ni z \text{ has a nonempty intersection with infinitely many of the sets } \mathcal{Z}(f_n)\} \tag{2.27}$$

Let us call an index k *dominant at z* if $|\lambda_k(z)| \geq |\lambda_l(z)|$ for all l ($1 \leq l \leq M$); and let us write

$$D_k \;=\; \{z \in D\colon\; k \text{ is dominant at } z\} \;. \tag{2.28}$$

Then the limiting zero sets can be completely characterized as follows:

Theorem 2.2 **[14–18]** *Let D be a domain in $\mathbb{C}$, and let $\alpha_1, \ldots, \alpha_M$, $\lambda_1, \ldots, \lambda_M$ ($M \geq 2$) be analytic functions on D, none of which is identically zero. Let us further assume a "no-degenerate-dominance" condition: there do not exist indices $k \neq k'$ such that $\lambda_k \equiv \omega \lambda_{k'}$ for some constant ω with $|\omega| = 1$ and such that D_k ($= D_{k'}$) has nonempty interior. For each integer $n \geq 0$, define f_n by*

$$f_n(z) \;=\; \sum_{k=1}^{M} \alpha_k(z)\, \lambda_k(z)^n \;.$$

Then $\liminf \mathcal{Z}(f_n) = \limsup \mathcal{Z}(f_n)$, and a point z lies in this set if and only if either

(a) There is a unique dominant index k at z, and $\alpha_k(z) = 0$; or

(b) There are two or more dominant indices at z.

Note that case (a) consists of isolated points in D, while case (b) consists of curves (plus possibly isolated points where all the λ_k vanish simultaneously). Henceforth we shall denote by $\mathcal{B}$ the locus of points satisfying condition (b).

We shall often refer to the functions λ_k as "eigenvalues", because that is how they arise in the transfer-matrix formalism.

3 Structural properties of the square-lattice transfer matrix

In this section we prove some structural results concerning the transfer matrices of square-lattice Potts models (and in particular chromatic polynomials) with free or cylindrical boundary conditions. We begin by proving some general results (Section 3.1) concerning the polynomial dependence in q of the transfer-matrix entries and the large-q behavior of the eigenvalues. Then we provide explicit closed-form expressions for the dominant diagonal entry of the transfer matrix with free or cylindrical boundary conditions (Sections 3.2 and 3.3).

3.1 General results

Let us begin by considering the case of the full Potts-model partition function. Indeed, we can be quite a bit more general, and consider any transfer matrix built out of operators of the form

$$\mathsf{H} \;=\; \sum_{A\subseteq\{1,\ldots,m\}} c_A \prod_{i\in A} \mathsf{J}_{i,i+1} \tag{3.1a}$$

$$\mathsf{V} \;=\; \sum_{B\subseteq\{1,\ldots,m\}} d_B \prod_{i\in B} \mathsf{D}_i \tag{3.1b}$$

with arbitrary coefficients $\{c_A\}$ and $\{d_B\}$. (Recall that site $m+1$ is to be understood as a synonym for site 1.) This general form includes as particular cases the square-lattice transfer matrix with free or cylindrical boundary conditions and arbitrary couplings $\{v_{i,i+1}\}$ and $\{v_i\}$.

Let us now recall that "id" denotes the partition of $\{1,\ldots,m\}$ in which each element is a singleton (i.e., $\{\{1\},\{2\},\ldots,\{m\}\}$). Let us call a partition $\mathcal{P}$ of $\{1,\ldots,m\}$ *non-trivial* if it is not "id".

Proposition 3.1 *For any operators* H *and* V *of the form (3.1), where the coefficients* $\{c_A\}$ *and* $\{d_B\}$ *are* numbers *(i.e., independent of q), the diagonal entry* $t_{\rm id}(m)$ *of the transfer matrix* $\mathsf{T}(m) = \mathsf{VH}$ *associated to the basis element* $\mathbf{e}_{\rm id}$ *is a polynomial in q of degree at most m, of the form*

$$t_{\rm id} \;=\; c_\emptyset\, d_{\{1,\ldots,m\}}\, q^m \;+\; \textit{terms of order at most } q^{m-1}\;. \tag{3.2}$$

All other entries of the transfer matrix $\mathsf{T}(m)$ *are polynomials in q of degree at most* $m-1$.

Remark. If H is a projection, then the diagonal entry $t'_{\rm id}(m)$ of the modified transfer matrix $\mathsf{T}'(m) = \mathsf{HVH}$ associated to the basis element $\mathbf{f}_{\rm id} = \mathsf{H}\mathbf{e}_{\rm id}$ is given by $t'_{\rm id} = t_{\rm id}$; indeed, *all* the entries of $\mathsf{T}'(m)$ are equal to the corresponding entries of $\mathsf{T}(m)$. This follows immediately from the fact that $\mathsf{T}\mathbf{e}_{\mathcal{P}} = \sum_{\mathcal{P}'} t_{\mathcal{P}\mathcal{P}'}\mathbf{e}_{\mathcal{P}'}$ implies $\mathsf{T}'\mathbf{f}_{\mathcal{P}} = \sum_{\mathcal{P}'} t_{\mathcal{P}\mathcal{P}'}\mathbf{f}_{\mathcal{P}'}$.

Proof of Proposition 3.1. First of all, it is obvious that each entry in the transfer matrix $\mathsf{T}(m)$ is a polynomial in q. Indeed, from (2.7)/(2.9) it is clear that we get a factor of q every time we apply the operator D_i to a partition in which i is a singleton. Indeed, we can *maximize* the number of factors of q by applying the vertical transfer matrix V to the vector $\mathbf{e}_{\rm id}$ that corresponds to the partition in which every site is a singleton. In particular, from (3.1b) we have

$$\begin{aligned}\mathsf{V}\mathbf{e}_{\rm id} &= \sum_{B\subseteq\{1,\ldots,m\}} d_B q^{|B|}\,\mathbf{e}_{\rm id} &\quad (3.3a)\\ &= \bigl(d_{\{1,\ldots,m\}}q^m + \text{terms of order at most } q^{m-1}\bigr)\,\mathbf{e}_{\rm id}\ . &\quad (3.3b)\end{aligned}$$

If we apply the vertical transfer matrix to any other partition, we get a polynomial in q of degree at most $m-1$.

Let us now consider the quantity $\mathsf{H}\mathbf{e}_{\rm id}$:

$$\begin{aligned}\mathsf{H}\mathbf{e}_{\rm id} &= \sum_{A\subseteq\{1,\ldots,m\}} c_A \left(\prod_{i\in A}\mathsf{J}_{i,i+1}\right)\mathbf{e}_{\rm id} &\quad (3.4a)\\ &= c_\emptyset\,\mathbf{e}_{\rm id} + \sum_{\mathcal{P}\text{ non-trivial}} a_{\mathcal{P}}\,\mathbf{e}_{\mathcal{P}}\ , &\quad (3.4b)\end{aligned}$$

for some quantities $a_{\mathcal{P}}$ that are polynomials in $\{c_A\}$ (and of course independent of q). Using (3.3)/(3.4) it is obvious that

$$\mathsf{V}\mathsf{H}\mathbf{e}_{\rm id} \;=\; c_\emptyset \sum_{B\subseteq\{1,\ldots,m\}} d_B\, q^{|B|}\,\mathbf{e}_{\rm id} + \sum_{\mathcal{P}} a'_{\mathcal{P}}(q)\,\mathbf{e}_{\mathcal{P}}\ , \qquad (3.5)$$

where the coefficients $a'_{\mathcal{P}}(q)$ are polynomials in q of degree at most $m-1$. ■

In view of Proposition 3.1, we shall henceforth refer to $t_{\rm id}$ (or $t'_{\rm id}$) as the "dominant diagonal entry" in the transfer matrix, as it is indeed dominant at large $|q|$. Furthermore, we can deduce from Proposition 3.1 the leading large-$|q|$ behavior of the eigenvalues. We begin with a simple perturbation lemma:

Lemma 3.2 *Consider an $N\times N$ matrix $M(\xi) = (M_{ij}(\xi))_{i,j=1}^N$ whose entries are analytic functions of ξ in some disc $|\xi| < R$. Suppose that $M_{11} = 1$ and that $M_{ij} = O(\xi)$ for $(i,j)\neq(1,1)$. Then, in some disc $|\xi| < R'$, $M(\xi)$ has a simple leading eigenvalue $\mu_\star(\xi)$ that is given by a convergent expansion*

$$\mu_\star(\xi) \;=\; 1 + \sum_{k=2}^{\infty}\alpha_k\xi^k \qquad (3.6)$$

[note that $\alpha_1 = 0$] with associated eigenvector

$$\mathbf{v}_\star(\xi) \;=\; \mathbf{e}_1 + \sum_{k=1}^{\infty}\mathbf{v}_k\xi^k\ , \qquad (3.7)$$

while all other eigenvalues are $O(\xi)$.

The key fact here is that the eigenvalue shift in (3.6) begins at order ξ^2, not order ξ.

PROOF. We have

$$\det[\mu - M(\xi)] \;=\; (\mu-1)\prod_{i=2}^{N}[\mu - M_{ii}(\xi)] \;+\; \xi^2 F(\mu,\xi)\;, \tag{3.8}$$

where $F(\mu,\xi)$ is a polynomial in μ whose coefficients are analytic functions of ξ for $|\xi| < R$. The polynomial $P(\mu) = (\mu-1)\prod_{i=2}^{N}[\mu - M_{ii}(\xi)]$ has, for all sufficiently small $|\xi|$, a simple root at $\mu = 1$ and roots (not necessarily simple) at $\mu = M_{ii}(\xi) = O(\xi)$. The simple root at $\mu = 1$ moves analytically [39] under the perturbation $\xi^2 F(\mu,\xi)$ — let us call this root $\mu_\star(\xi)$ — and so is given by the convergent expansion (3.6). The corresponding eigenvector also moves analytically under the perturbation $M(\xi) = \mathrm{diag}(1,0,\ldots,0) + O(\xi)$, which proves (3.7). To see that all other eigenvalues are $O(\xi)$, it suffices to consider the reduced matrix

$$M(\xi) \;-\; \mu_\star(\xi)\,\frac{\mathbf{v}_\star(\xi)\,\mathbf{v}_\star(\xi)^{\mathrm{T}}}{\mathbf{v}_\star(\xi)^{\mathrm{T}}\,\mathbf{v}_\star(\xi)} \tag{3.9}$$

and observe that all its entries are $O(\xi)$. ■

Remark. The "small" eigenvalues need not be analytic in ξ. For instance,

$$M(\xi) \;=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \xi \\ 0 & \xi^2 & 0 \end{pmatrix} \tag{3.10}$$

has eigenvalues $\mu = 1$ and $\mu = \pm\xi^{3/2}$. ■

To apply Lemma 3.2 to our transfer matrix T, we set $\xi = q^{-1}$ and $M = \mathsf{T}/t_{\mathrm{id}}$. We then have:

Corollary 3.3 *Consider operators* H *and* V *of the form (3.1) where the coefficients* $\{c_A\}$ *and* $\{d_B\}$ *are* numbers *(i.e., independent of* q*) and* $c_\emptyset d_{\{1,\ldots,m\}} \neq 0$*. Then* T *has a simple eigenvalue* $\lambda_\star$ *that is analytic for large* $|q|$ *and behaves there like* $c_\emptyset d_{\{1,\ldots,m\}} q^m$*: more precisely, it has a convergent expansion*

$$\frac{\lambda_\star}{t_{\mathrm{id}}} \;=\; 1 \;+\; \sum_{k=2}^{\infty} \alpha_k q^{-k} \tag{3.11}$$

[so that, in particular, $\lambda_\star - t_{\mathrm{id}} = O(q^{m-2})$*]. All other eigenvalues are* $O(q^{m-1})$*.*

Let us now return to the case of main interest, in which H and V are the transfer matrices (2.8)/(2.9) for the chromatic polynomial $v_i = v_{i,j} = -1$. In this case we can sharpen (3.2) by providing explicit expressions for the lower-order terms. We must now distinguish between free and cylindrical boundary conditions, and we shall treat each case in a separate subsection.

3.2 Free boundary conditions

Let us consider a square-lattice grid of fixed width $m \geq 1$ and free boundary conditions. Let us also assume that all horizontal edges have weights v and all vertical edges have weights v'; they need not be -1. The horizontal transfer matrix (2.8a) is thus

$$\mathsf{H} \;=\; \prod_{i=1}^{m-1} (1 + v\mathsf{J}_{i,i+1}) \tag{3.12}$$

and the vertical transfer matrix is

$$\mathsf{V} \;=\; \prod_{i=1}^{m} (v'I + \mathsf{D}_i) \;. \tag{3.13}$$

Consider first the action of H on the start vector $\mathbf{e}_{\rm id}$. It generates 2^{m-1} terms, each of which corresponds to a partition $\mathcal{P}$ in which all the blocks are sequential sets of vertices in $\{1, \ldots, m\}$ (we shall call these sets "polymers"). Furthermore, each polymer of size ℓ picks up a factor $v^{\ell-1}$.

Consider next the action of V on a basis vector $\mathbf{e}_{\mathcal{P}}$ corresponding to an arbitrary partition $\mathcal{P} = \{P_1, \ldots, P_k\}$. If we are to end up with the partition $\mathbf{e}_{\rm id}$, then for each block P_j we must either choose the delete operator D_i for all $i \in P_j$ (the last deletion gives a factor q) or else choose the delete operator for all but one $i \in P_j$ and choose $v'I$ for the last site (this can be done in $|P_j|$ ways). We therefore have

$$\mathsf{V}\mathbf{e}_{\mathcal{P}} \;=\; \left[\prod_{j=1}^{k} (q + v'|P_j|) \right] \mathbf{e}_{\rm id} \;+\; \hbox{other terms} \tag{3.14}$$

where "other terms" means terms involving $\mathbf{e}_{\mathcal{P}'}$ with $\mathcal{P}' \neq {\rm id}$. We thus obtain a factor $q + \ell v'$ for each block of size $\ell = |P_j| \geq 1$.

Putting these facts together, we conclude that

$$\mathsf{V}\mathsf{H}\mathbf{e}_{\rm id} \;=\; t_{\rm F}(m)\, \mathbf{e}_{\rm id} \;+\; \hbox{other terms}\;, \tag{3.15}$$

where $t_{\rm F}(m)$ is the partition function for a one-dimensional m-site polymer gas (with free boundary conditions) in which each site must be occupied by exactly one polymer, and each polymer of length $\ell \geq 1$ gets a fugacity $\mu_\ell = v^{\ell-1}(q + \ell v')$, i.e.

$$t_{\rm F}(m) \;=\; \sum_{k=1}^{\infty} \sum_{\substack{\ell_1, \ldots, \ell_k \geq 1 \\ \ell_1 + \ldots + \ell_k = m}} \prod_{j=1}^{k} v^{\ell_k - 1}(q + \ell_k v') \;. \tag{3.16}$$

To solve this polymer model, let us introduce the generating function ("grand partition function”)

$$\Phi_{\mathrm{F}}(z) \;\equiv\; \sum_{m=1}^{\infty} z^m t_{\mathrm{F}}(m) \tag{3.17a}$$

$$= \sum_{k=1}^{\infty} \sum_{\ell_1,\ldots,\ell_k \ge 1} \prod_{j=1}^{k} z^{\ell_j} v^{\ell_j - 1}(q + \ell_j v') \tag{3.17b}$$

$$= \frac{\Psi(z)}{1-\Psi(z)} \tag{3.17c}$$

where

$$\Psi(z) \;\equiv\; \sum_{\ell=1}^{\infty} z^{\ell} v^{\ell-1}(q+\ell v') \;=\; z\left[\frac{q}{1-zv} \;+\; \frac{v'}{(1-zv)^2}\right] \tag{3.18}$$

is the total weight for a single polymer of arbitrary size. We therefore have

$$\Phi_{\mathrm{F}}(z) \;=\; \frac{(q+v')z - qvz^2}{1-(q+2v+v')z + v(q+v)z^2} \;. \tag{3.19}$$

When $v = v' = -1$ this reduces to

$$\Phi_{\mathrm{F}}(z) \;=\; \frac{(q-1)z + qz^2}{1-(q-3)z-(q-1)z^2} \;. \tag{3.20}$$

As a check we have expanded (3.20) in powers of z, and verified that it agrees with available dominant diagonal elements $t_{\mathrm{F}}(m)$ for $1 \le m \le 11$ (see [5] for $m \le 8$).

The next step is to get an explicit expression for $t_{\mathrm{F}}(m)$. Using the notation $[z^m]P(z)$ for the m-th coefficient in a polynomial or power series, we have the alternate representations

$$[z^m]\frac{1}{1-az-bz^2} \;=\; \sum_{j=0}^{\lfloor m/2 \rfloor} \binom{m-j}{j} a^{m-2j} b^j \tag{3.21a}$$

$$= \; 2^{-m} \sum_{j=0}^{\lfloor m/2 \rfloor} \binom{m+1}{2j+1} a^{m-2j}(a^2+4b)^j \;. \tag{3.21b}$$

The first of these comes directly from $[z^m]\sum_{k=0}^{\infty}(az+bz^2)^k$, while the second is obtained by factoring the quadratic and using partial fractions. Using (3.20) we have

$$t_{\mathrm{F}}(m) \;=\; [z^m]\Phi_{\mathrm{F}}(z) \;=\; (q-1)[z^{m-1}]\frac{1}{1-az-bz^2} \;+\; q[z^{m-2}]\frac{1}{1-az-bz^2} \tag{3.22}$$

where $a = q-3$ and $b = q-1$. Inserting this into (3.21a) we have

$$t_{\mathrm{F}}(m) \;=\; \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} \binom{m-1-j}{j} (q-3)^{m-1-2j}(q-1)^{j+1} + q \sum_{j=0}^{\lfloor (m-2)/2 \rfloor} \binom{m-2-j}{j} (q-3)^{m-2-2j}(q-1)^{j} \;, \tag{3.23}$$

which is manifestly a polynomial in q of degree at most m. Furthermore, the term of order q^m comes only from $j=0$ in the first sum and has coefficient 1 (thereby confirming explicitly what we already knew from Proposition 3.1), so the degree is exactly m.

