Families of graphs with $W_r(\{G\},q)$ functions that are nonanalytic at $1/q=0$

Robert Shrock* and Shan-Ho Tsai†
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794-3840
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Denoting $P(G,q)$ as the chromatic polynomial for coloring an n-vertex graph G with q colors, and considering the limiting function $W(\{G\},q)=\lim_{n\to\infty}P(G,q)^{1/n}$, a fundamental question in graph theory is the following: is $W_r(\{G\},q)=q^{-1}W(\{G\},q)$ analytic or not at the origin of the $1/q$ plane (where the complex generalization of q is assumed)? This question is also relevant in statistical mechanics because $W(\{G\},q)=\exp(S_0/k_B)$, where S_0 is the ground state entropy of the q-state Potts antiferromagnet on the lattice graph $\{G\}$, and the analyticity of $W_r(\{G\},q)$ at $1/q=0$ is necessary for the large-q series expansions of $W_r(\{G\},q)$. Although W_r is analytic at $1/q=0$ for many $\{G\}$, there are some $\{G\}$ for which it is not; for these, W_r has no large-q series expansion. It is important to understand the reason for this nonanalyticity. Here we give a general condition that determines whether or not a particular $W_r(\{G\},q)$ is analytic at $1/q=0$ and explains the nonanalyticity where it occurs. We also construct infinite families of graphs with W_r functions that are nonanalytic at $1/q=0$ and investigate the properties of these functions. Our results are consistent with the conjecture that a sufficient condition for $W_r(\{G\},q)$ to be analytic at $1/q=0$ is that $\{G\}$ is a regular lattice graph Λ. (This is known not to be a necessary condition.) [S1063-651X(97)04110-X]

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I. INTRODUCTION

The chromatic polynomial $P(G,q)$ of an n-vertex graph G and the asymptotic limiting function

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

play important roles in both graph theory [1–6] and statistical mechanics [7–9]. Here $P(G,q)$ is defined as the number of ways of coloring the graph G with q colors such that no two adjacent vertices have the same color, and $\{G\}$ denotes the limit as $n\to\infty$ of the family of n-vertex graphs of type G. The connection with statistical mechanics is via the elementary equality $P(G,q)=Z(G,q,T=0)_{\rm PAF}$, where $Z(G,q,T=0)_{\rm PAF}$ is the partition function of the zero-temperature q-state Potts antiferromagnet (AF) [8,9] on the graph G, and the consequent equality (in the $n\to\infty$ limit) $W(\{G\},q)=\exp[S_0(\{G\},q)/k_B]$, where $S_0(\{G\},q)$ denotes the ground state entropy of the q-state Potts AF on $\{G\}$ (typically a regular lattice, $\{G\}=\Lambda$ with some specified boundary conditions). Given the fact that $P(G,q)$ is a polynomial, there is a natural generalization, which we assume here, of the variable q from integer to complex values. Since an obvious upper bound on $P(G,q)$ describing the coloring of an n-vertex graph with q colors is $P(G,q)\leqslant q^n$, and hence $W(\{G\},q)\leqslant q$, it is natural to define a reduced function

$$W_r(\{G\},q)=q^{-1}W(\{G\},q). \tag{1.2}$$

A fundamental question in graph theory concerns whether $W_r(\{G\},q)$ is analytic or not at the origin, $1/q=0$, of the $z=1/q$ plane. This question is important in both graph theory and statistical mechanics because a standard method for studying this function or equivalent reduced W functions is to calculate a large-q Taylor series expansion about the point $1/q=0$ [10–12]. However, if $W_r(\{G\},q)$ is nonanalytic at $1/q=0$, then one cannot carry out such a Taylor series expansion in the usual manner. Indeed, we recently discussed an example, namely, the bipyramid graph B_n, for which $W_r(\{B\},q)$ is not analytic at $1/q=0$ [13] (see also [14]).

Clearly it is important to understand better the differences between the families of graphs that yield $W_r(\{G\},q)$ functions analytic at $1/q=0$ and those which produce $W_r(\{G\},q)$ functions that are nonanalytic at $1/q=0$. In the present paper we shall address this problem. We shall give a general condition that determines whether or not a particular $W_r(\{G\},q)$ is analytic at $1/q=0$. This explains the source of the nonanalyticity in the cases where it occurs. We also construct infinite families of graphs with W_r functions that are nonanalytic at $1/q=0$. These serve as a very useful theoretical laboratory, and we study the properties of the resultant W_r functions in some detail. A salient point is that none of the $\{G\}$ that we construct with $W_r(\{G\},q)$ that are nonanalytic at $1/q=0$ is a regular lattice graph $\{G\}=\Lambda$. Thus, anticipating the later discussion in this paper, our work is consistent with the conjecture that (in the $n\to\infty$ limit) a sufficient condition that $W_r(\{G\},q)$ be analytic at $1/q=0$ is that $\{G\}=\Lambda$ is a regular lattice graph. (We know from our previous work [13] that this is not a necessary condition.) We state it as a conjecture since we are not aware of any proof of the analyticity at $1/q=0$ of $W_r(\Lambda,q)$ for a regular lattice Λ in the literature. Indeed, in Ref. [12], it was acknowledged that there was no general theory for the existence of the limit (1.1) and, hence also, in our notation, the reduced function W_r, even in the case of regular lattices.

Before proceeding, it is necessary to clarify the definition of $W(\{G\},q)$ for values of q that are not positive integers. As we discussed in Ref. [13], for certain ranges of real q,

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

$P(G,q)$ can be negative, and, of course, when q is complex, so is $P(G,q)$ in general. In these cases it may not be obvious, *a priori*, which of the n roots

$$P(G,q)^{1/n}=\{|P(G,q)|^{1/n}e^{2\pi ir/n}\},\quad r=0,1,\ldots,n-1 \tag{1.3}$$

to choose in Eq. (1.1). Consider the function $W(\{G\},q)$ defined via Eq. (1.1) starting with q on the positive real axis where $P(G,q)>0$, and consider the maximal region in the complex q plane that can be reached by analytic continuation of this function. We denote this region as R_1. Clearly, the phase choice in (1.3) for $q\in R_1$ is that given by $r=0$, namely, $P(G,q)^{1/n}=|P(G,q)|^{1/n}$. However, as we showed via exactly solved cases in Ref. [13], there are many families of graphs $\{G\}$ for which the areas of analyticity of $W(\{G\},q)$ include other regions not analytically connected to R_1, and in these regions, there is not, in general, any canonical choice of phase in Eq. (1.3).

