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The signless Laplacian coefficients and incidence energy of bicyclic graphs ☆

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ABSTRACT

Let $Q(G;x) = \det(xI - Q(G)) = \sum_{i=1}^{n}(-1)^i \varphi_i x^{n-i}$ be the characteristic polynomial of the signless Laplacian matrix of a graph G of order n. This paper investigates how the signless Laplacian coefficients (i.e., coefficients of $Q(G;x)$) change after some graph transformations. These results are used to prove that the set $(\mathcal{B}_n, \preceq)$ of all bicyclic graphs of order n has exactly two minimal elements with respect to the partial ordering of their coefficients. Furthermore, we present a sharp lower bound for the incidence energy of bicyclic graphs of order n and characterize all extremal graphs.

1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G)$. If $A(G)$ is the $(0,1)$ adjacency matrix and $D(G) = \mathrm{diag}(d(v_1), \ldots, d(v_n))$ is the degree diagonal matrix with the degree $d(v_i)$ of vertex v_i, then $L(G) = D(G) - A(G)$ is the *Laplacian matrix* of G. Related to the Laplacian matrix, the so-called *signless Laplacian matrix* of a graph is $Q(G) = D(G) + A(G)$. Moreover, the *Laplacian and signless Laplacian characteristic polynomials* of G are defined to be

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$$L(G;x)=\det\bigl(xI-L(G)\bigr)=\sum_{i=0}^{n}(-1)^i c_i(G)x^{n-i}$$

and

$$Q(G;x)=\det\bigl(xI-Q(G)\bigr)=\sum_{i=0}^{n}(-1)^i \varphi_i(G)x^{n-i}.$$

Let $\mathcal{G}_n$ be the set of all simple graphs of order n. For $G, H \in \mathcal{G}_n$, if $c_i(G) \leqslant c_i(H)$ for $i=1,\dots,n$, then we can say that $G \preceq' H$. Similarly, we say that $G \preceq H$, if $\varphi_i(G) \leqslant \varphi_i(H)$ for $i=1,\dots,n$.

The Laplacian matrix has been extensively studied (for example see [17] and the references therein). Recently, Mohar [13] defined a partial ordering among classes of Laplacian-cospectral trees of the same order n and proved that this poset has a unique minimal and a unique maximal element. Further he pointed it would be interesting to know how long the height and how large the width of this poset are. This paper motivated researchers to investigate the structures and properties of this poset [7–9,16,18]. For example, Ilić [9] characterized that the set of all trees of order n with fixed matching number m has a unique minimal element with this partial ordering $\preceq'$. Stevanović and Ilić [15] proved that the partial ordering set of all unicyclic graphs of order n with $\preceq'$ has a unique maximal and a unique minimal element. He and Shan [6] proved that there is only one minimal element in the partial ordering set of all bicyclic graphs with $\preceq'$.

The signless Laplacian matrix of G has attracted more and more attention, since it can discover more structure characterization of graphs than the Laplacian matrix in some ways. The reader may refer to three excellent surveys [2–4] on the signless Laplacian matrix for related information. Recently, Li, Tam, and Su [10] proved that there are two maximal elements and two minimal elements in the partial ordering set of all unicyclic graphs with $\preceq$. Mirzakhah and Kiani [12] studied the coefficients of the signless Laplacian matrix of a unicyclic graph. Motivated by all these works, we are devoted to study the structure and properties of the partial ordering set $(\mathcal{G}_n, \preceq)$, in particular for all bicyclic graphs of order n. In addition, the energy of a graph, which originated from Hückel Molecular Orbital Theory, has been widely investigated [11]. Nikiforov [14] extended the concept of graph energy to an arbitrary matrix. The *incidence energy* of a graph is defined to be the sum of the square root of all eigenvalues of $Q(G)$ [5]. It may be interesting to further study the relationship between the coefficients of the signless Laplacian matrix and the incidence energy.

A connected graph is called *bicyclic* if the size of its edges is equal to the size of its vertices plus one. It is easy to see that a connected graph G is bicyclic if and only if G can be obtained from a tree T with the same order by adding two new edges. The set of all bicyclic graphs of order n is denoted by $\mathcal{B}_n$. He and Shan [6] proved that the partial ordering set $(\mathcal{B}_n, \preceq')$ has a unique minimal element. Hence it may be guessed that $(\mathcal{B}_n, \preceq)$ has a unique minimal element. But it is not true. Let G_1 be a graph of order 5 by adding a pendent edge to a vertex of degree 3 of the diamond K_4-e, and G_2 be the complete bipartite graph $K_{2,3}$. Then

$$Q(G_1;x)=x^5-12x^4+49x^3-86x^2+64x-16,$$
$$Q(G_2;x)=x^5-12x^4+51x^3-92x^2+60x,$$

are the characteristic polynomials of the signless Laplacian matrices of the two minimal bicyclic graphs of order 5.

In this paper we focus on some structure properties of $(\mathcal{B}_n, \preceq)$. In particular, we prove that $(\mathcal{B}_n, \preceq)$ has only two minimal elements and characterize the two extremal graphs. Let B' be the graph of order n obtained by identifying the center of a star $K_{1,n-4}$ and a vertex of degree 3 of the diamond K_4-e. Let B'' be the graph of order n obtained from the complete bipartite graph $K_{2,3}$ by adding $n-5$ pendent vertices to a vertex of degree 3. The main results of this paper can be stated as follows:

Theorem 1.1. *B' and B'' are the only two minimal elements in the partial ordering set $(\mathcal{B}_n, \preceq)$.*

In addition, the extremal graphs with the minimal incidence energy among the set of all bicyclic graphs of order n are characterized.

