

## ARTICLES

## Families of graphs with chromatic zeros lying on circles

Robert Shrock\* and Shan-Ho Tsai†

*Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794-3840*

(Received 12 March 1997)

We define an infinite set of families of graphs, which we call  $p$ -wheels and denote  $(Wh)_n^{(p)}$ , that generalize the wheel ( $p=1$ ) and biwheel ( $p=2$ ) graphs. The chromatic polynomial for  $(Wh)_n^{(p)}$  is calculated, and remarkably simple properties of the chromatic zeros are found: (i) the real zeros occur at  $q=0, 1, \dots, p+1$  for  $n-p$  even and  $q=0, 1, \dots, p+2$  for  $n-p$  odd; and (ii) the complex zeros all lie, equally spaced, on the unit circle  $|q-(p+1)|=1$  in the complex  $q$  plane. In the  $n \rightarrow \infty$  limit, the zeros on this circle merge to form a boundary curve separating two regions where the limiting function  $W(\{(Wh)_n^{(p)}\}, q)$  is analytic, viz., the exterior and interior of the above circle. Connections with statistical mechanics are noted. [S1063-651X(97)01108-2]

PACS number(s): 05.20.-y, 75.10.Hk

## I. INTRODUCTION

The chromatic polynomial  $P(G, q)$  of a graph  $G$  plays a fundamental role in graph theory; it gives the number of ways of coloring this graph  $G$  with  $q$  colors such that no two adjacent vertices have the same color [1–5]. Since  $P(G, q) \leq q^n$  for a graph  $G$  with  $n$  vertices, it is natural to consider the asymptotic limiting function

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

where  $\{G\}$  denotes the limit as  $n \rightarrow \infty$  of the family of  $n$ -vertex graphs of type  $G$ . There is a natural generalization, which we assume here, of the variable  $q$  from integer to complex values. Recently, we calculated the  $W(\{G\}, q)$  functions for several families of graphs  $\{G\}$  [6] and studied their analytic properties. One of the interesting results that we found was that for three families of graphs, namely, circuit, wheel, and biwheel graphs, the zeros of the respective chromatic polynomials, i.e., the chromatic zeros of these graphs, lie at certain real integer values and on certain unit circles in the complex  $q$  plane. A question that occurred to us was the following: Can one generalize this finding and if so, can one thereby achieve a deeper understanding of the result? We have succeeded in finding a comprehensive generalization which does yield further insight into this result, and we present this here. Given the elementary relation that the chromatic polynomial  $P(G, q) = Z(G, q, T=0)_{\text{PAF}}$ , where  $Z(G, q, T=0)_{\text{PAF}}$  is the partition function of the zero-temperature  $q$ -state Potts antiferromagnet (AF) on the graph  $G$ , and the consequent relation, for the thermodynamic limit, between  $W(\{G\}, q)$  and the exponent of the ground state entropy of the Potts AF, our results also have implications

for statistical mechanical properties of the Potts antiferromagnet on a certain family of graphs.

To construct the  $p$ -wheel with  $n$  vertices, we start with a circuit with  $n-p$  vertices,  $C_{n-p}$ , and adjoin  $p$  points to each of the points on the circuit and to each other. Here, obviously,  $n-p \geq 1$  and, for a nontrivial circuit,  $n-p \geq 2$ . This process could be symbolized as the product  $K_p \times C_{n-p}$ , where  $K_p$  is the complete graph on  $p$  vertices. We denote the  $p$ -wheel as  $(Wh)_n^{(p)}$ . This generalizes the definitions of the  $n$ -vertex wheel and biwheel graphs  $(Wh)_n$  and  $U_n$ ; these are seen now as special cases of the  $p$ -wheel for the respective values  $p=1$  and  $p=2$ :  $(Wh)_n^{(1)} = (Wh)_n$  and  $(Wh)_n^{(2)} = U_n$ . The  $n$ -vertex circuit graph  $C_n$  is subsumed as the  $p=0$  special case:  $(Wh)_n^{(0)} = C_n$ . Thus each family  $K_p \times C_{n-p} = (Wh)_n^{(p)}$  forms an infinite set as one increases the number of vertices  $n$ . Clearly,