A second subtlety in the definition of $W(\{G\},q)$ concerns the fact that at certain special points q_s, the following limits do not commute [13] [for any choice of r in Eq. (1.3)]:

$$\lim_{n\to\infty}\lim_{q\to q_s}P(G,q)^{1/n}\neq\lim_{q\to q_s}\lim_{n\to\infty}P(G,q)^{1/n}. \tag{1.4}$$

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. (1.4):

$$W(\{G\},q_s)_{D_{qn}}\equiv\lim_{q\to q_s}\lim_{n\to\infty}P(G,q)^{1/n}. \tag{1.5}$$

As indicated, we shall denote this definition as D_{qn}, where the subscript indicates the order of the limits. 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 that one would get for $P(G,q_s)^{1/n}$ with finite-n graphs G. The definition based on the opposite order of limits,

$$W(\{G\},q_s)_{D_{nq}}\equiv\lim_{n\to\infty}\lim_{q\to q_s}P(G,q)^{1/n} \tag{1.6}$$

gives the expected results such as $W(\{G\},q_s)=0$ for $q_s=0,1$, and, for $G\supseteq\triangle$, $q=2$, as well as $W((\mathrm{tri})_n,q=3)=1$ (where $(\mathrm{tri})_n$ denotes a triangular lattice with n sites and boundary conditions that do not introduce frustration for $q=3$), but yields a function $W(\{G\},q)$ with discontinuities at the set of points $\{q_s\}$. In our results below, in order to avoid having to write special formulas for the points q_s, we shall adopt the definition D_{qn} but at appropriate places will take note of the noncommutativity of limits (1.4).

II. CONSTRUCTION OF FAMILIES WITH $W_r(\{G\},q)$ NONANALYTIC AT $1/q=0$

A. General algorithm and calculation of chromatic polynomial

In general, as discussed in Ref. [13], for a given family $\{G\}$, the corresponding $W(\{G\},q)$, at least as defined via the order of limits (1.5), is an analytic function in certain regions of the complex q plane. These regions are separated from each other by curves (or lines) comprising the union of boundaries $\mathcal{B}$. $W(\{G\},q)$ is nonanalytic on these boundaries. Clearly, $\mathcal{B}$ is the same for $W(\{G\},q)$ and $W_r(\{G\},q)$. Because $P(G,q)$ is a polynomial with real (actually integer) coefficients, it follows that $\mathcal{B}$ is invariant under complex conjugation, i.e.,

$$\mathcal{B}(q)=\mathcal{B}(q^*). \tag{2.1}$$

A basic question is whether, for a given family $\{G\}$, some portion of the boundary $\mathcal{B}$ extends to complex infinity in the q plane, so that $W_r(\{G\},q)$ is nonanalytic at $1/q=0$ in the $1/q$ plane. Related to this, an important question is whether there is a general algorithm for producing a family $\{G\}$ of graphs such that in the $n\to\infty$ limit, the boundary $\mathcal{B}$ extends to complex infinity in the q plane. We answer this question in the affirmative and present the following algorithm.

Consider a family of graphs $\{G\}$. If this family already has the property that the limiting function $W(\{G\},q)$ has a region boundary $\mathcal{B}$ that extends to complex infinity in the q plane (i.e., to $1/q=0$ in the $1/q$ plane), then we have no work to do to get such a boundary. So assume that $\{G\}$ is such that $W(\{G\},q)$ has a region boundary $\mathcal{B}$ that does not extend to complex infinity in the q plane. As discussed in Ref. [13] [Sec. III and theorem 1, Eq. (3.1)] a rather general form for the chromatic polynomial of a graph G is

$$P(G_n,q)=q(q-1)\left\{c_0(q)+\sum_{j=1}^{N_a}c_j(q)a_j(q)^n\right\}, \tag{2.2}$$

where $c_j(q)$ and $a_j(q)$ are polynomials in q. Here the $a_j(q)$ and $c_{j\neq 0}(q)$ are independent of n, while $c_0(q)$ may contain n-dependent terms, such as $(-1)^n$, but does not grow with n like a^n. Obviously, the reality of $P(G,q)$ for real q implies that $c_j(q)$ and $a_j(q)$ are real for real q. The condition that $\mathcal{B}$ does not extend an infinite distance from the origin in the q plane is equivalent to the condition that for sufficiently large $|q|$, there is one leading term $a_j(q)$ in Eq. (2.2). Here we recall that "leading term $a_\ell(q)$ at a point q" was defined in Ref. [13] as a term satisfying $|a_\ell(q)|\geq 1$ and $|a_\ell(q)|>|a_j(q)|$ for $j\neq\ell$. If the c_0 term is absent and $N_a=1$, then the sole $a_1(q)$ may be considered to be leading even if $|a_j(q)|<1$. We require sufficiently large $|q|$ so that, for our analysis, there is a switching between only two leading terms a_ℓ. In principle there might be such a switching between more than two, so that $\mathcal{B}$ would include more than two components running to complex infinity in the q plane. However, for the families that we have constructed via our algorithm and studied, we find, for sufficiently large $|\mathrm{Im}(q)|$, only two such components. As required by the symmetry (2.1), these components are mapped to each other under complex conjugation. Now adjoin a complete graph K_p to G_n in such a way that each vertex in K_p is adjacent, i.e., connected by bonds (edges), to each of the vertices of G_n. Here, recall that a p-vertex graph is defined as "complete" and labeled K_p if each vertex is completely connected by bonds with all the other vertices of the K_p graph. Denote the resultant graph as $(K_p\times G_n)$. A basic theorem of graph theory states that if a graph H is obtained by adjoining a vertex to a graph G such that this point is adjacent to all of the vertices of G, then the chromatic polynomials are related according to

$$P(H,q)=qP(G,q-1). \tag{2.3}$$

Applying this iteratively p times, we obtain the result that

$$P(K_p\times G_n,q)=\left[\prod_{s=0}^{p-1}(q-s)\right]P(G_n,q-p). \tag{2.4}$$

Next, we select one vertex in K_p and remove b bonds connecting it to other vertices of K_p. Since each vertex of K_p has $p-1$ bonds connecting it to other vertices of K_p, this implies that we can only remove this many such bonds, i.e.,

$$1\leqslant b\leqslant p-1. \tag{2.5}$$

We denote the resultant graph as $(K_p\times G_n)_{rb}$, where the subscript signifies the above removal (r) of b bonds. In order for this to be nontrivial, i.e., for $b\geqslant 1$, we thus require that

$$p\geqslant 2. \tag{2.6}$$

The conditions (2.6) and (2.5) will be assumed henceforth. Using Eq. (2.4) and r applications of the addition-contraction theorem [15], we obtain the important result

$$\begin{aligned}P((K_p\times G_n)_{rb},q)&=P(K_p\times G_n,q)+bP(K_{p-1}\times G_n,q)\\&=\left[\prod_{s=0}^{p-2}(q-s)\right]\{[q-(p-1)]\\&\quad\times P(G_n,q-p)+bP(G_n,q-(p-1))\}.\end{aligned} \tag{2.7}$$