Theorem 1.2. *Let $IE(G)$ be the incidence energy of a bicyclic graph G of order n.*

(1) *If $n \geqslant 31$, $IE(G) \geqslant IE(B') = (n-4)+\sqrt{2}+\sqrt{\alpha_1}+\sqrt{\alpha_2}+\sqrt{\alpha_3}$ with equality if and only if $G = B'$, where $\alpha_1 \geqslant \alpha_2 \geqslant \alpha_3$ are the roots of $x^3-(n+4)x^2+4nx-8=0$.*
(2) *If $n \leqslant 30$, then $IE(G) \geqslant IE(B'') = (n-6)+2\sqrt{2}+\sqrt{\beta_1}+\sqrt{\beta_2}+\sqrt{\beta_3}$ with equality if and only if $G = B''$, where $\beta_1 \geqslant \beta_2 \geqslant \beta_3$ are the roots of $x^3-(n+4)x^2+(5n-2)x-3n=0$.*

The rest of this paper is organized as follows. In Section 2, some preliminaries are introduced. In Section 3, two transformations of graphs with respect to $\preceq$ are introduced. In Section 4, the partial orderings of several special graphs are obtained. In Section 5, we present the proofs of Theorems 1.1 and 1.2.

2. Preliminaries

In this section, we introduce some notations and known results, which will be used in later sections. Let G be a graph of order n. A connected graph of order n is *odd unicyclic* if it has only one cycle whose length is odd. A spanning subgraph of G whose connected components are trees or odd unicyclic graphs is called a *TU-subgraph* of G. Let H be a TU-subgraph of G consisting of c odd unicyclic graphs and s trees $T_1,\dots,T_s$ of orders $n_1,\dots,n_s$, respectively. Then the weight of H is denoted by $W(H)=4^c\prod_{i=1}^{s}n_i$. If H contains no tree, then $W(H)=4^c$. According to the following theorem, the signless Laplacian coefficients of G can be expressed in terms of the weights of TU-subgraphs of G.

Theorem 2.1. *(See [1].) Let $Q(G;x)=\sum_{i=0}^{n}(-1)^i\varphi_i(G)x^{n-i}$ be the characteristic polynomial of the signless Laplacian matrix of a graph G of order n. Then*

$$\varphi_i(G)=\sum_{H_i}W(H_i),\quad i=1,\dots,n, \tag{1}$$

where the summation runs over all TU-subgraphs H_i of G with i edges.

A *pendent* edge is an edge which is incident to a vertex of degree 1. For any bicyclic graph G of order n, the base of G, denoted by $\overline{G}$, is the (unique) minimal bicyclic subgraph of G. It is easy to see that the base of a bicyclic graph can be obtained by consecutively deleting pendent edges. In addition, it is known that there are three types of bases of bicyclic graphs, $B(p,q)$ is obtained from two vertex-disjoint cycles C_p and C_q by identifying vertex u of C_p and vertex v of C_q, $B(p,l,q)$ is obtained from two vertex-disjoint cycles C_p and C_q by joining vertex u of C_p and vertex v of C_q by a path $uu_1u_2\cdots u_{l-1}v$ of length l ($l \geqslant 1$), $B(P_k,P_l,P_m)$ ($m \leqslant l \leqslant k$) is obtained from three pairwise internal disjoint paths of lengths k,l,m from vertices x to y (see Fig. 1). Note that $B(p,0,q)$ is exactly $B(p,q)$. Moreover, let

$$\mathcal{B}_1(n)=\{G \mid G\in\mathcal{B}_n,\ \overline{G}=B(p,q),\ p\geqslant 3,\ q\geqslant 3\},$$
$$\mathcal{B}_2(n)=\{G \mid G\in\mathcal{B}_n,\ \overline{G}=B(p,l,q),\ p,q\geqslant 3,\ l\geqslant 1\},$$
$$\mathcal{B}_3(n)=\{G \mid G\in\mathcal{B}_n,\ \overline{G}=B(P_k,P_l,P_m),\ 1\leqslant m\leqslant \min\{k,l\}\}.$$

Then $\mathcal{B}_n=\mathcal{B}_1(n)\cup\mathcal{B}_2(n)\cup\mathcal{B}_3(n)$. For any bicyclic graph G of order n, it is easy to see that $\varphi_0(G)=1$, $\varphi_1(G)=2(n+1)$.

3. Transformations

In this section, we introduce several transformations of graphs which still keep the partial ordering. Given a graph G and an edge $e\in E(G)$ (respectively, $e\notin E(G)$), we denote by $G-e$ (respectively, $G+e$) the graph obtained from G by deleting (respectively, adding) the edge e. Let $N_G(v)$ denote the neighbors of v in the graph G. He and Shan [6] introduced the following transformation:

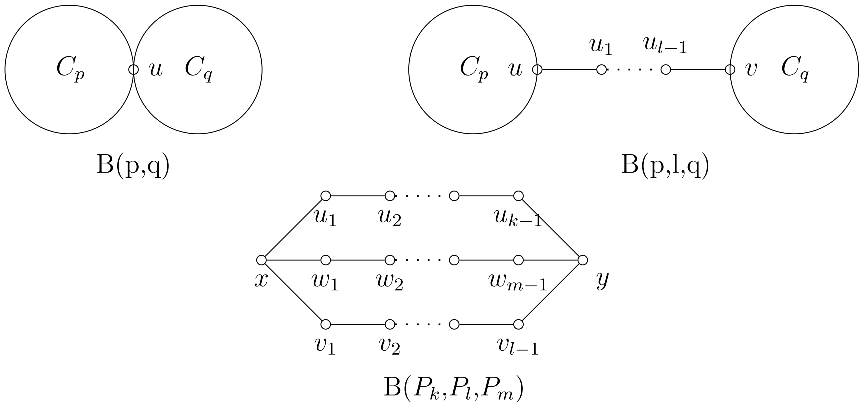

Fig. 1. Three types of bases of bicyclic graphs.

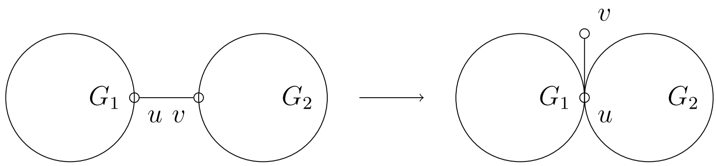

Fig. 2. α-transformation.