We may therefore write $t_F(m)$ explicitly as a polynomial in q with certain coefficients $a_k^{\rm F}(m)$:

$$t_{\rm F}(m) \;=\; \sum_{k=0}^{m} (-1)^k a_k^{\rm F}(m)\, q^{m-k} \;. \tag{3.24}$$

The next step is to obtain a closed formula for the coefficients $a_k^{\rm F}(m)$ with $m \ge 1$ and $0 \le k \le m$. We shall prove that, for each fixed $k \ge 0$, the coefficient $a_k^{\rm F}(m)$ is in fact a *polynomial* in m of degree exactly k.[7] We begin by expanding the binomials in (3.23):

$$\begin{aligned}
a_k^{\rm F}(m) \;&\equiv\; (-1)^k [q^{m-k}] t_{\rm F}(m) && \text{(3.25a)}\\
&=\; (-1)^k \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} \sum_{\ell=0}^{\infty} \binom{m-1-j}{j} \binom{m-1-2j}{m-k-\ell} \binom{j+1}{\ell} (-3)^{k+\ell-1-2j} (-1)^{j+1-\ell} \\
&\qquad +\, (-1)^k \sum_{j=0}^{\lfloor (m-2)/2 \rfloor} \sum_{\ell=0}^{\infty} \binom{m-2-j}{j} \binom{m-2-2j}{m-k-\ell-1} \binom{j}{\ell} (-3)^{k+\ell-1-2j} (-1)^{j-\ell} && \text{(3.25b)}\\
&=\; \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} \sum_{\ell=0}^{\infty} \binom{m-1-j}{j} \binom{m-1-2j}{k+\ell-1-2j} \binom{j+1}{\ell} (-1)^j 3^{k+\ell-1-2j} \\
&\qquad -\, \sum_{j=0}^{\lfloor (m-2)/2 \rfloor} \sum_{\ell=0}^{\infty} \binom{m-2-j}{j} \binom{m-2-2j}{k+\ell-1-2j} \binom{j}{\ell} (-1)^j 3^{k+\ell-1-2j} && \text{(3.25c)}
\end{aligned}$$

Let us consider the first sum in (3.25c):

$$\begin{aligned}
S^{(1)}(m,k) \;&=\; \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} \sum_{\ell=0}^{\infty} \binom{m-1-j}{j} \binom{m-1-2j}{k+\ell-1-2j} \binom{j+1}{\ell} (-1)^j 3^{k+\ell-1-2j} \\
&\equiv\; \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} \sum_{\ell=0}^{\infty} S_{j,\ell}^{(1)}(m,k) \;. && \text{(3.26)}
\end{aligned}$$

The goal is to substitute $\sum_{j=0}^{\lfloor (m-1)/2 \rfloor}$ by something independent of m, e.g., $\sum_{j=0}^{k}$. Indeed, if $k = \lfloor (m-1)/2 \rfloor$, the identity is trivial. Let us consider next the case $k < \lfloor (m-1)/2 \rfloor$. Then, if we prove that the sum

$$\sum_{j=k+1}^{\lfloor (m-1)/2 \rfloor} S_{j,\ell}^{(1)}(m,k) \;=\; 0 \,, \tag{3.27}$$

---

[7] More precisely, $a_k^{\rm F}(m)$ is the restriction to integers $m \ge \max(k,1)$ of such a polynomial.

then, we have not modified the result of (3.26) by changing the upper index in the sum over the variable j. The second binomial appearing in (3.26) vanishes whenever $k+\ell-1-2j<0$. On the other hand, the third binomial is *non-vanishing* only if $j \geq \ell-1$. Therefore, if $j>k$ and $j \geq \ell-1$, we have $k+\ell-1-2j<k+\ell-1-k-(\ell-1)=0$. So, $S^{(1)}(m,k)=0$ whenever $j>k$.[8] Finally, let us consider the third case $k>\lfloor(m-1)/2\rfloor$. Then, by making this change in the upper index in the sum over j, we are adding some extra terms

$$\sum_{j=\lfloor(m-1)/2\rfloor+1}^{k} S^{(1)}_{j,\ell}(m,k)\ . \tag{3.28}$$

In this case we have to focus on the first binomial of (3.26). This binomial is nonzero only when $0 \leq j \leq \lfloor(m-1)/2\rfloor$ or when $j \geq m$. The first of these do not appear in (3.28); and since $m \geq k$, the second appears only when $j=k=m$. The contribution of this extra term is 1. Thus, (3.26) reduces to

$$S^{(1)}(m,k)=\sum_{j=0}^{k}\sum_{\ell=0}^{\infty}\binom{m-1-j}{j}\binom{m-1-2j}{k+\ell-1-2j}\binom{j+1}{\ell}(-1)^j 3^{k+\ell-1-2j}-\delta_{km}\ . \tag{3.29}$$

Let us now consider the second sum in (3.25c):

$$\begin{aligned} S^{(2)}(m,k) &= \sum_{j=0}^{\lfloor(m-2)/2\rfloor}\sum_{\ell=0}^{\infty}\binom{m-2-j}{j}\binom{m-2-2j}{k+\ell-1-2j}\binom{j}{\ell}(-1)^j 3^{k+\ell-1-2j} \\ &\equiv \sum_{j=0}^{\lfloor(m-2)/2\rfloor}\sum_{\ell=0}^{\infty} S^{(2)}_{j,\ell}(m,k)\ . \end{aligned} \tag{3.30}$$

The goal is now to substitute $\sum_{j=0}^{\lfloor(m-2)/2\rfloor}$ by $\sum_{j=0}^{k-1}$. As before, the case $k-1=\lfloor(m-2)/2\rfloor$ is trivial. Let us now suppose that $k-1<\lfloor(m-2)/2\rfloor$. Then, the second binomial vanishes whenever $k+\ell-1-2j<0$, the third binomial is *non-vanishing* only if $j \geq \ell$. Therefore for $j>k-1$ and $j \geq \ell$ we have $k+\ell-1-2j<k+\ell-1-(k-1)-\ell=0$. So $S^{(2)}_{j,\ell}(m,k)=0$ whenever $j>k-1$. Let us finally consider the third case $k-1>\lfloor(m-2)/2\rfloor$. Then, we should consider the extra terms

$$\sum_{j=\lfloor(m-2)/2\rfloor+1}^{k-1} S^{(2)}_{j,\ell}(m,k)\ . \tag{3.31}$$

In this case we have to focus on the first binomial of (3.30). This binomial is nonzero only when $0 \leq j \leq \lfloor(m-2)/2\rfloor$ or when $j \geq m-1$. The first of these do not appear in (3.31); and since $m \geq k$, the second appears only when $j=k-1=m-1$. The

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[8] This is true even if m is treated as an algebraic indeterminate.

contribution of this extra term is again 1. Thus, (3.30) reduces to

$$S^{(2)}(m,k) = \sum_{j=0}^{k-1} \sum_{\ell=0}^{\infty} \binom{m-2-j}{j} \binom{m-2-2j}{k+\ell-1-2j} \binom{j}{\ell} (-1)^j 3^{k+\ell-1-2j} - \delta_{km} \,. \tag{3.32}$$

Putting together (3.29)/(3.32), we find that the two contributions δ_{km} cancel exactly, and that (3.25c) can be written as

$$\begin{aligned} a_k^{\rm F}(m) \;&=\; \sum_{j=0}^{k} \sum_{\ell=0}^{j+1} \binom{m-1-j}{j} \binom{m-1-2j}{k+\ell-1-2j} \binom{j+1}{\ell} (-1)^j 3^{k+\ell-1-2j} \\ &\qquad - \sum_{j=0}^{k-1} \sum_{\ell=0}^{j} \binom{m-2-j}{j} \binom{m-2-2j}{k+\ell-1-2j} \binom{j}{\ell} (-1)^j 3^{k+\ell-1-2j} \,, \end{aligned} \tag{3.33}$$

where the independent variable m does not appear in the summation limits. After some straightforward but lengthy algebra we can rewrite the above formula in the more compact form

$$\begin{aligned} a_k^{\rm F}(m) \;&=\; \sum_{p=0}^{k} (-1)^p \binom{m-1-p}{p} \sum_{r=0}^{k-p} 3^r \binom{m-1-2p}{r} \binom{p+1}{k-p-r} \\ &\qquad + \sum_{p=1}^{k} (-1)^p \binom{m-1-p}{p-1} \sum_{r=0}^{k-p} 3^r \binom{m-2p}{r} \binom{p-1}{k-p-r} \,. \end{aligned} \tag{3.34}$$

From (3.33) or (3.34) we see that $a_k^{\rm F}(m)$ is (the restriction of) a polynomial in m of degree at most k, as m appears only in the upper index of the binomials and

$$\binom{m}{j} \;=\; \frac{m^{\underline{j}}}{j!} \;=\; \frac{m(m-1)(m-2)\cdots(m-j+1)}{j!} \tag{3.35}$$

is a polynomial in m of degree j. [Here and in what follows, we use Knuth's [40] notation for falling powers: $x^{\underline{j}} = x(x-1)(x-2)\cdots(x-j+1)$.]

The degree of the polynomial $a_k^{\rm F}(m)$ is in fact exactly k. To see this, let us extract the term of order m^k from (3.34). The second sum in (3.34) does not contribute, as it is a polynomial in m of order at most $k-1$; the only contribution comes from the first sum:

$$[m^k] a_k^{\rm F}(m) \;=\; \sum_{p=0}^{k} \frac{(-1)^p 3^{k-p}}{p!(k-p)!} \;=\; \frac{2^k}{k!} \;\neq\; 0 \,. \tag{3.36}$$

We can summarize all this into the following proposition:

Proposition 3.4 *Let* H *and* V *be the transfer matrices (2.8a)/(2.9) for the chromatic polynomial* $v_i = v_{i,i+1} = -1$ *with free boundary conditions. Then the dominant diagonal entry in the transfer matrix can be written as*

$$t_{\rm F}(m) \;=\; \sum_{k=0}^{m} (-1)^k a_k^{\rm F}(m)\, q^{m-k} \tag{3.37}$$

where each $a_k^{\mathrm{F}}(m)$ *is a polynomial in* m *of degree* k *given by (3.34).*

For the first few values of k, we obtain

$$\begin{aligned}
a_0^{\mathrm{F}}(m) &= 1 && (3.38\text{a})\\
a_1^{\mathrm{F}}(m) &= 2m-1 && (3.38\text{b})\\
a_2^{\mathrm{F}}(m) &= 2m^2-3m+1 && (3.38\text{c})\\
a_3^{\mathrm{F}}(m) &= \tfrac{4}{3}m^3-4m^2+\tfrac{8}{3}m && (3.38\text{d})\\
a_4^{\mathrm{F}}(m) &= \tfrac{2}{3}m^4-\tfrac{10}{3}m^3+\tfrac{23}{6}m^2+\tfrac{5}{6}m-1 && (3.38\text{e})\\
a_5^{\mathrm{F}}(m) &= \tfrac{4}{15}m^5-2m^4+\tfrac{11}{3}m^3+\tfrac{3}{2}m^2-\tfrac{133}{30}m-2 && (3.38\text{f})\\
a_6^{\mathrm{F}}(m) &= \tfrac{4}{45}m^6-\tfrac{14}{15}m^5+\tfrac{23}{9}m^4+\tfrac{7}{6}m^3-\tfrac{733}{90}m^2-\tfrac{71}{15}m+12 && (3.38\text{g})
\end{aligned}$$

We find empirically the following amusing relationships:

$$\begin{aligned}
a_k^{\mathrm{F}}(k-1) &= 0 \qquad \text{for } k\ge 2 && (3.39\text{a})\\
a_k^{\mathrm{F}}(k-2) &= 0 \qquad \text{for } k\ge 3 && (3.39\text{b})\\
a_k^{\mathrm{F}}(k-3) &= 1 \qquad \text{for } k\ge 4 && (3.39\text{c})\\
a_k^{\mathrm{F}}(k-4) &= -(k-2) \quad \text{for } k\ge 5 && (3.39\text{d})\\
a_k^{\mathrm{F}}(k-5) &= \tfrac{1}{2}(k^2-5k-2) \qquad \text{for } k\ge 6 && (3.39\text{e})\\
a_k^{\mathrm{F}}(k-6) &= -\tfrac{1}{6}(k^2-6k-22)(k-3) \qquad \text{for } k\ge 7 && (3.39\text{f})
\end{aligned}$$

so that in particular $(m-k+1)(m-k+2)$ is a factor of $a_k^{\mathrm{F}}(m)$ for $k\ge 3$. We also find

$$\begin{aligned}
a_k^{\mathrm{F}}(k) &= F_{2k} \qquad \text{for } k\ge 1 && (3.40\text{a})\\
a_k^{\mathrm{F}}(k+1) &= \frac{(2k+1)F_{2k+2}-(k-4)F_{2k+1}}{5} && (3.40\text{b})
\end{aligned}$$

where

$$F_n = \frac{1}{\sqrt{5}}\left[\left(\frac{\sqrt{5}+1}{2}\right)^n - \left(\frac{\sqrt{5}-1}{2}\right)^n\right] \tag{3.41}$$

are the Fibonacci numbers. We have checked these relationships up to $k=100$.

Since we have proven that $a_k^{\mathrm{F}}(m)$ is a polynomial in m of degree k, it is also of interest to obtain explicit expressions for the coefficients of this polynomial, which we write as

$$a_k^{\mathrm{F}}(m) = \sum_{\ell=0}^{k} \frac{(-1)^\ell 2^{k-2\ell+1}}{(k-\ell)!(\ell+2)!}\, a_{k,\ell}^{\mathrm{F}}\, m^{k-\ell}\ ; \tag{3.42}$$

here the prefactors have been chosen to make many (though not all) of the coefficients $a^{\mathrm{F}}_{k,\ell}$ integers (in fact, all of them are integers for $\ell \le 5$, see below). Now we use the well-known expansion of the falling powers in terms of Stirling cycle numbers [40],

$$x^{\underline{r}} \;=\; \sum_{c \ge 0} \begin{bmatrix} r \\ c \end{bmatrix} (-1)^{r-c} x^c \;, \tag{3.43}$$

and expand all the binomials in (3.34) involving m. We arrive after some algebra at the following expression:

$$\begin{aligned}
a^{\mathrm{F}}_{k,\ell} \;&\equiv\; \frac{(k-\ell)!(\ell+2)!}{(-1)^{\ell} 2^{k-2\ell+1}} \, [m^{k-\ell}] a^{\mathrm{F}}_k(m) && \text{(3.44a)} \\
&=\; \frac{(k-\ell)!(\ell+2)!(-1)^k}{2^{k-2\ell+1}} \Bigg\{ \sum_{p=0}^{k} \sum_{r=0}^{k-p} \binom{p+1}{k-p-r} \frac{(-3)^r}{p!r!} \\
&\qquad \times \sum_{a=0}^{p} \sum_{c=0}^{r} \begin{bmatrix} p \\ a \end{bmatrix} \begin{bmatrix} r \\ c \end{bmatrix} \sum_{d=0}^{k-\ell} \binom{a}{k-\ell-d} \binom{c}{d} (1+2p)^{c-d} (1+p)^{a+d-k+\ell} \\
&\quad - \sum_{p=1}^{k} \sum_{r=0}^{k-p} \binom{p-1}{k-p-r} \frac{(-3)^r}{(p-1)!r!} \sum_{a=0}^{p-1} \sum_{c=0}^{r} \begin{bmatrix} p-1 \\ a \end{bmatrix} \begin{bmatrix} r \\ c \end{bmatrix} \\
&\qquad \times \sum_{d=0}^{k-\ell} \binom{a}{k-\ell-d} \binom{c}{d} (2p)^{c-d} (1+p)^{a+d-k+\ell} \Bigg\} \;. && \text{(3.44b)}
\end{aligned}$$

By computing (3.44b) for integers $k \ge \ell \ge 0$, we find *empirically* that $a^{\mathrm{F}}_{k,\ell}$ is in fact, for each fixed ℓ, (the restriction of) a *polynomial* in k of degree ℓ. The first few of these polynomials are:

$$\begin{aligned}
a^{\mathrm{F}}_{k,0} \;&=\; 1 && \text{(3.45a)} \\
a^{\mathrm{F}}_{k,1} \;&=\; 3k+3 && \text{(3.45b)} \\
a^{\mathrm{F}}_{k,2} \;&=\; 6k^2 - 14k + 52 && \text{(3.45c)} \\
a^{\mathrm{F}}_{k,3} \;&=\; 10k^3 - 100k^2 + 130k + 240 && \text{(3.45d)} \\
a^{\mathrm{F}}_{k,4} \;&=\; 15k^4 - 330k^3 + 845k^2 - 18k - 1928 && \text{(3.45e)} \\
a^{\mathrm{F}}_{k,5} \;&=\; 21k^5 - 805k^4 + 5005k^3 + 749k^2 + 8358k - 87360 && \text{(3.45f)} \\
a^{\mathrm{F}}_{k,6} \;&=\; 28k^6 - 1652k^5 + 20020k^4 - \tfrac{128156}{9}k^3 + \tfrac{278096}{3}k^2 \\
&\qquad + \tfrac{3141872}{9}k - \tfrac{3838336}{3} && \text{(3.45g)}
\end{aligned}$$

The fact that $a^{\mathrm{F}}_{k,0} = 1$ for all $k \ge 0$ is just a restatement of (3.36) [compare (3.42)].

3.3 Cylindrical boundary conditions

Let us now consider a square-lattice grid of fixed width $m \ge 1$ and cylindrical boundary conditions. (Please note that for $m = 1$ the horizontal edges are loops, and that for $m = 2$ there are *two* horizontal edges connecting the pair of sites in each row.) Let us also assume that all horizontal edges have weights v and all vertical edges have weights v'; they need not be -1. We proceed analogously to the preceding subsection, making the changes necessary to handle cylindrical rather than free boundary conditions.

Consider first the action of H on the start vector $\mathbf{e}_{\rm id}$. It generates 2^m terms, each of which corresponds to a partition $\mathcal{P}$ in which all the blocks are sequential sets of vertices on the m-cycle (we shall call these sets "polymers"). Furthermore, each polymer of size $\ell < m$ picks up a factor $v^{\ell-1}$, while a polymer of size m picks up a factor $v^m + mv^{m-1}$ (the v^m comes from the case in which all edges are occupied, while the mv^{m-1} comes from the m cases in which all edges but one are occupied). The action of V is identical to that for free boundary conditions.

The upshot is that we have

$$\mathsf{V}\mathsf{H}\mathbf{e}_{\rm id} \;=\; t_{\rm P}(m)\,\mathbf{e}_{\rm id} \,+\, \hbox{other terms}\;, \tag{3.46}$$

where $t_{\rm P}(m)$ is the partition function for a polymer gas on the m-cycle in which each polymer of length $\ell \geq 1$ gets a fugacity

$$\widehat{\mu}_\ell \;=\; \begin{cases} v^{\ell-1}(q+\ell v') & \hbox{for } 1 \leq \ell \leq m-1 \\ v^{m-1}(v+m)(q+mv') & \hbox{for } \ell = m \end{cases} \tag{3.47}$$

Please note that

$$\widehat{\mu}_\ell \;=\; \begin{cases} \mu_\ell & \hbox{for } 1 \leq \ell \leq m-1 \\ (v+m)\mu_m & \hbox{for } \ell = m \end{cases} \tag{3.48}$$

where μ_ℓ are the fugacities for free boundary conditions considered in the preceding subsection.

We can obtain the $t_{\rm P}(m)$ by using a simple recursion relating the periodic and free cases:

$$t_{\rm P}(m) \;=\; \sum_{k=1}^{m-1} k\mu_k t_{\rm F}(m-k) + \widehat{\mu}_m \;. \tag{3.49}$$

To see this, single out a site (e.g. 1) and let $k \geq 1$ be the size of the polymer placed on it. If $k \leq m-1$, we have k ways of placing this polymer such that the selected site belongs to it, with fugacity μ_k for each such placement; and for the rest of the ring, the total weight of all admissible polymer configurations is simply $t_{\rm F}(m-k)$. Finally, if $k = m$, there is only one way of placing the polymer, and it receives fugacity $\widehat{\mu}_m$. This proves (3.49).

In order to compute explicitly the $t_{\rm P}(m)$, it is convenient to introduce the generating function

$$\Phi_{\rm P}(z) \;=\; \sum_{m=1}^{\infty} z^m t_{\rm P}(m)\;. \tag{3.50}$$

Note next that the upper limit on the sum in (3.49) can be changed to ∞, provided that we define $t_{\rm F}(\ell) = 0$ for $\ell \leq 0$ [which is anyway implicit in the definition (3.17a) of the generating function $\Phi_{\rm F}(z)$]. Multiplying both sides of (3.49) by z^m and summing over m, we arrive easily at the equation

$$\begin{aligned} \Phi_{\rm P}(z) &= z\frac{d\Psi(z)}{dz}\,[1+\Phi_{\rm F}(z)] + v\Psi(z) && \text{(3.51a)} \\ &= \frac{z}{1-\Psi(z)}\,\frac{d\Psi(z)}{dz} + v\Psi(z) && \text{(3.51b)} \end{aligned}$$

where $\Psi(z) = \sum_{\ell=1}^{\infty} z^\ell \mu_\ell$ is defined in (3.18).[9] When $v = v' = -1$, we obtain the final formula

$$\begin{aligned} \Phi_{\rm P}(z) &= \left(\frac{z}{1+z}\right)^2 \frac{q^2-3q+3+2(q-1)^2 z + q(q-1)z^2}{1-(q-3)z-(q-1)z^2} && \text{(3.52a)} \\ &= -\,\frac{qz^2+(q+1)z+2}{(1+z)^2} + \frac{2-(q-3)z}{1-(q-3)z-(q-1)z^2}\ . && \text{(3.52b)} \end{aligned}$$

By expanding this function in powers of z, we have checked that it agrees with the known dominant diagonal elements $t_{\rm P}(m)$ for $m \le 13$ [5,6].

