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The Signless Laplacian Coefficients and the Incidence Energy of Graphs with a Given Bipartition

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Abstract. We consider two classes of the graphs with a given bipartition. One is trees and the other is unicyclic graphs. The signless Laplacian coefficients and the incidence energy are investigated for the sets of trees/unicyclic graphs with *n* vertices in which each tree/unicyclic graph has an (n_1, n_2) -bipartition, where n_1 and n_2 are positive integers not less than 2 and $n_1 + n_2 = n$. Four new graph transformations are proposed for studying the signless Laplacian coefficients. Among the sets of trees/unicyclic graphs considered, we obtain exactly, for each, the minimal element with respect to the quasi-ordering according to their signless Laplacian coefficients and the element with the minimal incidence energies.

1. Introduction

Let G = (V(G), E(G)) be a simple graph, where $V(G) = \{v_1, \dots, v_n\}$ and $E(G) = \{e_1, \dots, e_m\}$ are the vertex set and the edge set of G, respectively. The adjacency matrix of G is denoted by A(G). The energy of G, as introduced by Gutman [6], is defined as the sum of the absolute values of all the eigenvalues of A(G). Let B be a matrix with real entries. The singular values of B are the positive square roots of the eigenvalues of BB^t , where B^t is the transpose of B. Moreover, if B is a symmetric matrix, then its singular values are the absolute values of its eigenvalues. Nikiforov [18] extended the concept of energy to all matrices, defining the energy of a matrix as the sum of the singular values of the matrix.

We denote by I(G) the vertex-edge incidence matrix of G, where I(G) is an $(n \times m)$ -matrix whose (i, j)entry is 1 if the vertex v_i is incident with the edge e_j , and 0 otherwise. In 2009, Jooyandeh et al. [11] defined the incidence energy (IE) of a graph G as

$$IE(G) = \sum_{i=1}^{n} \sigma_i,\tag{1}$$

where $\sigma_1, \sigma_2, \cdots, \sigma_n$ are the singular values of I(G).

Let $D(G) = \text{diag}(d_G(v_1), d_G(v_2), \dots, d_G(v_n))$ be the degree diagonal matrix of G, where $d_G(v_i)$ $(1 \le i \le n)$ is the degree of vertex v_i of G. We refer to L(G) = D(G) - A(G) and Q(G) = D(G) + A(G) as the Laplacian

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matrix and the signless Laplacian matrix, respectively. Since $I(G)I^{t}(G) = D(G) + A(G) = Q(G)$, we get [7]

$$IE(G) = \sum_{i=1}^{n} \sqrt{q_i},$$
(2)

where q_1, q_2, \dots, q_n are the eigenvalues of the signless Laplacian matrix Q(G). It is noted that q_1, q_2, \dots, q_n are real and non-negative.

The IE of *G*, which origins from chemical graph theory, can help explain some phenomena of chemical molecule. The graphs having the extremal IEs are derived on basis of (5) and other methods. For the graphs with the extremal IEs and the upper and lower bounds of IE, one can refer to Refs. [5, 7, 10, 15, 20, 21, 24, 26, 27]. Kaya and Maden got some bounds for the generalized version of incidence energy [12].

The Laplacian and signless Laplacian characteristic polynomials of G are respectively defined as

$$L(G;x) = \det[xI - L(G)] = \sum_{i=0}^{n} (-1)^{i} c_{i}(G) x^{n-i},$$
(3)

$$Q(G;x) = \det[xI - Q(G)] = \sum_{i=0}^{n} (-1)^{i} \varphi_{i}(G) x^{n-i},$$
(4)

where *I* is the identity matrix of order *n*, and $c_i(G)$ and $\varphi_i(G)$ are coefficients of corresponding characteristic polynomials. It is known that Q(G) and L(G) are similar if and only if (iff) *G* is bipartite. Therefore, the Laplacian coefficients are the same as the signless Laplacian coefficients (SLCs) iff *G* is bipartite.

