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LETTER TO THE EDITOR

Ground-state entropy of the Potts antiferromagnet on cyclic strip graphs

Robert Shrock†§ and Shan-Ho Tsai‡‖

† Institute for Theoretical Physics, State University of New York, Stony Brook, NY 11794-3840, USA

‡ Department of Physics and Astronomy, University of Georgia, Athens, GA 30602, USA

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Abstract. We present exact calculations of the zero-temperature partition function (chromatic polynomial) and the (exponent of the) ground-state entropy S_0 for the q-state Potts antiferromagnet on families of cyclic and twisted cyclic (Möbius) strip graphs composed of p-sided polygons. Our results suggest a general rule concerning the maximal region in the complex q plane to which one can analytically continue from the physical interval where $S_0 > 0$. The chromatic zeros and their accumulation set $\mathcal{B}$ exhibit the rather unusual property of including support for $\mathrm{Re}\,(q) < 0$ and provide further evidence for a relevant conjecture.

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

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

where $n = v(G)$ is the number of vertices of G and $\{G\} = \lim_{n\to\infty} G$¶. Since $P(G, q)$ is a polynomial, one can generalize q from $\mathbb{Z}_+$ to $\mathbb{R}$ and to $\mathbb{C}$, and this is useful, just as the study of functions of a complex variable gives deeper insight into functions of a real variable in mathematics. The zeros of $P(G, q)$ in the complex q plane, called chromatic zeros, are of basic importance. Their accumulation set in the limit $n \to \infty$, denoted $\mathcal{B}$, is the continuous locus of points where $W(\{G\}, q)$ is nonanalytic. A fundamental question concerning the Potts AF is the maximal region in the complex q plane to which one can analytically continue the function $W(\{G\}, q)$ from physical values where there is nonzero ground-state entropy, i.e., $W > 1$. We denote this region as R_1. In this letter we present exact calculations of $P(G, q)$ and $W(\{G\}, q)$ for families of strip graphs with free transverse and periodic longitudinal boundary conditions. From these we infer an answer to the above question.

§ E-mail address: robert.shrock@sunysb.edu

‖ E-mail address: tsai@hal.physast.uga.edu

¶ Some previous works include [4–10].

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These results are of further interest because of a property of the chromatic zeros. For many years, no examples of chromatic zeros were found with negative real parts, leading to the conjecture that $\mathrm{Re}\,(q) \geqslant 0$ for any chromatic zero [11]. Although this was later shown to be false [12], very few cases of graphs with chromatic zeros having $\mathrm{Re}\,(q) < 0$ are known, and the investigation of such cases is thus valuable for the insight it yields into properties of chromatic zeros. Note that the condition that a graph has some chromatic zeros with $\mathrm{Re}\,(q) < 0$ is a necessary but not sufficient condition that it has an accumulation set $\mathcal{B}$ with support for $\mathrm{Re}\,(q) < 0$. For the graph families considered here we find that both the chromatic zeros and their accumulation set $\mathcal{B}$ include support for $\mathrm{Re}\,(q) < 0$.

We start with a cyclic strip of the square lattice comprised of m squares, with its longitudinal (transverse) direction taken to be horizontal (vertical). By cyclic, we mean that this strip has periodic boundary conditions in the longitudinal direction, which will extend to infinity in the $m \to \infty$ limit. Now add $k-2$ vertices to the upper edge and $k-2$ vertices to the lower edge of each square. We denote this graph as $(Ch)_{k,m,cyc.}$. The analogous graph with twisted periodic longitudinal boundary conditions is a Möbius strip, denoted $(Ch)_{k,m,cyc.,t}$. These graphs have $n = 2(k-1)m$ vertices and can be regarded as cyclic and twisted cyclic strips of m p-sided polygons, where $p = 2k$, such that each p-gon intersects the previous one on one of its edges, and intersects the next one on its opposite edge. For a given m, the $(Ch)_{k,m,cyc.}$ and $(Ch)_{k,m,cyc.,t}$ form separate homeomorphic families†. The girth (length of minimum closed path) is $g = p = 2k$ for both.