It is now easy to extract the partition function $t_{\rm P}(m)$: using (3.21a) we get

$$\begin{aligned} t_{\rm P}(m) \;=\; [z^m]\Phi_{\rm P}(z) \;=\;& (-1)^m(q-m-2) \\ &+ 2\sum_{j=0}^{\lfloor m/2\rfloor} \binom{m-j}{j} (q-3)^{m-2j}(q-1)^j \\ &- \sum_{j=0}^{\lfloor (m-1)/2\rfloor} \binom{m-1-j}{j} (q-3)^{m-2j}(q-1)^j\ , \qquad \text{(3.53)} \end{aligned}$$

which is manifestly a polynomial in q of degree m.

We can now define the coefficients $a_k^{\rm P}(m)$ in the same way as for free boundary conditions:

$$t_{\rm P}(m) \;=\; \sum_{k=0}^{m} (-1)^k a_k^{\rm P}(m)\, q^{m-k}\ , \qquad \text{(3.54)}$$

where k and m are integers satisfying $m \ge 1$ and $0 \le k \le m$. However, it is slightly more convenient to extract explicitly *part of* the term $(-1)^m(q-m-2)$ from (3.53), and define $\tilde{a}_k^{\rm P}(m)$ to be the coefficients in what remains:

$$t_{\rm P}(m) \;=\; (-1)^m(q-m-1) \;+\; \sum_{k=0}^{m} (-1)^k \tilde{a}_k^{\rm P}(m)\, q^{m-k}\ . \qquad \text{(3.55)}$$

Notice that the relation between $\tilde{a}_k^{\rm P}(m)$ and $a_k^{\rm P}(m)$ is rather simple: for fixed $m \ge 1$ we have that

$$a_k^{\rm P}(m) \;=\; \begin{cases} \tilde{a}_k^{\rm P}(m) & \text{for } 0 \le k \le m-2 \\ \tilde{a}_k^{\rm P}(m) - 1 & \text{for } k = m-1 \\ \tilde{a}_k^{\rm P}(m) - (m+1) & \text{for } k = m \end{cases}\ . \qquad \text{(3.56)}$$

---

[9] Note that the term of order z^1 in (3.51) vanishes whenever $v = -1$ (irrespective of the values of q and v'). This reflects the fact that $t_{\rm P}(1) = 0$ whenever $v = -1$ because of the loops at each vertex.

Expanding the binomials in (3.53), we have

$$\begin{aligned}\tilde{a}_k^{\mathrm{P}}(m) \;&=\; 2\sum_{j=0}^{\lfloor m/2\rfloor}\sum_{\ell=0}^{\infty}\binom{m-j}{j}\binom{m-2j}{k+\ell-2j}\binom{j}{\ell}(-1)^j 3^{k+\ell-2j} \\ &\quad-\sum_{j=0}^{\lfloor (m-1)/2\rfloor}\sum_{\ell=0}^{\infty}\binom{m-1-j}{j}\binom{m-2j}{k+\ell-2j}\binom{j}{\ell}(-1)^j 3^{k+\ell-2j}\,. \\ &\quad-\delta_{km} \end{aligned} \tag{3.57}$$

Again we want to substitute the m-dependent upper index in the sum over j by something independent of m: e.g., by k.

In the first sum there are two non-trivial cases: a) If $k < \lfloor m/2\rfloor$, then the second binomial vanishes whenever $k+\ell-2j<0$, and the third binomial is non-vanishing only if $j \geq \ell$. Therefore for $j>k$ and $j\geq \ell$ we have that $k+\ell-2j < k+\ell-k-\ell = 0$. So all these terms vanish. b) If $k > \lfloor m/2\rfloor$, then the first binomial does not vanish only when $0\leq j\leq \lfloor m/2\rfloor$ or when $j\geq m+1$. As we are adding terms with $\lfloor m/2\rfloor+1 \leq j\leq k-1\leq m-1$, none of them give rise to a non-vanishing contribution.

In the second sum we play a similar game: a) If $k<\lfloor (m-1)/2\rfloor$, the binomials involved are the same as for the first sum, so the same result applies here too. b) If $k>\lfloor (m-1)/2\rfloor$, then we are adding terms with $\lfloor (m-1)/2\rfloor+1\leq j\leq k-1$. The first binomial does not vanish only when $0\leq j\leq \lfloor (m-1)/2\rfloor$ or when $j\geq m$. The first of these do not appear in the extra terms; and since $m\geq k$, the second appears only when $j=k=m$, giving rise to an extra contribution equal to 1. This contribution cancels out exactly the term $-\delta_{km}$ in (3.57).

Putting all the pieces together, we end with the following expression for $\tilde{a}_k^{\mathrm{P}}(m)$:

$$\tilde{a}_k^{\mathrm{P}}(m) \;=\; \sum_{j=0}^{k}(-1)^j\left[2\binom{m-j}{j}-\binom{m-1-j}{j}\right]\sum_{\ell=0}^{\infty}\binom{m-2j}{k+\ell-2j}\binom{j}{\ell}3^{k+\ell-2j}\,, \tag{3.58}$$

where the independent variable m does not appear in the summation limits. After some straightforward but lengthy algebra we can rewrite the above formula in a more compact form:

$$\tilde{a}_k^{\mathrm{P}}(m) \;=\; 3^k\binom{m}{k}+\sum_{p=1}^{k}(-1)^p\,\frac{m}{p}\binom{m-p-1}{p-1}\sum_{r=0}^{k-p}3^r\binom{m-2p}{r}\binom{p}{k-p-r} \tag{3.59}$$

It is clear from (3.59) that $\tilde{a}_k^{\mathrm{P}}(m)$ is (the restriction of) a polynomial in m of degree at most k. To see that its degree is exactly k, let us extract the term of order m^k:

$$[m^k]\tilde{a}_k^{\mathrm{P}}(m) \;=\; \frac{3^k}{k!}+\sum_{p=1}^{k}\frac{(-1)^p 3^{k-p}}{p!(k-p)!} \;=\; \frac{3^k}{k!}+\frac{2^k-3^k}{k!} \;=\; \frac{2^k}{k!} \;\neq\; 0\,. \tag{3.60}$$

Let us also remark that the constant term in $\tilde{a}_k^{\mathrm{P}}(m)$ vanishes whenever $k\geq 1$:

$$[m^0]\tilde{a}_k^{\mathrm{P}}(m) \;=\; \delta_{k0} \;=\; \begin{cases}1 & \text{if } k=0\\ 0 & \text{if } k\geq 1\end{cases} \tag{3.61}$$

We can summarize the foregoing results in the following proposition:

Proposition 3.5 *Let* H *and* V *be the transfer matrices (2.8b)/(2.9) for the chromatic polynomial* $v_i = v_{i,i+1} = -1$ *with cylindrical boundary conditions. Then the dominant diagonal entry in the transfer matrix can be written as*

$$t_{\rm P}(m) \;=\; (-1)^m (q-m-1) \,+\, \sum_{k=0}^{m} (-1)^k \tilde{a}_k^{\rm P}(m)\, q^{m-k} \tag{3.62}$$

where each $\tilde{a}_k^{\rm P}(m)$ *is a polynomial in* m *of degree* k *given by (3.59).*

The first polynomials $\tilde{a}_k^{\rm P}(m)$ are given by

$$\tilde{a}_0^{\rm P}(m) \;=\; 1 \tag{3.63a}$$

$$\tilde{a}_1^{\rm P}(m) \;=\; 2m \tag{3.63b}$$

$$\tilde{a}_2^{\rm P}(m) \;=\; 2m^2 - m \tag{3.63c}$$

$$\tilde{a}_3^{\rm P}(m) \;=\; \tfrac{4}{3}m^3 - 2m^2 - \tfrac{1}{3}m \tag{3.63d}$$

$$\tilde{a}_4^{\rm P}(m) \;=\; \tfrac{2}{3}m^4 - 2m^3 - \tfrac{1}{6}m^2 + \tfrac{3}{2}m \tag{3.63e}$$

$$\tilde{a}_5^{\rm P}(m) \;=\; \tfrac{4}{15}m^5 - \tfrac{4}{3}m^4 + \tfrac{1}{3}m^3 + \tfrac{10}{3}m^2 - \tfrac{3}{5}m \tag{3.63f}$$

$$\tilde{a}_6^{\rm P}(m) \;=\; \tfrac{4}{45}m^6 - \tfrac{2}{3}m^5 + \tfrac{5}{9}m^4 + \tfrac{7}{2}m^3 - \tfrac{119}{45}m^2 - \tfrac{23}{6}m \tag{3.63g}$$

Since $\tilde{a}_k^{\rm P}(m)$ is a polynomial in m of degree k, we are again interested in obtaining the coefficients $\tilde{a}_{k,\ell}^{\rm P}$ defined by

$$\tilde{a}_k^{\rm P}(m) \;=\; \sum_{\ell=0}^{k} \frac{(-1)^\ell 2^{k-2\ell+1}}{(k-\ell)!(\ell+2)!}\, \tilde{a}_{k,\ell}^{\rm P}\; m^{k-\ell}\;. \tag{3.64}$$

With the help of (3.43), we obtain after some algebra the following result:

$$\begin{aligned} \tilde{a}_{k,\ell}^{\rm P} \;=\; & \frac{(k-\ell)!(\ell+2)!}{2^{k-2\ell+1}} \left\{ \frac{3^k}{k!} \begin{bmatrix} k \\ k-\ell \end{bmatrix} \right. \\ & + (-1)^k \sum_{p=1}^{k} \sum_{r=0}^{k-p} \frac{(-3)^r}{p!r!} \binom{p}{k-p-r} \sum_{a=0}^{p-1} \sum_{c=0}^{r} \begin{bmatrix} p-1 \\ a \end{bmatrix} \begin{bmatrix} r \\ c \end{bmatrix} \\ & \left. \times \sum_{d=0}^{k-\ell-1} \binom{c}{d} \binom{a}{k-\ell-d-1} (2p)^{c-d} (1+p)^{a-k+\ell+d+1} \right\}\;. \end{aligned} \tag{3.65}$$

By computing (3.65) for integers $k \geq \ell \geq 0$, we find *empirically* that $\tilde{a}_{k,\ell}^{\rm P}$ is in fact, for each fixed ℓ, (the restriction of) a *polynomial* in k of degree ℓ. The first few are:

$$\tilde{a}^{\mathrm{P}}_{k,0} = 1 \tag{3.66a}$$

$$\tilde{a}^{\mathrm{P}}_{k,1} = 3k - 3 \tag{3.66b}$$

$$\tilde{a}^{\mathrm{P}}_{k,2} = 6k^2 - 38k + 52 \tag{3.66c}$$

$$\tilde{a}^{\mathrm{P}}_{k,3} = 10k^3 - 160k^2 + 390k + 0 \tag{3.66d}$$

$$\tilde{a}^{\mathrm{P}}_{k,4} = 15k^4 - 450k^3 + 2405k^2 - 1450k - 7688 \tag{3.66e}$$

$$\tilde{a}^{\mathrm{P}}_{k,5} = 21k^5 - 1015k^4 + 10465k^3 - 16121k^2 - 37030k - 151200 \tag{3.66f}$$

$$\begin{aligned}\tilde{a}^{\mathrm{P}}_{k,6} = {} & 28k^6 - 1988k^5 + 34580k^4 - \tfrac{1100876}{9}k^3 - \tfrac{327376}{3}k^2 \\ & + \tfrac{480752}{9}k - \tfrac{1902976}{3}\end{aligned} \tag{3.66g}$$

The fact that $\tilde{a}^{\mathrm{P}}_{k,0} = 1$ for all $k \geq 0$ is just a restatement of (3.60).

4 Large-q expansion of the leading eigenvalue

In this section we compute the large-q expansion of the leading eigenvalue $\lambda_\star(m)$ for both free and cylindrical boundary conditions, and determine empirically some of its remarkable properties. In Section 5 we shall provide theoretical explanations of some (but not all!) of these empirical observations.

4.1 Overview of method and results

In the preceding section we computed in closed form the dominant diagonal entry in the transfer matrix, t_{id}, for a strip of width $m \geq 1$ with either free or cylindrical boundary conditions (denoted t_{F} and t_{P}, respectively). We found that this entry is in each case a polynomial in q of degree m:

$$t_{\mathrm{F}}(m) = \sum_{k=0}^{m} (-1)^k a^{\mathrm{F}}_k(m)\, q^{m-k} \tag{4.1a}$$

$$t_{\mathrm{P}}(m) = \sum_{k=0}^{m} (-1)^k a^{\mathrm{P}}_k(m)\, q^{m-k} \tag{4.1b}$$

$$= (-1)^m (q - m - 1) + \sum_{k=0}^{m} (-1)^k \tilde{a}^{\mathrm{P}}_k(m)\, q^{m-k} \tag{4.1c}$$

We furthermore computed in closed form the coefficients $a^{\mathrm{F}}_k(m)$ and $\tilde{a}^{\mathrm{P}}_k(m)$, which are in fact polynomials in m of degree k [cf. (3.34) and (3.59)]. For instance, the leading few terms for large $|q|$ are

$$\begin{aligned} t_{\rm F}(m) &= q^m - (2m-1)q^{m-1} + (2m^2-3m+1)q^{m-2} \\ &\qquad - (\tfrac{4}{3}m^3 - 4m^2 + \tfrac{8}{3}m)q^{m-3} + \ldots \quad \text{[for } m \ge 1\text{]} \end{aligned} \tag{4.2a}$$

$$\begin{aligned} t_{\rm P}(m) &= q^m - 2mq^{m-1} + (2m^2-m)q^{m-2} \\ &\qquad - (\tfrac{4}{3}m^3 - 2m^2 - \tfrac{1}{3}m)q^{m-3} + \ldots \quad \text{[for } m \ge 5\text{]} \end{aligned} \tag{4.2b}$$

In this section we want to carry out an analogous computation for the dominant *eigenvalue* of the transfer matrix, which we call $\lambda_\star^{\rm F/P}$. Already from Corollary 3.3 we can conclude that $\lambda_\star(m)$ has, for large $|q|$, a convergent expansion in powers of q^{-1},

$$\lambda_\star^{\rm F}(m) = \sum_{k=0}^{\infty} (-1)^k b_k^{\rm F}(m)\, q^{m-k} \tag{4.3a}$$

$$\lambda_\star^{\rm P}(m) = \sum_{k=0}^{\infty} (-1)^k b_k^{\rm P}(m)\, q^{m-k} \tag{4.3b}$$

and that the first two terms in this expansion coincide with those in the dominant diagonal entry:

$$\lambda_\star^{\rm F/P}(m) - t_{\rm F/P}(m) = O(q^{m-2}) \tag{4.4}$$

and hence

$$b_k^{\rm F/P}(m) = a_k^{\rm F/P}(m) \qquad \text{for } k = 0, 1\,. \tag{4.5}$$

Here we shall go further and compute the coefficients $b_k^{\rm F/P}(m)$ for $1 \le m \le 11_{\rm F}, 13_{\rm P}$ and $0 \le k \le 40$.[10] Somewhat surprisingly, we shall find that

$$b_k^{\rm F}(m) = a_k^{\rm F}(m) \qquad \text{for } k = 2, 3 \tag{4.6a}$$

$$b_k^{\rm P}(m) = a_k^{\rm P}(m) \qquad \text{for } k = 2, 3 \text{ and } m \ge k+2 \tag{4.6b}$$

so that

$$\lambda_\star^{\rm F}(m) - t_{\rm F}(m) = O(q^{m-4}) \tag{4.7a}$$

$$\lambda_\star^{\rm P}(m) - t_{\rm P}(m) = O(q^{m-4}) \qquad \text{for } m \ge 5 \tag{4.7b}$$

rather than merely $O(q^{m-2})$ as Corollary 3.3 shows.

For some purposes it is slightly more convenient to use, in place of the coefficients $b_k^{\rm P}(m)$, the modified coefficients $\tilde{b}_k^{\rm P}(m)$ defined by

$$\lambda_\star^{\rm P}(m) = (-1)^m (q-m-1) + \sum_{k=0}^{\infty} (-1)^k \tilde{b}_k^{\rm P}(m)\, q^{m-k} \tag{4.8}$$

---

[10] It would not be difficult to extend this computation to much larger values of k, if we really cared. Extension to larger values of m is, however, an extremely demanding computational task. The dimension of the transfer matrix for $m = 11_{\rm F}$ is 1142; for $m = 12_{\rm F}$ it is 2947, which is beyond the capabilities of our current computer facilities.

[analogously to (4.1c) for $t_{\mathrm{P}}(m)$]. Note that the relation between the coefficients $b_k^{\mathrm{P}}(m)$ and $\tilde{b}_k^{\mathrm{P}}(m)$ is the same as for the coefficients $a_k^{\mathrm{P}}(m)$ and $\tilde{a}_k^{\mathrm{P}}(m)$ [cf. (3.56)].

Most importantly, however, it is enlightening to pass from the eigenvalue $\lambda_\star(m)$ to its logarithm, which is a free energy, and define

$$\log \frac{\lambda_\star^{\mathrm{F/P}}(m)}{q^m} \;=\; \sum_{k=1}^{\infty} c_k^{\mathrm{F/P}}(m)\, q^{-k} \; . \tag{4.9}$$

For cylindrical boundary conditions it is slightly more efficient to define the modified coefficients $\tilde{c}_k^{\mathrm{P}}(m)$ by

$$\log \frac{\lambda_\star^{\mathrm{P}}(m) - (-1)^m(q-m-1)}{q^m} \;=\; \sum_{k=1}^{\infty} \tilde{c}_k^{\mathrm{P}}(m)\, q^{-k} \; . \tag{4.10}$$

In this section we shall see *empirically* that the coefficients $c_k(m)$ behave in a much simpler way than the $b_k(m)$: namely, while $b_k(m)$ is, for large enough m, (the restriction of) a polynomial *of degree k* in m, we shall find that $c_k(m)$ is, for large enough m, (the restriction of) a polynomial *of degree 1* in m. In Section 5 we shall discuss the theoretical interpretation of this empirical observation.

We shall proceed as follows: Using the methods of [5, 6] we shall compute the transfer matrices for strips of width $m \le 11$ for free boundary conditions and $m \le 13$ for cylindrical boundary conditions.[11] From these we can extract the dominant eigenvalue as a power series in q^{-1}, i.e. for each available m we can easily compute as many coefficients $b_k(m)$ and $c_k(m)$ as we please.[12] We then observe *empirically* that, for each $k \ge 0$, the coefficient $b_k(m)$ [resp. $c_k(m)$] is a polynomial B_k [resp. C_k] in m of degree k [resp. degree 1] *provided that we restrict to integers* $m \ge$ some $m_{\min}(k)$.[13] *Assuming* that this empirical observation is accurate (i.e., that the polynomial behavior persists to all larger m), we can infer the expressions for the polynomials B_k and C_k for $k \le 31$ (resp. $k \le 16$) for free (resp. cylindrical) boundary conditions.

4.2 Free boundary conditions

Using the methods just described, we have obtained the leading eigenvalue $\lambda_\star^{\mathrm{F}}(m)$ for $0 \le m \le 11$ as a power series in q^{-1} [cf. (4.3a)] through order $k = 40$. The resulting

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[11] In fact, this was already done in ref. [5] for $m \le 8$ with both boundary conditions, and in ref. [6] for $9 \le m \le 13$ with cylindrical boundary conditions. Therefore, the only new transfer matrices we need to compute here are $m = 9, 10, 11$ with free boundary conditions. See also Section 6 below for further results from this computation.

[12] To compute the dominant eigenvalue as a power series in q^{-1}, we have used the power method [41, Section 7.3.1] *in symbolic form*. Each iteration gives one additional term in the expansion of the dominant eigenvalue in powers of q^{-1}. We can therefore compute the *exact* expansion up to any desired order in a *finite* number of steps.