Let \mathcal{G}_n be the set of all the simple graphs of order *n*. For $G, H \in \mathcal{G}_n$, we write $G \leq H$ if $c_i(G) \leq c_i(H)$ with $0 \leq i \leq n$. Similarly, we denote $G \leq H$ if $\varphi_i(G) \leq \varphi_i(H)$ for $0 \leq i \leq n$. We write G <' H if $G \leq H$ with an integer *k* in such a way that $\varphi_k(G) < \varphi_k(H)$. Then we refer to this symbol \leq' as the quasi-ordering. Mirzakhah and Kiani [16] obtained

$$G \leq' H \Longrightarrow IE(G) \leq IE(H),$$
 (5)

$$G <' H \Longrightarrow IE(G) < IE(H). \tag{6}$$

The Laplacian matrix has been studied extensively. Among various classes of graphs, some results have been derived about the partial ordering according to \leq . For example, Laplacian-cospectral trees [17], trees with a fixed matching number [9], unicyclic graphs [19], and bicyclic graphs [8], etc.

The signless Laplacian matrix of *G* has attracted more and more attention due to it can be used to discover more structural characterization of graphs than the Laplacian matrix in some ways [24]. For the partial ordering according to \leq' , there are many interesting results. Mirzakhah and Kiani [16] studied the coefficients of the signless Laplacian matrix of unicyclic graphs. Li et al. [13] determined two maximal elements and two minimal elements among unicyclic graphs. Zhang and Zhang [24] got two minimal elements in bicyclic graphs. Among the unicyclic graphs having a fixed matching number, Zhang and Zhang [25] characterized all the minimal elements. In the connected graphs of *n* vertices and *m* edges without even cycles, Wang et al. [23] obtained the minimal element which has the minimum SLCs and the minimum IE. Among the unicyclic graphs with *n* vertices and *r* pendent vertices, where $n \ge 4$ and $r \ge 1$, Wang and Zhong [22] characterized a unique extremal graph which has the minimum SLCs and the minimum IE. For further information on the signless Laplacian matrix, one can refer to three surveys [2–4].

Let *G* be a connected bipartite graph with *n* vertices. Then *V*(*G*) can be partitioned into two subsets $V_1(G)$ and $V_2(G)$ in such a way that each edge in *E*(*G*) joins a vertex in $V_1(G)$ with a vertex in $V_2(G)$. Let $|V_1(G)| = n_1$ and $|V_2(G)| = n_2$ with $n_1 + n_2 = n$. We say that *G* has an (n_1, n_2) -bipartition. Let $\mathcal{T}_{n_1, n_2}/\mathcal{U}_{n_1, n_2}$ be the set of trees/unicyclic graphs with *n* vertices in which each tree/unicyclic graph has an (n_1, n_2) -bipartition, where n_1 and n_2 are positive integers not less than 2 and $n_1 + n_2 = n$.

Motivated by all the above-mentioned work, we will characterize, in the present study, the minimal graphs in terms of \leq' according to their SLCs, and then deduce the graphs with the minimal IEs in \mathcal{T}_{n_1,n_2} and \mathcal{U}_{n_1,n_2} .

The subdivision graph S(G) of a graph G is a graph obtained by inserting a new vertex on each edge of G. Among \mathcal{T}_{n_1,n_2} , by comparing the number of k-matchings of the subdivision graphs of the graphs considered, Lin and Yan [14] characterized the trees having the minimal and the second minimal Laplacian coefficients. In this paper, we will use the α -transformation (presented in Lemma 3.3 in Subsection 3.1) to obtain the graph with the minimal SLCs among \mathcal{T}_{n_1,n_2} . Since the graphs among \mathcal{T}_{n_1,n_2} and \mathcal{U}_{n_1,n_2} are bipartite, their Laplacian coefficients are the same as their SLCs. Thus, in this paper, another straightforward and simpler method is acquired to obtain the graph with the minimal Laplacian coefficients among \mathcal{T}_{n_1,n_2} (presented in Theorem 3.13 in Subsection 3.2), and the graph with the minimal Laplacian coefficients among \mathcal{U}_{n_1,n_2} is deduced (presented in Theorem 3.17 in Subsection 3.2).