This is our general formula for the chromatic polynomial of $(K_p\times G_n)_{rb}$, for an arbitrary n-vertex graph G_n. Substituting the expression (2.2), we obtain

$$\begin{aligned}P((K_p\times G_n)_{rb},q)=&\left[\prod_{s=0}^{p-2}(q-s)\right]\left[(q-p+1)(q-p)(q-p-1)\left\{c_0(q-p)+\sum_{j=1}^{N_a}c_j(q-p)a_j(q-p)^n\right\}\right.\\&\left.+b(q-p+1)(q-p)\left\{c_0(q-p+1)+\sum_{j=1}^{N_a}c_j(q-p+1)a_j(q-p+1)^n\right\}\right].\end{aligned} \tag{2.8}$$

B. Boundary $\mathcal{B}$ for $\{(K_p\times G)_{rb}\}$

We denote the $n\to\infty$ limit of the families $K_p\times G_n$ and $(K_p\times G_n)_{rb}$ as

$$\lim_{n\to\infty}K_p\times G_n=\{K_p\times G\} \tag{2.9}$$

and

$$\lim_{n\to\infty}(K_p\times G_n)_{rb}=\{(K_p\times G)_{rb}\}, \tag{2.10}$$

respectively. As discussed in Ref. [13], the boundary $\mathcal{B}$ for $W(\{G\},q)$ is the locus of points in the q plane where there is a switching between different leading terms a_{ℓ} in Eq. (2.2). Since $\{G\}$ was assumed not to have $\mathcal{B}$ extending to infinity in the q plane, it follows that for large enough $|q|$, there is a single leading term $|a_{\ell}(q)|$ in Eq. (2.2). Hence from Eq. (2.8), we see that at sufficiently large $|q|$, the boundary $\mathcal{B}$ for the limiting function $W(\{K_p\times G)_{rb}\},q)$ is determined by the equality

$$|a_{\ell}(q-p)|=|a_{\ell}(q-p+1)|. \tag{2.11}$$

Note that this is independent of b, so that

$$\mathcal{B}\text{ is independent of } b \text{ for } \{(K_p\times G)_{rb}\} \tag{2.12}$$

[given that the basic condition (2.5) is satisfied]. Let $q=q_R+iq_I$. One can next enumerate the various cases possible for $a_{\ell}(q)$. The basic theorem that the coefficient of the highest-order term, q^n, in the chromatic polynomial $P(G_n,q)$ of any n-vertex graph G_n is unity implies that if a dominant term $a_{\ell}(q)$ is a polynomial of degree $s_{\max}$,

$$a_{\ell}(q)=\sum_{s=0}^{s_{\max}}\alpha_s q^s \tag{2.13}$$

then

$$\alpha_{s_{\max}}=1. \tag{2.14}$$

Consider, for example, the case where $a_{\ell}(q)$ is a linear function of q: $a_{\ell}(q)=\alpha_1 q+\alpha_0$, which reduces to $a_{\ell}(q)=q+\alpha_0$ by Eq. (2.14). Then Eq. (2.11) yields

$$q_R=p-(\tfrac{1}{2}+\alpha_0)\quad\text{for } s_{\max}=1 \tag{2.15}$$

with q_I undetermined, i.e., a vertical line segment extending to $\pm i\infty+p-(\frac{1}{2}+\alpha_0)$ in the complex q plane. This type of behavior is exemplified by graphs involving K_p adjoined to trees or chains of triangles, in which one bond in the K_p subgraph is removed. We shall discuss these below.

If $a_{\ell}(q)$ is a quadratic function of q, $a_{\ell}(q)=q^2+\alpha_1 q+\alpha_0$, then Eq. (2.11) yields an equation that has, as its only acceptable solution,

$$q_R=p-\tfrac{1}{2}(1+\alpha_1) \quad \text{as } |q_I|\to\infty \quad \text{for } s_{\max}=2. \tag{2.16}$$

Hence, the boundary $\mathcal{B}$ in this case is, for sufficiently large $|q_I|$, again a vertical line in the complex q plane located at the value of q_R given by Eq. (2.16) and extending to $\pm i\infty$. This type of behavior is exemplified in our discussion below of graphs involving K_p adjoined to chains of squares (i.e., ladder graphs) with various boundary conditions, in which r bonds are removed from the K_p subgraph in the manner discussed above. In general, as we shall show, if one adjoins K_p to an open chain of k-gons arranged such that two adjacent k-gons intersect along one of their mutual edges, then the resultant chromatic polynomial has the form (2.8) with $s_{\max}=k-2$ and $c_0(q)=0$ (there should be no confusion in the notation of k for the k-gons and K for K_p).

This, then, is the algorithm for producing families of graphs depending on three parameters, p, b, and n, with the property that the limiting function W_r is nonanalytic at $1/q=0$. We have proved this by calculating first the chromatic polynomials for finite graphs and then their respective limiting functions W. The key ingredients in the construction are, first, the adjoining of the complete graph K_p to G_n, and second, the removal of b of the bonds connecting one vertex in K_p to other vertices of K_p. Together, these guarantee, via Eq. (2.7), that the equation for the degeneracy of the leading term a_{ℓ} is of the form (2.11), and the locus of points that solve this degeneracy equation extends to complex infinity in the q plane, as we have shown.

We next give some illustrations of the application of this algorithm.

