Invariant Factors of Graphs associated with Hyperplane Arrangements

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Abstract

A matrix called Varchenko matrix associated with a hyperplane arrangement was defined by Varchenko in 1991. Matrices that we shall call q-matrices are induced from Varchenko matrices. Many researchers are interested in the invariant factors of these q-matrices. In this paper, we associate this problem with a graph theoretic model. We will discuss some general properties and give some methods for finding the invariant factors of q-matrices of certain types of graphs. The proofs are elementary. The invariant factors of complete graphs, complete bipartite graphs, even cycles, some hexagonal systems, and some polygonal trees are found.

Key words and phrases : q-matrix, invariant factors, bipartite graph, hyperplane arrangement.

AMS 1991 subject classification : 05C30, 05C12

1. Introduction and background

Let $\mathfrak{H} = \{H_1, \ldots, H_t\}$ be an *arrangement* (or a *configuration*) *of hyperplanes* in $\mathbb{R}^n$. Let $r(\mathfrak{H}) = \{R_1, \ldots, R_m\}$ be the sets of regions in the complement of the union of elements in $\mathfrak{H}$. For any regions $R_i, R_j \in r(\mathfrak{H})$, let $s(R_i, R_j)$ be the set of hyperplanes in $\mathfrak{H}$ which separate R_i from R_j. Varchenko in [17] defined a matrix $B = B(\mathfrak{H})$, with rows and columns indexed by the regions in $r(\mathfrak{H})$ and $(B)_{i,j} = \prod\limits_{H \in s(R_i,R_j)} a_H$, where a_H is an indeterminate called the *weight* assigned to the hyperplane H. B is called *Varchenko matrix* of the arrangement $\mathfrak{H}$.

Varchenko matrix first appeared in the work of Schechtman and Varchenko [7]. That paper was initially a chapter of [18]. The nullspaces of the Varchenko matrices for some values of the indeterminates a_H's are of particular interest [17]. When we let $a_H = q$ for all $H \in \mathfrak{H}$, then the Varchenko matrix becomes a matrix over $\mathbb{Q}[q]$ (sometimes we consider this matrix over the field $\mathbb{C}(q)$), which is an Euclidean domain. Let us call this matrix a *q-matrix*. We can define the Smith normal form† of the q-matrix [16]. Entries appearing in the diagonal of a Smith normal form of

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†Smith normal form was discovered by H.J.S. Smith.

a matrix are called invariant factors. Applications of invariant factors of a q-matrix can be found in [3].

We are going to associate the q-matrices of hyperplane arrangements with a graph theoretic model. All graphs under consideration are finite, connected and simple. Any undefined graph theoretic and algebraic terminologies and notations used in this paper may be found in any textbook, for example [1, 5].

Let $\mathfrak{H}$ be an arrangement of hyperplanes in $\mathbb{R}^n$, $r(\mathfrak{H})$ be defined above and B be the Varchenko matrix of $\mathfrak{H}$. If we set $a_H = q$ for all $H \in \mathfrak{H}$, then B becomes a matrix, say Q, whose entries are in $\mathbb{Q}[q]$ (in fact in $\mathbb{Z}[q]$). For any $R_i, R_j \in r(\mathfrak{H})$, the (i, j)-entry (or the (R_i, R_j)-entry) of Q is given by $Q_{i,j} = q^{n(R_i,R_j)}$, where $n(R_i, R_j)$ is the number of hyperplanes in $\mathfrak{H}$ which separate R_i from R_j. We define a graph $G(\mathfrak{H})$ whose vertex set is $r(\mathfrak{H})$. Two vertices (regions) are adjacent if their closures have an $(n-1)$-dimensional common boundary. $G(\mathfrak{H})$ is called the *graph* of $\mathfrak{H}$. It is easy to see that $G(\mathfrak{H})$ contains no odd cycles, i.e., $G(\mathfrak{H})$ is a (connected) bipartite graph. Moreover, $G(\mathfrak{H})$ contains a cycle unless all the hyperplanes are parallel. For any $R_i, R_j \in r(\mathfrak{H}) = V(G(\mathfrak{H}))$, let $x \in R_i$ and $y \in R_j$. Any connected curve joining x and y must pass through all the hyperplanes in $\mathfrak{H}$ which separate R_i and R_j at least once and there is a connected curve joining x and y passing through those hyperplanes exactly once. Thus $n(R_i, R_j)$ is the distance between R_i and R_j in $G(\mathfrak{H})$.

Let $D_G = (d_{i,j})$ (or simply D) be the distance matrix of a graph G under an ordering of vertices. Let $Q_G(q) = \left(q^{d_{i,j}}\right)$ (or simply $Q(q)$, Q_G or Q; sometimes denoted as q^D), where q is an indeterminate. $Q_G(q)$ is called the *q-matrix* of G (it is unique up to isomorphism). If G is a graph of an arrangement of hyperplanes $\mathfrak{H}$, then $Q_G(q)$ is the q-matrix of the Varchenko matrix of $\mathfrak{H}$. We call it the *q-matrix* of $\mathfrak{H}$.

In this paper, we shall determine the invariant factors of q-matrices of some graphs, which in particular give the determinants of those q-matrices. This is important for applications to quantum groups and Knizhnik-Zamolodchikov equations [2, 3, 7, 17, 18]. The invariant factors of complete graphs, complete bipartite graphs, even cycles, hexagonal graphs and polygonal trees are described in Sections 3, 5 and 6. Some relationships between q-matrix of a graph and its subgraphs are established in Section 4. All the proofs are elementary.

2. Examples and invariant factor of a graph

In this section, we shall give some examples of hyperplane arrangements and their associated graphs and q-matrices. Some basic properties of q-matrices of graphs are given.

Example 2.1: Let $\mathfrak{H} = \{H_1, H_2, H_3\}$ be an arrangement of hyperplanes in $\mathbb{R}^2$ and $r(\mathfrak{H}) =$

$\{R_1, R_2, \ldots, R_7\}$ described in Figure 2.1(a). This example is selected from Example 1.1 of [3]. The graph $G = G(\mathfrak{H})$ is described in Figure 2.1(b) and Q_G is given by

$$Q_G = \begin{pmatrix} 1 & q & q^2 & q^3 & q^2 & q & q \\ q & 1 & q & q^2 & q^3 & q^2 & q^2 \\ q^2 & q & 1 & q & q^2 & q^3 & q \\ q^3 & q^2 & q & 1 & q & q^2 & q^2 \\ q^2 & q^3 & q^2 & q & 1 & q & q \\ q & q^2 & q^3 & q^2 & q & 1 & q^2 \\ q & q^2 & q & q^2 & q & q^2 & 1 \end{pmatrix}.$$

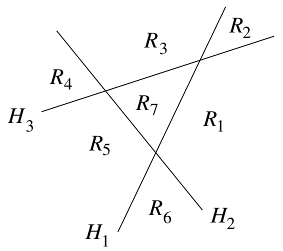

Figure 2.1(a): A hyperplane arrangement.

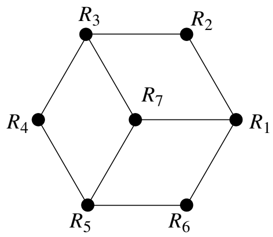

Figure 2.1(b): The graph of the arrangement.

Example 2.2: For $1 \leq i \leq n$, let $O_i = \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid x_i = 0\}$. Let $\mathfrak{O}_n = \{O_1, \ldots, O_n\}$ (see [2, 3]). Then $r(\mathfrak{O}_n)$ has 2^n regions and can be indexed by vectors $\alpha = (a_1, \ldots, a_n)$, where a_i is either 1 or -1. α corresponds to the region R_α which contains all points $(x_1, \ldots, x_n)$ where $x_i < 0$ if and only if $a_i = -1$. Then the graph of $\mathfrak{O}_n$ is isomorphic to the n-cube.