[13] By contrast, for the dominant diagonal entry we have *proven* that $a_k^{\mathrm{F}}(m)$ and $\tilde{a}_k^{\mathrm{P}}(m)$ are polynomials in m of degree k; and in this case the polynomial form holds for *all* allowable integers m, i.e. $m \ge \max(k, 1)$.

coefficients $b_k^{\mathrm{F}}(m)$ are displayed in Table 1, and the corresponding coefficients $c_k^{\mathrm{F}}(m)$ [cf. (4.9)] are displayed in Table 2. It is interesting to note that for all (k,m) that we have computed (i.e., $1 \le m \le 11$ and $0 \le k \le 40$), the coefficients $b_k^{\mathrm{F}}(m)$ and $kc_k^{\mathrm{F}}(m)$ are integers. We observe *empirically* that, for each fixed k, the coefficients $b_k^{\mathrm{F}}(m)$ are the restriction to integers m of a polynomial B_k^{F} in m of degree k, and that the coefficients $c_k^{\mathrm{F}}(m)$ are the restriction to integers m of a polynomial C_k^{F} in m of degree 1, *provided that we restrict attention to* $m \ge m_{\min}^{\mathrm{F}}(k)$ with

$$m_{\min}^{\mathrm{F}}(k) \;=\; \begin{cases} 1 & \text{if } 0 \le k \le 6 \\ \left\lceil \frac{k}{2} \right\rceil - 2 & \text{if } k \ge 7 \end{cases} . \tag{4.11}$$

Below this threshold $m_{\min}^{\mathrm{F}}(k)$, the coefficients deviate from polynomial behavior. With our available data together with a few tricks described below, we are able to determine these polynomials for $0 \le k \le 31$.

First we start by trying to fit the coefficients $b_k^{\mathrm{F}}(m)$ with $m \ge m_{\min}^{\mathrm{F}}(k)$ to a polynomial B_k^{F} in m of degree k. As we need $k+1$ coefficients for such a polynomial, we are able to obtain these polynomials only up to $k = 8$. Please note that in all cases we have at least one data point more than the number of unknowns, so every fit can be tested at least on one extra data point. Our results are:

$$B_0^{\mathrm{F}}(m) \;=\; 1 \tag{4.12a}$$

$$B_1^{\mathrm{F}}(m) \;=\; 2m - 1 \tag{4.12b}$$

$$B_2^{\mathrm{F}}(m) \;=\; 2m^2 - 3m + 1 \tag{4.12c}$$

$$B_3^{\mathrm{F}}(m) \;=\; \tfrac{4}{3}m^3 - 4m^2 + \tfrac{8}{3}m \tag{4.12d}$$

$$B_4^{\mathrm{F}}(m) \;=\; \tfrac{2}{3}m^4 - \tfrac{10}{3}m^3 + \tfrac{23}{6}m^2 + \tfrac{11}{6}m - 3 \tag{4.12e}$$

$$B_5^{\mathrm{F}}(m) \;=\; \tfrac{4}{15}m^5 - 2m^4 + \tfrac{11}{3}m^3 + \tfrac{7}{2}m^2 - \tfrac{433}{30}m + 9 \tag{4.12f}$$

$$B_6^{\mathrm{F}}(m) \;=\; \tfrac{4}{45}m^6 - \tfrac{14}{15}m^5 + \tfrac{23}{9}m^4 + \tfrac{19}{6}m^3 - \tfrac{2263}{90}m^2 + \tfrac{574}{15}m - 18 \tag{4.12g}$$

$$\begin{aligned} B_7^{\mathrm{F}}(m) \;=\; & \tfrac{8}{315}m^7 - \tfrac{16}{45}m^6 + \tfrac{62}{45}m^5 + \tfrac{16}{9}m^4 - \tfrac{1144}{45}m^3 + \tfrac{5947}{90}m^2 \\ & - \tfrac{15011}{210}m + 29 \end{aligned} \tag{4.12h}$$

$$\begin{aligned} B_8^{\mathrm{F}}(m) \;=\; & \tfrac{2}{315}m^8 - \tfrac{4}{35}m^7 + \tfrac{3}{5}m^6 + \tfrac{2}{3}m^5 - \tfrac{2131}{120}m^4 + \tfrac{4129}{60}m^3 \\ & - \tfrac{302017}{2520}m^2 + \tfrac{9041}{84}m - 49 \end{aligned} \tag{4.12i}$$

Notice that the three highest-order coefficients agree with those of the corresponding polynomial $a_k^{\mathrm{F}}(m)$, i.e.

$$B_k^{\mathrm{F}}(m) \;=\; \begin{cases} a_k^{\mathrm{F}}(m) & \text{for } 0 \le k \le 3 \\ a_k^{\mathrm{F}}(m) + O(m^{k-3}) & \text{for } k \ge 4 \end{cases} \tag{4.13}$$

However, there is a better way of extracting the desired information from our numerical data: instead of using the coefficients $b_k^{\mathrm{F}}(m)$ as our basic quantities, we can use the related coefficients $c_k^{\rm F}(m)$ [cf. (4.9)]. The latter coefficients are *empirically* found to be, for each fixed k, the restriction to integer m of a polynomial $C_k^{\rm F}$ in m *of degree 1*, i.e.

$$C_k^{\rm F}(m) \;=\; \alpha_k^{\rm F} m + \beta_k^{\rm F} \;, \tag{4.14}$$

provided that $m \geq$ the same $m_{\rm min}^{\rm F}(k)$ defined in (4.11). As we need only *two* coefficients for such a polynomial (i.e., $\alpha_k^{\rm F}$ and $\beta_k^{\rm F}$), we are able to obtain these polynomials up to $k = 22$ (if we want at least one extra data point to test the fit) or $k = 24$ (if we don't). Our results for $k \leq 10$ are:

$$\begin{aligned}
C_1^{\rm F}(m) &= -2m+1 && \text{(4.15a)}\\
C_2^{\rm F}(m) &= -m+\tfrac{1}{2} && \text{(4.15b)}\\
C_3^{\rm F}(m) &= \tfrac{1}{3}m-\tfrac{2}{3} && \text{(4.15c)}\\
C_4^{\rm F}(m) &= \tfrac{5}{2}m-\tfrac{11}{4} && \text{(4.15d)}\\
C_5^{\rm F}(m) &= \tfrac{28}{5}m-\tfrac{29}{5} && \text{(4.15e)}\\
C_6^{\rm F}(m) &= \tfrac{55}{6}m-\tfrac{28}{3} && \text{(4.15f)}\\
C_7^{\rm F}(m) &= \tfrac{89}{7}m-\tfrac{97}{7} && \text{(4.15g)}\\
C_8^{\rm F}(m) &= \tfrac{81}{4}m-\tfrac{243}{8} && \text{(4.15h)}\\
C_9^{\rm F}(m) &= \tfrac{505}{9}m-\tfrac{1019}{9} && \text{(4.15i)}\\
C_{10}^{\rm F}(m) &= \tfrac{1029}{5}m-\tfrac{4489}{10} && \text{(4.15j)}
\end{aligned}$$

The polynomials $C_k^{\rm F}$ for $11 \leq k \leq 22$ are reported in the MATHEMATICA file `data_FREE.m` that is included with the preprint version of this article at arXiv.org; they can also be read off from the results of Section 5 below [cf. (5.12)/(5.15)]. Finally, the polynomials $B_k^{\rm F}$ for $9 \leq k \leq 22$ can be determined from the $C_k^{\rm F}$ using (4.9).

Actually, we can do better than this. We believe that the coefficients $c_k^{\rm F}(m)$ are, for each fixed $k \geq 0$, the restriction to integers $m \geq m_{\rm min}^{\rm F}(k)$ of a polynomial $C_k^{\rm F}$ in m of degree 1. If we compute the difference

$$\Delta_k^{\rm F}(m) \;=\; c_k^{\rm F}(m) - C_k^{\rm F}(m) \tag{4.16}$$

between the numerical coefficients $c_k^{\rm F}(m)$ and the corresponding polynomials $C_k^{\rm F}$, we find, not surprisingly, that they are nonzero whenever $m < m_{\rm min}(k)$: see Table 3. If we could somehow guess an analytic form for at least some of these coefficients $\Delta_k^{\rm F}(m)$, we could then define improved coefficients $\hat{c}_k^{\rm F}(m)$ by

$$\hat{c}_k^{\rm F}(m) \;=\; c_k^{\rm F}(m) - \Delta_k^{\rm F}(m) \;, \tag{4.17}$$

so that these coefficients $\hat{c}_k^{\rm F}(m)$ would be, for each fixed k, the restriction to integers $m \geq \widehat{m}_{\rm min}^{\rm F}(k)$ of the same polynomial $C_k^{\rm F}$, with a *smaller* threshold $\widehat{m}_{\rm min}^{\rm F}(k) <$

$m^{\rm F}_{\rm min}(k)$. The important point here is that a smaller threshold $\widehat{m}^{\rm F}_{\rm min}(k)$ implies that we can obtain more polynomials $C^{\rm F}_k$ with the same raw data.

By inspecting Table 3, it is not difficult to realize that there are some patterns in $\Delta^{\rm F}_k(m)$ immediately below the threshold $m^{\rm F}_{\rm min}(k)$: for instance, for odd $k = 2p + 1$ with $3 \le p \le 10$, we have $\Delta^{\rm F}_{2p+1}(p-2) = 1$; and for even $k = 2p$ with $4 \le p \le 10$, we have $\Delta^{\rm F}_{2p}(p-3) = 3p - 2$. We then *assume* that this behavior holds true for all larger p. For other subsets of the nonzero values of $\Delta^{\rm F}_k(m)$ slightly farther below the boundary $m^{\rm F}_{\rm min}(k)$, we likewise find simple polynomial Ansätze. Our *empirical* results are:

$$\begin{aligned}
\Delta^{\rm F}_{2p+1}(p-2) &= 1\,, \quad \text{for } p \ge 3 && \text{(4.18a)}\\
\Delta^{\rm F}_{2p+1}(p-3) &= \tfrac{13}{2}p^2 - \tfrac{37}{2}p + 27\,, \quad \text{for } p \ge 4 && \text{(4.18b)}\\
\Delta^{\rm F}_{2p+1}(p-4) &= \tfrac{95}{8}p^4 - \tfrac{1265}{12}p^3 + \tfrac{2961}{8}p^2 - \tfrac{8515}{12}p + 917\,, \quad \text{for } p \ge 5 && \text{(4.18c)}
\end{aligned}$$

$$\begin{aligned}
\Delta^{\rm F}_{2p}(p-3) &= 3p - 2\,, \quad \text{for } p \ge 4 && \text{(4.18d)}\\
\Delta^{\rm F}_{2p}(p-4) &= \tfrac{59}{6}p^3 - 66p^2 + \tfrac{817}{6}p - 17\,, \quad \text{for } p \ge 5 && \text{(4.18e)}\\
\Delta^{\rm F}_{2p}(p-5) &= \tfrac{473}{40}p^5 - \tfrac{2207}{12}p^4 + \tfrac{9023}{8}p^3 - \tfrac{38413}{12}p^2 + \tfrac{29763}{10}p + 2941\,,\\
&\qquad \text{for } p \ge 7 && \text{(4.18f)}
\end{aligned}$$

We are able to test each fit on at least one additional data point. Notice that in (4.18f), the condition $p \ge 7$ does *not* follow the expected behavior from the previous correction terms (i.e., one would have expected $p \ge 6$). The new threshold $\widehat{m}^{\rm F}_{\rm min}(k)$ is given by

$$\widehat{m}^{\rm F}_{\rm min}(k) = \begin{cases} 1 & \text{if } 0 \le k \le 11 \\ 2 & \text{if } 12 \le k \le 14 \\ \lceil \frac{k}{2} \rceil - 5 & \text{if } k \ge 15 \end{cases} \tag{4.19}$$

By this method, we can obtain the polynomials $C^{\rm F}_k$ (and therefore the polynomials $B^{\rm F}_k$) up to $k = 28$. Indeed, the fits to obtain the polynomials $C^{\rm F}_k$ with $k \le 28$ were tested on at least one additional data point.

If we do not demand to have at least one extra data point to test the fits, we can extend this computation up to $k = 30$. We can then guess one further correction term $\Delta^{\rm F}_k(m)$ (again with no additional test for the fit):

$$\begin{aligned}
\Delta^{\rm F}_{2p+1}(p-5) &= \tfrac{161}{16}p^6 - \tfrac{43693}{240}p^5 + \tfrac{21757}{16}p^4 - \tfrac{86909}{16}p^3 + \tfrac{110297}{8}p^2 - \tfrac{433772}{15}p\\
&\qquad +42719\,, \quad \text{for } p \ge 8\,. && \text{(4.20)}
\end{aligned}$$

With this additional correction, the new threshold $\widehat{m}^{\rm F}_{\rm min}$ is

$$\widehat{m}^{\rm F}_{\rm min}(k) \;=\; \begin{cases} 1 & \text{if } 0 \le k \le 11 \\ 2 & \text{if } 12 \le k \le 14 \\ 3 & \text{if } 15 \le k \le 17 \\ \left\lfloor \frac{k}{2} \right\rfloor - 5 & \text{if } k \ge 18 \end{cases} \tag{4.21}$$

so the computation of the polynomials $C^{\rm F}_k$ can be extended up to $k = 31$ (with no extra data points to test the fit).

4.3 Cylindrical boundary conditions

We have likewise obtained the leading eigenvalue $\lambda^{\rm P}_\star(m)$ for $0 \le m \le 13$ as a power series in q^{-1} [cf. (4.3b)] through order $k = 40$. The resulting coefficients $b^{\rm P}_k(m)$ are displayed in Table 4, and the corresponding coefficients $c^{\rm P}_k(m)$ are displayed in Table 6. As for free boundary conditions, we note that for all (k, m) that we have computed (i.e., $1 \le m \le 13$ and $0 \le k \le 40$), the coefficients $b^{\rm P}_k(m)$ and $kc^{\rm P}_k(m)$ are integers.

We observe *empirically* that, for each fixed k, the coefficients $b^{\rm P}_k(m)$ are the restriction to integers m of a polynomial $B^{\rm P}_k$ in m of degree k, and that the coefficients $c^{\rm P}_k(m)$ are the restriction to integers m of a polynomial $C^{\rm P}_k$ in m of degree 1, *provided that we restrict attention to* $m \ge m^{\rm P}_{\rm min}(k) = k + 2$. Below this threshold the coefficients deviate from polynomial behavior. The polynomial behavior can be extended downwards by two steps, i.e. to $m = k$, if we use the coefficients $\widetilde{b}^{\rm P}_k(m)$ [cf. (4.8)] in place of $b^{\rm P}_k(m)$. With our available data together with the tricks described in the preceding subsection, we are able to determine these polynomials for $0 \le k \le 15$. The coefficients $\widetilde{b}^{\rm P}_k(m)$ are displayed in Table 5.

We begin, as before, by fitting $\widetilde{b}^{\rm P}_k(m)$ for $m \ge k$ to a polynomial $B^{\rm P}_k$ of degree k. With our data we can do this for $0 \le k \le 6$; we also have, in each case, at least one extra data point to test the fit. Our results are:

$$B^{\rm P}_0(m) \;=\; 1 \tag{4.22a}$$

$$B^{\rm P}_1(m) \;=\; 2m \tag{4.22b}$$

$$B^{\rm P}_2(m) \;=\; 2m^2 - m \tag{4.22c}$$

$$B^{\rm P}_3(m) \;=\; \tfrac{4}{3}m^3 - 2m^2 - \tfrac{1}{3}m \tag{4.22d}$$

$$B^{\rm P}_4(m) \;=\; \tfrac{2}{3}m^4 - 2m^3 - \tfrac{1}{6}m^2 + \tfrac{5}{2}m \tag{4.22e}$$

$$B^{\rm P}_5(m) \;=\; \tfrac{4}{15}m^5 - \tfrac{4}{3}m^4 + \tfrac{1}{3}m^3 + \tfrac{16}{3}m^2 - \tfrac{28}{5}m \tag{4.22f}$$

$$B^{\rm P}_6(m) \;=\; \tfrac{4}{45}m^6 - \tfrac{2}{3}m^5 + \tfrac{5}{9}m^4 + \tfrac{11}{2}m^3 - \tfrac{614}{45}m^2 + \tfrac{55}{6}m \tag{4.22g}$$

Notice that the three highest-order coefficients agree with those of the corresponding polynomial $\tilde{a}_k^{\rm P}(m)$, i.e.

$$B_k^{\rm P}(m) \;=\; \begin{cases} \tilde{a}_k^{\rm P}(m) & \text{for } 0 \le k \le 3 \\ \tilde{a}_k^{\rm P}(m) + O(m^{k-3}) & \text{for } k \ge 4 \end{cases} \tag{4.23}$$

Note also that the constant term vanishes in all these polynomials except $B_0^{\rm P}$.

As in the previous subsection, we can extract the desired information more efficiently by analyzing the coefficients $c_k^{\rm P}(m)$, which are found empirically to be, for each fixed k, a polynomial $C_k^{\rm P}$ in m *of degree 1* for $m \ge m_{\rm min}^{\rm P}(k) = k+2$, i.e.

$$C_k^{\rm P}(m) \;=\; \alpha_k^{\rm P} m + \beta_k^{\rm P} \;, \tag{4.24}$$

As we need only two coefficients for such a polynomial, we can obtain these polynomials up to $k = 9$ (if we want at least one extra data point to test the fit) or $k = 10$ (if we don't).

However, we can do slightly better if we consider instead of the coefficients $c_k^{\rm P}(m)$ the modified coefficients $\tilde{c}_k^{\rm P}(m)$ defined by (4.10). We find empirically that $k\tilde{c}_k^{\rm P}(m)$ is an integer for all the computed values of (k, m): see Table 7. We also find empirically that $\tilde{c}_k^{\rm P}(m)$ is, for each fixed k, the restriction to integers $m \ge \widetilde{m}_{\rm min}^{\rm P}(k)$ of the same polynomial $C_k^{\rm P}$ with a *smaller* threshold $\widetilde{m}_{\rm min}^{\rm P}(k) = \max(k, 2) < m_{\rm min}^{\rm P}(k)$. In this way we can obtain the polynomials $C_k^{\rm P}$ up to $k = 11$ or $k = 12$, depending on whether or not we insist on having an extra data point to test the fit. Our results for $k \le 10$ are:

$$C_1^{\rm P}(m) \;=\; -2m \tag{4.25a}$$

$$C_2^{\rm P}(m) \;=\; -m \tag{4.25b}$$

$$C_3^{\rm P}(m) \;=\; \tfrac{1}{3}m \tag{4.25c}$$

$$C_4^{\rm P}(m) \;=\; \tfrac{5}{2}m \tag{4.25d}$$

$$C_5^{\rm P}(m) \;=\; \tfrac{28}{5}m \tag{4.25e}$$

$$C_6^{\rm P}(m) \;=\; \tfrac{55}{6}m \tag{4.25f}$$

$$C_7^{\rm P}(m) \;=\; \tfrac{89}{7}m \tag{4.25g}$$

$$C_8^{\rm P}(m) \;=\; \tfrac{81}{4}m \tag{4.25h}$$

$$C_9^{\rm P}(m) \;=\; \tfrac{505}{9}m \tag{4.25i}$$

$$C_{10}^{\rm P}(m) \;=\; \tfrac{1029}{5}m \tag{4.25j}$$

The polynomials $C_k^{\rm P}$ for $k = 11, 12$ are reported in the MATHEMATICA file `data_CYL.m` that is included with the preprint version of this article at arXiv.org. Please note that the constant term vanishes in all these polynomials, while the term linear in m is the same as for free boundary conditions [cf. (4.15)]:

$$\alpha_k^{\rm P} \;=\; \alpha_k^{\rm F} \tag{4.26a}$$

$$\beta_k^{\rm P} \;=\; 0 \tag{4.26b}$$

in all cases that we are able to test (namely, $1 \leq k \leq 12$). Finally, the polynomials B_k^{P} for $7 \leq k \leq 12$ can be determined from the C_k^{P} using (4.10).