$$(Wh)_{p+1}^{(p)} = K_{p+1}. \quad (2)$$

II. THEOREMS ON CHROMATIC ZEROS OF  $(Wh)_n^{(p)}$ 

In general, the chromatic polynomial  $P(G, q)$  for a (non-empty) graph  $G$  has zeros at the discrete values  $q=0$ ,  $q=1$ , and, if  $G$  contains one or more triangles ( $\triangle$ ), also the value  $q=2$ . Furthermore, since  $P(G, q)$  is real for real  $q$ , it follows that the zeros of this polynomial (i.e., the chromatic zeros) are invariant under the complex conjugation  $q \rightarrow q^*$ . We consider an  $n$ -vertex graph  $G$  in a particular family  $\{G\}$  of graphs for which, as  $n \rightarrow \infty$ , aside from the above-mentioned discrete zeros at  $q=0, 1$  and, for  $G \supseteq \triangle$ ,  $q=2$ , the remaining zeros merge to form the union of boundaries  $\mathcal{B}$  separating various regions in the complex  $q$  plane [7]. A general question that one may ask about this latter set of zeros is whether all, or a subset of them, lie exactly on the boundary curves  $\mathcal{B}$  even for finite  $n$ . (Some of the set of discrete zeros may also lie on  $\mathcal{B}$ .) Clearly, the fact that a subset of zeros merges to form the boundary  $\mathcal{B}$  in the  $n \rightarrow \infty$  limit does not imply

\*Electronic address: shrock@insti.physics.sunysb.edu

†Electronic address: tsai@insti.physics.sunysb.edu

that, for finite graphs  $G$ , some subset of zeros will lie precisely on  $\mathcal{B}$ . We have investigated this question and have found that there do exist some families of graphs  $\{G\}$  for which the zeros of  $P(G, q)$  (aside from a certain discrete set) lie exactly on the respective boundary curves  $\mathcal{B}$ . Furthermore, we find that these families of graphs also provide an answer to the question posed at the beginning of this paper, concerning a generalization of the property that  $\mathcal{B}$  comprises a (unit) circle.

Our main results are contained in the following two theorems [as noted above, for a nontrivial circuit  $C_{n-p}$  in  $(Wh)_n^{(p)}$ ,  $n-p \geq 2$ ].

Theorem 1. The chromatic polynomial for the  $p$ -wheel is

$$P((Wh)_n^{(p)}, q) = \left[ \prod_{l=0}^{p-1} (q-l) \right] [(q-p-1)^{n-p} + (-1)^{n-p}(q-p-1)]. \quad (3)$$

Proof. We use the theorem that if a graph  $H$  is obtained from a graph  $G$  by adding a vertex which is adjacent to all of the vertices of  $G$  (i.e., connected to them by bonds of the graph), then (e.g., Ref. [4])

$$P(H, q) = qP(G, q-1). \quad (4)$$

We take  $G = C_{n-p}$ , the circuit with  $n-p$  vertices, and apply Eq. (4) iteratively  $p$  times to get

$$P((Wh)_n^{(p)}, q) = \left[ \prod_{l=0}^{p-1} (q-l) \right] P(C_{n-p}, q-p). \quad (5)$$

Substituting the basic result  $P(C_n, q) = (q-1)^n + (-1)^n(q-1)$  then yields Eq. (3). ■

Theorem 2. The real zeros of the chromatic polynomial of the  $p$ -wheel,  $P((Wh)_n^{(p)}, q)$ , occur at  $q=0, 1, \dots, p+1$  for  $n-p$  even and  $q=0, 1, \dots, p+2$  for  $n-p$  odd, while the complex zeros all lie on the unit circle  $|q-(p+1)|=1$  in the complex  $q$  plane. Furthermore, the zeros are equally spaced around this circle, and in the  $n \rightarrow \infty$  limit, the density  $g(\{(Wh)_n^{(p)}\}, \theta)$  of zeros on the circle  $q=p+1+e^{i\theta}$ ,  $-\pi < \theta \leq \pi$ , is a constant, independent of  $\theta$ .