The paper is organized as follows. In Subsection 3.1, four new transformations (see Lemmas 3.1–3.11) which keep the bipartition unchanged are derived. In Subsection 3.2, by the four transformations proposed in this paper, we obtain exactly, among \mathcal{T}_{n_1,n_2} and \mathcal{U}_{n_1,n_2} , one minimal element with respect to the quasi-ordering \prec' according to their SLCs and we get the graph with the minimal IEs.

2. Preliminaries

Let *G* be a graph of order *n*. A connected graph of order *n* is an odd unicyclic graph if it has only one cycle with an odd length. 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 *s* odd unicyclic graphs and *t* trees T_1, T_2, \dots, T_t of orders n_1, n_2, \dots, n_t , respectively. Then the weight of *H* is denoted by

$$W(H) = 4^s \prod_{i=1}^t n_i.$$
 (7)

If *H* contains no trees, then $W(H) = 4^s$. If *H* contains no cycles, then $W(H) = \prod_{i=1}^t n_i$. Note that isolated vertices in *H* may be ignored since they do not contribute to W(H).

To obtain the main results of this paper, Lemma 2.1 is introduced as follows.

Lemma 2.1. [1] Let $Q(G, x) = det[xI - Q(G)] = \sum_{i=0}^{n} (-1)^{i} \varphi_{i}(G) x^{n-i}$ be the characteristic polynomial of the signless Laplacian matrix of a graph G with order n. Then

$$\varphi_i(G) = \sum_{H_i} W(H_i), \qquad (i = 0, 1, 2, \cdots, n), \tag{8}$$

where the summation runs over all TU-subgraphs H_i of G with i edges. In particular, $\varphi_0(G) = 1$, $\varphi_1(G) = 2m$ and $\varphi_2(G) = 2m^2 - m - \frac{1}{2}\sum_{i=1}^n d_G^2(v_i)$.

By Lemma 2.1, we get the following property, which is used to obtain our transformations in Subsection 3.1. Let G_1 and G_2 be two connected graphs with n vertices. Let i be a fixed number with $2 \le i \le n$. Let $\mathcal{H}_1 = \{H^1, H^2, \ldots, H^s\}$ and $\mathcal{H}_2 = \{\widehat{H}^1, \widehat{H}^2, \ldots, \widehat{H}^t\}$ be the sets of all the TU-subgraphs of G_1 and of G_2 with i edges exactly, respectively, where $s \le t$. Then $\varphi_i(G_1) = \sum_{j=1}^s W(H^j)$ and $\varphi_i(G_2) = \sum_{j=1}^t W(\widehat{H}^j)$. If there exists a mapping f from \mathcal{H}_1 to \mathcal{H}_2 satisfying $W(H^k) \le W(\widehat{H}^k)$, where $1 \le k \le s$, then we have $\varphi_i(G_1) = W(H^1) + \ldots + W(H^s) \le W(\widehat{H}^1) + \cdots + W(\widehat{H}^t) = \varphi_i(G_2)$.

3. Main results

3.1. Four transformations for studying the SLCs of graphs considered

In this subsection, we will introduce four new transformations for studying the SLCs of the graphs with a given bipartition, which are shown in Lemmas 3.1–3.11. The bipartition for the graphs among T_{n_1,n_2} and U_{n_1,n_2} keeps unchanged within the framework of the four transformations.



Figure 1: α -transformation from A_n to A_n^*

For a subset *M* of E(G), G - M denotes the graph obtained from *G* by deleting all the edges in *M*. For an edge set M^* satisfying $M^* \cap E(G) = \emptyset$, $G + M^*$ denotes the graph obtained from *G* by adding all the edges in M^* . If $M = \{e\}$ and $M^* = \{e\}$, then G - M and $G + M^*$ are rewritten as G - e and G + e, respectively. For a subgraph *H* of *G*, G - H denotes the subgraph of *G* induced by the vertices not in *H*.