III. FAMILIES OF GRAPHS WITH W_r NONANALYTIC AT $1/q=0$

A. $(K_p\times T_n)_{rb}$

Perhaps the simplest illustration is for the family $K_p\times T_n$ formed by adjoining a succession of p vertices to each of the n vertices of a tree graph T_n and to each other. Removing b bonds connecting a vertex of K_p to other vertices of K_p in the manner described above yields the graph $(K_p\times T_n)_{rb}$. From Eq. (2.7), we calculate

$$P((K_p\times T_n)_{rb},q)=\left[\prod_{s=0}^{p}(q-s)\right][(q-p-1)^{n-1}+b(q-p)^{n-2}]. \tag{3.1}$$

Our general analysis in Eqs. (2.11)–(2.15) applies with $s_{\max}=1$, $\alpha_0=-1$, and $c_0(q)=0$ so that, from the general formula (2.15) we have

$$q_R=p+\tfrac{1}{2} \quad \text{for } G=(K_p\times T)_{rb}. \tag{3.2}$$

Hence, the boundary $\mathcal{B}$ consists of the vertical line (3.2) with $-i\infty\le q_I\le i\infty$. The diagram describing the regions of analyticity of the limiting function $W(\{(K_p\times T)_{rb}\},q)$ consists of two regions,

$$R_1:\mathrm{Re}(q)>p+\tfrac{1}{2} \tag{3.3}$$

and

$$R_2:\mathrm{Re}(q)<p+\tfrac{1}{2}. \tag{3.4}$$

Mapped to the $1/q$ plane (a conformal transformation), the image of the vertical line is a closed curve, which crosses the real axis at the inverse of q_R in Eq. (3.2) and at the origin. In the $1/q$ plane, the image of region R_1 is a compact region enclosed by this closed curve, while its complement is the image of the region R_2. We find that

$$W(\{(K_p\times T)_{rb}\},q)=q-p \quad \text{for } q\in R_1, \tag{3.5}$$

i.e., $W_r(\{(K_p\times T)_{rb}\},q)=1-p/q$. For $q\in R_2$, if q is real, $P((K_p\times T_n)_{rb},q)$ alternates in sign as n increases through even and odd integers, so, strictly speaking, the limit as $n\to\infty$ does not exist. Of course, there is also a corresponding variation in phases in this limit for the case of complex $q\in R_2$. As we have discussed before, in such a situation, at least the magnitude does have a well-defined limit:

$$|W(\{(K_p\times T)_{rb}\},q)|=|q-p-1| \quad \text{for } q\in R_2 \tag{3.6}$$

or equivalently $|W_r(\{(K_p\times T)_{rb}\},q)|=|1-(p+1)/q|$. This simple example thus explicitly illustrates the nonanalyticity at $1/q=0$; even aside from the choice of the phase in region R_2, the two expressions above for the magnitude of the reduced W_r functions are different. The nonanalyticity in the W_r function thus involves [for any choice of phases in Eq. (1.3) in R_2] a discontinuity in the first derivative dW_r/dz, where $z=1/q$ at $z=0$.

Although these are all exact results for the $n\to\infty$ limit, it is of some interest to see how these boundaries develop by studying chromatic zeros for finite n. Here, we recall the definition that the ''chromatic zeros'' of a graph G are the zeros of the chromatic polynomial $P(G,q)$ for this graph. We carried out these types of studies for a number of families of graphs in Refs. [13] and [16]. A general question that we investigated was the following: excluding a well-understood subset of chromatic zeros at certain discrete real integer values, and considering the remainder, how close are these remaining zeros, for finite n, to the boundary $\mathcal{B}$ that obtains in the $n\to\infty$ limit? From our study of the bipyramid graph, in Ref. [13] (see also Ref. [14]), it was found that the chromatic zeros near to the real axis in the q plane (aside from the discrete zeros at $q=0$ and 1 and a zero very near to $q=Be_5=2.618,\ldots$) lie on or near to the arcs forming the boundary curves $\mathcal{B}(R_1,R_3)$ and $\mathcal{B}(R_2,R_3)$ [defined in greater generality in Eqs. (3.11), (3.12) below], but the outer zeros do not lie very close to the line segments of $\mathcal{B}(R_1,R_2)$, given by the $p=2$ special case of Eq. (3.13) below, and only approach these line segments slowly as n increases. We inferred that this latter behavior was connected with the fact that this component of the boundary extends to complex infinity in the q plane and observed that this type of deviation

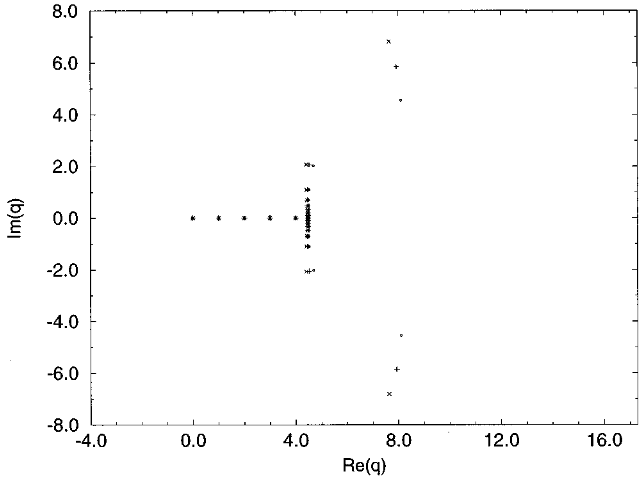

FIG. 1. Chromatic zeros of $(K_p\times T_n)_{rb}$ for $p=4$, $n=18$, and $b=1$ $(\cdot)$, 2 $(+)$, and 3 $(\times)$, where the symbols for the points are given in parentheses. In the $n\to\infty$ limit, our exact results give the continuous region boundary $\mathcal{B}$ as the $p=4$ special case of Eq. (3.2), i.e., the vertical line with $\mathrm{Re}(q)=9/2$ and $\mathrm{Im}(q)$ arbitrary, independent of b by Eq. (2.12).

did not occur for families of graphs whose boundaries $\mathcal{B}$ were compact and did not extend to complex infinity.

Here we have carried out an analogous study of the chromatic zeros of $(K_p\times T_n)_{rb}$ and we find similar behavior as a function of n. Since an interesting feature here is the dependence of the locations of chromatic zeros on b, we focus on this. In Fig. 1 we show the results for $p=4$ and $n=18$ for $b=1$,2, and 3, the full range allowed by Eq. (2.5). The outermost zero and its complex conjugate do not lie very near to the vertical line with $q_R=9/2$ given by the $p=4$ special case of Eq. (3.2). As b increases from 1 to 3, this outermost zero moves to larger $|q_I|$ and slightly smaller q_R, and hence slowly toward the above-mentioned vertical line. From Eq. (3.1), it follows that for $p=4$, there are also discrete chromatic zeros at $q=0,\ 1,\ 2,\ 3$, and 4, and these are evident in Fig. 1.