These results can be improved in the same way as we did in the previous subsection. First we compute the difference $\Delta_k^{\mathrm{P}}(m) = \tilde{c}_k^{\mathrm{P}}(m) - C_k^{\mathrm{P}}(m)$: see Table 8. We then try to guess an analytic form for some of the coefficients $\Delta_k^{\mathrm{P}}(m)$, and we define improved coefficients $\hat{c}_k^{\mathrm{P}}(m)$ [as in (4.17)] so that the $\hat{c}_k^{\mathrm{P}}(m)$ will be, for each fixed k, the restriction to integers $m \geq \widehat{m}_{\mathrm{min}}^{\mathrm{P}}(k)$ of the polynomial C_k^{P}, with a *smaller* threshold $\widehat{m}_{\mathrm{min}}^{\mathrm{P}}(k) < \widetilde{m}_{\mathrm{min}}^{\mathrm{P}}(k)$. As in the case of free boundary conditions, we find empirically that the coefficients $\Delta_k^{\mathrm{P}}(m)$ closest to the boundary $\widetilde{m}_{\mathrm{min}}^{\mathrm{P}}(k)$ are the restriction to integers m of certain polynomials:

$$\Delta_k^{\mathrm{P}}(k-1) \;=\; (-1)^{k-1}\left(\tfrac{3}{2}k^2 - \tfrac{11}{2}k + 4\right) , \quad \text{for } k \geq 4 \tag{4.27a}$$

$$\Delta_k^{\mathrm{P}}(k-2) \;=\; (-1)^{k-2}\left(\tfrac{11}{6}k^3 - 10k^2 + \tfrac{73}{6}k + 1\right) , \quad \text{for } k \geq 6 \tag{4.27b}$$

$$\Delta_k^{\mathrm{P}}(k-3) \;=\; (-1)^{k-3}\left(\tfrac{35}{24}k^4 - \tfrac{199}{12}k^3 - \tfrac{1837}{24}k^2 - \tfrac{2201}{12}k + 191\right) , \quad \text{for } k \geq 8 \tag{4.27c}$$

Again, each fit can be tested on at least an extra data point. The new threshold $\widehat{m}_{\mathrm{min}}^{\mathrm{P}}$ is

$$\widehat{m}_{\mathrm{min}}^{\mathrm{P}}(k) \;=\; \begin{cases} 2 & \text{if } k \leq 2 \\ \lfloor \frac{k}{2} \rfloor + 1 & \text{if } 3 \leq k \leq 8 \\ k-3 & \text{if } k \geq 9\,, \end{cases} \tag{4.28}$$

By this method, we can obtain the polynomials C_k^{P} (and therefore the polynomials B_k^{P}) up to $k = 14$, with at least one extra data point to test the fit.

If we do not insist on having an extra data point to test the fit, we can extend this computation of C_k^{P} up to $k = 15$. We can then guess one further correction term $\Delta_k^{\mathrm{P}}(m)$ (again with no additional test for the fits):

$$\Delta_k^{\mathrm{P}}(k-4) \;=\; (-1)^{k-4}\left(\tfrac{33}{40}k^5 - \tfrac{115}{8}k^4 + \tfrac{741}{8}k^3 - \tfrac{1821}{8}k^2 - \tfrac{729}{20}k + 695\right) , \quad \text{for } k \geq 10\,. \tag{4.29}$$

With this correction the new threshold is

$$\widehat{m}_{\mathrm{min}}^{\mathrm{P}}(k) \;=\; \begin{cases} 2 & \text{if } k \leq 2 \\ \lfloor \frac{k}{2} \rfloor + 1 & \text{if } 3 \leq k \leq 10 \\ k-4 & \text{if } k \geq 11 \end{cases} \tag{4.30}$$

so the computation of the polynomials C_k^{P} can be extended up to $k = 16$ (with no extra data points to test the fit).

The polynomials C_k^{P} for $10 \leq k \leq 16$ also have a zero constant term, and the relation (4.26) between periodic and free boundary conditions continues to hold.

5 Thermodynamic limit ($m \to \infty$)

In previous sections we have dealt with semi-infinite square-lattice strips of fixed width m. In this section we will study the thermodynamic limit $m \to \infty$ of the free energy of our model.

In Section 5.1 we introduce some preliminary definitions and discuss the expected behavior of the strip free energies per unit length, $f_m^{\mathrm{F}}(q)$ and $f_m^{\mathrm{P}}(q)$, as a function of the strip width m. We then discuss the large-$|q|$ expansion of the bulk free energy that was calculated by Bakaev and Kabanovich [42]. In Section 5.2 we obtain (using the polynomials c_k^{F}) a large-$|q|$ expansion for the limiting free energy $f_m(q)$ of a semi-infinite strip of width m and free boundary conditions. We find that this expansion contains two terms: a bulk term (independent of m and in full agreement with the series in Ref. [42]) and a surface term (linear in $1/m$). Our result gives an independent check of 31 out of the 36 terms of the series in Ref. [42], and provides many terms of the large-$|q|$ expansion of the surface free energy for free boundary conditions. Finally, in Section 5.3 we repeat the computation with cylindrical boundary conditions. We find that the bulk contribution is the same as for free boundary conditions and that there is *no* surface free energy. These results provide a theoretical interpretation of the behavior found in the preceding section for C_k^{F} and C_k^{P} [cf. (4.15)/(4.25) and (4.26)].

5.1 Generalities

Corollary 3.3 shows that, for each width m and each boundary condition (free or cylindrical), the transfer matrix has, for sufficiently large $|q|$, a *single* dominant eigenvalue $\lambda_\star(q)$ that moreover is an analytic function of q (in fact, it is q^m times an analytic function of q^{-1}). However, Corollary 3.3 gives no information about *how large* $|q|$ has to be for this behavior to occur; in particular, there is no guarantee that this large-q domain is uniform in m. However, the uniformity in m can be proven by invoking the following theorem:

Theorem 5.1 [43, Corollary 5.3 and Proposition 5.4] *Let $G = (V, E)$ be a loopless finite undirected graph of maximum degree Δ. Then all the zeros of the chromatic polynomial $P_G(q)$ lie in the disc $|q| < 7.963907\Delta$.*

Let us remark that this theorem has been recently improved by Fernández and Procacci [44, Corollary 2]: they showed that the constant 7.963907 in Theorem 5.1 can be replaced by 6.907652.

For the square lattice with any of the standard boundary conditions (free, cylindrical, cyclic or toroidal) we have $\Delta = 4$, so we can conclude that all chromatic roots lie inside the disc $|q| < 7.963907 \times 4 = 31.855628$. Actually, by [43, Corollary 5.3 and Table 1], we have for $\Delta = 4$ the slightly stronger bound $|q| < C(4) \leq 29.081607$. With the improved result of Fernández and Procacci, we get $|q| < 6.907652 \times 4 = 27.630607$; and for the particular case $\Delta = 4$ these authors [44, Corollary 1] obtained the slightly better bound $|q| < C^\star(4) \leq 24.443218$.

It follows that the limiting curves $\mathcal{B}_m$ must also lie inside the disc $|q| \le 24.443218$ for all widths m: for if part of the limiting curve were to lie outside the (closed) disc, then the Beraha–Kahane–Weiss theorem (Theorem 2.2) would imply that chromatic roots would also lie outside the disc for $m \times n$ strips of all sufficiently large lengths n. Furthermore, using again the Beraha–Kahane–Weiss theorem we can conclude that, outside this disc, the transfer matrix for each width m must have one and only one eigenvalue of largest modulus. Since this dominant eigenvalue cannot collide with any other eigenvalue, it must be an analytic function of q outside the given disc.

In summary, the transfer matrix for a square-lattice strip of width m and with free or cylindrical boundary conditions has a single dominant eigenvalue $\lambda_{\star,m}^{\rm F/P}(q)$ that is an analytic function of q (in fact, q^m times an analytic function of q^{-1}) whenever $|q| > 24.443218$.

Let us now introduce the free energy per site for a finite strip with free or cylindrical boundary conditions,

$$f_{m,n}^{\rm F/P}(q) \;=\; \frac{1}{mn} \log P_{G_{m_{\rm F/P} \times n_{\rm F}}}(q) \;, \tag{5.1}$$

and its limiting value for a semi-infinite strip,

$$f_{m}^{\rm F/P}(q) \;=\; \lim_{n\to\infty} \frac{1}{mn} \log P_{G_{m_{\rm F/P} \times n_{\rm F}}}(q) \;. \tag{5.2}$$

Finally, let us introduce the free energy per site for the infinite lattice,

$$f^{\rm F/P}(q) \;=\; \lim_{m,n\to\infty} \frac{1}{mn} \log P_{G_{m_{\rm F/P} \times n_{\rm F}}}(q) \;. \tag{5.3}$$

Here we are assuming that the indicated limits exist and that in (5.3) the limit is independent of the way that m and n tend to infinity. Furthermore, it is natural to expect that in (5.3) the limiting free energy is independent of boundary conditions, in which case we can omit the superscripts F or P and write simply $f(q)$.

In fact, some of these assumptions can be proven. Indeed, the above discussion guarantees that at least for $|q| > 24.443218$, the limiting strip free energy $f_m(q)$ exists for all m and is given by

$$f_{m}^{\rm F/P}(q) \;=\; \frac{1}{m} \log \lambda_{\star,m}^{\rm F/P}(q) \;, \tag{5.4}$$

which in particular is an analytic function of q in the indicated domain. Moreover, Procacci *et al.* [45, Theorem 2] have proven that, when $|q|$ is large enough (namely, $|q| > 8e^3 \approx 160.684295$), the infinite-volume limiting free energy $f(q)$ exists and is analytic in $1/q$ and is the same for all reasonable sequences of graphs $G_{m\times n}$ (in particular, it is the same for free, cylindrical, cyclic and toroidal boundary conditions and is independent of the way that m and n tend to infinity). In this paper we will take $n \to \infty$ first and then take $m \to \infty$, so that

$$f(q) \;=\; \lim_{m\to\infty} f_{m}^{\rm F/P}(q) \;. \tag{5.5}$$

For simplicity, we shall focus on the *real part* of the free energy, in order to avoid any ambiguity due to branch cuts in the definition of the logarithm in (5.1)–(5.3).

Finite-size-scaling theory [46, Section 2.5] gives a rather precise prediction for the form of the free energy (5.1)/(5.2) for a finite (or semi-infinite) system away from a critical point (in the absence of soft modes). In particular, for a system defined on a two-dimensional surface of linear size m with bulk correlation length $\xi_{\rm bulk} \ll m$, the predicted behavior is

$$f_m \;=\; f_{\rm bulk} + \frac{1}{m}\, f_{\rm surf} + \frac{1}{m^2}\, f_{\rm corner} + O(e^{-m/\xi_{\rm bulk}}) \tag{5.6}$$

where $f_{\rm bulk}$, $f_{\rm surf}$ and $f_{\rm corner}$ are, respectively, the contributions of the bulk, free surfaces and corners of the system. For a semi-infinite strip $m \times \infty$, the corner contribution vanishes, i.e. $f_{\rm corner} = 0$; and if we impose periodic boundary conditions on the transverse (finite) direction, the surface contribution also vanishes, i.e. $f_{\rm surf} = 0$. We thus obtain the following predictions for semi-infinite strips of width m according to the transverse boundary conditions:

$$f_m \;=\; \begin{cases} f_{\rm bulk} + \frac{1}{m} f_{\rm surf} + O(e^{-m/\xi_{\rm bulk}}) & \text{free} \\ f_{\rm bulk} + O(e^{-m/\xi_{\rm bulk}}) & \text{cylindrical} \end{cases} \tag{5.7}$$

The relation (5.7) of course holds for the chromatic polynomials at *fixed* large q. But we can also argue heuristically what it should imply for the series expansion in powers of $1/q$. It is not difficult to see that, for large q, we have

$$e^{-1/\xi_{\rm bulk}(q)} \;=\; \frac{1}{q} + O\Big(\frac{1}{q^2}\Big) \tag{5.8}$$

(just as for a *one-dimensional* Potts antiferromagnet at zero temperature).[14] We can therefore interpret $O(e^{-m/\xi_{\rm bulk}(q)})$ as meaning $O(q^{-m})$. Therefore, we expect that

$$f_m(q) \;=\; f_{\rm bulk}(q) \;+\; \frac{1}{m} f^{\rm F}_{\rm surf}(q) \;+\; O(q^{-m}) \;, \tag{5.9}$$

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[14] Let $G = (V, E)$ be a finite graph (let us suppose for simplicity that it has no loops or multiple edges) with n vertices and m edges; then one sees immediately from the Fortuin–Kasteleyn representation (2.4) that its Potts-model partition function has the large-q expansion

$$Z_G(q,v) \;=\; q^n \;+\; mq^{n-1} \;+\; \frac{m(m-1)}{2} q^{n-2} \;+\; O(q^{n-3}) \;.$$

When G is a finite piece of a regular lattice, the corresponding expansion for $|V|^{-1} \log Z_G(q,v)$ gives in the infinite-volume limit the large-q expansion for the bulk free energy $f(q,v)$.

Now let i,j be vertices of G; then the unnormalized 2-point correlation function $Z_G\langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle = Z_G\langle (q\delta_{\sigma_i,\sigma_j} - 1)/(q-1) \rangle$ is given by a representation like (2.4) but with the constraint that i and j must belong to the same connected component. The dominant terms of the large-q expansion are the ones in which this component has the minimal number of vertices and all other components are isolated vertices; one therefore gets

$$Z_G\langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle \;=\; Q_G(v;i,j) \left(\frac{v}{q}\right)^{d_G(i,j)} q^n \left[1 + O(q^{-1})\right]$$

where $d_G(i,j)$ is the length of the shortest path in G from i to j, and $Q_G(v;i,j)$ is a polynomial in v that enumerates the connected subgraphs of G that contain i and j and have exactly $d_G(i,j)+1$

or in other words we predict $m_{\rm min}^{\rm F/P}(k) = k+1$. Of course, we should not take too seriously the "+1" here, since the *amplitude* of the correction term in (5.7) could be proportional to a positive or negative power of q. But we do predict that $m_{\rm min}^{\rm F/P}(k) \approx k$ in the sense that $\lim_{k\to\infty} m_{\rm min}^{\rm F/P}(k)/k = 1$. This is indeed what we found for cylindrical boundary conditions (Section 4.3). For free boundary conditions (Section 4.2), however, we found the *faster* convergence $m_{\rm min}^{\rm F/P}(k) \approx k/2$, for which we lack at present any theoretical explanation.

Bakaev and Kabanovich [42] obtained in 1994 the expansion in powers of q^{-1} of the infinite-volume free energy $f(q)$ for the square-lattice chromatic polynomial. Their results can be summarized as follows: as $|q| \to \infty$, the exponential of the free energy per site for an infinite square lattice is given by the series expansion

$$e^{f(q)} \;=\; \frac{(q-1)^2}{q} \left[1 + z^3 + z^7 + 3z^8 + 4z^9 + 3z^{10} + 3z^{11} + 11z^{12} + 24z^{13} + O(z^{14})\right] \;, \tag{5.10}$$

where z is defined as

$$z \;=\; \frac{1}{q-1} \;. \tag{5.11}$$

We have here copied the first few terms; the series reported in [42] contains terms up to order z^{37}. The series for the bulk free energy $f(q) = f_{\rm bulk}(q)$ in terms of the

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vertices [with a weight v for each edge beyond the minimum number $d_G(i,j)$]. In particular, if G is triangle-free, these subgraphs are simply shortest paths from i to j. In general $Q_G(v;i,j)$ can grow exponentially in $d_G(i,j)$ [when e.g. G is an infinite regular lattice]; but if G is a piece of the square lattice and $i-j$ lies *along an axis direction*, then $Q_G(v;i,j) = 1$. It follows that the exponential decay rate of correlations along an axis is

$$e^{-1/\xi_{\rm bulk}(q,v)} \;=\; \left|\frac{v}{q}\right| + O\Big(\frac{1}{|q|^2}\Big) \;.$$

For $v=-1$ this gives (5.8).

It is instructive to ask how these results would be seen in the transfer-matrix formalism. Ordinarily one has $e^{-1/\xi_{\rm bulk}} = |\lambda_2/\lambda_\star|$, where $\lambda_\star$ is the dominant eigenvalue and λ_2 is the first subleading eigenvalue. But when one performs the computation using our transfer matrices, one finds $\lambda_2/\lambda_\star = \alpha_m^{\rm F/P}(v)/q^2 + O(1/q^3)$ for suitable polynomials $\alpha_m^{\rm F/P}$ — *not* the predicted v/q. (Indeed, for width $m=1$ — i.e., a one-dimensional Potts model — the transfer matrix is of size 1×1, i.e. there is *no* subleading eigenvalue at all.) What is going on here?

The point is that the exponential decay rate in the correlation function $\langle \boldsymbol{\sigma}_0 \cdot \boldsymbol{\sigma}_x \rangle$ is controlled by a "colored" intermediate state, i.e. the state obtained by applying the field $\boldsymbol{\sigma}_0$ to the vacuum. The corresponding eigenvalue λ_2 would be seen in a transfer matrix in the *spin representation* [5, Section 3.1]; but it is not seen in our transfer matrix in the *Fortuin–Kasteleyn representation*, which represents only "colorless" states (i.e., states invariant under the Potts global symmetry group S_q). Rather, the first subleading eigenvalue of the latter transfer matrix corresponds to a "colorless" two-particle state, hence has $\lambda_2/\lambda_\star$ of order $1/q^2$. More precisely, for square-lattice strips of widths $m \geq 4$ (resp. $m \geq 3$) with cylindrical (resp. free) boundary conditions, we find (at least up to $m = 9_{\rm P}, 7_{\rm F}$) that there are *at least two* subleading eigenvalues of order $1/q^2$. Some of these satisfy $\lambda_2/\lambda_\star = (v/q)^2 + O(q^{-3})$, and the others satisfy $\lambda_2/\lambda_\star = (1+v)(v/q)^2 + O(q^{-3})$; note that the latter ones vanish at order $1/q^2$ for the chromatic polynomial $v=-1$. All other eigenvalues are $O(q^{-3})$.

variable q can be easily deduced from the results reported in [42]: we have

$$\begin{aligned} f(q) \;=\; & \log q - \tfrac{2}{q} - \tfrac{1}{q^2} + \tfrac{1}{3q^3} + \tfrac{5}{2q^4} + \tfrac{28}{5q^5} + \tfrac{55}{6q^6} + \tfrac{89}{7q^7} + \tfrac{81}{4q^8} + \tfrac{505}{9q^9} + \tfrac{1029}{5q^{10}} + \tfrac{7742}{11q^{11}} \\ & + \tfrac{25291}{12q^{12}} + \tfrac{73552}{13q^{13}} + \tfrac{197755}{14q^{14}} + \tfrac{508036}{15q^{15}} + \tfrac{632129}{8q^{16}} + \tfrac{2984620}{17q^{17}} + \tfrac{6229711}{18q^{18}} + \tfrac{9466083}{19q^{19}} \\ & + \tfrac{1683}{2q^{20}} - \tfrac{73176046}{21q^{21}} - \tfrac{179849385}{11q^{22}} - \tfrac{1186642912}{23q^{23}} - \tfrac{1001526407}{8q^{24}} - \tfrac{5740022997}{25q^{25}} \\ & - \tfrac{3575642890}{13q^{26}} - \tfrac{3813364151}{27q^{27}} - \tfrac{20139149153}{28q^{28}} - \tfrac{266971823494}{29q^{29}} - \tfrac{57261174745}{q^{30}} \\ & - \tfrac{7630985910267}{31q^{31}} - \tfrac{13030951687759}{16q^{32}} - \tfrac{69034388820418}{33q^{33}} - \tfrac{63973396203381}{17q^{34}} \\ & - \tfrac{9963329876758}{5q^{35}} - \tfrac{614621388337219}{36q^{36}} + O(q^{-37}) \end{aligned} \tag{5.12}$$

The large-q series of the strip free energy $f_m(q)$ depends on the boundary conditions. We will treat free and cylindrical boundary conditions in separate sections.