Define

$$D_k = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s}. \tag{2}$$

By iterated use of the deletion–contraction theorem [5], we obtain the chromatic polynomials

$$P((Ch)_{k,m,cyc.}, q) = c_0 + (a_1)^m + (q-1)[(a_2)^m + (a_3)^m] \tag{3}$$

$$P((Ch)_{k,m,cyc.,t}, q) = c_0^{(t)} + (a_1)^m + (-1)^k (q-1)[(a_2)^m - (a_3)^m] \tag{4}$$

with $c_0 = q^2 - 3q + 1$, $c_0^{(t)} = -1$,

$$a_1 = D_{2k} \tag{5}$$

$$a_2 = (-1)^{k+1} D_{k+1} + D_k \tag{6}$$

$$a_3 = (-1)^{k+1} D_{k+1} - D_k. \tag{7}$$

In the lowest case, $k = 2$ (cyclic and twisted cyclic ladder graphs), equations (3), (4) reduce to known results [8, 12]. In [17] we have calculated $\mathcal{B}$ and W for these cases, as part of the general studies in [14–22]. P always has a factor $q(q-1)$; in addition, $P((Ch)_{k,m,cyc.}, q)$ has a $(q-2)$ factor for $(k,m) = (e,o)$ and $P((Ch)_{k,m,cyc.,t}, q)$ has a factor D_k^2 for odd k, $(q-2)D_k^2$ for $(k,m) = (e,e)$ and D_k^2 for (e,o), where e = even and o = odd. (For odd k, D_k has a factor $(q-2)$.) These are in accord with the values of the chromatic number χ (minimum q to colour the graph with the above constraint): for $(k,m) = (e,e)$, (o,e), and (o,o), $\chi((Ch)_{k,m,cyc.}) = 2$ and $\chi((Ch)_{k,m,cyc.,t}) = 3$ while for $(k,m) = (e,o)$, $\chi((Ch)_{k,m,cyc.}) = 3$ and $\chi((Ch)_{k,m,cyc.,t}) = 2$.

Taking m and hence n to infinity, we determine W. For special points q_s (e.g., $q_s = 0, 1$) where the limits $n \to \infty$ and $q \to q_s$ do not commute, we use the order of limits in equation (1.5) of [17], i.e. $n \to \infty$, then $q \to q_s$. For a given $q \in \mathbb{C}$, $W(q)$ is determined by the term a_j which is 'leading', i.e., has maximal $|a_j| > 1$ over the j, and if $|a_j| < 1$,

† Two graphs G and H are homeomorphic to each other if one of them, say H, can be obtained from the other, G, by successive insertions of degree-two vertices on bonds of G (e.g., [13–15]).