B. $(K_p\times C_n)_{rb}$

A second illustration is provided by the family of graphs $(K_p\times C_n)_{rb}$ obtained by starting with the p-wheel $K_p\times C_n$ with $p\geqslant 2$, where C_n is the n-vertex circuit graph, and removing b bonds connecting a vertex in K_p to other vertices in K_p. From the general formula Eq. (2.7) we calculate

$$P((K_p\times C_n)_{rb},q)=\left[\prod_{s=0}^{p-2}(q-s)\right][(q-p+1)(q-p-1)\times\{(q-p-1)^{n-1}+(-1)^n\}+b(q-p)\{(q-p)^{n-1}+(-1)^n\}]. \quad (3.7)$$

Our general analysis in Eqs. (2.11)–(2.15) applies with $s_{\max}=1$ and $\alpha_0=-1$ so that again, for sufficiently large $|q|$, $\mathcal{B}$ contains the vertical lines extending to $\pm i\infty$ with $q_R=p+1/2$, as was the case with $W(\{(K_p\times T)_{rb}\},q)$. However, because the $c_0(q)$ terms are nonzero in this case, the region boundaries in the vicinity of the real axis differ from the simple vertical line found for $W(\{(K_p\times T)_{rb}\},q)$. By methods similar to those that we used in Ref. [13] (i.e., working out the conditions for the degeneracy of the leading terms in P), we find that the region diagram for $W(\{(K_p\times C)_{rb}\},q)$ consists of three regions:

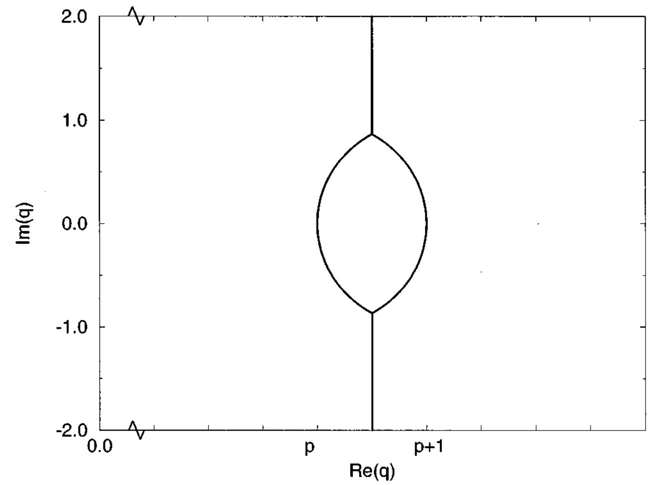

FIG. 2. Diagram showing regional boundaries comprising $\mathcal{B}$ for $W(\{(K_p\times C)_{rb}\},q)$. Breaks in the horizontal axis indicate that p is an arbitrary integer $\geqslant 2$.

$$R_1:\ \mathrm{Re}(q)>p+\tfrac{1}{2}\quad\text{and}\quad |q-p|>1, \quad (3.8)$$

$$R_2:\ \mathrm{Re}(q)<p+\tfrac{1}{2}\quad\text{and}\quad |q-(p+1)|>1, \quad (3.9)$$

and

$$R_3:\ |q-p|<1\quad\text{and}\quad |q-(p+1)|<1. \quad (3.10)$$

The boundaries between these regions are thus the two circular arcs

$$\mathcal{B}(R_1,R_3):q=p+e^{i\theta},\quad -\frac{\pi}{3}<\theta<\frac{\pi}{3} \quad (3.11)$$

and

$$\mathcal{B}(R_2,R_3):q=p+1+e^{i\phi},\quad \frac{2\pi}{3}<\phi<\frac{4\pi}{3} \quad (3.12)$$

together with the semi-infinite vertical line segments

$$\mathcal{B}(R_1,R_2)=\{q\}:Re(q)=p+\tfrac{1}{2}\quad\text{and}\quad |\mathrm{Im}(q)|>\frac{\sqrt{3}}{2}. \quad (3.13)$$

These meet at the intersection points

$$q_{int.}=p+\frac{1}{2}\pm i\frac{\sqrt{3}}{2}. \quad (3.14)$$

The arcs $\mathcal{B}(R_1,R_3)$ and $\mathcal{B}(R_2,R_3)$ cross the real axis at $q=p+1$ and $q=p$, respectively. The region diagram for $W(\{(K_p\times C)_{rb}\},q)$ is shown in Fig. 2.

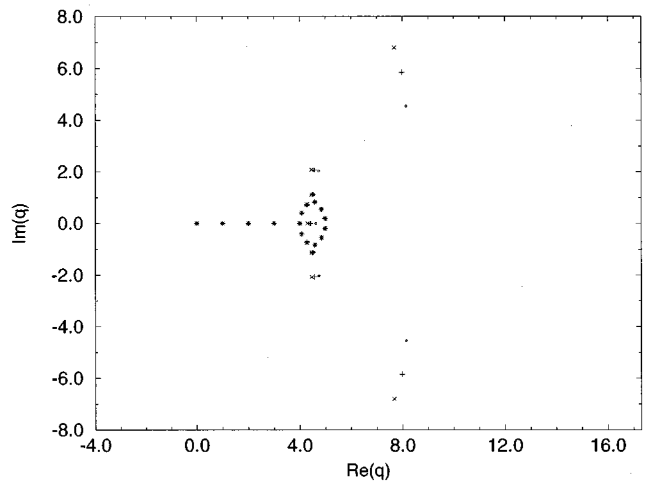

FIG. 3. Chromatic zeros of $(K_p \times C_n)_{rb}$ for $p=4$, $n=18$, and $b=1$ $(\cdot)$, 2 $(+)$, and 3 $(\times)$. In the $n\to\infty$ limit, our exact results give the continuous region boundary $\mathcal{B}$ as the $p=4$ special case of Fig. 2.