Definition 3.1. (See [6].) Let G be a simple connected graph with n vertices, and uv be a non-pendent edge which is not contained in any cycles of G. Let G_{uv} be obtained from G by changing all edges (except uv) incident with v into new edges between u and $N_G(v)\backslash\{u\}$. In other words, $G_{uv} = G - \{vx \mid x \in N_G(v)\backslash\{u\}\} + \{ux \mid x \in N_G(v)\backslash\{u\}\}$ (see Fig. 2). We say that G_{uv} is an α-transformation of G.

Lemma 3.2. *Let G be a connected graph of order $n \geqslant 4$, and G_{uv} be obtained from G by α-transformation. Then $G_{uv} \preceq G$, i.e.,*

$$\varphi_i(G_{uv}) \leqslant \varphi_i(G), \quad i = 0, 1, \ldots, n,$$

with equality if and only if either $i \in \{0, 1, n\}$ when G is non-bipartite, or $i \in \{0, 1, n-1, n\}$ for otherwise.

Proof. If G is bipartite, then the assertion follows from [6]. Now we assume that G is not bipartite. Clearly, $\varphi_0(G) = \varphi_0(G_{uv}), \varphi_1(G) = \varphi_1(G_{uv})$ and $\varphi_n(G) = \varphi_n(G_{uv})$. For $2 \leqslant i \leqslant n-1$, let $\mathcal{H}_i$ and $\mathcal{H}'_i$ be the sets of all TU-subgraphs of G and G_{uv} with exactly i edges, respectively. For an arbitrary TU-subgraph $H'_i \in \mathcal{H}'_i$, let R' be the component of H'_i containing u. Let $f : \mathcal{H}'_i \to \mathcal{H}_i$, $H_i = f(H'_i)$, where $V(H_i) = V(G)$ and $E(H_i) = E(H'_i) - \{ux \mid x \in N_{R'}(u) \cap N_G(v)\} + \{vx \mid x \in N_{R'}(u) \cap N_G(v)\}$. Then f is injective from $\mathcal{H}'_i \to \mathcal{H}_i$. Now we consider the following three cases.

Case 1: $uv \in E(H'_i)$. Then H'_i and H_i have the same components except for R'. Moreover, H_i has a component containing u which corresponds to R'. Clearly the two components have the same orders. Hence $W(H'_i) = W(H_i)$.

Case 2: $uv \notin E(H'_i)$ and u is contained in an odd unicyclic component U' of H'_i. Then H'_i and H_i have the same components except for two components U' and $\{v\}$ in H'_i. Since uv is a cut edge in G, H_i has an odd unicyclic component corresponding to the component U' in H'_i. Moreover, H_i has a tree component of order $a \geqslant 1$ corresponding to the component $\{v\}$ in H'_i. Hence $W(H'_i) = 4 \cdot 1 \cdot N$ and $W(H_i) = 4 \cdot a \cdot N$ for some constant value N. So $W(H'_i) \leqslant W(H_i)$ with equality if and only if $a = 1$.

Case 3: $uv \notin E(H'_i)$ and u is contained in a tree component T' of H'_i. Then H'_i and H_i have the same components except for two components T' and $\{v\}$ in H'_i. Assume that $G - uv$ has two components

G_1 and G_2. Denote by $|V(T')\cap V(G_1)|=b$ and $|V(T')\cap V(G_2)|=c$. Then H_i has a tree component of order b corresponding to the component T' of order $b+c$. Moreover, H_i has a tree component of order $c+1$ corresponding to the component $\{v\}$ in H_i'. Hence $W(H_i')=(b+c)N$ and $W(H_i)=b(c+1)N$ for some constant value N. So $W(H_i')\leqslant W(H_i)$ with equality if and only if $b=1$ or $c=0$. Therefore,

$$\varphi_i(G_{uv})=\sum_{H_i'\in\mathcal{H}_i'}W\big(H_i'\big)\leqslant\sum_{H_i\in\mathcal{H}_i}W(H_i)=\varphi_i(G),\quad i=2,\dots,n-1,$$

with equality if and only if $i=n-1$ and G is bipartite. □

Remark. It is easy to see that Lemma 3.2 is a generalization of Theorem 2.7 in [12]. Using the transformation of Definition 3.1 consecutively, every graph in $\mathcal{B}_2(n)$ can be transformed into some graph which belongs to $\mathcal{B}_1(n)$, and keep all the signless Laplacian coefficients not increased. Hence for any bicyclic graph G of order n, there exists a bicyclic graph $H\in\mathcal{B}_1(n)\cup\mathcal{B}_3(n)$ such that $\varphi_i(G)\geqslant\varphi_i(H)$.

Definition 3.3. Let $G=(V,E)$ be a connected graph with one cycle C of length at least 5, and u,v,w be three consecutive vertices in C which satisfy $N_G(u)\cap N_G(v)=\emptyset$, $N_G(v)\cap N_G(w)=\emptyset$, $N_G(u)\cap N_G(w)=\{v\}$. Let the graph $G'(u,v,w)$ be obtained from G by deleting all edges vz for $z\in N_G(v)\setminus\{u,w\}$, wz for $z\in N_G(w)$, and adding all edges uz for $z\in(N_G(v)\cup N_G(w))\setminus\{u,v\}$. In other words,

$$\begin{aligned}G'(u,v,w)=G&-\big\{vz\,\big|\,z\in N_G(v)\setminus\{u,w\}\big\}-\big\{wz\,\big|\,z\in N_G(w)\big\}\\&+\big\{uz\,\big|\,z\in\big(N_G(v)\cup N_G(w)\big)\setminus\{u,v\}\big\}.\end{aligned}$$

We say that $G'(u,v,w)$ is a β-transformation of G.