Proof. Defining  $x = q - (p+1)$ , we can write the second expression in Eq. (5) as

$$x[x^{n-p-1} + (-1)^{n-p}]. \quad (6)$$

It follows that the complex zeros of  $P((Wh)_n^{(p)}, q)$  are the complex solutions to the equation  $x^{n-p-1} + (-1)^{n-p} = 0$ , which clearly lie on the unit circle  $|x|=1$ , i.e.,  $|q-(p+1)|=1$ . Specifically, for  $n-p$  even,  $x=-1$ , i.e.,  $q=p$  is a root, and the  $n-p-2$  complex roots are given by

$$q = p+1 + e^{i\pi + 2s\pi/[n-(p+1)]}, \quad s = 1, \dots, n-p-2 \quad (7)$$

while for  $n-p$  odd,  $x = \pm 1$ , i.e.,  $q=p, p+2$  are real roots, while the  $n-p-3$  complex roots are

$$q = p+1 + e^{2s\pi/[n-(p+1)]}, \quad s = 1, \dots, n-p-2, \quad s \neq \frac{n-p-1}{2} \quad (8)$$

where the (integer) value  $(n-p-1)/2$  is omitted because this root is real. These complex roots obviously come in complex conjugate pairs; a factorization which makes this explicit is, for  $n-p$  even,

$$\begin{aligned} P((Wh)_n^{(p)}, q)_{n-p \text{ even}} &= \left[ \prod_{l=0}^{p+1} (q-l) \right] \prod_{j=0}^{(n-p)/2-2} \{q - (p+1 + e^{(2j+1)\pi i/[n-(p+1)]})\} \\ &\quad \times \{q - (p+1 + e^{-(2j+1)\pi i/[n-(p+1)]})\} \end{aligned} \quad (9)$$

and for  $n-p$  odd,

$$\begin{aligned} P((Wh)_n^{(p)}, q)_{n-p \text{ odd}} &= \left[ \prod_{l=0}^{p+2} (q-l) \right] \prod_{j=1}^{(n-p-1)/2-1} \{q - (p+1 + e^{2j\pi i/[n-(p+1)]})\} \\ &\quad \times \{q - (p+1 + e^{-2j\pi i/[n-(p+1)]})\}. \end{aligned} \quad (10)$$

The complex factors in Eqs. (9) and (10) follow immediately from Eqs. (7) and (8). This proves the second part of our theorem, that the complex roots lie on the unit circle  $|x|=1$  with equal spacing. In particular, in the  $n \rightarrow \infty$  limit, it follows that the density  $g(\{(Wh)_n^{(p)}\}, \theta)$  of zeros on the circle  $q=p+1+e^{i\theta}$ ,  $-\pi < \theta \leq \pi$  is a constant, independent of  $\theta$ . If one normalizes this density according to

$$\int_{-\pi}^{\pi} g(\{(Wh)_n^{(p)}\}, \theta) d\theta = 1 \quad (11)$$

then

$$g(\{(Wh)_n^{(p)}\}, \theta) = \frac{1}{2\pi}. \quad (12)$$

Concerning the product of real integer roots, we observe that for  $n-p$  even, Eq. (6) has the real factors  $x$  and  $x+1$ , i.e.,  $q-(p+1)$  and  $q-p$  which, combined with the factor  $\prod_{l=0}^{p-1} (q-l)$  in Eq. (3), yield the factor  $\prod_{l=0}^{p+1} (q-l)$  in Eq. (9). For  $n-p$  odd, Eq. (6) has the real factors  $x$ ,  $x+1$ , and  $x-1$ , i.e.,  $q-(p+1)$ ,  $q-p$ , and  $q-(p+2)$  which, combined again with the factor  $\prod_{l=0}^{p-1} (q-l)$  in Eq. (3), yield the factor  $\prod_{l=0}^{p+2} (q-l)$  in Eq. (10). This proves the first part of the theorem, which specifies the real roots of  $P((Wh)_n^{(p)}, q)$ . This completes the proof of both parts of the theorem. ■