Mapped to the $1/q$ plane, the image of the vertical line is a curve in the right-hand half-plane, which passes vertically through the origin, enclosing the image of R_1. The enclosed region R_3 remains enclosed, while the left-hand region R_2 in the q plane maps to the region exterior to the images of R_1 and R_3 in the $1/q$ plane. The case $p=2$ is the bipyramid family of graphs [13,14]. We find that

$$W(\{(K_p \times C)_{rb}\},q) = q-p \quad \text{for } q \in R_1. \tag{3.15}$$

For the other regions, we have, in general,

$$|W(\{(K_p \times C)_{rb}\},q)| = \begin{cases} |q-(p+1)| & \text{for } q \in R_2 \\ 1 & \text{for } q \in R_3. \end{cases} \tag{3.16}$$

The W_r functions in regions R_1 and R_2 are the same as those in the corresponding regions for the previous family, $\{(K_p \times T)_{rb}\}$, while region R_3 has no analog for that family. As before, the nonanalyticity in W_r is most conveniently discussed in the $1/q$ plane. There are two regions contiguous across the image of $\mathcal{B}$ at the origin, $1/q=0$, namely, the images under inversion of regions R_1 and R_2. The nature of the nonanalyticity in W_r at $1/q=0$ is the same as that in the $\{(K_p \times T)_{rb}\}$ family.

Again, it is of interest to calculate the chromatic zeros for some finite graphs in these families and see how close they lie to the locus of zeros in the $n\to\infty$ limit. We have carried out such a study. As an illustration, in Fig. 3, we show the chromatic zeros for $(K_p \times C_n)_{rb}$ with $p=4$, and $n=18$ for $b=1$, 2, and 3. This may be compared with the $p=4$ special case of the plot of the region diagram in Fig. 2 [which is the same for all b, by the result (2.12)]. Note that the discrete chromatic zeros at $q=0$, 1, 2, and 3 are not part of the continuous locus of zeros forming $\mathcal{B}$ in the $n\to\infty$ limit. For comparison, the previously mentioned bipyramid graph is the case $p=2$, for which only the single value $b=1$ is allowed. We find that the complex chromatic zeros near the real axis lie on or close to the arcs $\mathcal{B}(R_1,R_3)$ and $\mathcal{B}(R_2,R_3)$, but the outer zeros do not lie very close to the line segments of $\mathcal{B}(R_1,R_2)$ given by the $p=4$ special case of (3.13), namely, $q_R=9/2$, $|q_I| \geq \sqrt{3}/2$ and only approach these line segments slowly as n increases. Evidently, the behavior of the chromatic zeros as functions of b is qualitatively similar to that which we observed in Fig. 1. We have carried out analogous studies of the chromatic zeros for other families of graphs constructed via our algorithm to have region boundaries $\mathcal{B}$ extending to complex infinity and have found similar results.

C. $[K_p \times (Ch)_{k,n}]_{rb}$

We define an open chain of m k-gons constructed such that a given k-gon intersects with the next k-gon in the chain along one of their mutual edges as $(Ch)_{k,n}$ where the number of vertices is

$$n=(k-2)m+2. \tag{3.17}$$

The chromatic polynomial for the open chain of m k-gons is

$$P((Ch)_{k,n},q) = q(q-1)D_k(q)^m, \tag{3.18}$$

where

$$D_k(q) = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s}. \tag{3.19}$$

Next, consider the graph $K_p \times (\mathrm{Ch})_{k,n}$ obtained by adjoining K_p to the chain of m k-gons, $(\mathrm{Ch})_{k,n}$, where n is again given by Eq. (3.17). From Eq. (2.4), we have

$$P(K_p \times (\mathrm{Ch})_{k,n},q) = \left[\prod_{s=0}^{p+1} (q-s)\right] D_k(q-p)^m. \tag{3.20}$$

The chromatic polynomial $P([K_p \times (\mathrm{Ch})_{k,n}]_{rb},q)$ is then obtained by substitution of Eq. (3.20) into Eq. (2.7). Note that

$$D_k(q) = a_{\ell}(q) \tag{3.21}$$

in Eqs. (2.8), (2.11), and (2.13) general class of graphs. From the above substitution, we find that the resultant chromatic polynomial is of the form (2.8) with

$$c_0(q)=0, \quad s_{\max}=k-2 \quad \text{for } [K_p \times (\mathrm{Ch})_{k,n}]_{rb}. \tag{3.22}$$

For sufficiently large $|q_I|$, the region boundary $\mathcal{B}$ for $W(\{[K_p \times (\mathrm{Ch})_k]_{rb}\},q)$ consists of complex-conjugate vertical line segments extending to $\pm i\infty$ with $Re(q)=q_R$ equal to

$$q_R = p + \frac{k}{2(k-2)} \quad \text{for } \{[K_p \times (\mathrm{Ch})_k]_{rb}\} \quad \text{with } k \geq 3 \tag{3.23}$$

where the notation convention of Eq. (2.10) is used. Note that if one considers chains of k-gons with k progressively larger and larger, this approaches the limit $\lim_{k\to\infty} q_R = p+1/2$. As defined in the Introduction, the region to the right of this boundary is R_1, and we denote the region to the left as R_2. In general (in particular, for $k \geq 5$)

there will be other regions within which $W(\{[K_p \times(\mathrm{Ch})_k]_{rb}\},q)$ is analytic but we only need R_1 and R_2 for our discussion of the nonanalyticity at $1/q=0$ since it is only the images under inversion of these two regions that border the origin of the $1/q$ plane. For the resultant limiting functions W we calculate

$$W(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)=D_k(q-p+1)^{1/(k-2)} \quad \text{for } q\in R_1, \tag{3.24}$$

$$|W(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)|=|D_k(q-p)|^{1/(k-2)} \quad \text{for } q\in R_2. \tag{3.25}$$

Hence

$$W_r(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)=\left(1-\frac{p-1}{q}\right)\left[\sum_{s=0}^{k-2}(-1)^s\binom{k-1}{s}(q-p+1)^{-s}\right]^{1/(k-2)} \quad \text{for } q\in R_1, \tag{3.26}$$

$$|W_r(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)|=\left|\left(1-\frac{p}{q}\right)\left[\sum_{s=0}^{k-2}(-1)^s\binom{k-1}{s}(q-p)^{-s}\right]\right|^{1/(k-2)} \quad \text{for } q\in R_2. \tag{3.27}$$

For $k\geqslant 4$, these have the expansions near $1/q=0$

$$W_r(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)=1-\left(p-1+\frac{k-1}{k-2}\right)q^{-1}+O(q^{-2}) \quad \text{as } 1/q\to 0 \quad \text{with } q\in R_1 \tag{3.28}$$

(e.g., $1/q\to 0^+$ through real values) and

$$|W_r(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)|=\left|1-\left(p+\frac{k-1}{k-2}\right)q^{-1}+O(q^{-2})\right| \quad \text{as } 1/q\to 0 \quad \text{with } q\in R_2. \tag{3.29}$$

These expressions also apply for the case $k=3$ but terminate with the $O(q^{-1})$ term, since $D_3(q)$ is linear and the exponent $1/(k-2)$ in Eqs. (3.24) and (3.25) is just unity. Thus, for all $k\geqslant 3$, these results indicate explicitly the nature of the nonanalyticity of the reduced function $W_r(\{[K_p\times(\mathrm{Ch})_k]_{rb}\},q)$ at $1/q=0$. As in our earlier examples, this nonanalyticity involves, in general, the sudden onset of a complex phase and apart from this, even for the magnitude, a discontinuity in the first derivative dW_r/dz at $z=1/q=0$.