Let G_1 , G_2 and G_3 be three mutually disjoint graphs in which u_i is a vertex of G_i ($1 \le i \le 3$). We denote by $G_1 + u_1u_2 + G_2$ the graph obtained from G_1 and G_2 by adding an edge u_1u_2 between u_1 of G_1 with u_2 of G_2 . Similarly, $G_1 + u_1u_2 + G_2 + u_2u_3 + G_3$ is the graph obtained from G_1 , G_2 and G_3 by adding an edge u_1u_2 between u_1 of G_1 with u_2 of G_2 and adding an edge u_2u_3 between u_2 of G_2 with u_3 of G_3 .

We denote by $N_G(v)$ the neighbors of v in the graph G.

Let *Q* be a connected graph with a vertex *x*, and T_v and T_w two trees with $v \in V(T_v)$ and $w \in V(T_w)$. Let $P_3 = uvw$ be a path of length 2. Let A_n be the graph with *n* vertices obtained from *Q* by first identifying *x* of *Q* with *u* of $P_3 = uvw$, then identifying *v* of T_v with *v* of P_3 and identifying *w* of T_w with *w* of P_3 . Let A_n^* be the graph obtained from A_n by replanting T_w from *w* to *u*. A_n and A_n^* are shown in Figs. 1(a) and 1(b), respectively. In other words,

$$A_n^* = A_n - \{wy \mid y \in N_{T_w}(w)\} + \{uy \mid y \in N_{T_w}(w)\}.$$
(9)

The transformation from A_n to A_n^* in (9) is called α -transformation.

Lemma 3.1. Let A_n and A_n^* be the two graphs as defined in Fig. 1. If Q is a connected unicyclic graph, then we have $\varphi_i(A_n) \ge \varphi_i(A_n^*)$ for $0 \le i \le n$, where the equalities do not hold for all *i*.

Proof. It follows from Lemma 2.1 that $\varphi_i(A_n) = \varphi_i(A_n^*)$ for i = 0, 1. Next, let $2 \le i \le n$. For a fixed *i*, let \mathcal{H}^* and \mathcal{H} be the sets of all the TU-subgraphs of A_n^* and of A_n with *i* edges exactly, respectively.

For an arbitrary TU-subgraph $H^* \in \mathcal{H}^*$, let

$$f_1: \mathcal{H}^* \to \mathcal{H}, H^* \to H = f_1(H^*),$$

with $V(H) = V(H^*)$ and

$$E(H) = E(H^*) - \{ux \mid x \in N_{T_m}(u) \cap V(H^*)\} + \{wx \mid x \in N_{T_m}(u) \cap V(H^*)\}.$$

Obviously, f_1 is a bijection from \mathcal{H}^* to \mathcal{H} .

For the sake of conciseness, a tree component, an odd unicyclic component, an arbitrary component, and the same component are abbreviated as a TC, an OUC, an AC, and the SC, respectively. Let *N* be the weight of all the components of H^* not containing *u*, *v* or *w*. In A_n^* , let $uv = e_1$ and $vw = e_2$. Three cases are considered as follows.

Case (I) $e_1, e_2 \notin E(H^*)$.

In this case, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by R_u^* , R_v^* and R_w^* the connected components of H^* containing u, v and w, respectively. Since $e_1, e_2 \notin E(H^*)$, R_u^* , R_v^* and $R_w^* = \{w\}$ are mutually

(10)

disjoint; and R_v^* and R_w^* are TCs. Let $|V(Q) \cap V(R_u^*) \setminus \{u\} = a$, $|V(T_w) \cap V(R_u^*) \setminus \{u\} = b$ and $|V(T_v) \cap V(R_v^*) \setminus \{v\} = c$. Thus, we get

$$|V(R_{w}^{*})| = a + b + 1, \quad |V(R_{w}^{*})| = c + 1, \quad |V(R_{w}^{*})| = 1.$$
(11)

By the bijection f_1 , in H, there exist three components, denoted by R_u , R_v and R_w , which correspond to R_u^* , R_v^* and R_w^* , respectively. It is noted that R_u , R_v and R_w contain u, v and w in H, respectively; R_v and R_w are TCs; and R_u , R_v and R_w are mutually disjoint. Obviously, we have

$$|V(R_u)| = a + 1, \quad |V(R_v)| = c + 1, \quad |V(R_w)| = b + 1.$$
(12)

Furthermore, we have the following statement:

Fact 3.2. Except for the component(s) containing u, v and w in H^* , an AC of H^* corresponds to the SC of H.