Example 2.3: For $1 \leq i < j \leq n$, let $H_{i,j} = H_{j,i} = \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid x_i = x_j\}$. Let $\mathfrak{A}_n = \{H_{i,j} \mid 1 \leq i < j \leq n\}$ (see [2, 3]). It is called the *braid arrangement*. Then $r(\mathfrak{A}_n)$ has $n!$ regions and can be indexed by permutations $\sigma \in S_n$. σ corresponds to the region $R_\sigma = \{(x_1, \ldots, x_n) \mid x_{\sigma(1)} < x_{\sigma(2)} < \cdots < x_{\sigma(n)}\}$. Then the graph of $\mathfrak{A}_n$ is isomorphic to the Cayley graph $\varGamma(S_n, T)$, where T is the generating set which is the set of all transpositions.

Let $Q_G(q) = Q$ be a q-matrix of a connected graph G of order n. Then Q is an $n \times n$ (symmetric) matrix over $\mathbb{Q}[q]$. There exist two invertible matrices U and V over $\mathbb{Q}[q]$ such that $UQV = \mathrm{diag}\{s_1(q), s_2(q), \cdots, s_n(q)\} = S(q)$ and $s_i(q)|s_{i+1}(q)$, $1 \leq i \leq n-1$, where $s_i(q) \in \mathbb{Q}[q]$. Since $Q(z)$ is not a zero matrix for any $z \in \mathbb{C}$, $\mathrm{rank}Q(z) \geq 1$. Hence $s_1(q) \in \mathbb{Q}$ (it can be assumed to be 1). $S(q)$ is called the *Smith normal form* of Q and the polynomials $s_i(q)$ are called the *invariant factors* of Q (see [4, p.79-84], [5, p.175-179], [6, p.63]). $S(q)$ and $s_i(q)$ are also called the *Smith normal form* and the *invariant factors* of G, respectively. We shall denote the **multiset** of all the invariant factors of G by $\mathrm{Inv}(G)$. From now on, all sets are considered as multisets and all the set operations are considered as multiset operations.

Example 2.4: Consider the arrangement given in Example 2.1. By using elementary row and column operations, we have

$$\mathrm{Inv}(G) = \left\{1,\ (1-q^2),\ (1-q^2),\ (1-q^2),\ (1-q^2)^2,\ (1-q^2)^2,\ (1-q^2)^2\right\}.$$

Theorem 2.1: *Let G be any graph. Then $1-q$ is a divisor of each invariant factor of G except the first one.*

Proof: It follows from $\mathrm{rank} Q_G(1) = 1$. □

Theorem 2.2: *Let G be a bipartite graph. If $f(q)$ is an irreducible divisor of an invariant factor of G with multiplicity α, then $f(-q)$ is an irreducible divisor of the same invariant factor with the same multiplicity α.*

Proof: Let (X, Y) be the bipartition of G. Let $X = \{x_1, \ldots, x_m\}$ and $Y = \{y_1, \ldots, y_n\}$. Let D be the distance matrix of G. We choose the order of vertices as $x_1, \ldots, x_m, y_1, \ldots, y_n$. Then $D = \left(\begin{smallmatrix} A_1 & B \\ B^T & A_2 \end{smallmatrix}\right)$, for some $A_1 \in M_m(\mathbb{Z})$, $A_2 \in M_n(\mathbb{Z})$ and $B \in M_{m,n}(\mathbb{Z})$. Since any entry of A_1 or A_2 is even and any entry of B is odd, $Q(-q) = \left(\begin{smallmatrix} q^{A_1} & -(q^B) \\ -(q^B)^T & q^{A_2} \end{smallmatrix}\right)$. Let $P = \left(\begin{smallmatrix} I_m & O_{m,n} \\ O_{n,m} & -I_n \end{smallmatrix}\right)$, where I_t is the $t \times t$ identity matrix and $O_{m,n}$ is the $m \times n$ zero matrix. Then $PQ(q)P = Q(-q)$. Therefore $Q(q)$ and $Q(-q)$ have the same invariant factors. □

Corollary 2.3: *Let G be a bipartite graph. Every invariant factor of G is of the form $f(q^2)$ for some $f(q) \in \mathbb{Q}[q]$. Hence $1-q^2$ is a divisor of each invariant factor of G except the first one.*

Corollary 2.4: *Let G be a bipartite graph. If $f(q)$ is an eigenvalue of Q_G for some expression f then so is $f(-q)$.*

Proof: Since P, defined in the proof of Theorem 2.2, is symmetric and orthogonal, the corollary follows. □

For any graph G, there are some questions:

1. What is the determinant of Q_G?
2. What are the multiplicities of $1-q$ and $1+q$ in the invariant factors of G respectively?
3. What is the spectrum of Q_G?
4. What is the Smith normal form of G?

There is a well-known method for computing the invariant factors of an $m \times n$ matrix over a principal ideal domain. This method can be found in many linear algebra or algebra textbooks, for example [5, p.175-179]. Before we state that theorem, we have to introduce some notation and terminology. Let A be an $m \times n$ matrix over a principal ideal domain, $r_1 < \cdots < r_t$, $c_1 < \cdots < c_t$, $t \le \min\{m, n\}$. Let $A\begin{bmatrix} r_1 & \cdots & r_t \\ c_1 & \cdots & c_t \end{bmatrix}$ denote the $t \times t$ submatrix obtained from A by deleting all rows except rows $r_1, \ldots, r_t$ and deleting all columns except columns $c_1, \ldots, c_t$. If $(r_1, \ldots, r_t) = (c_1, \ldots, c_t)$ then we simply denote it by $A[r_1 \ \cdots \ r_t]$. The determinant of $A\begin{bmatrix} r_1 & \cdots & r_t \\ c_1 & \cdots & c_t \end{bmatrix}$ is called a *t-rowed minor* of A. Two matrices A and B over a ring R are called *equivalent* if there are two invertible matrices U and V over R such that $B = UAV$.

Theorem 2.5: *Let A be an $m \times n$ matrix over a principal ideal domain $\mathbb{D}$ and suppose that the rank of A is r. Suppose $s_1, s_2, \ldots, s_r$ are the nonzero invariant factors of A. For each i, $1 \le i \le r$, let Δ_i be the g.c.d. of all the i-rowed minors of A. Then any set of invariant factors of A differ by unit multipliers from the elements $s_1 = \Delta_1,\ s_2 = \Delta_2\Delta_1^{-1},\ \ldots,\ s_r = \Delta_r\Delta_{r-1}^{-1}$.*

Note that the invariant factors are invariant up to equivalence. Also the invariant factors do not change if we consider A as a matrix over any principal ideal domain containing $\mathbb{D}$.

Let A be an $n \times n$ matrix over a principal ideal domain. If A is equivalent to a diagonal matrix B, then the multiset of entries in the diagonal of B is called a *pre-invariant factor set* of A. If A is a q-matrix of a graph G, then a pre-invariant factor set of A is called a *pre-invariant factor set* of G. The elements of such set are called *pre-invariant factors* of G. Clearly this set is not unique.