5.2 Free boundary conditions

We can check the results of Bakaev and Kabanovich [42] by computing the large-$|q|$ expansion of the limiting free energy for a semi-infinite strip:

$$\begin{aligned} f_m(q) &= \frac{1}{m} \log \lambda^{\rm F}_{\star,m}(q) \\ &= \log q + \frac{1}{m} \log \left[\sum_{k=0}^{\infty} (-1)^k b^{\rm F}_k(m) q^{-k} \right] \\ &= \log q + \frac{1}{m} \sum_{k=1}^{\infty} (-1)^k c^{\rm F}_k(m) q^{-k} \end{aligned} \tag{5.13}$$

If $m \geq m^{\rm F}_{\rm min}(k)$, we can replace the coefficients $c^{\rm F}_k(m)$ by the corresponding polynomials $C^{\rm F}_k(m)$ [cf. (4.15)]. These polynomials $C^{\rm F}_k$ are of degree 1 in m for $1 \leq k \leq 31$, and we have conjectured that this behavior holds for all values of $k \geq 1$. Thus, $f_m(q)$ contains only two terms: a bulk term $f_{\rm bulk}(q) = f(q)$ that is independent of m, and a surface free energy energy $f^{\rm F}_{\rm surf}(q)$ that is of order $1/m$:

$$f_m(q) \;\cong\; f_{\rm bulk}(q) \;+\; \frac{1}{m} f^{\rm F}_{\rm surf}(q) \; . \tag{5.14}$$

Here $\cong$ denotes that the two sides agree at each order q^{-k} of the expansion in powers of q^{-1}, but we require this only for $m \geq m^{\rm F}_{\rm min}(k)$. The computations reported here thus provide an independent check of the first 31 terms of the series (5.12). They also provide the first 31 terms in the large-q expansion of the surface free energy $f^{\rm F}_{\rm surf}$ for free boundary conditions:

$$\begin{aligned} f^{\rm F}_{\rm surf}(q) \;=\; & \tfrac{1}{q} + \tfrac{1}{2q^2} - \tfrac{2}{3q^3} - \tfrac{11}{4q^4} - \tfrac{29}{5q^5} - \tfrac{28}{3q^6} - \tfrac{97}{7q^7} - \tfrac{243}{8q^8} - \tfrac{1019}{9q^9} - \tfrac{4489}{10q^{10}} - \tfrac{17280}{11q^{11}} \\ & - \tfrac{14654}{3q^{12}} - \tfrac{183143}{13q^{13}} - \tfrac{550885}{14q^{14}} - \tfrac{1641827}{15q^{15}} - \tfrac{4863283}{16q^{16}} - \tfrac{14046504}{17q^{17}} - \tfrac{38484965}{18q^{18}} \\ & - \tfrac{97576171}{19q^{19}} - \tfrac{225286241}{20q^{20}} - \tfrac{475452259}{21q^{21}} - \tfrac{488026665}{11q^{22}} - \tfrac{2328851061}{23q^{23}} - \tfrac{314331005}{q^{24}} \\ & - \tfrac{29043846754}{25q^{25}} - \tfrac{108019100461}{26q^{26}} - \tfrac{350862625046}{27q^{27}} - \tfrac{941375883585}{28q^{28}} \\ & - \tfrac{1890755493699}{29q^{29}} - \tfrac{1783943165791}{30q^{30}} + \tfrac{5699142939376}{31q^{31}} + O(q^{-32}) \, . \end{aligned} \tag{5.15}$$

We can slightly extend this latter series by using the series (5.12) for $f_{\rm bulk}$ as an *input*: in this case, each polynomial $C_k^{\rm F}$ contains a single unknown coefficient to be determined (rather than two unknown coefficients). We then obtain the coefficient of the term q^{-32} in $f_{\rm surf}^{\rm F}$:

$$\left[q^{-32}\right] f_{\rm surf}^{\rm F} \;=\; \tfrac{35810617213837}{32} \,. \tag{5.16}$$

5.3 Cylindrical boundary conditions

The large-$|q|$ expansion of the free energy for a semi-infinite strip with cylindrical boundary conditions is

$$\begin{aligned} f_m(q) &= \frac{1}{m} \log \lambda_{\star,m}^{\rm P}(q) \\ &= \log q + \frac{1}{m} \log \left[\sum_{k=0}^{\infty} (-1)^k b_k^{\rm P}(m) q^{-k} \right] \\ &= \log q + \frac{1}{m} \sum_{k=1}^{\infty} (-1)^k c_k^{\rm P}(m) q^{-k} \end{aligned} \tag{5.17}$$

Once again, if m is large enough (depending on k), we can replace the coefficients $c_k^{\rm P}(m)$ by the corresponding polynomials $C_k^{\rm P}(m)$ [cf. (4.25)]. These polynomials $C_k^{\rm P}$ are of degree 1 in m with a zero constant term for $1 \le k \le 16$, and we conjecture that this behavior holds for every $k \ge 1$. Thus, $f_m(q)$ contains only a single m-independent term $f_{\rm bulk}(q) = f(q)$; the surface free energy $f_{\rm surf}^{\rm P}(q)$ is *zero*. This result is not in fact surprising, as an infinitely long cylinder has no boundary. Our data show that the series for $f_{\rm bulk}$ is the *same*, up to the order we are able to compute (namely, q^{-16}), for free and periodic boundary conditions; in particular, it agrees with (5.12). We also find that $f_{\rm surf}^{\rm P}$ vanishes to this same order.

If we use the bulk free-energy series (5.12) as input, we can compute the term of order q^{-17} in the surface free energy: as expected, we find that it vanishes.

6 Numerical results for widths $m = 9_{\rm F}, 10_{\rm F}, 11_{\rm F}$

As part of this work, we have computed the transfer matrices for square-lattice strips with free boundary conditions and widths $m = 9, 10, 11$. (Widths $m \le 8$ were computed in a previous paper [5].) In this section we use these newly-computed transfer matrices to study the real and complex roots of the chromatic polynomials $P_{m_{\rm F} \times n_{\rm F}}(q)$ for $m = 9, 10, 11$, focussing on the behavior in the infinite-length limit ($n \to \infty$). In Section 6.1 we discuss the limiting curve $\mathcal{B}_m$ and the isolated limiting points for each width m. In Section 6.2 we study the behavior of the real crossing points $q_0(m)$ and attempt to extract $q_0({\rm sq}) = \lim\limits_{m\to\infty} q_0(m)$. In Section 6.3 we discuss the *real* chromatic roots for finite lattices $m_{\rm F} \times n_{\rm F}$.

6.1 Limiting curves and isolated limiting points

Having computed the transfer matrices for $m = 9_{\rm F}, 10_{\rm F}, 11_{\rm F}$, we can analyze them as in [5–9] to extract the chromatic roots for finite-length lattices ($n < \infty$) as well as the limiting curves and isolated limiting points in the infinite-length limit ($n \to \infty$). Unfortunately, we have not been able to compute the full limiting curves $\mathcal{B}_m$, as this would have required a major computational effort. However, we have tried to locate the most important points on each of them, i.e. crossings of the real axis and endpoints near the real axis, using the direct-search method [5]. These results are summarized in Table 11. (Furthermore, the chromatic roots for $n = 5m$ and $n = 10m$ shown in Figures 1–3 give a fairly good idea of the general shape of the curve $\mathcal{B}_m$.) Finally, for all these strips there are real isolated limiting points at the Beraha numbers $q = 0, 1, 2, B_5$, and for $m = 9, 11$ there also appear to be complex isolated limiting points (we cannot, however, guarantee that we have found all of them). In Figures 1–3 these points are marked with a × sign.

For $m = 9$, the dimension of the transfer matrix is 179. In Figure 1 we have plotted the chromatic zeros in the complex q-plane for the strips $9_{\rm F} \times 45_{\rm F}$ and $9_{\rm F} \times 90_{\rm F}$. The limiting curve crosses the real q-axis at a single point:

$$q_0(9) \;\approx\; 2.70165995678\,. \tag{6.1}$$

Figure 1 also suggests that there is a complex-conjugate pair of isolated limiting points at $q \approx 2.5946 \pm 0.5963\, i$.

For $m = 10$, the dimension of the transfer matrix is 435. In Figure 2 we have plotted the chromatic zeros for the strips $10_{\rm F} \times 50_{\rm F}$ and $10_{\rm F} \times 100_{\rm F}$. In this case the limiting curve does not cross the real q-axis; rather, there is a pair of complex-conjugate endpoints very close to the real q-axis, at

$$q_0(10) \;\approx\; 2.7343903604 \pm 0.0003924978\, i\,. \tag{6.2}$$

Finally, for $m = 11$, the dimension of the transfer matrix is 1142. In Figure 3 we have plotted the chromatic zeros for the strips $11_{\rm F} \times 55_{\rm F}$ and $11_{\rm F} \times 110_{\rm F}$. The limiting curve crosses the real q-axis at

$$q_0(11) \;\approx\; 2.7608973951\,. \tag{6.3}$$

Figure 3 also suggests that there are two complex-conjugate pairs of isolated limiting points at $q \approx 2.6555 \pm 0.4978\, i$ and $q \approx 2.4648 \pm 1.1380\, i$.

In view of the results reported in Table 11, we conjecture that the limiting curve $\mathcal{B}_m$ crosses the real axis for all odd m and has a complex-conjugate pair of endpoints very near the real axis for all even $m \geq 8$.

6.2 Value of $q_0(\mathrm{sq})$

We can try to use the results reported in Table 11 to obtain the value of $q_0(\mathrm{sq}) = \lim\limits_{m\to\infty} q_0(m)$. As just discussed, there are clear parity effects: the limiting curve $\mathcal{B}_m$ crosses the real q-axis for odd m but not for even m. We have therefore split the data into two sets according to the parity of m, and analyzed each set separately. The data for $q_0(m)$ are essentially exact: there is a tiny *non-statistical* error of order 10^{-10} in their numerical estimates. In order to keep to the standard notation in finite-size-scaling theory, we here denote the strip width by L instead of m.

For each data set we have considered several Ansätze, and for a given Ansatz with k free parameters, we have taken into account the points with $L = L_{\rm min}, L_{\rm min} + 2, \ldots, L_{\rm min} + 2(k-1)$. So in each fit there are no degrees of freedom. From the variation of the estimates as $L_{\rm min}$ is increase, we can roughly estimate the error bar.

If we use the power-law Ansatz for the data coming from odd L

$$q_0(L) \;=\; q_0({\rm sq}) + BL^{-\Delta} \tag{6.4}$$

we obtain the following estimates using $L_{\rm min} = 7$

$$q_0({\rm sq}) \;=\; 2.999(6) \tag{6.5a}$$
$$\Delta \;=\; 1.108(4) \tag{6.5b}$$

where the error bars are twice the distance from these estimates and those obtained with $L_{\rm min} = 5$.

If we play the same game for the quantity ${\rm Re}\, q$ for even L, we arrive at the estimates for $L_{\rm min} = 6$

$$q_0({\rm sq}) \;=\; 2.97(7) \tag{6.6a}$$
$$\Delta \;=\; 1.25(12) \tag{6.6b}$$

where again the error bars are twice the difference with respect to the estimates for $L_{\rm min} = 4$. The convergence in this case is not very good, so we cannot trust these results too much.

These above results (6.5)/(6.6) are consistent (especially the former one) with the conjecture [6, Conjecture 4.3]:

$$q_0({\rm sq}) \;=\; 3 \tag{6.7a}$$
$$\Delta \;=\; 1 \tag{6.7b}$$

In particular, the value of $q_0({\rm sq}) = q_c({\rm sq}) = 3$ is (as expected) the same for both free and cylindrical boundary conditions. Moreover, very recent work [9, Section 5.1] gives strong evidence that this equality holds also for toroidal boundary conditions.[15]

Better fits can in principle be obtained by imposing the values (6.7). In particular, we expect the following Ansatz to describe better the data points:

$$q_0(L) \;=\; 3 - BL^{-1} - CL^{-2} \tag{6.8}$$

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[15] The authors of Ref. [9] found that for toroidal square-lattice strips of *odd* widths $3 \le L \le 11$, the value of $q_0(L)$ is *exactly* equal to the expected limiting value $q_0({\rm sq}) = 3$, while for toroidal strips of *even* widths $2 \le L \le 12$, the fits of the numerical data to the Ansatz (6.4) gave $q_0({\rm sq}) = 2.999 \pm 0.012$ and $\nu = 0.49 \pm 0.02$, in agreement with the conjectured behavior (6.7).

However the results are not very stable: for odd L we find that for $L_{\rm min} = 7$, $B \approx 2.436$, and $C \approx 2.243$, while for $L_{\rm min} = 9$, $B \approx 2.283$, and $C \approx 2.719$. A similar behavior is found for even L: for $L_{\rm min} = 6$, $B \approx 2.387$, and $C \approx 2.665$, while for $L_{\rm min} = 8$, $B \approx 2.409$, and $C \approx 2.473$. We conclude that our numerical data are not accurate enough to be able to accurately determine corrections to scaling to the behavior of $q_0(L)$.

6.3 Real chromatic roots

It is also of interest to study the real chromatic roots for lattices of finite length n. For every length n there are, of course, roots at $q = 0$ and $q = 1$; and there are also roots converging (exponentially rapidly) as $n \to \infty$ to the isolated limiting point at $q = 2$. Here we shall concentrate on the roots converging to the isolated limiting point at $q = B_5 = (3+\sqrt{5})/2$ and, for $m = 9$ and 11, to the real crossing point $q_0(m)$.

For width $m = 10$, the real roots converging to B_5 do so monotonically from below; we refrain from presenting the details. There are no real roots above B_5.

For widths $m = 9$ and 11, by contrast, two interesting things happen (see Tables 9 and 10). On the one hand, the real roots converging to B_5 do so with parity $(-1)^{n+1}$, i.e. alternating from above and below (starting from $n = 39$ and $n = 23$, respectively). On the other hand, for odd lengths n, there are also real roots converging to $q_0(m)$ from below. We conjecture that these behaviors will persist for all larger odd widths m.

These results for $m = 9, 11$ provide a (presumably infinite) family of counterexamples to a conjecture made in [5] concerning the real chromatic roots of bipartite planar graphs. For further discussion and for a revised conjecture, see Appendix A.

An important question is the rate of convergence of these real zeros towards the limiting values B_5 and $q_0(m)$. For B_5 we expect an exponentially rapid convergence (as with all isolated limiting points in the Beraha–Kahane–Weiss theorem); for $q_0(m)$, by contrast, we expect a $1/n$ convergence. We have tested these predictions by fitting the given real roots q_n to a power-law Ansatz

$$q \;=\; q_\infty + A n^{-\Delta} \;, \tag{6.9}$$

using the data points $n \geq$ a variable threshold $n_{\rm min}$. For the sequences of zeros converging to B_5, the estimates of the power Δ appear to increase without bound as $n_{\rm min}$ is increased (e.g. $\Delta \gtrsim 45$), suggesting that the convergence is indeed exponentially fast. For the sequences converging to $q_0(m)$, by contrast, we obtain powers $\Delta \approx 1.1$ for small values of $n_{\rm min}$, which slowly decrease toward 1 as we increase $n_{\rm min}$. In particular, for $n_{\rm min} = 99$ we obtain $\Delta \approx 1.023$ for $m = 9$ and $\Delta \approx 1.037$ for $m = 11$. This is consistent with the $1/n$ behavior expected from the Beraha–Kahane–Weiss theorem.

A Upper zero-free interval for bipartite planar graphs

Let G be a loopless planar graph. Then it is not hard to prove that $P_G(q) > 0$ for all *integers* $q \geq 5$;[16] moreover, one of the most famous theorems of graph theory — the Four-Color Theorem [48–52] — asserts that $P_G(q) > 0$ holds in fact for all integers $q \geq 4$.

It is natural to ask whether these results can be extended from integer q to *real* q. The answer is yes, at least in part: Birkhoff and Lewis [53] proved in 1946 that if G is a loopless planar graph, then $P_G(q) > 0$ for all real numbers $q \geq 5$.[17] Furthermore, they conjectured that $P_G(q) > 0$ also for $4 < q < 5$; and while no one has yet found a proof, no one has found a counterexample either, so it seems plausible (in the light of the Four-Color Theorem) that the conjecture is true.

Now, some planar graphs can be colored with three or even two colors; this means that their chromatic polynomials $P_G(q)$ are strictly positive for *integers* $q \geq 3$ or $q \geq 2$, respectively. Can *these* bounds can be extended to real q? That is, if G is a k-colorable planar graph, do we have $P_G(q) > 0$ for all real $q \geq k$? Woodall [54, p. 142] conjectured that the answer is yes. For $k = 4$, this is the conjecture of Birkhoff and Lewis mentioned above. For $k = 3$, however, Thomassen [55, pp. 505–506] has shown that Woodall's conjecture is false: there exist 3-colorable (and in fact 2-degenerate[18]) planar graphs with real chromatic roots greater than 3. Indeed, by combining Thomassen's construction [55, proof of Theorem 3.9] with Royle's [56] recent construction of planar graphs with real chromatic roots arbitrarily close to 4, we see that there exist 3-colorable (and in fact 2-degenerate) planar graphs with real chromatic roots arbitrarily close to 4.

In Ref. [5] we showed that Woodall's conjecture is false also for $k = 2$: there exist 2-colorable (i.e. bipartite) planar graphs with real chromatic roots greater than 2. For example, the $4_{\rm P} \times 6_{\rm F}$ square lattice has chromatic roots at $q \approx 2.009978$ and $q \approx 2.168344$. For the cases $8_{\rm F} \times n_{\rm F}$ and $8_{\rm P} \times n_{\rm F}$, we also observed numerically [5] that there are real chromatic roots tending to $B_5 = (3 + \sqrt{5})/2 \approx 2.618034$ from below as $n \to \infty$. This led us to modify Woodall's conjecture as follows [5, Conjecture 7.5]:

Conjecture A.1 **[5]** *Let G be a bipartite planar graph. Then $P_G(q) > 0$ for real $q \geq B_5 = (3 + \sqrt{5})/2$.*

However, the numerical results reported in the present paper (see Tables 9 and 10) now show that this conjecture is also false. Indeed, it appears that all strip graphs

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[16] This is the Five-Color Theorem, which goes back to Heawood in 1890. For a proof, see e.g. [47, Theorem V.8, pp. 154–155]; or for an elegant alternate proof of an even stronger result, see [47, Theorem V.12, pp. 161–163].

[17] See also Woodall [54, Theorem 1] and Thomassen [55, Theorem 3.1 ff.] for alternate proofs of a more general result.

[18] A graph G is said to be *k-degenerate* if every subgraph $H \subseteq G$ has at least one vertex of degree $\leq k$. It is not difficult to prove [47, Theorem V.1, p. 148] that every k-degenerate graph is $(k + 1)$-colorable.

$9_{\mathrm{F}} \times n_{\mathrm{F}}$ (with *odd* $n \geq 39$) and $11_{\mathrm{F}} \times n_{\mathrm{F}}$ (with *odd* $n \geq 23$) have *two* real roots greater than B_5.

So, not only is Conjecture A.1 false; it is actually false for *two distinct reasons*. First of all, the real roots converging to the isolated limiting point B_5 need not do so only from below. (Empirically we find that, for $m = 9$ and 11, these roots converge to B_5 with parity $(-1)^{n+1}$.) Secondly, real roots can converge to the real crossing point $q_0(m) > B_5$ when one exists.[19] (Empirically we find that such a crossing point exists at least for *odd* widths m and that the roots converging to it exist for sufficiently large *odd* lengths n.)

We expect both of these behaviors to persist for all larger *odd* widths m. In particular, since we expect that $q_0(m) \uparrow 3$ as $m \to \infty$ (see Section 6.2), we expect that $m_{\mathrm{F}} \times n_{\mathrm{F}}$ square-lattice strips with m, n both odd and large can have real chromatic roots arbitrarily close to 3. However, in the vast majority of cases of which we are aware [5–9, 56], the convergence of real chromatic roots to $q_0(m)$ occurs only *from below*.[20] Therefore, the following weakened version of Conjecture A.1 is plausible:

Conjecture A.2 *Let G be a bipartite planar graph. Then $P_G(q) > 0$ for real $q \geq 3$.*

(Note that the honeycomb lattice, which is bipartite and planar, has $q_c = B_5 < 3$.)