Remark. After performing β-transformation in Definition 3.3, $G'(u,v,w)$ is bipartite (non-bipartite) if G is bipartite (non-bipartite). Moreover, the length of at least one cycle of $G'(u,v,w)$ decreases by 2.

Lemma 3.4. *Let $G=(V,E)$ be a bicyclic graph of order n with base $\overline{G}=B(P_k,P_l,P_m)$ (see Fig. 1). For $k\geqslant l\geqslant m\geqslant 3$ or $k\geqslant l\geqslant 3>m=2$, let $G'(w_j,w_{j+1},w_{j+2})$ be the graph obtained from G by β-transformation to the vertices w_j,w_{j+1},w_{j+2}, $0\leqslant j\leqslant m-2$ (according to Fig. 1, $x=w_0$, $y=w_m$). Then $G'(w_j,w_{j+1},w_{j+2})\preceq G$, i.e.,*

$$\varphi_i\big(G'(w_j,w_{j+1},w_{j+2})\big)\leqslant\varphi_i(G),\quad i=0,1,\dots,n,$$

with equality if and only if $i\in\{0,1\}$ when G is non-bipartite, and $i\in\{0,1,n\}$ when G is bipartite.

Proof. Clearly $\varphi_i(G)=\varphi_i(G'(w_j,w_{j+1},w_{j+2}))$, for $i=0,1$. Moreover, $\varphi_n(G)=\varphi_n(G'(w_j,w_{j+1},w_{j+2}))=0$ for bipartite graph. Now we assume that $2\leqslant i\leqslant n$. For convenience, let $\mathcal{H}'$ and $\mathcal{H}$ be the sets of all TU-subgraphs of $G'(w_j,w_{j+1},w_{j+2})$ and G with exactly i edges, respectively. For an arbitrary TU-subgraph $H'\in\mathcal{H}'$, denote by R' the connected component of H' containing w_j. Furthermore let $f:\mathcal{H}'\to\mathcal{H}$, $H'\to H=f(H')$, where $V(H)=V(H')$ and

$$\begin{aligned}E(H)=E\big(H'\big)&-\big\{w_jx\,\big|\,x\in N_{R'}(w_j)\cap N_G(w_{j+1})\big\}\\&-\big\{w_jx\,\big|\,x\in N_{R'}(w_j)\cap N_G(w_{j+2})\setminus\{w_{j+1}\}\big\}\\&+\big\{w_{j+1}x\,\big|\,x\in N_{R'}(w_j)\cap N_G(w_{j+1})\big\}\\&+\big\{w_{j+2}x\,\big|\,x\in N_{R'}(w_j)\cap N_G(w_{j+2})\setminus\{w_{j+1}\}\big\}.\end{aligned}$$

Then f is injective from $\mathcal{H}'\to\mathcal{H}$. If w_j,w_{j+1},w_{j+2} belong to one component R' of H', then $f(R')$ is a component of H and has the same order as R'. So $W(H)=W(H')$. Hence assume that w_j,w_{j+1},w_{j+2} belong to at least 2 components of H'. Now we consider the following two cases.

Case 1: w_j is not in an odd unicyclic component of H'. Then w_j is contained in a tree component of H'. Suppose that there are a_1+1 vertices in the connected component containing w_j in

$H - w_j w_{j+1}$ and $a_2 + 1$ vertices in the component containing w_{j+2} in $H - w_{j+1}w_{j+2}$, $a_3 + 1$ vertices in the component containing w_{j+1} in $H - w_{j+1}w_{j+2} - w_j w_{j+1}$ ($a_1, a_2, a_3 \geqslant 0$). Denote by N the weight of all components of H' containing no w_j, w_{j+1}, w_{j+2}.

Subcase 1.1: $w_j w_{j+1} \in H'$, $w_j w_{j+2} \notin H'$. Then $W(H') = (a_1 + a_2 + a_3 + 2) \cdot 1 \cdot N$ and $W(H) = (a_1 + a_3 + 2) \cdot (a_2 + 1) \cdot N$. Hence $W(H) - W(H') = [a_2 \cdot (a_1 + a_3 + 1)] \cdot N \geqslant 0$ with equality if and only if $a_2 = 0$.

Subcase 1.2: $w_j w_{j+1}, w_j w_{j+2} \notin H'$. Then $W(H') = (a_1 + a_2 + a_3 + 1) \cdot 1 \cdot 1 \cdot N$ and $W(H) = (a_1 + 1) \cdot (a_2 + 1) \cdot (a_3 + 1) \cdot N$. Hence $W(H) - W(H') \geqslant 0$ with equality if and only if there are at least 2 zeros among a_1, a_2, a_3.

Subcase 1.3: $w_j w_{j+1} \notin H'$, $w_j w_{j+2} \in H'$. Then $W(H') = (a_1 + a_2 + a_3 + 2) \cdot 1 \cdot N$ and $W(H) = (a_2 + a_3 + 2) \cdot (a_1 + 1) \cdot N$. Hence $W(H) - W(H') = [a_1 \cdot (a_2 + a_3 + 1)] \cdot N \geqslant 0$ with equality if and only if $a_1 = 0$.

Case 2: w_j belongs to an odd unicyclic component R' of H'. Without loss of generality, assume C' is a subgraph of R', and corresponds to an odd cycle C in G.

Subcase 2.1: $w_j w_{j+1}, w_j w_{j+2} \notin H'$. Then H' and H have the same components except for R', $\{w_{j+1}\}$, $\{w_{j+2}\}$ in H' which correspond to two trees R_1 containing w_j, w_{j+2} of order at least $g(C) - 1$, and R_2 containing w_{j+1} of order at least 1 in H. Therefore $W(H') = 4 \cdot 1 \cdot 1 \cdot N$ and $W(H) \geqslant (g(C) - 1) \cdot 1 \cdot N$ for some constant value N. Hence $W(H) - W(H') \geqslant (g(C) - 5) \cdot N \geqslant 0$ by the girth of G being at least 5.