Corollary 2.6: *Let A be an $m \times n$ matrix of rank r over a principal ideal domain with nonzero invariant factors $s_1, s_2, \ldots, s_r$, where $s_i | s_{i+1}, 1 \le i \le r-1$. Suppose $\{f_1, \ldots, f_r, 0, \ldots, 0\}$ is a pre-invariant factor set of A, where $f_i \neq 0$. Let ϕ be an irreducible factor of $f_1 f_2 \cdots f_r$. Denote the multiplicities of ϕ in the factors f_j's by $0 \le a_1 \le a_2 \le \cdots \le a_r$. Then the multiplicity of ϕ in s_j is a_j.*

The sequence $a_1, a_2, \ldots, a_r$ is called the *multiplicity sequence* of ϕ with respect to $\{f_1, \ldots, f_r\}$. Because of Corollary 2.6, if the eigenvalues of Q_G are polynomials of q (over any extension field of $\mathbb{Q}$) then question 4 can be solved in principle.

3. Computational results of some bipartite graphs (1)

In this section, we give some examples to illustrate how to use Corollary 2.6 to find the invariants factors of some graphs.

3.1. Complete bipartite graphs

Let $J_{m,n}$ be the $m \times n$ matrix whose entries are 1 and let $J_n = J_{n,n}$. The q-matrix of $K_{m,n}$ is

$$Q = \left(\begin{array}{c|c} q^2 J_m + (1-q^2) I_m & q J_{m,n} \\ \hline q J_{n,m} & q^2 J_n + (1-q^2) I_n \end{array}\right).$$

After applying row operations $-q^2 r_1 + r_j$, $2 \le j \le m$; $-q r_1 + r_j$, $m+1 \le j \le m+n$ and the same column operations, Q becomes

$$Q_1 = \left(\begin{array}{cc|c} 1 & O_{1,m-1} & O_{1,n} \\ O_{m-1,1} & (1-q^2)(q^2 J_{m-1} + I_{m-1}) & q(1-q^2) J_{m-1,n} \\ \hline O_{n,1} & q(1-q^2) J_{n,m-1} & (1-q^2) I_n \end{array}\right).$$

For convenience, we omit to write the first row and first column of Q_1 and divide each of the remaining entries by $1-q^2$. After applying row operations $-q r_{m+j} + r_i$, $1 \le j \le n$, $2 \le i \le m$ and the same column operations, the matrix becomes

$$Q_2 = \left(\begin{array}{c|c} (1-n) q^2 J_{m-1} + I_{m-1} & O_{m-1,n} \\ \hline O_{n,m-1} & I_n \end{array}\right).$$

We omit to write the last n rows and columns of Q_2. Applying column operations $-c_3 + c_2$, $-c_4 + c_3$, $\ldots$, $-c_m + c_{m-1}$ and $r_3 + r_2$, $r_4 + r_3$, $\ldots$, $r_m + r_{m-1}$ in proper order, the matrix becomes

$$\left(\begin{array}{c|c} & (1-n)q^2 \\ & 2(1-n)q^2 \\ I_{m-2} & \vdots \\ & (m-2)(1-n)q^2 \\ \hline O_{1,m-2} & 1 + (m-1)(1-n)q^2 \end{array}\right).$$

After clearing the non-diagonal entries, the original matrix Q becomes

$$\mathrm{diag}\{1,\ \overbrace{1-q^2,\ \cdots,\ 1-q^2}^{m-2 \text{ times}},\ (1-q^2)(1-(m-1)(n-1)q^2),\ \overbrace{1-q^2,\ \cdots,\ 1-q^2}^{n \text{ times}}\}.$$

Thus the invariant factors of $K_{m,n}$ are $1,\ 1-q^2$ [$m+n-2$ times], $(1-q^2)(1-(m-1)(n-1)q^2)$.

3.2. Composition of even cycles with null graphs

Let G and H be two graphs. The composition $G \circ H$ of G with H is the graph with vertex set $V(G) \times V(H)$ in which (u_1, v_1) is adjacent to (u_2, v_2) if and only if $u_1 u_2 \in E(G)$ or $u_1 = u_2$ and $v_1 v_2 \in E(H)$.

Consider $C_{2s} \circ N_n$, where C_{2s} is the cycle of order $2s$ and N_n is the null graph of order n. We write the vertex set of $C_{2s} \circ N_n$ as $\mathbb{Z}_n \times \mathbb{Z}_{2s} = \{(i,j) \mid 0 \le i \le n-1,\ 0 \le j \le 2s-1\}$.

$\{(x_1, y_1),\ (x_2, y_2)\}$ is an edge if and only if $y_1 \equiv y_2 \pm 1 \pmod{2s}$. Before computing the spectrum of the q-matrix of $C_{2s} \circ N_n$ we introduce some notations.

Let $\mathbb{F}$ be any field. Let $\beta = (b_0, \ldots, b_{n-1}) \in \mathbb{F}^n$ and $R(\beta)$ be the $n \times n$ right cyclic (circulant) matrix whose first row is β. It is known that (see [8]) the spectrum of $R(\beta)$ is

$$\left\{ \sum_{j=0}^{n-1} b_j,\ \sum_{j=0}^{n-1} b_j \zeta^j,\ \sum_{j=0}^{n-1} b_j \zeta^{2j},\ \ldots,\ \sum_{j=0}^{n-1} b_j \zeta^{(n-1)j} \right\}, \tag{3.1}$$

where ζ is a primitive n-th root of unity over $\mathbb{F}$.

Let q be an indeterminate. For $\alpha = (a_0, \ldots, a_{n-1}) \in \mathbb{Z}^n$ we write $q^\alpha = (q^{a_0}, \ldots, q^{a_{n-1}})$. We shall consider $R(q^\alpha)$ as a matrix over $\mathbb{C}(q)$.

Now we come back to consider the graph $G = C_{2s} \circ N_n$. If we arrange the vertices in lexicographic order (0 is the first), then the distance matrix of G is a right cyclic matrix of order $2sn$ whose first row is

$$\begin{aligned} \alpha &= ((0,1,2,3,\cdots,s,\cdots,3,2,1), \overbrace{(2,1,2,3,\cdots,s,\cdots,3,2,1), \cdots\cdots (2,1,2,3,\cdots,s,\cdots,3,2,1)}^{n-1 \text{ times}}) \\ &= (a_0,\ a_1,\ \ldots,\ a_{2sn-1}). \end{aligned}$$

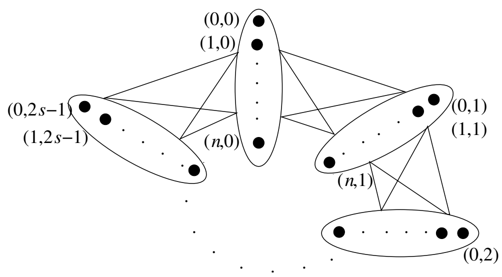

Figure 3.1: $C_{2s} \circ N_n$.

Hence the spectrum of Q_G is

$$\left\{ \sum_{j=0}^{2sn-1} q^{a_j},\ \sum_{j=0}^{2sn-1} q^{a_j} \zeta^j,\ \ldots,\ \sum_{j=0}^{2sn-1} q^{a_j} \zeta^{kj},\ \ldots,\ \sum_{j=0}^{2sn-1} q^{a_j} \zeta^{(2sn-1)j} \right\},$$

where ζ is a primitive $2sn$-th root of 1 over $\mathbb{C}$. That is, if we let $f_{s,n}(q, \lambda) = \sum_{j=0}^{2sn-1} q^{a_j} \lambda^j \in \mathbb{C}[q, \lambda]$, then the spectrum of Q_G is $\left\{ f_{s,n}(q, \zeta^k) \mid 0 \le k \le 2sn-1 \right\}$. It is a pre-invariant factor set of G.