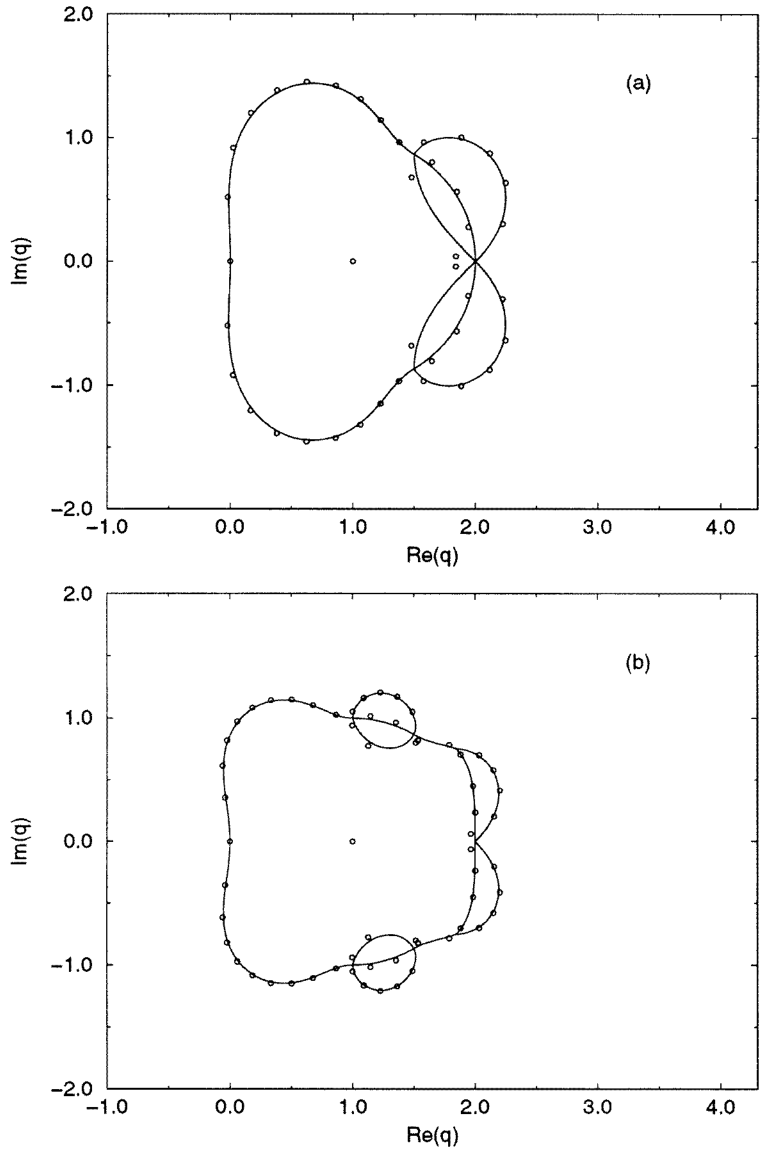

Figure 1. $\mathcal{B}$ for $\lim_{m\to\infty}(Ch)_{k,m,cyc.(t)}$ with $k = (a)\ 3$, $(b)\ 4$. Chromatic zeros are shown for the cyclic case with $m = 10$, i.e., $n = (a)\ 40$, $(b)\ 60$.

then W is determined by c_0, and $|W| = 1$. The locus $\mathcal{B}$ is determined by the degeneracy of leading a_j. From equations (3), (4), it follows that W and $\mathcal{B}$ are the same for $(Ch)_{k,m=\infty,cyc.}$ and $(Ch)_{k,m=\infty,cyc.,t}$ (indicated in the figure captions by (t)).

This locus is shown in figures 1 and 2 for $3 \leqslant k \leqslant 6$ together with chromatic zeros for long finite strips for comparison. We note the following theorems: $\mathcal{B}$ (i) separates the q plane into various regions; (ii) is compact in this plane; and (iii) for $k \geqslant 3$, contains support for $\mathrm{Re}\,(q) < 0$. Theorem (i) is proved by explicit solution of the equations for the boundary $\mathcal{B}$. Theorem (ii) is proved by recasting the degeneracy equations in the variable $z = 1/q$ and