Subcase 2.2: $w_j w_{j+1} \notin H'$ and $w_j w_{j+2} \in H'$; or $w_j w_{j+2} \notin H'$ and $w_j w_{j+1} \in H'$. Then H' and H have the same components except for two components R', $\{w_{j+1}\}$ or $\{w_{j+2}\}$ in H' which correspond to one tree R containing w_j, w_{j+1}, w_{j+2} of order at least $g(C)$. Therefore $W(H') = 4 \cdot 1 \cdot N$ and $W(H) \geqslant g(C) \cdot N$ for some constant value N. Hence $W(H) - W(H') \geqslant (g(C) - 4) \cdot N > 0$. Therefore,

$$\varphi_i\big(G'(u_j, u_{j+1}, u_{j+2})\big) = \sum_{H' \in \mathcal{H}'} W\big(H'\big) \leqslant \sum_{H \in \mathcal{H}} W(H) = \varphi_i(G), \quad i = 2, \ldots, n,$$

with equality if and only if $i = n$ and G is bipartite. □

Lemma 3.5. *Let $G = (V, E)$ be a bicyclic graph of order n whose base is $\overline{G} = B(P_k, P_l, P_m)$ with $k \geqslant l \geqslant m$. For either $m = 1$ and $k \geqslant 4$, or $m = l = 2$ and $k \geqslant 4$, let $G'(u_j, u_{j+1}, u_{j+2})$ be the graph obtained from G by β-transformation to the three vertices u_j, u_{j+1}, u_{j+2}, $0 \leqslant j \leqslant k - 2$, where, according to Fig. 1, $x = u_0$ and $y = u_k$. Then $G'(u_j, u_{j+1}, u_{j+2}) \preceq G$, i.e.,*

$$\varphi_i\big(G'(u_j, u_{j+1}, u_{j+2})\big) \leqslant \varphi_i(G), \quad i = 0, 1, \ldots, n,$$

with equality if and only if $i \in \{0, 1\}$ when G is non-bipartite and $i \in \{0, 1, n\}$ when G is bipartite.

Proof. The proof is similar to that of Lemma 3.4 and omitted. □

Lemma 3.6. *Let $G = (V, E)$ be a bicyclic graph of order n with base $\overline{G} = B(p, q)$. Denote by the cycle C_p: $uu_1 \cdots u_{p-1}u$. For $p \geqslant 5$, $q \geqslant 3$, let $G'(u_j, u_{j+1}, u_{j+2})$ be the graph obtained from G by β-transformation to the three vertices u_j, u_{j+1}, u_{j+2}, $0 \leqslant j \leqslant p - 3$ (according to Fig. 1, $u = u_0$). Then $G'(u_j, u_{j+1}, u_{j+2}) \preceq G$, i.e.,*

$$\varphi_i\big(G'(u_j, u_{j+1}, u_{j+2})\big) \leqslant \varphi_i(G), \quad i = 0, 1, \ldots, n,$$

with equality if and only if $i \in \{0, 1\}$ when G is non-bipartite and $i \in \{0, 1, n\}$ for otherwise.

Proof. The proof is similar to that of Lemma 3.4 and omitted. □

Now we present the main result of this section.

Theorem 3.7. *Let G be a bicyclic graph of order n. Then there exists a bicyclic graph G' of order n such that $G' \preceq G$, where the base of G' is one of the following eight bases $B(3,3)$, $B(3,4)$, $B(4,4)$, $B(P_2, P_2, P_1)$, $B(P_3, P_2, P_1)$, $B(P_3, P_3, P_1)$, $B(P_2, P_2, P_2)$ and $B(P_3, P_2, P_2)$; and the remaining vertices of G' except the vertices of the base are pendent vertices.*

Proof. If the base of G is $B(p,l,q)$, then by performing a series of α-transformations, there exists a bicyclic graph G_1 with base $B(p,q)$ such that $G_1 \preceq G$ by Lemma 3.2. If the base of G is $B(P_k, P_l, P_m)$, then by performing a series of β-transformations, there exists a bicyclic graph G_2 such that $G_2 \preceq G$ by Lemmas 3.4–3.6, where the base of G_2 is one of the following eight bases $B(3,3)$, $B(3,4)$, $B(4,4)$, $B(P_2,P_2,P_1)$, $B(P_3,P_2,P_1)$, $B(P_3,P_3,P_1)$, $B(P_2,P_2,P_2)$ and $B(P_3,P_2,P_2)$. If the base of G is $B(p,q)$, by performing a series of β-transformations, there exists a bicyclic graph G_3 such that $G_3 \preceq G$ by Lemmas 3.6, where the base of G_3 is one of $B(3,3)$, $B(3,4)$, $B(4,4)$. Further, by performing a series of α-transformations to G_2 and G_3, there exist bicyclic graphs G_4 (respectively, G_5) such that $G_4 \preceq G_2$, $G_5 \preceq G_3$, where the base of G_4 or G_5 is one of the above eight bases and the remaining vertices except the vertices of the base are pendent vertices, so the assertion holds. □

4. The orderings of graphs in eight special bicyclic graphs

In this section, we investigate the coefficients of the eight graphs in Theorem 3.7. For convenience, let $B_1(a,b,c,d,e)$, $B_2(a,b,c,d,e,f)$, $B_3(a,b,c,d,e,f,g)$, $B_4(a,b,c,d)$, $B_5(a,b,c,d,e)$, $B_6(a,b,c,d,e,f)$, $B_7(a,b,c,d,e)$ and $B_8(a,b,c,d,e,f)$ be bicyclic graphs whose bases are $B(3,3)$, $B(3,4)$, $B(4,4)$, $B(P_2,P_2,P_1)$, $B(P_3,P_2,P_1)$, $B(P_3,P_3,P_1)$, $B(P_2,P_2,P_2)$ and $B(P_3,P_2,P_2)$, respectively, and whose remaining vertices are pendent vertices (see Fig. 3).