We can also give some plausible "physics" considerations that provide additional support for a slightly weakened version of Conjecture A.2. Some two-dimensional antiferromagnetic models at zero temperature have the remarkable property that they can be mapped onto a "height" (or "interface" or "SOS-type") model (see e.g. [57] and the references cited there). Experience tells us that when such a representation exists, the corresponding zero-temperature spin model is nearly always critical.[21] In particular, when the q-state zero-temperature Potts antiferromagnet on a lattice $\mathcal{L}$ admits a height representation, one expects that $q = q_c(\mathcal{L})$.[22] This prediction is confirmed in all heretofore-studied cases: 3-state square-lattice [57,58,60,61], 3-state Kagomé [62,63], 4-state triangular [64], and 4-state on the line graph (= covering lattice) of the square lattice [63,65]. Now, the height representation of the square-lattice zero-temperature 3-state Potts antiferromagnet (i.e., the square-lattice chromatic polynomial at $q = 3$), as presented in [57], generalizes immediately from the square lattice to an arbitrary finite or infinite plane quadrangulation G. This suggests that $q_c(\mathcal{L}) = 3$ for all infinite

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[19] A similar phenomenon was exploited recently by Royle [56] to provide examples of plane triangulations with real chromatic roots converging to 4 from below. His graphs are $4_{\mathrm{P}} \times n_{\mathrm{F}}$ triangular lattices with carefully chosen endgraphs adjoined at top and bottom. The key fact underlying this construction is that $q_0(\mathrm{tri}, 4_{\mathrm{P}}) = 4$.

[20] The only exceptions we know are several triangular-lattice strips: $m = 2, 4, 5$ with cyclic boundary conditions [8] and $m = 3$ with toroidal boundary conditions [9].

[21] Some exceptions are the constrained square-lattice 4-state antiferromagnetic Potts model [58] and the triangular-lattice antiferromagnetic spin-s Ising model for large enough s [59], both of which appear to lie in a non-critical ordered phase at zero temperature.

[22] Here $q_c(\mathcal{L})$ is the value (which is conjectured to exist) such that for $q > q_c(\mathcal{L})$ the antiferromagnetic Potts model has exponential decay of correlations uniformly at all temperatures, including zero temperature, while for $q = q_c(\mathcal{L})$ the model has a zero-temperature critical point.

periodic lattices that are plane quadrangulations. It in turn provides some support for the following weakened version of Conjecture A.2:

Conjecture A.3 *Let G be a plane quadrangulation. Then $P_G(q) > 0$ for real $q \geq 3$.*

Surprisingly, however, we know of a potential counterexample to Conjectures A.2 and A.3! Consider the diced lattice [66, Figure 15], which is the dual of the Kagomé lattice and is a plane quadrangulation. Even though there exists a height representation for the 3-state Potts antiferromagnet on the diced lattice, this model appears to be in a non-critical ordered phase at zero temperature. Indeed, Feldmann *et al.* [67] found (by dualizing the numerical data of Ref. [68] for the Kagomé-lattice Potts model) that the 3-state diced-lattice Potts model has a critical point at $v_c = -0.8607 \pm 0.0008$, which lies at *nonzero* temperature in the physical antiferromagnetic region $-1 \leq v \leq 0$. (By contrast, the 4-state model was found to have its antiferromagnetic critical point in the unphysical region at $v_c = -1.18 \pm 0.02$, so that the 4-state antiferromagnet is disordered for all temperatures, including zero temperature.) We have very recently [69] confirmed this general scenario by Monte Carlo simulations: for $q = 3$ we find a critical point at nonzero temperature (fairly near to the predicted value), and for $q = 4$ we find a finite correlation length uniformly in the region $-1 \leq v \leq 0$. These numerical results give strong evidence that $3 < q_c(\text{diced}) < 4$, contrary to our prediction that $q_c = 3$ for all (regular) plane quadrangulations; indeed, linear interpolation from the predictions of [67] would suggest $q_c(\text{diced}) \approx 3.44$.

Now, one strongly expects that finite pieces of the diced lattice with free or cylindrical boundary conditions will have chromatic roots tending to $q_c(\text{diced})$ in the infinite-volume limit. What is less clear, however, is whether the roots converging to q_c will necessarily be *real* roots. If they are, then a sufficiently large finite piece of the diced lattice, with boundary conditions arranged so that the graph is a plane quadrangulation (or at least planar and bipartite), would provide a counterexample to Conjecture A.3 (or at least to Conjecture A.2). It would be very interesting to undertake a transfer-matrix study of the diced-lattice chromatic polynomial along the lines of [5–9] in order to test whether this is the case.

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m	b_0^{F}	b_1^{F}	b_2^{F}	b_3^{F}	b_4^{F}	b_5^{F}	b_6^{F}	b_7^{F}	b_8^{F}	b_9^{F}	b_{10}^{F}	b_{11}^{F}	b_{12}^{F}	b_{13}^{F}	b_{14}^{F}	b_{15}^{F}
1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	3	3	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	5	10	8	1	-1	1	-2	6	-16	35	-61	69	42	-583	2371
4	1	7	21	32	23	3	-2	-1	6	-14	28	-54	102	-172	145	695
5	1	9	36	80	102	66	10	-9	6	-6	14	-38	97	-218	361	-75
6	1	11	55	160	290	322	192	26	-19	2	15	-35	77	-160	241	-5
7	1	13	78	280	655	1017	1011	556	75	-59	21	-6	32	-84	103	107
8	1	15	105	448	1281	2541	3486	3153	1617	201	-151	22	64	-73	24	132
9	1	17	136	672	2268	5460	9492	11741	9785	4697	550	-436	96	103	-97	67
10	1	19	171	960	3732	10548	22128	34468	39006	30223	13652	1461	-1190	229	316	-221
11	1	21	210	1320	5805	18819	46149	86346	122436	128142	92975	39640	3874	-3318	650	881

Table 1: Coefficients $b_k^{\mathrm{F}}(m)$ of the large-q expansion of the dominant eigenvalue $\lambda_\star^{\mathrm{F}}$ for free boundary conditions. For each $1 \le m \le 11$, we include all coefficients $b_k^{\mathrm{F}}(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_FREE.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \ge m_{\mathrm{min}}^{\mathrm{F}}(k)$ [cf. (4.11)].

m	c_1^{F}	$2c_2^{\mathrm{F}}$	$3c_3^{\mathrm{F}}$	$4c_4^{\mathrm{F}}$	$5c_5^{\mathrm{F}}$	$6c_6^{\mathrm{F}}$	$7c_7^{\mathrm{F}}$	$8c_8^{\mathrm{F}}$	$9c_9^{\mathrm{F}}$	$10c_{10}^{\mathrm{F}}$	$11c_{11}^{\mathrm{F}}$	$12c_{12}^{\mathrm{F}}$	$13c_{13}^{\mathrm{F}}$	$14c_{14}^{\mathrm{F}}$	$15c_{15}^{\mathrm{F}}$
1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
2	−3	−3	0	9	27	54	81	81	0	−243	−729	−1458	−2187	−2187	0
3	−5	−5	1	19	55	109	170	243	496	1685	5957	17449	39463	57430	−21119
4	−7	−7	2	29	83	164	259	405	1001	3743	13688	42548	111078	240401	393557
5	−9	−9	3	39	111	219	348	567	1506	5801	21430	67839	184617	437890	898368
6	−11	−11	4	49	139	274	437	729	2011	7859	29172	93130	258169	635645	1406389
7	−13	−13	5	59	167	329	526	891	2516	9917	36914	118421	331721	833400	1914425
8	−15	−15	6	69	195	384	615	1053	3021	11975	44656	143712	405273	1031155	2422461
9	−17	−17	7	79	223	439	704	1215	3526	14033	52398	169003	478825	1228910	2930497
10	−19	−19	8	89	251	494	793	1377	4031	16091	60140	194294	552377	1426665	3438533
11	−21	−21	9	99	279	549	882	1539	4536	18149	67882	219585	625929	1624420	3946569

Table 2: Coefficients $kc_k^{\mathrm{F}}(m)$ of the large-q expansion of $\log(q^{-m}\lambda_\star^{\mathrm{F}})$ where $\lambda_\star^{\mathrm{F}}$ is the dominant eigenvalue for free boundary conditions. For each $1 \leq m \leq 11$, we include all coefficients $c_k^{\mathrm{F}}(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_FREE.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \geq m_{\min}^{\mathrm{F}}(k)$ [cf. (4.11)].

m	Δ_6^{F}	Δ_7^{F}	Δ_8^{F}	Δ_9^{F}	Δ_{10}^{F}	Δ_{11}^{F}	Δ_{12}^{F}	Δ_{13}^{F}	Δ_{14}^{F}	Δ_{15}^{F}	Δ_{16}^{F}	Δ_{17}^{F}	Δ_{18}^{F}	Δ_{19}^{F}	Δ_{20}^{F}	Δ_{21}^{F}
1	0	1	10	57	243	867	2777	8430	$\frac{50447}{2}$	75586	224939	650699	$\frac{3583917}{2}$	4637373	$\frac{22526941}{2}$	$\frac{78375472}{3}$
2	0	0	0	1	13	97	548	2604	10942	41717	146333	476291	$\frac{2896101}{2}$	4142266	$\frac{22531163}{2}$	29609731
3	0	0	0	0	0	1	16	150	1075	6440	33513	154727	643296	2438443	8522559	27772788
4	0	0	0	0	0	0	0	1	19	216	1883	13595	84238	458660	2235421	9900665
5	0	0	0	0	0	0	0	0	0	1	22	295	3031	25574	183804	1155646
6	0	0	0	0	0	0	0	0	0	0	0	1	25	387	4578	44167
7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	28	492
8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 3: Coefficients $\Delta_k^{\mathrm{F}}(m)$ for free boundary conditions [cf. (4.16)] for $6 \leq k \leq 21$ and $1 \leq m \leq 11$. For $0 \leq k \leq 6$ and $1 \leq m \leq 11$, the coefficients $\Delta_k^{\mathrm{F}}(m)$ vanish. For the whole data set up to $k = 22$, see the Mathematica file `data_FREE.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \geq m_{\min}^{\mathrm{F}}(k)$ [cf. (4.11)] and are therefore zero.

m	$b_0^{\rm P}$	$b_1^{\rm P}$	$b_2^{\rm P}$	$b_3^{\rm P}$	$b_4^{\rm P}$	$b_5^{\rm P}$	$b_6^{\rm P}$	$b_7^{\rm P}$	$b_8^{\rm P}$	$b_9^{\rm P}$	$b_{10}^{\rm P}$	$b_{11}^{\rm P}$	$b_{12}^{\rm P}$	$b_{13}^{\rm P}$	$b_{14}^{\rm P}$	$b_{15}^{\rm P}$
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	3	3	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	6	14	13	0	0	0	0	0	0	0	0	0	0	0	0
4	1	8	28	51	45	2	−8	10	2	2	−192	980	−2942	6164	−7566	−9986
5	1	10	45	115	174	141	20	−45	20	50	15	−400	670	930	−8155	27400
6	1	12	66	214	441	575	428	81	−119	−45	210	35	−396	−122	1075	2106
7	1	14	91	357	924	1617	1868	1275	273	−287	−210	294	532	−679	−539	−609
8	1	16	120	552	1716	3744	5748	5991	3777	812	−636	−634	280	1096	724	−3022
9	1	18	153	807	2925	7623	14505	19962	19034	11140	2313	−1497	−1374	−360	1662	4377
10	1	20	190	1130	4675	14144	32005	54340	68085	59999	32790	6375	−3660	−2760	−1792	215
11	1	22	231	1529	7106	24453	64009	128777	198330	228866	187901	96306	17336	−9537	−5093	−4367
12	1	24	276	2012	10374	39984	118702	275460	501213	708868	760164	585131	282358	46638	−25822	−9177
13	1	26	325	2587	14651	62491	207285	544232	1139450	1899300	2490423	2499471	1813122	826359	124540	−71760

Table 4: Coefficients $b_k^{\rm P}(m)$ of the large-q expansion of the dominant eigenvalue $\lambda_\star^{\rm P}$ for cylindrical boundary conditions. For each $1 \leq m \leq 13$, we include all coefficients $b_k^{\rm F}(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_CYL.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \geq m_{\rm min}^{\rm P}(k) = k + 2$.

m	$\tilde{b}^{\mathrm{P}}_0$	$\tilde{b}^{\mathrm{P}}_1$	$\tilde{b}^{\mathrm{P}}_2$	$\tilde{b}^{\mathrm{P}}_3$	$\tilde{b}^{\mathrm{P}}_4$	$\tilde{b}^{\mathrm{P}}_5$	$\tilde{b}^{\mathrm{P}}_6$	$\tilde{b}^{\mathrm{P}}_7$	$\tilde{b}^{\mathrm{P}}_8$	$\tilde{b}^{\mathrm{P}}_9$	$\tilde{b}^{\mathrm{P}}_{10}$	$\tilde{b}^{\mathrm{P}}_{11}$	$\tilde{b}^{\mathrm{P}}_{12}$	$\tilde{b}^{\mathrm{P}}_{13}$	$\tilde{b}^{\mathrm{P}}_{14}$	$\tilde{b}^{\mathrm{P}}_{15}$
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	4	6	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	6	15	17	0	0	0	0	0	0	0	0	0	0	0	0
4	1	8	28	52	50	2	−8	10	2	2	−192	980	−2942	6164	−7566	−9986
5	1	10	45	115	175	147	20	−45	20	50	15	−400	670	930	−8155	27400
6	1	12	66	214	441	576	435	81	−119	−45	210	35	−396	−122	1075	2106
7	1	14	91	357	924	1617	1869	1283	273	−287	−210	294	532	−679	−539	−609
8	1	16	120	552	1716	3744	5748	5992	3786	812	−636	−634	280	1096	724	−3022
9	1	18	153	807	2925	7623	14505	19962	19035	11150	2313	−1497	−1374	−360	1662	4377
10	1	20	190	1130	4675	14144	32005	54340	68085	60000	32801	6375	−3660	−2760	−1792	215
11	1	22	231	1529	7106	24453	64009	128777	198330	228866	187902	96318	17336	−9537	−5093	−4367
12	1	24	276	2012	10374	39984	118702	275460	501213	708868	760164	585132	282371	46638	−25822	−9177
13	1	26	325	2587	14651	62491	207285	544232	1139450	1899300	2490423	2499471	1813123	826373	124540	−71760

Table 5: Coefficients $\tilde{b}^{\mathrm{P}}_k(m)$ of the large-q expansion of the dominant eigenvalue $\lambda^{\mathrm{P}}_\star$ for cylindrical boundary conditions. For each $1 \leq m \leq 13$, we include all coefficients $\tilde{b}^{\mathrm{F}}_k(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_CYL.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \geq k$.

m	c_1^{P}	$2c_2^{\mathrm{P}}$	$3c_3^{\mathrm{P}}$	$4c_4^{\mathrm{P}}$	$5c_5^{\mathrm{P}}$	$6c_6^{\mathrm{P}}$	$7c_7^{\mathrm{P}}$	$8c_8^{\mathrm{P}}$	$9c_9^{\mathrm{P}}$	$10c_{10}^{\mathrm{P}}$	$11c_{11}^{\mathrm{P}}$	$12c_{12}^{\mathrm{P}}$	$13c_{13}^{\mathrm{P}}$	$14c_{14}^{\mathrm{P}}$	$15c_{15}^{\mathrm{P}}$
2	−3	−3	0	9	27	54	81	81	0	−243	−729	−1458	−2187	−2187	0
3	−6	−8	−3	16	34	−59	−622	−2464	−6843	−14648	−24118	−28595	−24342	−59256	−386483
4	−8	−8	7	52	162	493	1595	4764	11383	15722	−31303	−360503	−1801119	−6704573	−19871718
5	−10	−10	5	46	120	155	−325	−2914	−10984	−27430	−37245	62971	649587	2559421	6057120
6	−12	−12	6	60	173	360	765	2644	11922	49003	170840	505212	1251225	2440055	2788766
7	−14	−14	7	70	196	379	581	742	385	−4074	−32123	−167537	−694721	−2340051	−6229223
8	−16	−16	8	80	224	440	719	1352	4652	21864	96762	384848	1421716	4975913	16390643
9	−18	−18	9	90	252	495	801	1450	4473	17622	61032	166635	307107	−34941	−3730356
10	−20	−20	10	100	280	550	890	1620	5059	20670	78685	266050	836335	2622628	8719855
11	−22	−22	11	110	308	605	979	1782	5555	22628	85052	276485	789910	2016223	4478441
12	−24	−24	12	120	336	660	1068	1944	6060	24696	92915	303624	884886	2400080	6337977
13	−26	−26	13	130	364	715	1157	2106	6565	26754	100646	328771	956020	2567903	6567418

Table 6: Coefficients $kc_k^{\mathrm{P}}(m)$ of the large-q expansion of $\log(q^{-m}\lambda_\star^{\mathrm{P}})$ where $\lambda_\star^{\mathrm{P}}$ is the dominant eigenvalue for cylindrical boundary conditions. For each $2 \le m \le 13$, we include all coefficients $c_k^{\mathrm{P}}(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_CYL.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \ge m_{\mathrm{min}}^{\mathrm{P}}(k) = k + 2$.

m	$\tilde{c}^{\mathrm{P}}_1$	$2\tilde{c}^{\mathrm{P}}_2$	$3\tilde{c}^{\mathrm{P}}_3$	$4\tilde{c}^{\mathrm{P}}_4$	$5\tilde{c}^{\mathrm{P}}_5$	$6\tilde{c}^{\mathrm{P}}_6$	$7\tilde{c}^{\mathrm{P}}_7$	$8\tilde{c}^{\mathrm{P}}_8$	$9\tilde{c}^{\mathrm{P}}_9$	$10\tilde{c}^{\mathrm{P}}_{10}$	$11\tilde{c}^{\mathrm{P}}_{11}$	$12\tilde{c}^{\mathrm{P}}_{12}$	$13\tilde{c}^{\mathrm{P}}_{13}$	$14\tilde{c}^{\mathrm{P}}_{14}$	$15\tilde{c}^{\mathrm{P}}_{15}$
2	−4	−4	8	56	176	368	416	−544	−4672	−15424	−33664	−42112	33536	386816	1346048
3	−6	−6	3	6	−111	−705	−2463	−6090	−11580	−20001	−49836	−195861	−767643	−2515155	−6905922
4	−8	−8	4	40	182	880	3674	12096	30586	51852	−5024	−534920	−3020324	−12012568	−38506486
5	−10	−10	5	50	140	125	−1130	−8030	−32125	−92520	−188000	−169195	584925	3408080	8106710
6	−12	−12	6	60	168	330	807	4148	23001	101778	360304	1038354	2394614	3965607	1844286
7	−14	−14	7	70	196	385	623	686	−2198	−25704	−148624	−642719	−2239797	−6350183	−13989773
8	−16	−16	8	80	224	440	712	1296	4724	26024	135790	619232	2490264	8897768	28169498
9	−18	−18	9	90	252	495	801	1458	4545	17532	54663	100467	−131058	−2239899	−12715191
10	−20	−20	10	100	280	550	890	1620	5050	20580	78795	275410	943000	3394462	12965290
11	−22	−22	11	110	308	605	979	1782	5555	22638	85162	276353	776611	1851289	3184016
12	−24	−24	12	120	336	660	1068	1944	6060	24696	92904	303492	885042	2418448	6584247
13	−26	−26	13	130	364	715	1157	2106	6565	26754	100646	328783	956176	2567721	6542653

Table 7: Coefficients $k\tilde{c}^{\mathrm{P}}_k(m)$ defined in (4.10). For each $2 \leq m \leq 13$, we include all coefficients $c^{\mathrm{P}}_k(m)$ up to $k = 15$. For the whole data set up to $k = 40$, see the MATHEMATICA file `data_CYL.m` included in the on-line version of the paper at arXiv.org. Those data points below the stair-case-like line satisfy $m \geq \widetilde{m}^{\mathrm{P}}_{\min}(k) = \max(k, 2)$.