Two subcases are considered according to the fact R_u^* is a TC or an OUC. **Subcase (I.i)** R_u^* is a TC. In this subcase, R_u is a TC. By Fact 3.2, (7), (11), and (12), we obtain

$$W(f_1(H^*)) - W(H^*) = (a+1)(b+1)(c+1)N - (a+b+1)(c+1)N$$

= Nab(c+1) \ge 0, (13)

with the third equality iff a = 0 or b = 0.

Subcase (I.ii) R_{μ}^{*} is an OUC.

In this subcase, R_u is an OUC. By Fact 3.2, (7), (11), and (12), we get

$$W(f_1(H^*)) - W(H^*) = 4(b+1)(c+1)N - 4(c+1)N = 4Nb(c+1) \ge 0,$$
(14)

with the third equality iff b = 0.

Case (II) $e_1 \in E(H^*)$ and $e_2 \notin E(H^*)$.

Let $R_{u,v}^* = R_u^* + uv + R_v^*$ and $R_{u,v} = R_u + uv + R_v$. Obviously, by (11) and (12), $R_{u,v}^*$ is a component of order a + b + c + 2 containing u, v in H^* and $R_{u,v}$ is a component of order a + c + 2 containing u, v of H. Since $e_1 \in E(H^*)$ and $e_2 \notin E(H^*)$, by the bijection $f_1, R_{u,v}^*$ and $\{w\}$ in H^* correspond to $R_{u,v}$ and R_w in H, respectively. Two subcases are considered according to the fact $R_{u,v}^*$ is a TC or an OUC.

Subcase (II.i) $R_{u,v}^*$ is a TC.

In this subcase, $R_{u,v}$ is a TC. By Fact 3.2, (7), (11), and (12), we get

$$W(f_1(H^*)) - W(H^*) = (a + c + 2)(b + 1)N - (a + b + c + 2)N$$

= Nb(a + c + 1) \ge 0, (15)

with the third equality iff b = 0. We denote

 $\mathcal{H}_1^* = \{ H^* \in \mathcal{H}^* \mid e_1 \in E(H^*), e_2 \notin E(H^*) \text{ and } R^*_{u,v} \text{ is a TC} \}.$

Subcase (II.ii) $R_{u,v}^*$ is an OUC.

In this subcase, $R_{u,v}$ is an OUC. It follows from Fact 3.2, (7) and (12) that

$$W(f_1(H^*)) - W(H^*) = 4(b+1)N - 4N = 4Nb \ge 0,$$
(16)

with the third equality iff b = 0.

Case (III) $e_1 \notin E(H^*)$ and $e_2 \in E(H^*)$.

Since $e_1 \notin E(H^*)$ and $e_2 \in E(H^*)$, by the bijection f_1 , R_u^* and $R_{v,w}^* = R_v^* + vw + R_w^*$ in H^* correspond to R_u and $R_{v,w} = R_v + vw + R_w$ in H, respectively. Obviously, by (11) and (12), $R_{v,w}^*$ is a TC of order c + 2 containing v and w in H^* and $R_{v,w}$ is a TC of order b + c + 2 containing v and w in H. Two subcases are considered according to the fact R_u^* is a TC or an OUC. **Subcase (III.i)** R_u^* is a TC.

In this subcase, R_u is a TC. By Fact 3.2, (7), (11), and (12), we have

$$W(f_1(H^*)) - W(H^*) = (a+1)(b+c+2)N - (a+b+1)(c+2)N$$

= Nb(a-c-1). (17)

We denote

 $\mathcal{H}_2^* = \{ H^* \in \mathcal{H}^* \mid e_1 \notin E(H^*), e_2 \in E(H^*) \text{ and } R_u^* \text{ is a TC} \}.$