First we assume $s > 2$. For $i \notin \{0, 2, s\}$, if $a_k = i$ then $k = 2sj + i$ or $2sj - i$ for some $0 \le j \le n$. If $a_k = 2$ then $k = 2sj + 2, 2sj - 2$ or $2sj'$ for some $0 \le j \le n, 1 \le j' \le n-1$. Thus when $i \notin \{0, 2, s\}$ the coefficient of q^i of $f_{s,n}(q, \zeta^k)$ is

$$\sum_{j=0}^{n-1} \zeta^{2skj+ki} + \sum_{j=1}^{n} \zeta^{2skj-ki} = (\zeta^{ki} + \zeta^{-ki}) \sum_{j=0}^{n-1} \zeta^{2skj}.$$

The coefficient of q^s of $f_{s,n}(q,\zeta^k)$ is

$$\sum_{j=0}^{n-1} \zeta^{2skj+ks} = \zeta^{ks} \sum_{j=0}^{n-1} \zeta^{2skj}.$$

The coefficient of q^2 of $f_{s,n}(q,\zeta^k)$ is

$$\sum_{j=0}^{n-1} \zeta^{2skj+2k} + \sum_{j=1}^{n} \zeta^{2skj-2k} + \sum_{j=1}^{n-1} \zeta^{2skj} = -1 + \left(\zeta^{2k} + \zeta^{-2k} + 1\right) \sum_{j=0}^{n-1} \zeta^{2sjk}.$$

It is known that

$$\sum_{j=0}^{n-1} \zeta^{2skj} = \begin{cases} 0 & \text{if } k \not\equiv 0 \pmod{n}, \\ n & \text{if } k \equiv 0 \pmod{n}. \end{cases}$$

Therefore, for $k \not\equiv 0 \pmod{n}$, $f_{s,n}(q,\zeta^k) = 1 - q^2$; and for $0 \le k \le 2s-1$,

$$\begin{aligned} f_{s,n}(q,\zeta^{nk}) =& 1 + (n-1)q^2 + (-1)^k n q^s + n \sum_{i=1}^{s-1} (\zeta^{nki} + \zeta^{-nki}) q^i \\ =& 1 - 2n + (n-1)q^2 + (-1)^k n q^s + n[1 - (-1)^k q^s] \left[\frac{1}{1-\zeta^{nk} q} + \frac{1}{1-\zeta^{-nk} q} \right]. \end{aligned} \tag{3.2}$$

In particular,

$$f_{s,n}(q,1) = 1 + (n-1)q^2 + 2n \sum_{i=1}^{s-1} q^i + n q^s = (1+q) \left(1 + (n-1)q + n \sum_{i=1}^{s-1} q^i \right)$$

and $f_{s,n}(1,1) \neq 0$. Clearly, $f_{s,n}(q,\zeta^k) = f_{s,n}(q,\zeta^{2sn-k})$, i.e., $f_{s,n}(q,\zeta^k) \in \mathbb{R}[q]$.

If $s = 2$ then the coefficient of q^2 of $f_{2,n}(q,\zeta^k)$ is

$$\sum_{j=1}^{2n-1} \zeta^{2kj} = -1 + \sum_{j=0}^{2n-1} \zeta^{2kj}.$$

Thus $f_{2,n}(q,1) = 1 + 2nq + (2n-1)q^2 = (1+q)[1 + (2n-1)q]$; $f_{2,n}(q,\zeta^k) = 1 - q^2$ if $k \not\equiv 0 \pmod{n}$; and $f_{2,n}(q,\zeta^n) = 1 - q^2 = f_{2,n}(q,\zeta^{3n})$, $f_{2,n}(q,\zeta^{2n}) = 1 - 2nq + (2n-1)q^2 = (1-q)[1 - (2n-1)q]$.

Example 3.1: Let $s = 4$ and $n = 2$, i.e., $G = C_8 \circ N_2$.

For brevity's sake, we write f for $f_{4,2}$.

$$\begin{aligned} f(q,1) &= 1 + 4q + 5q^2 + 4q^3 + 2q^4 = (1+q)(1 + 3q + 2q^2 + 2q^3); \\ f(q,\zeta^k) &= 1 - q^2 \text{ if } k \text{ is odd}, 1 \le k \le 15; \\ f(q,\zeta^2) = f(q,\zeta^{14}) &= 1 + 2(\zeta^2 + \zeta^{-2})q + q^2 + 2(\zeta^6 + \zeta^{-6})q^3 - 2q^4 = (1-q^2)(1+\sqrt{2}q)^2; \\ f(q,\zeta^4) = f(q,\zeta^{12}) &= 1 - 3q^2 + 2q^4 = (1-q^2)(1-2q^2); \\ f(q,\zeta^6) = f(q,\zeta^{10}) &= 1 + 2(\zeta^6 + \zeta^{-6})q + q^2 + 2(\zeta^2 + \zeta^{-2})q^3 - 2q^4 = (1-q^2)(1-\sqrt{2}q)^2; \\ f(q,\zeta^8) = f(q,-1) &= 1 - 4q + 5q^2 - 4q^3 + 2q^4 = (1-q)(1 - 3q + 2q^2 - 2q^3). \end{aligned}$$

By applying Corollary 2.6,

$$\begin{aligned}\mathrm{Inv}(C_8 \circ N_2) = \{1,\ &\overbrace{(1-q^2),\ \ldots,\ (1-q^2)}^{11\text{ times}},\ (1-q^2)(1-2q^2),\ (1-q^2)(1-2q^2),\\ &(1-q^2)(1-2q^2)^2,\ (1-q^2)(1-2q^2)^2(1-5q^2-8q^4-4q^6)\}.\end{aligned}$$

We want to know whether $q=1$ or $q=-1$ is a multiple root of $f_{s,n}(q,\zeta^k)$. Since $f_{s,n}(-q,\zeta^k) = f_{s,n}(q,\zeta^{n(k+s)})$ and $f_{s,n}(q,\zeta^k) = 1-q^2$ if $k \not\equiv 0 \pmod n$, we only need to consider the multiplicity of $q=1$ in $f_{s,n}(q,\zeta^{nk})$ when $1 \le k \le 2s-1$ (1 is not a root of $f_{s,n}(q,1)$).

For $1 \le k \le 2s-1$, from (3.2) we have $f_{s,n}(1,\zeta^{nk}) = 0$ and

$$f'_{s,n}(1,\zeta^{nk}) = 2n-2+\frac{n[1-(-1)^k]}{\cos\frac{k\pi}{s}-1} = \begin{cases} 2n-2 & \text{if } k \text{ is even,}\\ 2n-2+\dfrac{2n}{\cos\frac{k\pi}{s}-1} & \text{if } k \text{ is odd,}\end{cases}$$

where f' is the derivative of f with respect to q. Thus we have the following lemma.

Lemma 3.1: *For $1 \le k \le 2s-1$, 1 is a double root of $f_{s,n}(q,\zeta^{nk})$ if and only if either k is even and $n=1$, or k is odd and $\cos\frac{k\pi}{s} = \frac{1}{1-n}$.*

Proof: From the previous paragraph we know that 1 is a multiple root of $f_{s,n}(q,\zeta^{nk})$ if and only if when k is even and $n=1$, or k is odd and $\cos\frac{k\pi}{s} = \frac{1}{1-n}$.

$$f''(1,\zeta^{nk}) = 2(n-1)+\frac{2ns(-1)^{k+1}-n+(-1)^k n}{\cos\frac{k\pi}{s}-1} = \begin{cases} 2(n-1)+\dfrac{2ns}{1-\cos\frac{k\pi}{s}} & \text{if } k \text{ is even,}\\ 2(n-1)+\dfrac{2n-2ns}{1-\cos\frac{k\pi}{s}} & \text{if } k \text{ is odd,}\end{cases}$$

where f'' is the second derivative of f with respect to q.