Since the lowest two cases, $k=3,4$ exhibit particularly simple boundaries $\mathcal{B}$, we give a few explicit results for them. For $k=3$ we find

$$P([K_p\times(\mathrm{Ch})_{3,n}]_{rb},q)=\left[\prod_{s=0}^{p}(q-s)\right][(q-p-1)(q-p-2)^m+b(q-p-1)^m], \tag{3.30}$$

where from Eq. (3.17), $m=n-2$. This has the form of our general Eq. (2.8) with linear $a_{\not\ell}(q)$, $\alpha_0=-2$, and $c_0(q)=0$ so that in the $n\to\infty$ limit, by Eq. (2.15), it follows that the boundary $\mathcal{B}$ consists of the vertical line

$$q_R=p+\tfrac{3}{2} \quad \text{for } \{[K_p\times(\mathrm{Ch})_3]_{rb}\}. \tag{3.31}$$

The general formulas (3.26) and (3.27) reduce to the simple expressions

$$W_r(\{[K_p\times(\mathrm{Ch})_3]_{rb}\},q)=1-\frac{p+1}{q} \quad \text{for } q\in R_1 \tag{3.32}$$

and

$$|W_r(\{[K_p\times(\mathrm{Ch})_3]_{rb}\},q)|=\left|1-\frac{p+2}{q}\right| \quad \text{for } q\in R_2. \tag{3.33}$$

For the $k=4$ case, $D_4(q)=a_{\not\ell}(q)=q^2-3q+3$, so that Eq. (3.23) or the quadratic special case Eq. (2.16) with $\alpha_1=-3$ and $c_0(q)=0$ applies and yields

$$q_R=p+1 \quad \text{for } W(\{[K_p\times(\mathrm{Ch})_4]_{rb}\},q). \tag{3.34}$$

Using Eqs. (3.20) and (2.7), we determine that the region boundary of $W(\{[K_p\times(\mathrm{Ch})_4]_{rb}\},q)$ is again precisely the vertical line with q_R given by Eq. (3.34) and $|q_I|$ arbitrary. Note that this holds even though $D_4(q)=a_{\not\ell}(q)$ is quadratic. However, the generic behavior for higher k is that in the vicinity of the real axis, $\mathcal{B}$ is more complicated, and the complex-conjugate vertical line segments with q_R given by Eq. (3.23) apply for $|q_I|>\kappa_k$, where κ_k is a k-dependent constant.

From Eqs. (3.26) and (3.27) we have

$$W_r(\{[K_p\times(\mathrm{Ch})_4]_{rb}\},q) =[1-(2p+1)q^{-1}+(p^2+p+1)q^{-2}]^{1/2} \quad \text{for } q\in R_1 \tag{3.35}$$

and

$$|W_r(\{[K_p\times(\mathrm{Ch})_4]_{rb}\},q)| = |[1-(2p+3)q^{-1}+(p^2+3p+3)q^{-2}]|^{1/2} \quad \text{for } q\in R_2. \tag{3.36}$$

D. $(K_p\times L_{n,bc})_{rb}$

A slightly more complicated illustration is provided by starting with an n-vertex ladder graph, i.e., chain of squares, as in the $k=4$ case discussed above, but with periodic or twisted boundary conditions (rather than open boundary conditions) denoted $L_{n,\mathrm{pbc}}$ and $L_{n,\mathrm{tbc}}$, respectively. Note that any even number of twists is equivalent to no twist and any odd number of twists is equivalent to one twist. Following our general algorithm in (2.7), we adjoin K_p to this ladder graph and then remove b of the bonds connecting a vertex in the K_p graph to other vertices in K_p. Using the basic results

$$P(L_{n,\mathrm{pbc}},q)=(q^2-3q+3)^{n/2}+(q-1)\times\{(3-q)^{n/2}+(1-q)^{n/2}\}+q^2-3q+1 \tag{3.37}$$

and

$$P(L_{n,\mathrm{tbc}},q)=(q^2-3q+3)^{n/2}+(q-1)\times\{(3-q)^{n/2}-(1-q)^{n/2}\}-1 \tag{3.38}$$

we can apply our general analysis above. First, we note that because the terms raised to the nth power, which can be leading terms as discussed in conjunction with Eq. (2.2), are the same for $P(L_{n,\mathrm{pbc}},q)$ and $P(L_{n,\mathrm{tbc}},q)$, it follows that

$$W(\{(K_p\times L_{\mathrm{pbc}})_{rb}\},q)=W(\{(K_p\times L_{\mathrm{tbc}})_{rb}\},q) \tag{3.39}$$

and hence the boundaries $\mathcal{B}$ are identical for these two functions. In both cases, from our general results, it follows that $\mathcal{B}$ contains complex-conjugate vertical line segments that extend to $\pm i\infty$ with

$$q_R=p+1 \tag{3.40}$$

as for the case of free boundary conditions, Eq. (3.34). These line segments extend outward to $q_I=\pm\infty$ from the intersection points

$$q_{\mathrm{int}},q_{\mathrm{int}}^*=p+1\pm i\sqrt{3}. \tag{3.41}$$

At these intersection points, the boundary bifurcates into two, which extend down and cross the real axis at

$$q_{R,\mathrm{cross}}=p,p+\sqrt{2}. \tag{3.42}$$

In Fig. 4 we show a plot of the region diagram for $W(\{(K_p\times L_{\mathrm{pbc}})_{rb}\},q)=W(\{(K_p\times L_{\mathrm{tbc}})_{rb}\},q)$; again, by Eq. (2.12), it is independent of b.