We construct a mapping ξ_1 from \mathcal{H}_2^* to \mathcal{H}_1^* as follows. For $H^* \in \mathcal{H}_2^*$, let

$$\xi_1: H^* \to \xi_1(H^*) = H^* - e_2 + e_1. \tag{18}$$

Obviously, ξ_1 is bijective. Thus, there exists a one-to-one relationship between \mathcal{H}_2^* and \mathcal{H}_1^* . Namely, for an arbitrary $H^* \in \mathcal{H}_2^*$, we can find, by ξ_1 , a unique element $\xi_1(H^*) \in \mathcal{H}_1^*$ corresponding to it, and vice versa. For $H^* \in \mathcal{H}_2^*$, by (17) and (15), we obtain

$$[W(f_1(H^*)) - W(H^*)] + [W(f_1(\xi_1(H^*))) - W(\xi_1(H^*))] = 2Nab \ge 0.$$
⁽¹⁹⁾

Furthermore, by (19), we get

$$\sum_{H^* \in \mathcal{H}_2^*} [W(f_1(H^*)) - W(H^*)] + \sum_{H^* \in \mathcal{H}_1^*} [W(f_1(H^*)) - W(H^*)]$$

=
$$\sum_{H^* \in \mathcal{H}_2^*} [W(f_1(H^*)) - W(H^*) + W(f_1(\xi_1(H^*))) - W(\xi_1(H^*))] \ge 0.$$
 (20)

Subcase (III.ii) R_u^* is an OUC.

In this subcase, R_u is an OUC. By Fact 3.2 and (7), we obtain

$$W(f_1(H^*)) - W(H^*) = 4(b+c+2)N - 4(c+2)N = 4Nb \ge 0,$$
(21)

with the third equality iff b = 0.

Case (IV) $e_1, e_2 \in E(H^*)$.

We have three facts: (i) u, v and w of H^* are contained in a component of H^* (denoted by $R^*_{u,v,w}$); (ii) $R^*_{u,v,w}$ corresponds to a component (denoted by $R_{u,v,w}$) of H containing u, v and w; and (iii) $R^*_{u,v,w}$ and $R_{u,v,w}$ are TCs or OUCs simultaneously and have the same order. Therefore, it follows from Fact 3.2 and (7) that

$$W(f_1(H^*)) = W(H^*).$$
 (22)

By (13), (14), (16), and (20)–(22), for a fixed $i (2 \le i \le n)$, we finally get

$$\sum_{H^* \in \mathcal{H}^*} W(f(H^*)) \ge \sum_{H^* \in \mathcal{H}^*} W(H^*).$$
(23)

The inequality in (23) holds when at least one of the inequalities in (14), (16) and (21) holds for $b \ge 1$. Therefore, by Lemma 2.1, for $0 \le i \le n$, we obtain $\varphi_i(A_n) \ge \varphi_i(A_n^*)$ and the equality holds iff i = 0, 1. Thus, we obtain Lemma 3.1. \Box

In A_n and A_n^* , if Q is a tree, then by deleting the proofs for Subcases (I.ii), (II.ii) and (III.ii) in Lemma 3.1, we can easily get Lemma 3.3 as follows.

Lemma 3.3. Let A_n and A_n^* be the two graphs as defined in Fig. 1. If Q is a tree, then we have $\varphi_i(A_n) \ge \varphi_i(A_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all i.



Figure 2: β -transformation from B_n to B_n^*

Remark 3.4. After performing the α -transformation once from A_n to A_n^* in Lemma 3.1, A_n and A_n^* have the same bipartition, and the number of pendent vertices of A_n^* is one more than that of A_n .

Let B_n be the graph shown in Fig. 2(a), where B_n satisfies the following conditions: (i) v and w are two adjacent vertices at C_l of B_n ; (ii) u is not at C_l and u is adjacent to v; (iii) u, v and w are identified with u' of a tree T_3 , v' of a tree T_1 and w' of a tree T_2 , respectively; and (iv) The other vertices at C_l of B_n (except for v and w) may be or maybe not attached by trees. Let B_n^* be the graph obtained from B_n by replanting T_3 from u to w, where B_n^* is shown in Fig. 2(b). In other words,

$$B_n^* = B_n - \{ uy \mid y \in N_{T_3}(u') \} + \{ wy \mid y \in N_{T_3}(u') \}.$$
(24)

The transformation from B_n to B_n^* in (24) is called β -transformation.