Lemma 4.1. *Let $B_1(a,b,c,d,e)$ be the bicyclic graph of order n. Then $B_1(a+b+c+d+e,0,0,0,0) \preceq B_1(a,b,c,d,e)$. In other words,*

$$\varphi_i\big(B_1(a+b+c+d+e,0,0,0,0)\big) \leqslant \varphi_i\big(B_1(a,b,c,d,e)\big), \quad i=0,1,\dots,n,$$

with equalities for all $i=0,\dots,n$ holds if and only if $b=c=d=e=0$.

Proof. For convenience, let $G = B_1(a,b,c,d,e)$ and $G' = B_1(a+b+c+d+e,0,0,0,0)$. Further, for $2 \leqslant i \leqslant n$, let $\mathcal{H}'$ and $\mathcal{H}$ be the set of all TU-subgraphs of G' and G with exactly i edges, respectively. Let

$$\mathcal{H}'^{(1)} = \big\{H' \in \mathcal{H}' \bigm| H' \text{ contains no odd cycle}\big\},$$
$$\mathcal{H}'^{(2)} = \big\{H' \in \mathcal{H}' \bigm| H' \text{ contains an odd cycle}\big\}.$$

Similarly for $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$. Let $f : \mathcal{H}' \to \mathcal{H}$ with $H' \to H = f(H')$, where $V(H) = V(H')$ and

$$\begin{aligned} E\big(H'\big) &= E(H) - \big\{u_1x \bigm| x \in N_{R'}(u_1) \cap N_G(u_2) \setminus \{u_3\}\big\} - \big\{u_1x \bigm| x \in N_{R'}(u_1) \cap N_G(u_3) \setminus \{u_2\}\big\} \\ &\quad - \big\{u_1x \bigm| x \in N_{R'}(u_1) \cap N_G(u_4) \setminus \{u_5\}\big\} - \big\{u_1x \bigm| x \in N_{R'}(u_1) \cap N_G(u_5) \setminus \{u_4\}\big\} \\ &\quad + \big\{u_2x \bigm| x \in N_{R'}(u_1) \cap N_G(u_2) \setminus \{u_3\}\big\} + \big\{u_3x \bigm| x \in N_{R'}(u_1) \cap N_G(u_3) \setminus \{u_2\}\big\} \\ &\quad + \big\{u_4x \bigm| x \in N_{R'}(u_1) \cap N_G(u_4) \setminus \{u_5\}\big\} + \big\{u_5x \bigm| x \in N_{R'}(u_1) \cap N_G(u_5) \setminus \{u_4\}\big\}, \end{aligned}$$

for R' being a component of H' containing u_1. Clearly f is injective and $f(\mathcal{H}'^{(j)}) \subseteq \mathcal{H}^{(j)}$ for $j=1,2$. By Lemma 3.5 in [6], we have

$$\sum_{H' \in \mathcal{H}'^{(1)}} W\big(H'\big) < \sum_{H \in \mathcal{H}^{(1)}} W(H).$$

For $H' \in \mathcal{H}'^{(2)}$, without loss of generality, we assume that R' contains $C_3 : u_1u_2u_3u_1$ as a subgraph. It is easy to see that $W(f(H')) - W(H') \geqslant 0$. Hence

$$\varphi_i\big(G'\big) = \sum_{H' \in \mathcal{H}'^{(1)}} W\big(H'\big) + \sum_{H' \in \mathcal{H}'^{(2)}} W\big(H'\big) < \sum_{H \in \mathcal{H}^{(1)}} W(H) + \sum_{H \in \mathcal{H}^{(2)}} W(H).$$