If k is even, then clearly $f''(1,\zeta^{kn}) > 0$. If k is odd, then 1 is a multiple root only if when $\cos\frac{k\pi}{s} = \frac{1}{1-n}$. In this case $f''(1,\zeta^{nk}) = 2(n-1)(2-s)$. If $f''(1,\zeta^{nk}) = 0$ then $s=2$ and then $k=1$. But this is not a case. □

Corollary 3.2: *1 is a double root of $f_{s,n}(q,-1)$ if and only if either $n=1$ and s is even, or $n=2$ and s is odd.*

Corollary 3.3: *For $0 \le k \le 2s-1$ and $k \ne s$, -1 is a double root of $f_{s,n}(q,\zeta^{nk})$ if and only if either $k+s$ is even and $n=1$, or $k+s$ is odd and $\cos\frac{k\pi}{s} = \frac{1}{n-1}$.*

Corollary 3.4: *-1 is a double root of $f_{s,n}(q,1)$ if and only if either $n=1$ and s is even, or $n=2$ and s is odd.*

By applying Corollary 2.6, when $n = 2$ and s is even, the multiplicities of $1-q^2$ in the invariant factors are $0,\ \overbrace{1,\ \ldots,\ 1}^{s-1 \text{ times}}$; when $n = 2$ and s is odd, the multiplicities of $1 - q^2$ are $0,\ \overbrace{1,\ \ldots,\ 1}^{s-2 \text{ times}},\ 2$. For $n \geq 3$, if $\cos\frac{k\pi}{s} = \frac{1}{1-n}$ has a solution k which is odd (in this case $2s - k$ is also a solution and that equation has at most 2 solutions) then the multiplicities of $1 - q^2$ in the invariant factors are $0,\ \overbrace{1,\ \ldots,\ 1}^{s-3 \text{ times}},\ 2,\ 2$, otherwise they are $0,\ \overbrace{1,\ \ldots,\ 1}^{s-1 \text{ times}}$. In general, the invariant factors of $C_{2s} \circ N_n$ seem difficult to express when $n \geq 2$. For $n = 1$, they can be expressed. We will consider this case in the following subsection.

3.3. Even cycles

The invariant factors of even cycle C_{2s} were computed in [2, Theorem 5.2]. In this subsection we shall use an elementary method to compute the invariant factors of C_{2s}. C_{2s} is a special case of $C_{2s} \circ N_n$ when $n = 1$. We try to factorize the polynomials $f_{s,1}(q, \zeta^k)$. Note that $\deg(f_{s,1}) = s$. Suppose $\pm k + j \not\equiv 0 \pmod{2s}$ and $k + j$ is even. For $0 \leq j \leq 2s - 1$,

$$f_{s,1}(\zeta^j, \zeta^k) = 2 + \sum_{i=1}^{s-1}(\zeta^{(k+j)i} + \zeta^{(-k+j)i}) = \sum_{i=0}^{s-1}(\zeta^{(k+j)i} + \sum_{i=0}^{s-1}\zeta^{(-k+j)i}).$$

Since $\zeta^{k+j}\sum_{i=0}^{s-1}\zeta^{(k+j)i} = \sum_{i=1}^{s}\zeta^{(k+j)i} = \sum_{i=0}^{s-1}\zeta^{(k+j)i}$, $\sum_{i=0}^{s-1}\zeta^{(k+j)i} = 0$. Similarly, $\sum_{i=0}^{s-1}\zeta^{(-k+j)i} = 0$.

Thus $f_{s,1}(\zeta^j, \zeta^k) = 0$ when $\pm k + j \not\equiv 0 \pmod{2s}$ and $k + j$ is even.

For a fixed k there are $s-2$ solutions for j. Let us consider the particular case that both s and k are even. There are $s-2$ possibilities for j (including $j = 0$ and $j = s$) such that $f_{s,1}(\zeta^j, \zeta^k) = 0$. In this case $q = 1$ and $q = -1$ are double roots of $f_{s,1}(q, \zeta^k)$. So we have found all roots of $f_{s,1}(q, \zeta^k)$. Similarly, we can find all roots of $f_{s,1}(q, \zeta^k)$ for the other cases. Combining the results above, we have the multiplicity sequences of irreducible factors of $f_{s,1}(q, \zeta^k)$'s with respect to the spectrum of $Q_{C_{2s}}$ as follows:

$$\begin{aligned} 1 - q:&\quad 0,\ \overbrace{1,\ \ldots,\ 1}^{s \text{ times}},\ \overbrace{2,\ \ldots,\ 2}^{s-1 \text{ times}}. \\ j \neq 0 \text{ or } s, \zeta^j - q:&\quad \overbrace{0,\ \ldots,\ 0}^{s+2 \text{ times}},\ \overbrace{1,\ \ldots,\ 1}^{s-2 \text{ times}}. \end{aligned}$$

The sequence of $1 + q$ is same as that of $1 - q$. Therefore we have the following result.

Theorem 3.5: *The invariant factor set of C_{2s} is*

$$\{1,\ \overbrace{(1-q^2),\ \ldots,\ (1-q^2)}^{s \text{ times}},\ (1-q^2)^2,\ \overbrace{(1-q^2)(1-q^{2s}),\ \ldots,\ (1-q^2)(1-q^{2s})}^{s-2 \text{ times}}\}.$$

Note that one can use the character theory of the cyclic group to establish Theorem 3.5.

4. Reductive methods

The natural question to ask is: can we find the invariant factors of a graph G if the invariant factors or pre-invariant factors of some subgraphs of G are known? In other word, can we reduce the problem of finding invariant factors of G to some of its subgraphs? Note that, suppose that H and K are subgraphs of G. The definitions of the union $H \cup K$ and the intersection $H \cap K$ of H and K are referred to [1]. We have some results below.

Theorem 4.1: *Let H and K be two subgraphs of G such that $G = H \cup K$ and $H \cap K \cong P_2$, the path of order 2. If H is bipartite, then $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \{1, 1-q^2\}$ is a pre-invariant factor set of G.*

Proof: Let uw be the common edge of H and K. Let $U = \{x \in V(H) \setminus \{u, w\} \mid d(x, u) < d(x, w)\}$ and $W = \{y \in V(H) \setminus \{u, w\} \mid d(y, w) < d(y, u)\}$, where $d(x, y)$ denotes the distance between vertices x and y. Clearly U and W are disjoint. Since H is bipartite $U \cup W = V(H) \setminus \{u, w\}$. Note that if $d(z, u) < d(z, w)$ where $z \in V(G)$ then $d(z, u) + 1 = d(z, w)$. It is easy to see that for any $z \in V(K)$ and $x \in U$, $d(x, z) = d(x, u) + d(u, z)$. Similarly, for any $z \in V(K)$ and $y \in W$, $d(y, z) = d(y, w) + d(w, z)$.