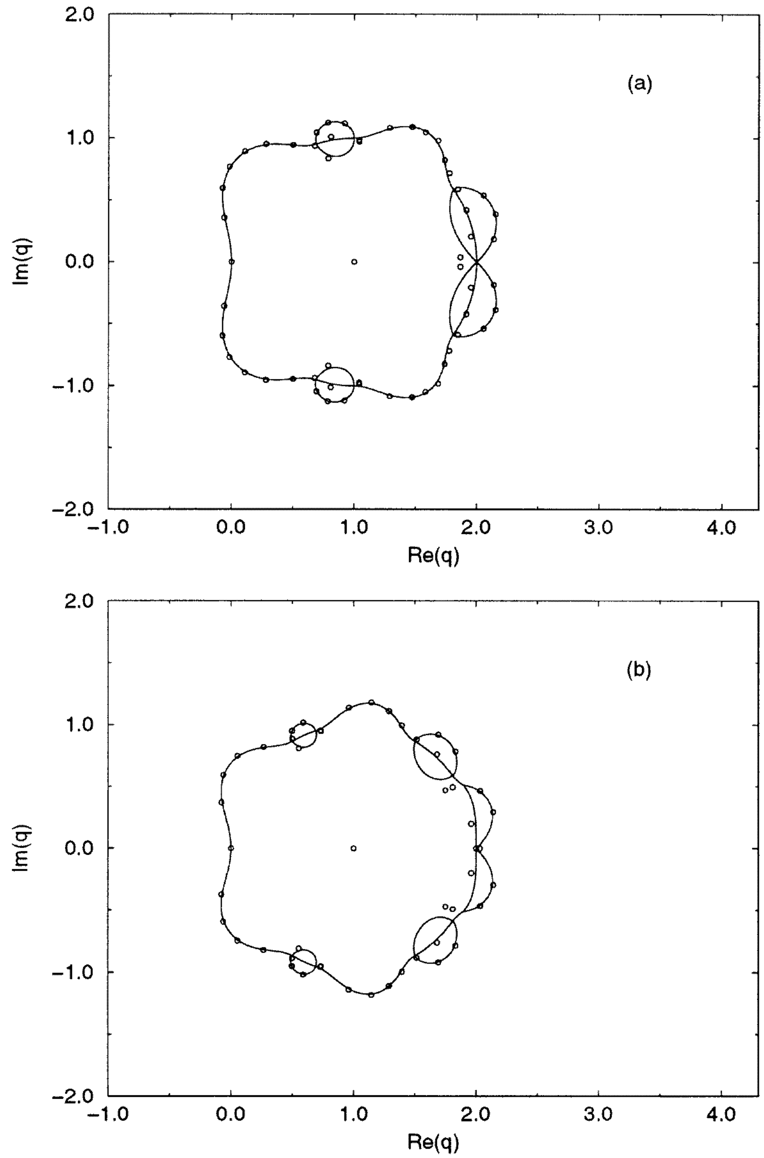

Figure 2. $\mathcal{B}$ for $\lim_{m\to\infty}(Ch)_{k,m,cyc.(t)}$ with $k = (a)\ 5$, $(b)\ 6$. Chromatic zeros are shown for the cyclic case with (*a*) $m = 8$ ($n = 64$), (*b*) $m = 5$ ($n = 50$).

showing that they have no solution for $z = 0$. Theorem (iii) is proved below.

We find the following regions and forms for W: first, R_1, which includes the real intervals $q \geqslant 2$ and $q < 0$ and surrounds all of $\mathcal{B}$. Here

$$W = (D_{2k})^{\frac{1}{2(k-1)}} \qquad \text{for} \quad q \in R_1. \tag{8}$$

For real $q \geqslant 2$ and a given k, W increases monotonically from 1 at $q = 2$, approaching q from below as $q \to \infty$: $W(q \to \infty) = q[1 - (2k-1)(2k-2)^{-1}q^{-1} + \mathrm{O}(q^{-2})]$. For a fixed q in this interval, W is a monotonically increasing function of k. This can be understood physically in the case of integral $q \geqslant 2$ since an increase in k increases the girth and thereby weakens the colouring constraint. As $q \to 0^-$ in R_1, $W \to (2k-1)^{\frac{1}{2(k-1)}}$. For regions $R_j \neq R_1$, only the magnitude $|W|$ can be determined [17]. The innermost region, denoted R_2, includes the interval $0 < q < 2$. Here, respectively,

$$|W| = |a_{2,3}|^{\frac{1}{2(k-1)}} \qquad \text{for} \quad q \in R_2 \qquad \text{and} \qquad k \text{ even, odd.} \tag{9}$$

The condition of degeneracy of leading terms in the vicinity of $q = 0$ is $|a_1| = |a_2|$ for even k and $|a_1| = |a_3|$ for odd k. Expanding these for fixed k and $r \to 0$, where $q = r\mathrm{e}^{\mathrm{i}\theta}$, we get

$$\cos\theta = -\frac{(k^2-3k+1)r}{2(2k-1)} + \mathrm{O}(r^2). \tag{10}$$

Hence, in the vicinity of $q = 0$, the curve $\mathcal{B}$ is concave toward the right (bends to the upper and lower right) for $k = 2$ but is concave to the left for $k \geqslant 3$. This proves theorem (iii), which, in turn, implies that for a given $k \geqslant 3$, and for sufficiently large n, these families have chromatic zeros with $\mathrm{Re}\,(q) < 0$ (as is evident from figures 1 and 2), which become dense, as $n \to \infty$, to form the part of the respective $\mathcal{B}$ with $\mathrm{Re}\,(q) < 0$. For $k = 3, 4$ and 5, chromatic zeros of $(Ch)_{k,m,cyc.}$ and $(Ch)_{k,m,cyc.,t}$ with $\mathrm{Re}\,(q) < 0$ occur first for strip lengths $m = 6, 4$, and 3, respectively; when k reaches the value $k = 6$, they occur already for the minimum nontrivial strip length, $m = 2$.

The fact that these families combine properties (ii) and (iii) is of particular interest since we have previously found a number of families of graphs with $\mathrm{Re}\,(q) < 0$ for some chromatic zeros and part of $\mathcal{B}$, but in these cases, $\mathcal{B}$ was noncompact (unbounded in the q plane) [22]. The property (i) also contrasts with the situation for homogeneous open strips, where we found [15, 21] that $\mathcal{B}$ does not enclose regions in the q plane.