IV. A GENERAL CONDITION GOVERNING THE (NON)ANALYTICITY OF $W_r(\{G\},q)$ AT $1/q=0$

As we stated at the end of Sec. II, the key ingredient in our algorithm to construct families of graphs $\{G\}$ with the property that $\mathcal{B}$ extends to complex infinity in the q plane

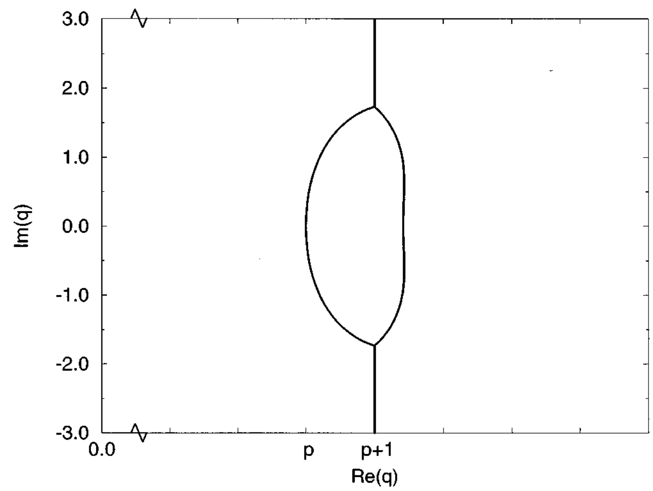

FIG. 4. Diagram showing regional boundaries comprising $\mathcal{B}$ for $W(\{(K_p\times L_{\mathrm{xbc}})_{rb}\},q)$ where xbc denotes periodic or twisted boundary conditions (pbc, tbc). Breaks in the horizontal axis indicate that p is an arbitrary integer ≥ 2.

and hence that $W_r(\{G\},q)$ is nonanalytic at $1/q=0$ is to produce a chromatic polynomial with the feature that there are two leading terms with a degeneracy condition (2.11). From Eq. (2.7), these leading terms are actually the same function, just evaluated at arguments that differ by unity, as is evident in Eq. (2.11). Here we generalize from this study to state the following theorem:

Theorem. Consider a family of n-vertex graphs and its $n\to\infty$ limit $\{H\}$. With $P(H_n,q)$ in the form of Eq. (2.2), the region boundary $\mathcal{B}$ of the resultant asymptotic limiting function $W(\{H\},q)$ extends to complex infinity in the q plane, and hence $W_r(\{H\},q)$ is nonanalytic at $1/q=0$ in the $1/q$ plane, if and only if the locus of solutions of the degeneracy condition of leading terms

$$|a_{\ell}(q)|=|a'_{\ell}(q)| \tag{4.1}$$

extends to complex infinity.

Of course, this locus of points obeys the condition (2.1). Our algorithm yields the family of graphs $(K_p\times G_n)_{rb}$, depending on p and b, whose $n\to\infty$ limit, $\{(K_p\times G)_{rb}\}$ satisfies the above condition.

A general feature of our results is that for the families of graphs we have constructed and studied, for which $\mathcal{B}$ extends to complex infinity in the q plane, the image, under inversion, of $\mathcal{B}$ passes through the origin of the $1/q$ plane with an infinite tangent, i.e., vertically. This reflects the property that the portion of $\mathcal{B}$ that extends to complex infinity is comprised of a vertical line segment and its complex conjugate, with a fixed value of $Re(q)$.

One salient feature of our study is clearly that none of our families of graphs with $W_r(\{G\},q)$ nonanalytic at $1/q=0$ is a regular lattice graph. Our results are therefore consistent with the assumption underlying the original series calculations, that a sufficient condition for $W_r(\{G\},q)$ to be analytic at $1/q=0$ is that $\{G\}$ be a regular lattice graph Λ. We state this formally as the following conjecture:

Conjecture: Let $\{G\}$ denote the infinite-n limit of a family of graphs G_n. A sufficient condition for the resultant reduced functions $W_r(\{G\},q)$ to be analytic at $1/q=0$ is that $\{G\}$ is a regular lattice graph $\{G\}=\Lambda$.

It is clear from Ref. [13] that the property that $\{G\}$ be a regular lattice is not a necessary condition for the associated $W_r(\{G\},q)$ to be analytic at $1/q=0$; in that work we calculated $W(\{G\},q)$ functions for a number of families $\{G\}$ which are not regular lattice graphs, but for which the corresponding $W_r(\{G\},q)$ functions are analytic at $1/q=0$.

For a regular lattice Λ with coordination number ζ, a natural reduced function is defined by

$$W(\{G\},q)=q(1-q^{-1})^{\zeta/2}\overline{W(}\Lambda,y) \tag{4.2}$$

for which the large-q Taylor series expansion is [10–12]

$$\overline{W(}\Lambda,y)=1+\sum_{n=1}^{\infty} w_{\Lambda,n}y^n, \quad y=\frac{1}{q-1}. \tag{4.3}$$

Clearly, $\overline{W(}\Lambda,y)$ is analytic at $y=0$ if and only if $W_r(\Lambda,q)$ is analytic at $1/q=0$. In Refs. [13,17,18] we have made detailed comparisons of existing large-q series expansions with high-precision Monte Carlo measurements of $W(\Lambda,q)$ as well as rigorous lower bounds that we have derived [19] and have found excellent agreement for $q\geqslant 4$ on a number of different lattices, including both homopolygonal (e.g., square and honeycomb) lattices and heteropolygonal Archimedean lattices (composed of regular polygons of more than one type, such that all vertices are equivalent), viz., the $4\cdot 8^2$ lattice, for which we have calculated a large-q series). This excellent agreement provides motivation to include lattices involving packings with different regular polytopes under the term ‘‘regular lattice’’ in the above conjecture (here, polytope is the general mathematical object that subsumes the polygon in two dimensions and polyhedron in three dimensions [20]).

V. CONCLUSIONS

In this paper we have addressed a fundamental problem in graph theory with important implications for statistical mechanics, namely, the question of the analyticity of $W_r(\{G\},q)$ at $1/q=0$. In order to understand the phenomenon of nonanalyticity of this function at $1/q=0$ better, we have constructed a general algorithm for producing infinitely many families of graphs, each depending on two parameters p and b, with W_r functions that are nonanalytic at $1/q=0$. We have studied the properties of several of these families. We have also stated a general necessary and sufficient condition on the chromatic polynomial of a family of graphs such that the resultant $W_r(\{G\},q)$ is nonanalytic at $1/q=0$. This condition explains the source of the nonanalyticity in the cases where it occurs. The results of our study are consistent with the conjecture that a sufficient condition (we know that this is not a necessary condition) for $W_r(\{G\},q)$ to be analytic at $1/q=0$ is that $\{G\}=\Lambda$ is a regular lattice graph.

ACKNOWLEDGMENT

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