So the assertion holds. □

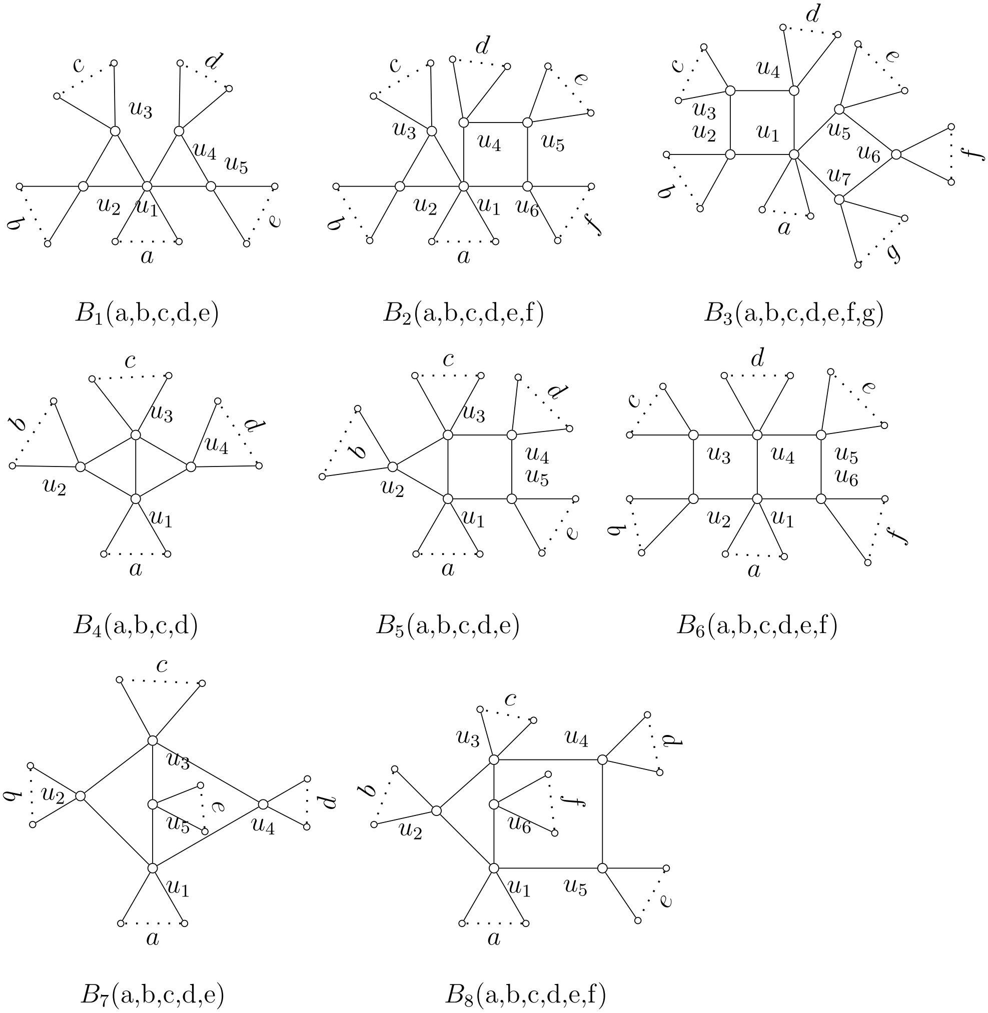

Fig. 3. Eight bicyclic graphs.

Lemma 4.2.

(1) $B_2(a+b+c+d+e+f,0,0,0,0) \preceq B_2(a,b,c,d,e,f)$ *with equality if and only if* $b=c=d=e=f=0$.
(2) $B_3(a+b+c+d+e+f+g,0,0,0,0,0) \preceq B_3(a,b,c,d,e,f,g)$ *with equality if and only if* $b=c=d=e=f=g=0$.
(3) $B_4(a+b+c+d,0,0,0) \preceq B_4(a,b,c,d)$ *with equality if and only if* $b=c=d=0$ *or* $a=b=d=0$.
(4) $B_5(a+b+c+d+e,0,0,0,0) \preceq B_5(a,b,c,d,e)$ *with equality if and only if* $b=c=d=e=0$ *or* $a=b=d=e=0$.
(5) $B_6(a+b+c+d+e+f,0,0,0,0,0) \preceq B_6(a,b,c,d,e,f)$ *with equality if and only if* $b=c=d=e=f=0$ *or* $a=b=c=e=f=0$.
(6) $B_7(a+b+c+d+e,0,0,0,0) \preceq B_7(a,b,c,d,e)$ *with equality if and only if* $b=c=d=e=0$ *or* $a=b=d=e=0$.
(7) $B_8(a+b+c+d+e+f,0,0,0,0) \preceq B_8(a,b,c,d,e,f)$ *with equality if and only if* $b=c=d=e=f=0$ *or* $a=b=d=e=f=0$.

Proof. The proof is similar to that of Lemma 4.2 and omitted. □

Lemma 4.3.

(1) $B_4(n-4,0,0,0) \preceq B_1(n-5,0,0,0,0)$.
(2) $B_4(n-4,0,0,0) \preceq B_5(n-5,0,0,0,0) \preceq B_2(n-6,0,0,0,0,0)$.
(3) $B_4(n-4,0,0,0) \preceq B_8(n-6,0,0,0,0,0)$.
(4) $B_7(n-5,0,0,0,0) \preceq B_6(n-6,0,0,0,0,0) \preceq B_3(n-7,0,0,0,0,0,0)$.

Proof. By [2], it is easy to see that the characteristic polynomials of these graphs are as follows:

$$\begin{aligned}
&Q\left(B_1(n-5,0,0,0,0);x\right) = (x-1)^{n-4}(x-3)\left[x^3-(n+3)x^2+3nx-8\right],\\
&Q\left(B_2(n-6,0,0,0,0,0);x\right)\\
&\quad = (x-1)^{n-6}(x-2)\left[x^5-(n+6)x^4+7(n+1)x^3-2(7n-1)x^2+2(3n+8)x-8\right],\\
&Q\left(B_4(n-4,0,0,0);x\right) = (x-1)^{n-4}(x-2)\left[x^3-(n+4)x^2+4nx-8\right],\\
&Q\left(B_5(n-5,0,0,0,0);x\right)\\
&\quad = (x-1)^{n-6}\left[x^6-(n+8)x^5+9(n+2)x^4-(27n+10)x^3\right.\\
&\qquad \left.+(31n+10)x^2-(11n+32)x+16\right],\\
&Q\left(B_8(n-6,0,0,0,0,0);x\right)\\
&\quad = (x-1)^{n-7}(x-2)\left[x^6-(n+7)x^5+(9n+8)x^4-(26n-22)x^3\right.\\
&\qquad \left.+(27n-30)x^2-(8n+8)x+8\right].
\end{aligned}$$

Hence

$$\begin{aligned}
&Q\left(B_1(n-5,0,0,0,0);x\right) - Q\left(B_4(n-4,0,0,0);x\right)\\
&\quad = (x-1)^{n-4}\left(x^2-nx+8\right),\\
&Q\left(B_2(n-6,0,0,0,0,0);x\right) - Q\left(B_5(n-5,0,0,0,0);x\right)\\
&\quad = x(x-1)^{n-6}\left[x^3-(n+2)x^2+(3n+2)x-(n+8)\right],\\
&Q\left(B_5(n-5,0,0,0,0);x\right) - Q\left(B_4(n-4,0,0,0);x\right)\\
&\quad = x(x-1)^{n-6}\left[(n-3)x^3-(6n-20)x^2+(9n-30)x-(3n-8)\right],\\
&Q\left(B_8(n-6,0,0,0,0,0);x\right) - Q\left(B_4(n-4,0,0,0);x\right)\\
&\quad = x(x-2)(x-1)^{n-7}\left[(2n-7)x^3-(11n-43)x^2+(14n-58)x-(4n-16)\right].
\end{aligned}$$