### III. ANALYTIC STRUCTURE OF $W(\{(Wh)_n^{(p)}\}, q)$

We next consider the limiting function  $W(\{(Wh)_n^{(p)}\}, q)$ . As we have discussed in Ref. [6], Eq. (1) is not, in general, adequate to define this function because of a noncommutativity that occurs at certain special values of  $q$ , which we denote  $q_s$ , where

$$\lim_{n \rightarrow \infty} \lim_{q \rightarrow q_s} P(G, q)^{1/n} \neq \lim_{n \rightarrow \infty} \lim_{q \rightarrow q_s} P(G, q)^{1/n}. \quad (13)$$

The origin of this noncommutativity of limits is an abrupt change in the behavior of  $P(G, q)$  in the vicinity of such a point  $q_s$ ; for  $q \neq q_s$ ,  $P(G, q)$  grows exponentially as the number of vertices  $n$  in  $G$  goes to infinity:  $P(G, q) \sim a^n$  for some nonzero  $a$ , whereas precisely at  $q = q_s$ , it has a completely different type of behavior; typically,  $P(G, q_s) = c_0(q_s)$  where  $c_0(q)$  may be a constant, independent of  $n$  or may depend on  $n$ , but in a way that does not involve exponential growth, such as  $(-1)^n$ . The set of special points  $\{q_s\}$  includes  $q = 0$ ,  $q = 1$ , and, if  $G \supseteq \Delta$ , also  $q = 2$ ; at these points,  $P(G, q_s) = 0$ .

In the present case, we find that for a fixed  $p$ , in the  $n \rightarrow \infty$  limit, the zeros on the unit circle  $|q - (p+1)| = 1$  merge to form a (complete) circle with a density given by Eq. (12). This circle thus constitutes the boundary curve  $\mathcal{B}$  and divides the complex  $q$  plane into two regions:

$$R_1: q \text{ such that } |q - (p+1)| > 1 \quad (14)$$

and

$$R_2: q \text{ such that } |q - (p+1)| < 1. \quad (15)$$

The set of special points  $\{q_s\}$  associated with the noncommutativity in Eq. (13) are the real integral zeros of  $P((Wh)_n^{(p)}, q)$ , i.e.,  $\{q_s\} = 0, 1, \dots, p+1$  for  $n-p$  even and  $\{q_s\} = 0, 1, \dots, p+2$  for  $n-p$  odd. We find that

$$W(\{(Wh)^{(p)}\}, q) = q - (p+1) \quad \text{for } q \in R_1 \text{ and } q \notin \{q_s\}. \quad (16)$$

Because of the noncommutativity (13), the formal definition (1) is, in general, insufficient to define  $W(\{G\}, q)$  at the set of special points  $\{q_s\}$ ; at these points, one must also specify the order of the limits in Eq. (13). One can maintain the analyticity of  $W(\{G\}, q)$  at these special points  $q_s$  of  $P(G, q)$  by choosing the order of limits in the right-hand side of Eq. (13):

$$W(\{G\}, q_s)_{D_{qn}} \equiv \lim_{q \rightarrow q_s} \lim_{n \rightarrow \infty} P(G, q)^{1/n}. \quad (17)$$

As indicated, we shall denote this definition as  $D_{qn}$ . Although this definition maintains the analyticity of  $W(\{G\}, q)$  at the special points  $q_s$ , it produces a function  $W(\{G\}, q)$  whose values at the points  $q_s$  differ significantly from the values which one would get for  $P(G, q_s)^{1/n}$  with finite- $n$  graphs  $G$ . The definition based on the opposite order of limits,

$$W(\{G\}, q_s)_{D_{nq}} \equiv \lim_{n \rightarrow \infty} \lim_{q \rightarrow q_s} P(G, q)^{1/n} \quad (18)$$

gives the expected results like  $W(G, q_s) = 0$  for  $q_s = 0, 1$ , and, for  $G \supseteq \Delta$ ,  $q = 2$ , but yields a function  $W(\{G\}, q)$  with discontinuities at the set of points  $\{q_s\}$ . Following our convention in Ref. [6], if no subscript is used,  $W(G, q) = W(G, q)_{D_{qn}}$ . In the present case, we have

$$W(\{(Wh)^{(p)}\}, q)_{D_{nq}} = 0 \quad \text{for } q \in R_1 \text{ and } q \in \{q_s\}. \quad (19)$$

while

$$W(\{(Wh)^{(p)}\}, q)_{D_{qn}} = q - (p+1)$$

$$\text{for } q \in R_1 \text{ and } q \in \{q_s\}. \quad (20)$$

For  $q \in R_2$  there is no canonical choice of phase to use in the  $n$ th root (1) [6]; however, for the complex amplitude we have

$$|W(\{(Wh)^{(p)}\}, q)| = 1 \quad \text{for } q \in R_2 \text{ and } q \notin \{q_s\}. \quad (21)$$