Let $U = \{x_1, \ldots, x_s\}$ and $W = \{y_1, \ldots, y_t\}$ and $V(K) = \{u, w, z_1, \ldots, z_r\}$. We arrange the vertices in the following order $x_1, \ldots, x_s, y_1, \ldots, y_t, u, w, z_1, \ldots, z_r$. Let D be the distance matrix of G under this vertex ordering. Note that $D_H = D[x_1 \ \cdots \ x_s \ y_1 \ \cdots \ y_t \ u \ w]$ and $D_K = [u \ w \ z_1 \ \cdots \ z_r]$ are distance matrices of H and K, respectively. Namely

$$D = \left(\begin{array}{cc|cc|c} \multicolumn{2}{c|}{\multirow{2}{*}{D_1}} & A_{11} & A_{12} & B_1 \\ & & A_{21} & A_{22} & B_2 \\ \hline A_{11}^T & A_{21}^T & 0 & 1 & \multirow{2}{*}{C} \\ A_{12}^T & A_{22}^T & 1 & 0 & \\ \hline B_1^T & B_2^T & \multicolumn{2}{c|}{C^T} & D_2 \end{array}\right)$$

where $D_1 \in M_{s+t}(\mathbb{Z})$, $D_2 \in M_r(\mathbb{Z})$, $A_{11}, A_{12} \in M_{s,1}(\mathbb{Z})$, $A_{21}, A_{22} \in M_{t,1}(\mathbb{Z})$, $B_1 \in M_{s,r}(\mathbb{Z})$, $B_2 \in M_{t,r}(\mathbb{Z})$ and $C \in M_{2,r}(\mathbb{Z})$. Moreover, $(A_{11})_{i1} = d(x_i, u)$, $(A_{12})_{i1} = d(x_i, w)$, $(A_{21})_{j1} = d(y_j, u)$, $(A_{22})_{j1} = d(y_j, w)$, $(B_1)_{ik} = d(x_i, u) + d(u, z_k)$, $(B_2)_{jk} = d(y_j, w) + d(w, z_k)$, $C_{1k} = d(u, z_k)$ and $C_{2k} = d(w, z_k)$. Then $A_{11} + J_{s,1} = A_{12}$ and $A_{22} + J_{t,1} = A_{21}$.

Let $Q = q^D$.

Step 1: Do the row operations $-q^{d(x_i,u)} r_u + r_{x_i}$, $1 \le i \le s$ and $-q^{d(y_j,w)} r_w + r_{y_j}$, $1 \le j \le t$, on Q; and then do the same column operations.

Then Q becomes

$$Q_1 = \left(\begin{array}{c|c|c} Q' & O_{s+t,2} & O_{s+t,r} \\ \hline O_{2,s+t} & \begin{matrix} 1 & q \\ q & 1 \end{matrix} & q^C \\ \hline O_{r,s+t} & (q^C)^T & q^{D_2} \end{array}\right).$$

Step 2: Do $-qr_u + r_w$ and $-qc_u + c_w$ on Q_1.

If we apply Step 2, then Q_1 will become

$$Q_2 = \left(\begin{array}{c|c|c} Q' & O_{s+t,2} & O_{s+t,r} \\ \hline O_{2,s+t} & \begin{matrix} 1 & 0 \\ 0 & 1-q^2 \end{matrix} & Q'' \\ \hline O_{r,s+t} & (Q'')^T & q^{D_2} \end{array}\right).$$

Note that $Q_2[x_1 \ \cdots \ x_s \ y_1 \ \cdots \ y_t \ u \ w]$ can be obtained by performing Step 1 and Step 2 to q^{D_H}. Thus 1 and $1-q^2$ are pre-invariant factors of H. We convert Q' to the Smith normal form. By Corollary 2.3, all the entries of the resulting Q' are divisible by $1-q^2$. Then $\{1, 1-q^2\} \subseteq \mathrm{Inv}(H)$. Thus the invariant factors of Q' is $\mathrm{Inv}(H) \setminus \{1, 1-q^2\}$. Since $Q_{22} = Q_2[u \ w \ z_1 \ \cdots \ z_r]$ is equivalent to q^{D_K}, we obtain $\mathrm{Inv}(K)$ from Q_{22}. Therefore, $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \{1, 1-q^2\}$ is a pre-invariant factor set of G. □

By a similar proof of Theorem 4.1 we have

Theorem 4.2: *Let H and K be two subgraphs of G such that $G = H \cup K$ and H and K have one vertex in common. Then* $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \{1\}$ *is a pre-invariant factor set of G.*

Corollary 4.3: *Let G be a bipartite graph. Suppose $v \in V(G)$ of degree* 1. *Then* $\mathrm{Inv}(G) = \mathrm{Inv}(G-v) \cup \{1-q^2\}$.

Proof: Let u be the vertex adjacent to v. Let H be the path uv and $K = G - v$. They are bipartite. Thus $\mathrm{Inv}(H) = \{1, 1-q^2\}$ and $\mathrm{Inv}(K) = \{1, 1-q^2, \dots\}$. By Theorem 4.2, Corollary 2.3 and since $1-q^2$ is an invariant factor of G, the corollary follows. □

By using Corollary 4.3, one can easily compute the invariant factors of tree with n vertices is $\{1, (1-q^2)[n-1 \text{ times}]\}$.

The following theorem is a generalization of Theorem 4.1.

Theorem 4.4: *Let H and K be two subgraphs of G such that $G = H \cup K$ and $H \cap K$ is connected. Let* $\mathrm{Inv}(H \cap K) = \{1, f_2, \dots, f_t\}$. *If* $\mathrm{Inv}(H \cap K)$ *is the first t invariant factors of H and for any*

$x \in V(H)$ *there exists* $y \in V(H \cap K)$ *such that for any* $z \in V(K)$, $d(x,z) = d(x,y) + d(y,z)$, *then* $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \mathrm{Inv}(H \cap K)$ *is a pre-invariant factor set of* G.

Proof: Let $Y = V(H \cap K)$, $X = V(H) \setminus Y$ and $Z = V(K) \setminus Y$. We arrange the vertices in the following order: Vertices of X first, Y second and Z last. Then the Q_G is formed as

$$\begin{pmatrix} Q_X & Q_{XY} & Q_{XZ} \\ Q_{XY}^T & Q_Y & Q_{YZ} \\ Q_{XZ}^T & Q_{YZ}^T & Q_Z \end{pmatrix},$$

where all block matrices are of their corresponding sizes. By the hypothesis, for each $x \in X$ there exists $y \in Y$ such that $d(x,z) = d(x,y) + d(y,z)$ for all $z \in Y \cup Z$. We apply the row operation $-q^{d(x,y)} r_y + r_x$ and the column operation $-q^{d(x,y)} c_y + c_x$ for each $x \in X$. Then Q becomes

$$Q_1 = \begin{pmatrix} Q'_X & O & O \\ O & Q_Y & Q_{YZ} \\ O & Q_{YZ}^T & Q_Z \end{pmatrix}.$$

Since $\mathrm{Inv}(H \cap K) = \{1, f_2, \ldots, f_t\}$, there exist two invertible matrices P, P' such that $PQ_YP' = \mathrm{diag}\{1, f_2, \ldots, f_t\} = Q'_Y$. Then

$$\begin{pmatrix} I_{|X|} & O & O \\ O & P & O \\ O & O & I_{|Z|} \end{pmatrix} Q_1 \begin{pmatrix} I_{|X|} & O & O \\ O & P' & O \\ O & O & I_{|Z|} \end{pmatrix} = \begin{pmatrix} Q'_X & O & O \\ O & Q'_Y & PQ_{YZ} \\ O & P'Q_{YZ}^T & Q_Z \end{pmatrix}. \tag{4.1}$$

Since $\mathrm{Inv}(H \cap K)$ is the first t invariant factors of H, similar to the proof of Theorem 4.1 the assertion holds. □

Theorem 4.5: *Let* H *and* K *be two subgraphs of* G *such that* $G = H \cup K$ *and* $H \cap K$ *is connected. If Inv*$(H \cap K) \subseteq \mathrm{Inv}(H) \cap \mathrm{Inv}(K)$ *and for any* $x \in V(H)$ *there exists* $y \in V(H \cap K)$ *such that for any* $z \in V(K)$, $d(x,z) = d(x,y) + d(y,z)$, *then* $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \mathrm{Inv}(H \cap K)$ *is a pre-invariant factor set of* G.