Hence $B_4(n-4,0,0,0) \preceq B_1(n-5,0,0,0,0)$, $B_4(n-4,0,0,0) \preceq B_5(n-5,0,0,0,0) \preceq B_2(n-6,0,0,0,0,0)$ and $B_4(n-4,0,0,0) \preceq B_8(n-6,0,0,0,0,0)$. Moreover,

$$\begin{aligned}
&Q\left(B_3(n-7,0,0,0,0,0,0);x\right)\\
&\quad = x(x-1)^{n-8}(x-2)^2\left(x^2-4x+2\right)\left[x^3-(n+2)x^2+2(2n-3)x-2n\right],\\
&Q\left(B_6(n-6,0,0,0,0,0);x\right)\\
&\quad = x(x-1)^{n-6}(x-3)\left[x^4-(n+5)x^3+(7n-1)x^2-(13n-17)x+5n\right],\\
&Q\left(B_7(n-5,0,0,0,0);x\right) = x(x-1)^{n-6}(x-2)^2\left[x^3-(n+4)x^2+(5n-2)x-3n\right].
\end{aligned}$$

Hence

$$Q\left(B_3(n-7,0,0,0,0,0,0);x\right)-Q\left(B_6(n-6,0,0,0,0,0);x\right)$$
$$=x(x-1)^{n-8}\left[x^5-(n+4)x^4+(6n+1)x^3-(11n-6)x^2+3(2n+1)x-n\right],$$
$$Q\left(B_6(n-6,0,0,0,0,0);x\right)-Q\left(B_7(n-5,0,0,0,0);x\right)$$
$$=x(x-1)^{n-6}\left[(n-4)x^3-(7n-28)x^2+(12n-43)x-3n\right].$$

Therefore, $B_7(n-5,0,0,0,0)\preceq B_6(n-6,0,0,0,0,0)\preceq B_3(n-7,0,0,0,0,0,0)$. So the assertion holds. □

5. The proofs of Theorems 1.1 and 1.2

In this section, we present the proofs of Theorems 1.1 and 1.2.

Proof of Theorem 1.1. Let G be a bicyclic graph of order n. We consider the following two cases.

Case 1: G contains an odd cycle. Then by Theorem 3.7, there exists a bicyclic graph G_1 of order n such that $G_1\preceq G$, where the base of G_1 is one of $B(3,3)$, $B(3,4)$, $B(P_2,P_2,P_1)$, $B(P_3,P_2,P_1)$ and $B(P_3,P_2,P_2)$, since G_1 can be obtained from G by a series of α- and β-transformations which still has an odd cycle. Further by Lemmas 4.1–4.3, we have $B_4(n-4,0,0,0)\preceq G_1\preceq G$ with equality if and only if $G=B_4(n-4,0,0,0)$.

Case 2: G contains no odd cycle. Then by Theorem 3.7, there exists a bicyclic graph G_2 of order n such that $G_2\preceq G$, where the base of G_2 is one of $B(4,4)$, $B(P_3,P_3,P_1)$ and $B(P_2,P_2,P_2)$, since G_2 is obtained from G by a series of α- and β-transformations which still contains no odd cycle. Further by Lemmas 4.2 and 4.3, we have $B_7(n-5,0,0,0,0)\preceq G_2\preceq G$ with equality if and only if $G=B_7(n-5,0,0,0,0)$. Note that B' is just $B_4(n-4,0,0,0)$ and B'' is just $B_7(n-5,0,0,0,0)$. Hence the assertion holds. □

From the proof of Theorem 1.1, in fact we obtain the following corollary.

Corollary 5.1. *Let $\mathcal{B}_n^{(1)}$ and $\mathcal{B}_n^{(2)}$ be the sets of all non-bipartite bicyclic graphs of order n and bipartite bicyclic graphs of order n, respectively. Then B' is the minimal element in $(\mathcal{B}_n^{(1)},\preceq)$ and B'' is the minimal element in $(\mathcal{B}_n^{(2)},\preceq)$.*

Proof of Theorem 1.2. By Theorem 1.1, it is follows from Theorem 4.2 in [12] that

$$IE(G)\geqslant \min\left\{IE\left(B'\right),IE\left(B''\right)\right\}.$$

Moreover, by Lemma 4.3, we have

$$IE\left(B'\right)=(n-4)+\sqrt{2}+\sqrt{\alpha_1}+\sqrt{\alpha_2}+\sqrt{\alpha_3},$$
$$IE\left(B''\right)=(n-6)+2\sqrt{2}+\sqrt{\beta_1}+\sqrt{\beta_2}+\sqrt{\beta_3},$$

where $\alpha_1\geqslant\alpha_2\geqslant\alpha_3$ are the roots of $x^3-(n+4)x^2+4nx-8=0$, $\beta_1\geqslant\beta_2\geqslant\beta_3$ are the roots of $x^3-(n+4)x^2+(5n-2)x-3n=0$.

Hence if $n\leqslant 30$, by Matlab 7.0 it is easy to see $IE(B')>IE(B'')$ holds.

If $n\geqslant 31$, it is easy to see that $n\leqslant\alpha_1\leqslant n+0.01$, $3.93\leqslant\alpha_2\leqslant 4$, $0\leqslant\alpha_3\leqslant 0.066$, and $n-1\leqslant\beta_1\leqslant n-0.995$, $4.27\leqslant\beta_2\leqslant 4.31$, $0.697\leqslant\beta_3\leqslant 0.726$, and $0.5899\leqslant\sum_{i=1}^{3}(\sqrt{\beta_i}-\sqrt{\alpha_i})\leqslant 1$. Then we have $IE(B'')-IE(B')=\sqrt{2}-2+\sum_{i=1}^{3}(\sqrt{\beta_i}-\sqrt{\alpha_i})\geqslant 0$. So the assertion holds. □

Corollary 5.2. *Let G be a bicyclic graph of order $n\geqslant 31$. Then $IE(G)>n+\sqrt{n}-\frac{2}{3}$.*

Proof. It is easy from the proof of Theorem 1.2 that $IE(B')>n-4+\sqrt{2}+\sqrt{n}+\sqrt{3.93}>n+\sqrt{n}-\frac{2}{3}$. By Theorem 1.2, the assertion holds. □

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