The region  $R_2$  contains the point  $q = p+1$  which is a member of the set of discrete zeros  $\{q_s\}$ ; for  $q = p+1$ , the two orders of limits give  $W(\{(Wh)^{(p)}\}, q)_{D_{nq}} = 0$  and  $|W(\{(Wh)^{(p)}\}, q)_{D_{qn}}| = 1$ . The limiting function  $W(\{(Wh)^{(p)}\}, q)$  is nonanalytic on the boundary circle  $|q - (p+1)| = 1$ .

In Ref. [6] (see also Ref. [8]) we discussed the quantity  $q_c(\{G\})$ , the maximal (finite) real point of nonanalyticity of  $W(\{G\}, q)$ , and inferred the values of  $q_c$  for certain lattices  $\{G\} = \Lambda$ . A corollary of our theorems above is that

$$q_c(\{(Wh)^{(p)}\}) = p+2. \quad (22)$$

As was the case with the lattices previously considered, we infer that for integer  $q$  above this critical value, i.e., here,  $q > p+2$ , the Potts antiferromagnet on the infinite- $n$  limit of the  $p$ -wheel graph has a nonzero ground state entropy  $S_0 = k_B \ln W(\{(Wh)^{(p)}\})$ . For integer  $q \leq p-1$ , the model is frustrated because of the impossibility of assigning different colors (i.e., spin states in the Potts AF) to all of the adjacent vertices of the  $K_p$  subgraph. It would be interesting to investigate further the properties of the Potts antiferromagnet on the infinite- $n$  limits of  $p$ -wheel graphs.

Because of the connection to statistical mechanics, it is worthwhile to contrast our theorem with the famous Yang-Lee circle theorem [9]. Yang and Lee considered the Ising model partition function  $Z = \sum_{\{\sigma_r\}} e^{-\beta \mathcal{H}}$  at temperature  $T$  in an external magnetic field  $H$ , for which the Hamiltonian is  $\mathcal{H} = -\sum_{r,r'} \sigma_r J_{r,r'} \sigma_{r'} - H \sum_r \sigma_r$ , where  $\sigma_r = \pm 1$  and  $\beta = (k_B T)^{-1}$ . They proved that for an arbitrary (finite as well as infinite) lattice with spin-spin couplings which are ferromagnetic,  $J_{r,r'} \geq 0$ , but not necessarily nearest neighbor (and physical temperature  $0 \leq T \leq \infty$ ), the zeros of  $Z$  in the variable  $\mu = e^{-2\beta H}$  lie on the unit circle  $|\mu| = 1$  in the  $\mu$  plane. In the thermodynamic limit, these zeros merge, becoming dense and forming an arc  $\mu = e^{i\theta}$  for  $\theta_0(T) \leq |\theta| \leq \pi$ , where  $\pm \theta_0(T)$  denote the angles at the end points of this arc. The free energy is nonanalytic across the arc. For temperature  $T > T_c$ , the arc leaves a gap which includes the positive real axis in the  $\mu$  plane, but as  $T$  decreases through the critical temperature  $T_c$ , this arc closes, pinching the real axis at  $\mu = 1$ . For  $0 \leq T \leq T_c$  the zeros continue to form a full closed unit circle. Our theorem shares with the Yang-Lee theorem the property of zeros lying on a unit circle and of being true for finite graphs as well as in the limit  $n \rightarrow \infty$ . However, there are several important differences: (i) first, in the Yang-Lee circle theorem, all of the zeros of  $Z$  lie on the fixed unit circle  $|\mu| = 1$ , whereas in contrast, in our theorem, only a subset do and, moreover, the center of the circle is at a different position,  $q = p+1$  for each respective family of