Proof: By the same proof of Theorem 4.4, we have the matrix described in (4.1). We convert the matrix $\begin{pmatrix} Q'_Y & PQ_{YZ} \\ P'Q_{YZ}^T & Q_Z \end{pmatrix}$ to Smith normal form S_K. Since $\mathrm{Inv}(H \cap K) \subseteq \mathrm{Inv}(K)$, $1,\ f_2,\ \ldots,\ f_t$ are elements of the diagonal of S_K. By suitably exchanging rows and columns, we can move $1,\ f_2,\ \ldots,\ f_t$ to the first t elements of the diagonal of S_K. That is, the matrix in (4.1) becomes

$$\begin{pmatrix} Q'_X & O & O \\ O & Q'_Y & O \\ O & O & Q'_Z \end{pmatrix},$$

where Q'_Z is a diagonal matrix. Convert the matrix $\begin{pmatrix} Q'_X & O \\ O & Q'_Y \end{pmatrix}$ to Smith normal form S_H. Since $\mathrm{Inv}(H \cap K) \subseteq \mathrm{Inv}(H)$, $1,\ f_2,\ \ldots,\ f_t$ also are elements of the diagonal of S_H. Thus $\mathrm{Inv}(K) \cup \mathrm{Inv}(H) \setminus \mathrm{Inv}(H \cap K)$ is a pre-invariant factor set of G. $\square$

A *polyomino* is a graph obtained from the grid $P_m \times P_n$ by deleting some squares and all the bounded faces are 4-faces. Figure 4.1 shows a polyomino. By using Theorem 4.4, one can compute the invariant factors of any polyomino. We leave it to the reader as an exercise.

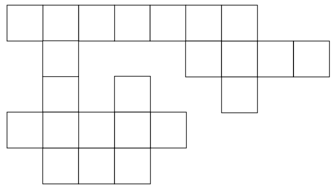

Figure 4.1: A polyomino.

5. Computation results of some bipartite graphs (2)

In this section we will compute some bipartite graphs, for example the hexagonal trees, which is a class of well-known molecular graphs.

A graph G is called a *polygonal tree* if it consists of finitely many regular polygons (we assume any two distinct polygons are not coplanar) and has the following two properties.

1. Any two distinct polygons are disjoint or have exactly one edge in common (such edge can be a common edge of several polygons).
2. The diagram obtained by joining the centroids of the polygons to the mid-point of the common edge has no closed curve.

If all polygons of a polygonal tree G are the same, say s-gons, then G is called a *s-gonal tree*. 6-gonal tree is called *hexagonal tree*. Consider the diagram defined in the condition 2. If we let the centroids and the mid-points of common edges of some polygons as "red" vertices and "green" vertices respectively and the straight line segments as edges of a bipartite graph. Then this graph is a tree.

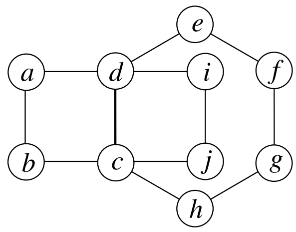

Figure 5.1: A polygonal tree.

Example 5.1: Let G be the graph described in Figure 5.1. Let $H = G[a, b, c, d, i, j]$ the induced subgraph of G. By Theorems 3.5 and 4.1 we have

$$\mathrm{Inv}(H) = \{1,\ 1-q^2,\ 1-q^2,\ 1-q^2,\ (1-q^2)^2,\ (1-q^2)^2\}.$$

By Theorems 3.5 and 4.1 again, a pre-invariant factor set of G is

$$\{1-q^2,\ 1-q^2,\ (1-q^2)^2,\ (1-q^2)^2\} \cup \{1,\ 1-q^2,\ 1-q^2,\ 1-q^2,\ (1-q^2)^2,\ (1-q^2)(1-q^6)\}.$$

By Corollary 2.6, $\mathrm{Inv}(G) = \{1,\ 1-q^2\ [5\text{ times}],\ (1-q^2)^2\ [\text{thrice}],\ (1-q^2)(1-q^6)\}$.

In general, we have the following theorem.

Theorem 5.1: *Suppose G is a polygonal tree consisting of $C_{2s_1}, C_{2s_2}, \ldots, C_{2s_n}$. Let $r_1 > r_2 > \cdots > r_t \geq 2$ be distinct values of $s_1, s_2, \ldots, s_n$ with multiplicities $n_1, n_2, \ldots, n_t$, respectively. Then the invariant factors of G are*

1 [*once*],

$1 - q^2$ [$n_1r_1 + \cdots + n_tr_t - n + 1 = s_1 + \cdots + s_n - n + 1$ *times*],

$(1-q^2)^2$ [$n_2r_2 + \cdots + n_tr_t - n + 2n_1$ *times*],

$(1-q^2)^2\left(\frac{1-q^{2r_1}}{1-q^2}\right)$ [$n_1(r_1-2) - n_2(r_2-2)$ *times*],

$\vdots$

$(1-q^2)^2\left(\frac{1-q^{2r_1}}{1-q^2}\right)\left(\frac{1-q^{2r_2}}{1-q^2}\right)\cdots\left(\frac{1-q^{2r_{t-1}}}{1-q^2}\right)$ [$n_{t-1}(r_{t-1}-2) - n_t(r_t-2)$ *times*],

$(1-q^2)^2\left(\frac{1-q^{2r_1}}{1-q^2}\right)\left(\frac{1-q^{2r_2}}{1-q^2}\right)\cdots\left(\frac{1-q^{2r_t}}{1-q^2}\right)$ [$n_t(r_t-2)$ *times*].

Proof: Let T be the tree described in the condition 2. Each red vertex represents a polygon. Choose a red leaf of T, apply Theorems 4.1 and 3.5 and remove it. Repeat this process until all red leaves are removed. Then remove all green leaves. Repeat the process until all vertices are removed. By Corollary 2.6, the theorem follows. □

Thus we have many non-isomorphic graphs whose invariant factors are the same.

Corollary 5.2: *The invariant factors of a $2s$-gonal tree consisting of n $2s$-cycles are*

1 [*once*],

$1 - q^2$ [$sn - n + 1$ *times*],

$(1-q^2)^2$ [n *times*],

$(1-q^2)^2(1-q^{2s})$ [$(s-2)n$ *times*].

Example 5.2: The invariant factors of a hexagonal tree with n hexagons is

$$\{1, \overbrace{1-q^2, \ \cdots, \ 1-q^2}^{2n+1 \text{ times}}, \overbrace{(1-q^2)^2, \ \cdots, \ (1-q^2)^2}^{n \text{ times}}, \overbrace{(1-q^2)^2(1-q^6), \ \cdots, \ (1-q^2)^2(1-q^6)}^{n \text{ times}}\}.$$

One can compute some pericondensed benzenoid molecular system graphs by using Theorem 4.4. For example, hexagonal nets, hexagonal parallelisums etc., which were defined in [9–14].