m	Δ_2^{P}	Δ_3^{P}	Δ_4^{P}	Δ_5^{P}	Δ_6^{P}	Δ_7^{P}	Δ_8^{P}	Δ_9^{P}	Δ_{10}^{P}	Δ_{11}^{P}	Δ_{12}^{P}	Δ_{13}^{P}	Δ_{14}^{P}	Δ_{15}^{P}	Δ_{16}^{P}
2	0	2	9	24	43	34	$-\frac{217}{2}$	$-\frac{1894}{3}$	-1954	-4468	$-\frac{15449}{2}$	-8736	-621	$\frac{109992}{5}$	$\frac{133695}{4}$
3	0	0	-6	-39	-145	-390	-822	-1455	$-\frac{5235}{2}$	-6642	$-\frac{45289}{2}$	-76023	-222030	-562002	-1284432
4	0	0	0	14	110	474	1431	3174	4362	-3272	-53007	-254964	-914542	$-\frac{8107726}{3}$	$-\frac{12999385}{2}$
5	0	0	0	0	-25	-225	-1105	-3850	-10281	-20610	$-\frac{49275}{2}$	16705	$\frac{345615}{2}$	371102	$-\frac{916875}{2}$
6	0	0	0	0	0	39	397	2219	8943	28532	73884	150254	$\frac{397011}{2}$	-80262	$-\frac{3442249}{2}$
7	0	0	0	0	0	0	-56	-637	-4011	-18438	-68313	-211897	-552462	-1169735	-1737302
8	0	0	0	0	0	0	0	76	956	6714	34742	146296	522552	1607014	4237541
9	0	0	0	0	0	0	0	0	-99	-1365	-10596	-61002	-287121	-1152501	-4024251
10	0	0	0	0	0	0	0	0	0	125	1875	15960	101208	525662	2333070
11	0	0	0	0	0	0	0	0	0	0	-154	-2497	-23144	-160292	-909502
12	0	0	0	0	0	0	0	0	0	0	0	186	3242	32521	244227
13	0	0	0	0	0	0	0	0	0	0	0	0	-221	-4121	-44499

Table 8: Modified coefficients $\Delta_k^{\mathrm{P}}(m)$ for cylindrical boundary conditions for $2 \leq k \leq 16$ and $2 \leq m \leq 13$. For $k = 1$ and $2 \leq m \leq 13$, the coefficients $\Delta_k^{\mathrm{P}}(m)$ vanish. Those data points below the stair-case-like line satisfy $m \geq \widetilde{m}_{\mathrm{min}}^{\mathrm{P}}(k) = \max(k, 2)$ and are therefore zero.

n	4th Zero - B_5	5th Zero
30	$-8.9459389900 \times 10^{-3}$	
32	$-5.6487223660 \times 10^{-3}$	
34	$-3.1962919070 \times 10^{-3}$	
36	$-1.5712164060 \times 10^{-3}$	
38	$-6.6617400470 \times 10^{-4}$	
39	$5.8575529850 \times 10^{-4}$	2.6298556468
40	$-2.5161135990 \times 10^{-4}$	
41	$1.7270275260 \times 10^{-4}$	2.6345567384
42	$-8.8890257250 \times 10^{-5}$	
43	$5.5346483490 \times 10^{-5}$	2.6384105545
44	$-3.0434570840 \times 10^{-5}$	
45	$1.8199961300 \times 10^{-5}$	2.6417380816
46	$-1.0281765140 \times 10^{-5}$	
47	$6.0420071920 \times 10^{-6}$	2.6446771074
48	$-3.4539716110 \times 10^{-6}$	
49	$2.0135551740 \times 10^{-6}$	2.6473078802
50	$-1.1574596530 \times 10^{-6}$	
51	$6.7216127470 \times 10^{-7}$	2.6496845069
52	$-3.8744221380 \times 10^{-7}$	
53	$2.2455458550 \times 10^{-7}$	2.6518466022
54	$-1.2962041990 \times 10^{-7}$	
55	$7.5047689080 \times 10^{-8}$	2.6538246782
56	$-4.3353170180 \times 10^{-8}$	
57	$2.5086443380 \times 10^{-8}$	2.6556430336
58	$-1.4497910190 \times 10^{-8}$	
59	$8.3866240660 \times 10^{-9}$	2.6573214747
60	$-4.8479232330 \times 10^{-9}$	
61	$2.8038883660 \times 10^{-9}$	2.6588764247
62	$-1.6210151380 \times 10^{-9}$	
63	$9.3745081850 \times 10^{-10}$	2.6603216811
64	$-5.4201053100 \times 10^{-10}$	
65	$3.1343270220 \times 10^{-10}$	2.6616689582
66	$-1.8122675760 \times 10^{-10}$	
67	$1.0479599710 \times 10^{-10}$	2.6629282884
68	$-6.0594535690 \times 10^{-11}$	
69	$3.5038676450 \times 10^{-11}$	2.6641083276
70	$-2.0260148680 \times 10^{-11}$	
∞	0	2.7016599568

Table 9: Fourth and fifth real chromatic zeros for a strip $9_{\rm F} \times n_{\rm F}$ with free boundary conditions. As the fourth zero converges rapidly to B_5, we show their difference. The last row (labelled with $n = \infty$) shows the infinite-length limit; in particular, the value of $q_0(9)$.

n	4th Zero - B_5	5th Zero
14	$-3.6516138320 \times 10^{-2}$	
16	$-1.9375298640 \times 10^{-2}$	
18	$-8.1115634110 \times 10^{-3}$	
20	$-2.2141892360 \times 10^{-3}$	
22	$-3.6952234840 \times 10^{-4}$	
23	$2.7283542170 \times 10^{-4}$	2.6360127941
24	$-4.7440730960 \times 10^{-5}$	
25	$2.3461500250 \times 10^{-5}$	2.6467690175
26	$-5.5660625770 \times 10^{-6}$	
27	$2.2973640450 \times 10^{-6}$	2.6554417441
28	$-6.2842068380 \times 10^{-7}$	
29	$2.3500000310 \times 10^{-7}$	2.6628475620
30	$-6.9454825890 \times 10^{-8}$	
31	$2.4549166270 \times 10^{-8}$	2.6693333011
32	$-7.5798800910 \times 10^{-9}$	
33	$2.5935418370 \times 10^{-9}$	2.6750988717
34	$-8.2103756740 \times 10^{-10}$	
35	$2.7571779370 \times 10^{-10}$	2.6802756665
36	$-8.8542077070 \times 10^{-11}$	
37	$2.9415010300 \times 10^{-11}$	2.6849567990
38	$-9.5240493620 \times 10^{-12}$	
39	$3.1444559750 \times 10^{-12}$	2.6892116307
40	$-1.0229343110 \times 10^{-12}$	
41	$3.3652761350 \times 10^{-13}$	2.6930937453
42	$-1.0977435000 \times 10^{-13}$	
43	$3.6039742950 \times 10^{-14}$	2.6966457592
44	$-1.1774405610 \times 10^{-14}$	
45	$3.8610612020 \times 10^{-15}$	2.6999024444
46	$-1.2625636940 \times 10^{-15}$	
47	$4.1373846520 \times 10^{-16}$	2.7028928687
48	$-1.3536187010 \times 10^{-16}$	
49	$4.4340363840 \times 10^{-17}$	2.7056419158
50	$-1.4511035420 \times 10^{-17}$	
51	$4.7522986580 \times 10^{-18}$	2.7081713766
52	$-1.5555245880 \times 10^{-18}$	
53	$5.0936147060 \times 10^{-19}$	2.7105007206
54	$-1.6674076830 \times 10^{-19}$	
∞	0	2.7608973951

Table 10: Fourth and fifth real chromatic zeros for a strip $11_{\rm F} \times n_{\rm F}$ with free boundary conditions. As the third zero converges rapidly to B_5, we show their difference. The last row (labelled with $n = \infty$) shows the infinite-length limit; in particular, the value of $q_0(11)$.

m_{F}	$\mathrm{Re}\, q_0$	$\lvert \mathrm{Im}\, q_0 \rvert$	Type
3_{F}	2	0	S
4_{F}	2.2283590792	0	+
5_{F}	2.4284379020	0	S
6_{F}	2.5286467909	0	+
7_{F}	2.6062482130	0	S
8_{F}	2.6602596816	1.257×10^{-3}	D
9_{F}	2.7016599568	0	S
10_{F}	2.7343903604	3.925×10^{-4}	D
11_{F}	2.7608973951	0	S

Table 11: Values of $q_0(m)$ for square-lattice strips with free boundary conditions. Type "S" means that the limiting curve $\mathcal{B}_m$ crosses the real axis at a single point, "D" means that the limiting curve does not cross the real q-axis but has two complex-conjugate endpoints nearby, and "+" means that the limiting curve contains a segment on the real q-axis (we define q_0 as the lower end of that segment). For points of type "D", we also show the imaginary part. The data for $m \leq 8$ are taken from [5].

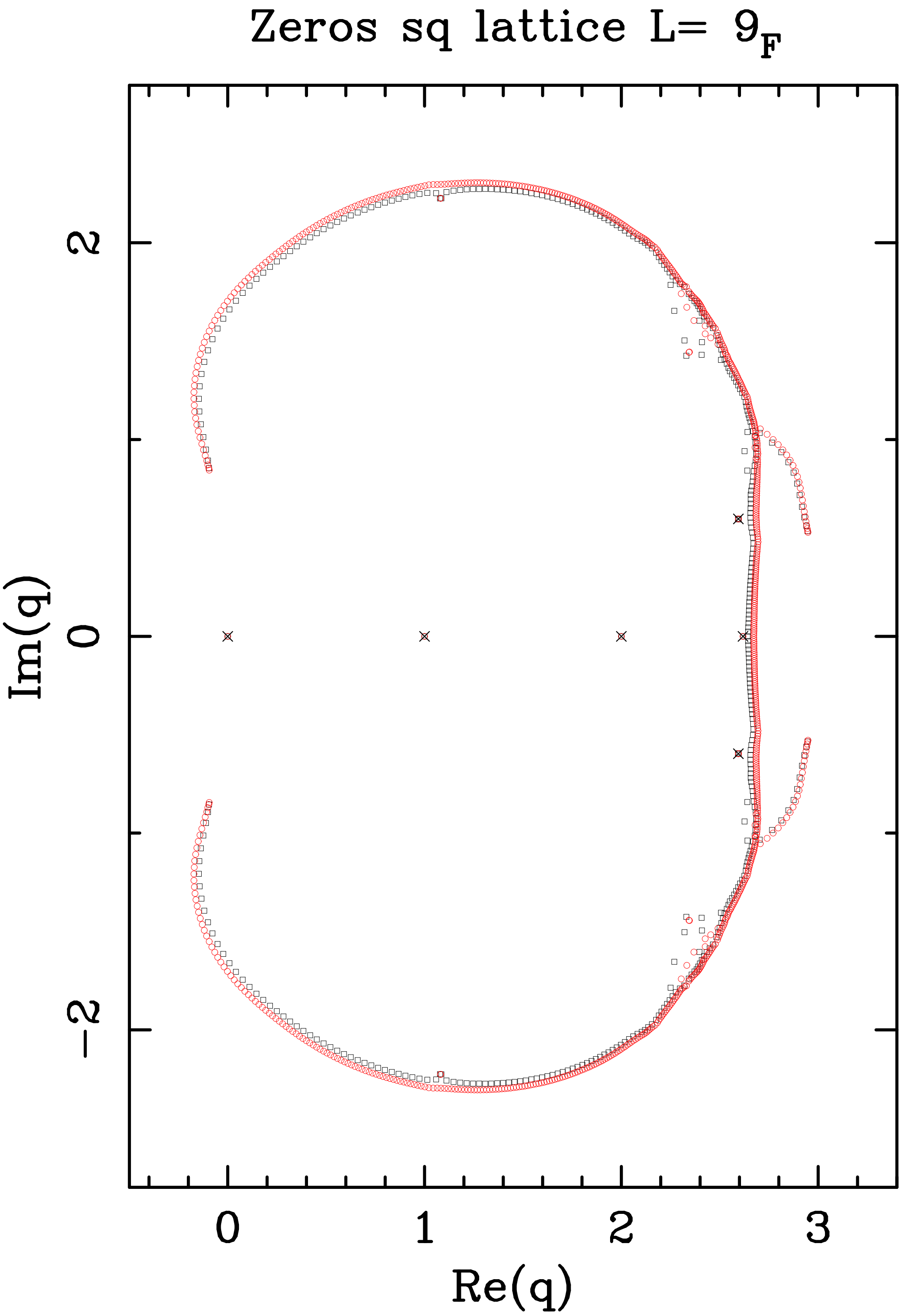

Figure 1: Zeros of the chromatic polynomial for the square lattices $9_F \times 45_F$ (□ black) and $9_F \times 90_F$ (○ red). Isolated limiting points are depicted as ×.

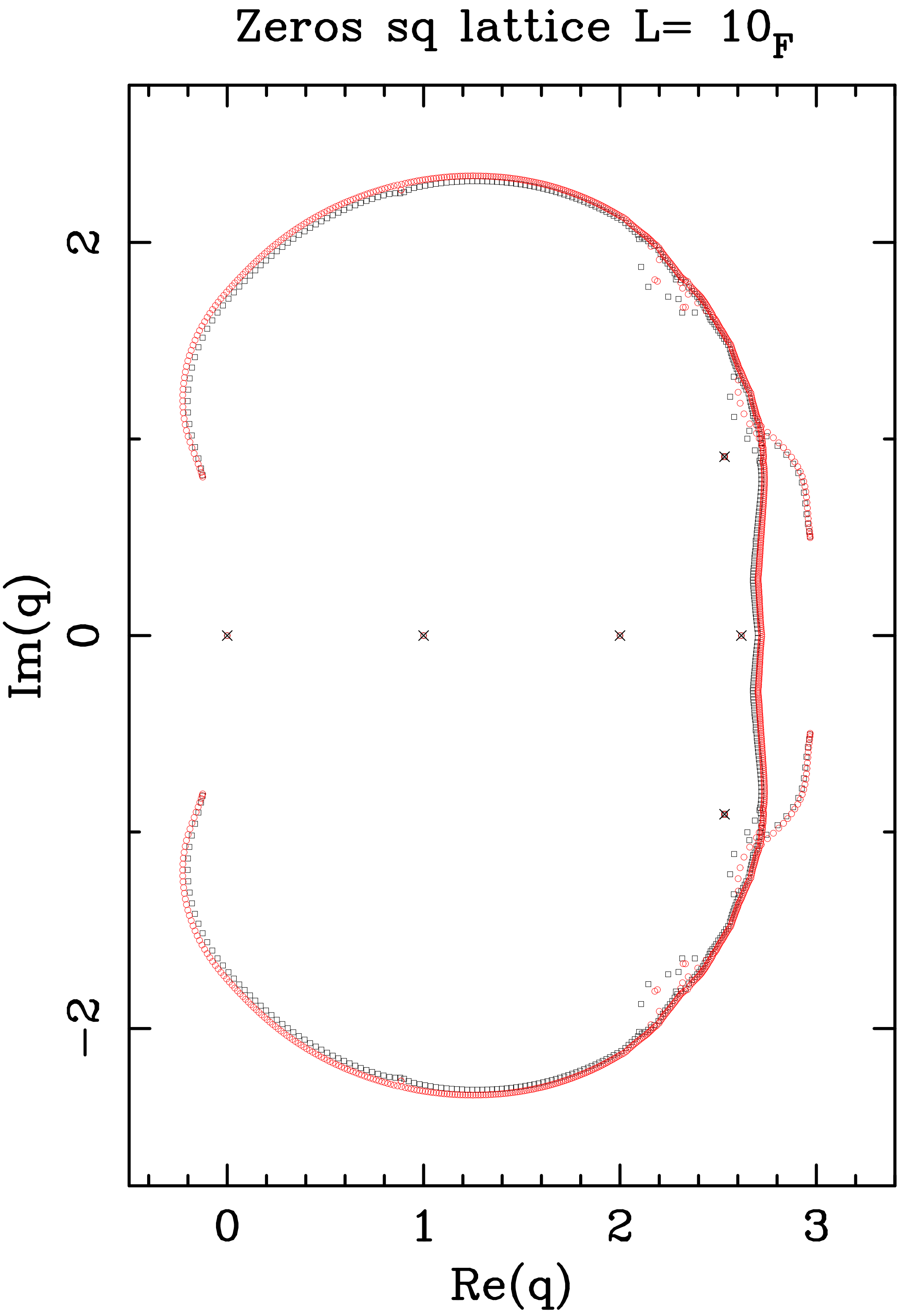

Figure 2: Zeros of the chromatic polynomial for the square lattices $10_F \times 50_F$ (□ black) and $10_F \times 100_F$ (∘ red). Isolated limiting points are depicted as ×.

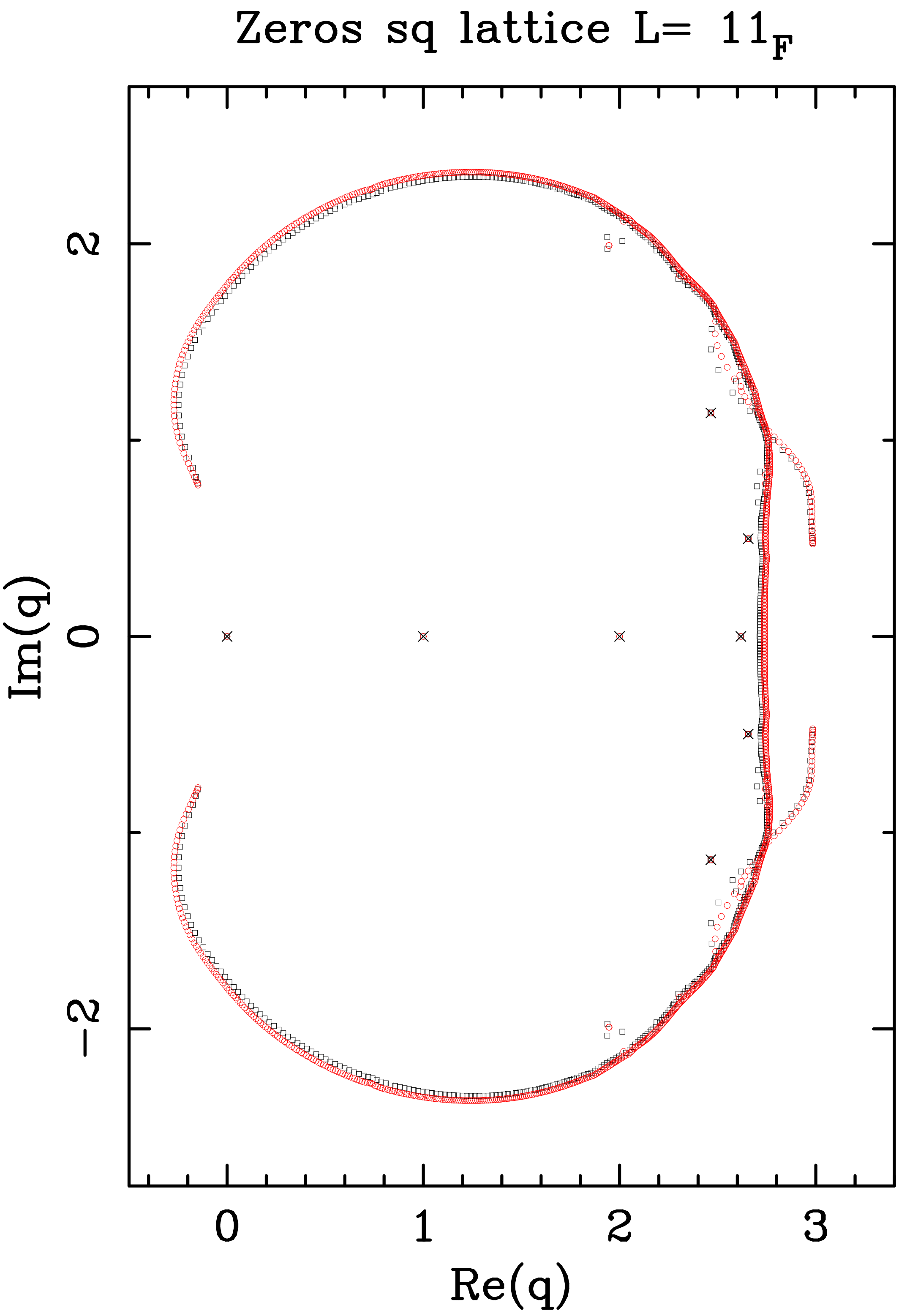

Figure 3: Zeros of the chromatic polynomial for the square lattices $11_F \times 55_F$ (□ black) and $11_F \times 110_F$ (○ red). Isolated limiting points are depicted as ×.