$p$ -wheel graphs,  $(Wh)_n^{(p)}$ ; (ii) the Yang-Lee theorem describes a multivariable problem, dealing with the zeros of  $Z$  in the complex  $\mu$  plane, which depend parametrically on the temperature  $T$ , and it requires in its premise that all  $J_{r,r'} \geq 0$ , whereas in our case, once  $p$  is specified, i.e., one specializes to a given  $p$ -wheel graph  $(Wh)_n^{(p)}$ , the zeros in the complex variable  $q$  are fixed; (iii) thus, while in the  $n \rightarrow \infty$  limit, the Yang-Lee zeros merge to form an arc which does not form a closed circle for  $T > T_c$ , the subset of chromatic zeros that we show lie on the unit circle  $|q - (p+1)| = 1$  always close to form a complete circle in the  $n \rightarrow \infty$  limit; and (iv) on the Yang-Lee arc, the density of zeros is not, in general, a constant, independent of  $\theta$ , whereas the density  $g(\{(Wh)_n^{(p)}\}, \theta)$  in our case is, in fact, independent of  $\theta$ . Despite these differences, the properties that our theorem and the Yang-Lee circle theorem share in common, namely, that they both apply to a finite graph and imply zeros lying on a unit circle, show a very interesting connection between these results.

#### IV. CONCLUSIONS

In conclusion, we have constructed a set of families of graphs which we call  $p$ -wheels,  $(Wh)_n^{(p)}$ , and calculated

their chromatic polynomials. We have proved that these provide a (countably infinite) generalization of the behavior that we had found previously for the circuit, wheel, and biwheel graphs (which are seen as the special cases  $p=0,1$ , and  $2$ , respectively), namely, that a subset of the chromatic zeros lies exactly on the unit circle  $|q - (p+1)| = 1$  in the complex  $q$  plane, and in the limit as the number of vertices  $n \rightarrow \infty$ , these zeros merge to form the full circle  $|q - (p+1)| = 1$  with density independent of position on the circle. Since the chromatic zeros lie exactly on this circle even for finite  $n$ , the families also constitute a constructive answer to another question that we posed, namely, to find families of graphs such that chromatic zeros lie precisely on the asymptotic boundary curve  $\mathcal{B}$ . We have compared our results with the Yang-Lee circle theorem and remarked on the connections with zero-temperature Potts antiferromagnets. Our present theorems provide a deeper and unified understanding of our previous findings in Ref. [6].

#### ACKNOWLEDGMENT

This research was supported in part by NSF Grant No. PHY-93-09888.

- 
- [1] G. D. Birkhoff, *Ann. Math.* **14**, 42 (1912).
  - [2] H. Whitney, *Ann. Math.* **33**, 688 (1932); *Bull. Am. Math. Soc.* **38**, 572 (1932).
  - [3] G. D. Birkhoff and D. C. Lewis, *Trans. Am. Math. Soc.* **60**, 355 (1946).
  - [4] R. C. Read and W. T. Tutte, in *Selected Topics in Graph Theory*, 3, edited by L. W. Beineke and R. J. Wilson (Academic Press, New York, 1988).
  - [5] W. T. Tutte, in *Graph Theory*, Encyclopedia of Mathematics and its Applications Vol. 21, edited by G. C. Rota (Addison-Wesley, New York, 1984).
  - [6] R. Shrock and S.-H. Tsai, *Phys. Rev. E* **55**, 5165 (1996).
  - [7] This sort of behavior does not occur for all graphs; for example, the chromatic zeros of the complete graph on  $n$  vertices,  $K_n$ , occur at the values  $0, 1, \dots, n-1$  and hence do not contain a subset which merges to form a continuous boundary curve in the  $n \rightarrow \infty$  limit.
  - [8] R. Shrock and S.-H. Tsai, *J. Phys. A* **30**, 495 (1997); *Phys. Rev. E* **55**, 6791 (1997).
  - [9] C. N. Yang and T. D. Lee, *Phys. Rev.* **87**, 404 (1952); T. D. Lee and C. N. Yang, *ibid.* **87**, 410 (1952).