6. Computation results of some non-bipartite graphs

6.1. Complete graphs

The distance matrix of K_s is a right cyclic matrix whose first row is $(0, 1, 1, \ldots, 1)$. Similar to

Section 3.2, we obtain the spectrum of Q_{K_s} is $\{f(q,\zeta^k) \mid 0 \le k \le s-1\}$ where $f(q,\lambda) = 1+q\sum_{j=1}^{s-1}\lambda^j$ and ζ is a primitive s-th root of 1. It is easy to compute that the eigenvalues are $1+(s-1)q$, $1-q$ [$s-1$ times]. Thus the invariant factors of K_s are 1, $1-q$ [$s-2$ times] and $(1-q)(1+(s-1)q)$.

6.2. Odd cycles

From (3.1) a set of pre-invariant factors of $C_{2s+1} \circ N_n$ is

$$g_{s,n}(q,\zeta^k) = 1-q^2,\ k \not\equiv 0 \pmod{n}$$

and

$$g_{s,n}(q,\zeta^{nk}) = 1+(n-1)q^2 + n\sum_{i=1}^{s}(\zeta^{nki}+\zeta^{-nki})q^i,\ 0 \le k \le 2s,$$

where ζ is a $(2s+1)$-th primitive root of 1.

Consider the $(2s+1)$-cycle, i.e., when $n=1$, a set of pre-invariant factors of C_{2s+1} is

$$f_{2s+1}(q,\zeta^k) = g_{s,1}(q,\zeta^k) = 1+\sum_{i=1}^{s}(\zeta^{ki}+\zeta^{-ki})q^i,\ 0 \le k \le 2s.$$

They seem difficult to be factorized in general. Let us consider two special cases.

Example 6.1: A set of pre-invariant factors of C_3 is $f_3(q,1) = 1+2q$, $f_3(q,\omega) = 1-q = f_3(q,\omega^2)$, where ω is a primitive root of $x^3 = 1$. Thus the invariant factors of C_3 are 1, $1-q$, $(1-q)(1+2q)$.

Example 6.2: A set of pre-invariant factors of C_5 is $f_5(q,1) = 1+2q+2q^2$, $f_5(q,\zeta) = f_5(q,\zeta^4) = 1+(\zeta+\zeta^{-1})q+(\zeta^2+\zeta^{-2})q^2 = (1-q)(1-(\zeta^2+\zeta^{-2})q)$, $f_5(q,\zeta^2) = f_5(q,\zeta^3) = (1-q)(1-(\zeta+\zeta^{-1})q)$, where ζ is a primitive root of $x^5 = 1$. Thus the invariant factors of C_5 are 1, $1-q$, $1-q$, $(1-q)(1+q-q^2)$, $(1-q)(1+q-q^2)(1+2q+2q^2)$.

6.3. Miscellaneous

Example 6.3: Consider $C_{2s} \circ K_n$. Similar to Section 3.2, a set of pre-invariant factors of $C_{2s} \circ K_n$ is $f(q,\zeta^k) = 1-q^2$, $k \not\equiv 0 \pmod{n}$; and $f(q,\zeta^{nk}) = 1+(n-1)q+(-1)^k q^s + n\sum_{i=1}^{s-1}(\zeta^{nki}+\zeta^{-nki})q^i$, $0 \le k \le 2s-1$, where ζ is a primitive $2s$-th root of 1.

For $n=2$ and $s=2$. A set of pre-invariant factors of $C_4 \circ K_2$ (Figure 6.1) is $f(q,1) = 1+5q+2q^2$, $f(q,\zeta) = f(q,\zeta^3) = f(q,\zeta^5) = f(q,\zeta^7) = 1-q^2$, $f(q,\zeta^2) = (1-q)(1+2q) = f(q,\zeta^6)$, $f(q,\zeta^4) = (1-q)(1-2q)$. Thus the invariant factors of $C_4 \circ K_2$ are 1, $1-q$, $1-q$, $1-q$, $1-q^2$, $1-q^2$, $(1-q^2)(1+2q)$, $(1-q^2)(1-4q^2)(1+5q+2q^2)$.

Example 6.4: Consider the graph G described in Figure 6.2. By Theorem 3.5 and Example 6.1 we have $\mathrm{Inv}(C_4) = \{1, 1-q^2, 1-q^2, (1-q^2)^2\}$ and $\mathrm{Inv}(C_3) = \{1, 1-q, (1-q)(1+2q)\}$. Applying

Theorem 4.1, a pre-invariant factor set of G is $\{1-q^2, (1-q^2)^2, 1, 1-q, (1-q)(1+2q)\}$. Hence

$$\mathrm{Inv}(G) = \{1,\ 1-q,\ 1-q,\ 1-q^2,\ (1-q^2)^2(1+2q)\}.$$

Example 6.5: Consider the graph G described in Figure 6.3. Applying Theorem 4.2 and the results of Examples 6.1 and 6.2, a pre-invariant factor set of G is

$$\{1,\ 1-q,\ (1-q)(1+2q),\ 1-q,\ 1-q,\ (1-q)(1+q-q^2),\ (1-q)(1+q-q^2)(1+2q+2q^2)\}.$$

Thus the invariant factors are

$$1,\ 1-q,\ 1-q,\ 1-q,\ 1-q,\ (1-q)(1+q-q^2),\ (1-q)(1+q-q^2)(1+2q+2q^2)(1+2q).$$

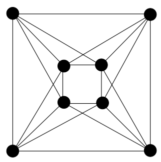

Figure 6.1: $C_4 \circ K_2$.

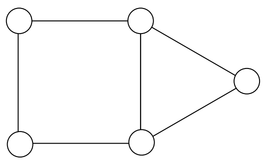

Figure 6.2.

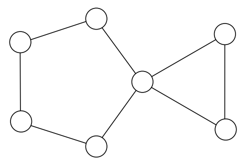

Figure 6.3.

Finally, we consider the first example (Example 2.1) again.

Example 6.6: Consider the graph G in Example 2.1. Let $H = G[R_1, R_2, R_3, R_7] \cong C_4$ and $K = G \setminus \{R_2\} \cong P_2 \times P_3$. Then $H \cap K \cong P_3$. From Example 5.1,

$$\mathrm{Inv}(K) = \{1,\ 1-q^2,\ 1-q^2,\ 1-q^2,\ (1-q^2)^2,\ (1-q^2)^2\}.$$

By Theorem 4.4 and Corollary 2.6,

$$\mathrm{Inv}(G) = \{1,\ 1-q^2,\ 1-q^2,\ 1-q^2,\ (1-q^2)^2,\ (1-q^2)^2,\ (1-q^2)^2\}.$$

7. Conclusion

This paper has presented some methods to find the invariant factors of graphs. This is the initial work on the problem. Invariant factors of some graphs derived from hyperplane arrangements have not been found yet, for example the Cayley graph described in Example 2.3. Recently, the invariant factors of Cartesian product of graphs have been discussed. The invariant factors of some Cartesian product graphs, such as $C_{2s} \times P_n$, $P_{s_1} \times P_{s_2} \times \cdots \times P_{s_n}$, $C_{2s} \times C_{2t}$ etc., are found [15]. We are also interested on other bipartite graphs (or general graphs), for example, complete n-partite graphs, etc. Some of these graphs were derived from projective arrangements of hyperplanes. Namely, a projective arrangement of hyperplanes amounts to take an affine arrangement where all hyperplanes have a common point, and considered two opposite regions as only one region. It is known that the graph G of an affine arrangement is antipodal and the graph of the projective arrangement is the quotient of G by relation of antipodality. For example, the 3-cube gives the complete graph K_4, the 4-cube gives complete bipartite graph $K_{4,4}$, etc. The general position of $n \geq 3$ points on the projective line gives an n-cycle. The general position of 4 lines in the projective plane gives $K_{3,4}$, the general position of 5 lines in the projective plane gives the Micielski graph of order 11, etc.

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