We next comment on the other regions. At the point $q = 2$ ($\equiv q_c$, where q_c is the maximal value of real $q \in \mathcal{B}$ [16, 17]) one branch of $\mathcal{B}$ crosses the real axis vertically. To the upper and lower right of q_c, there are two complex-conjugate (c.c.) regions, denoted $R_{q_c,r}$ and $R^*_{q_c,r}$ ($r =$ 'right'); here, $|W| = |a_3|^{1/[2(k-1)]}$ for even k and $|W| = |a_2|^{1/[2(k-1)]}$ for odd k. In the latter case of odd k, there are two additional c.c. regions adjacent to q_c to the upper and lower left, denoted $R_{q_c;\ell}$, $R^*_{q_c;\ell}$ ($\ell =$ 'left'); in these regions, $|W| = 1$. Thus, for even and odd k, four and six curves on $\mathcal{B}$ intersect at q_c, respectively. As is evident from figures 1 and 2, for $k \geqslant 4$ there are further c.c. pairs of regions, each consisting of a pair on either side of the 'main' part of $\mathcal{B}$; here, in the outer parts, $|W| = |a_3|^{1/[2(k-1)]}$ for even k and $|W| = |a_2|^{1/[2(k-1)]}$ for odd k, while in the inner parts, $|W| = 1$ for both even and odd k. From our findings here we infer that the total number of regions is $2k$.

Define the outer envelope $\mathcal{E}$ of $\mathcal{B}$ to be the set of $q \in \mathcal{B}$ with maximal value of $|q-1|$; this is the inner boundary of region R_1. We observe that this envelope $\mathcal{E}$ always lies outside of the unit circle $|q-1| = 1$. As k increases, $\mathcal{B}$ lies closer to this circle.

Our present results strengthen the evidence for our conjectures [21, 22] that on a graph with well-defined lattice directions, a necessary property for there to be chromatic zeros and, in the $n \to \infty$ limit, a locus $\mathcal{B}$ including support for $\mathrm{Re}\,(q) < 0$, is that the graph has at least one global circuit, defined as a route along a lattice which is topologically equivalent to the circle, S^1. (This is known not to be a sufficient property, as shown, e.g., by the circuit and ladder graphs, which have such global circuits, but whose chromatic zeros and loci $\mathcal{B}$ have support only for $\mathrm{Re}\,(q) \geqslant 0$.) Note that in the second conjecture, the length of this global circuit, $L_{g.c.}$, must $\to \infty$ as $n \to \infty$ in order for some chromatic zeros and part of the locus $\mathcal{B}$ to include support for $\mathrm{Re}\,(q) < 0$. For the family $(Ch)_{k,m,cyc.}$ there are two such global circuits, along the upper and lower sides of the strip†.

† We have also calculated P, W, and $\mathcal{B}$ for the cyclic strips of the square lattice with width $L_y = 3$ and the Kagomé lattice with $L_y = 2$, and again these yield chromatic zeros and $\mathcal{B}$ with support for $\mathrm{Re}\,(q) < 0$ and have $\mathcal{B}$ separating the q plane into different regions.

This letter, combined with our earlier calculations [17–22], suggests an answer to the basic question of how large is the region R_1 to which one can analytically continue W from the interval in q where $S_0 > 0$ for graphs with regular lattice directions: a sufficient condition that in the $n \to \infty$ limit the locus $\mathcal{B}$ separates the q plane into two or more regions is that the graph has a global circuit with $\lim_{n\to\infty} \ell_{g.c.} = \infty$†. Thus, for graphs (with regular lattice directions), a necessary condition that R_1 includes the full q plane (except for the set of measure zero occupied by $\mathcal{B}$) is that the graphs do not contain any such global circuits.

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† That this is not a necessary condition is shown by our results on inhomogeneous open strip graphs [21]. Moreover, $\mathcal{B}$ includes the point $q = 0$ for the families $(Ch)_{k,m=\infty,cyc.}$; however, our results in [18, 19, 22] show, and explain why, in cases where there are global circuits, $\mathcal{B}$ does not necessarily include the point $q = 0$.