Lemma 3.5. For $0 \le i \le n$, we have $\varphi_i(B_n) \ge \varphi_i(B_n^*)$ where the equality does not hold for all *i*.

Proof. By Lemma 2.1, $\varphi_i(B_n) = \varphi_i(B_n^*)$ for i = 0, 1. Next, we assume $2 \le i \le n$.

For a fixed *i*, we denote by \mathcal{H}^* and \mathcal{H} the sets of all the TU-subgraphs of B_n^* and of B_n with exactly *i* edges, respectively. For an arbitrary TU-subgraph $H^* \in \mathcal{H}^*$, let

$$f_2: \mathcal{H}^* \to \mathcal{H}, H^* \to H = f_2(H^*), \tag{25}$$

with $V(H) = V(H^*)$ and

$$E(H) = E(H^*) - \{wx \mid x \in N_{T_3}(u') \cap V(H^*)\} + \{ux \mid x \in N_{T_3}(u') \cap V(H^*)\}$$

Obviously, f_2 is bijective from \mathcal{H}^* to \mathcal{H} .

Let *N* be the weight of all the components of H^* not containing *u*, *v* or *w*. Next, four cases are considered as follows.

Case (I) $uv, vw \notin E(H^*)$.

Two subcases are considered as follows.

Subcase (I.i) v and w of H^* are not contained in a SC.

In this subcase, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by \overline{R}_u , \overline{R}_v and \overline{R}_w the connected components of H^* containing u, v and w, respectively. Since uv, $vw \notin E(H^*)$, $\overline{R}_u = \{u\}$, \overline{R}_v and \overline{R}_w are TCs and they are mutually disjoint. Let $|V(\overline{R}_v - v)| = a$, $|V(\overline{R}_w - T_3 - w)| = b$ and $|V(T_3) \cap V(\overline{R}_w) \setminus \{w\}| = c$. Thus, we get

$$|V(\tilde{R}_u)| = 1, \quad |V(\tilde{R}_v)| = a + 1, \quad |V(\tilde{R}_w)| = b + c + 1.$$
(26)

By the bijection f_2 , in H, there exist three components, denoted by R'_u , R'_v and R'_w , which correspond to \widetilde{R}_u , \widetilde{R}_v and \widetilde{R}_w , respectively. Obviously, we have: (i) R'_u , R'_v and R'_w contain u, v and w in H, respectively; (ii) R'_u , R'_v and R'_w are TCs and they are mutually disjoint; and (iii) R'_v is \widetilde{R}_v . Furthermore, we have

$$|V(R'_{u})| = c + 1, \quad |V(R'_{v})| = a + 1, \quad |V(R'_{w})| = b + 1.$$
(27)

We have the following statement:

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Fact 3.6. Except for the component(s) containing u, v and w in H^* , an AC of H^* corresponds to the SC of H.

Therefore, by Fact 3.6, (7), (26), and (27), we obtain

$$W(f_2(H^*)) - W(H^*) = (a+1)(b+1)(c+1)N - (a+1)(b+c+1)N$$

= N(a+1)bc \ge 0, (28)

with the third equality iff b = 0 or c = 0.

Subcase (I.ii) v and w of H^* are contained in a SC.

In this subcase, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by \widetilde{R}_1 the connected component of H^* containing v and w. Since $vw \notin E(H^*)$, \widetilde{R}_1 is a TC. Since $uv \notin E(H^*)$, u of H^* is contained in $\widetilde{R}_u = \{u\}$. Let $|V(\widetilde{R}_1 - T_3 - v - w)| = h$ and $|V(T_3) \cap V(\widetilde{R}_1) \setminus \{w\}| = c$. Thus, we get

$$|V(\tilde{R}_1)| = h + c + 2, \quad |V(\tilde{R}_n)| = 1.$$
⁽²⁹⁾

By the bijection f_2 , we obtain that \widetilde{R}_1 and \widetilde{R}_u in H^* correspond to a TC (denoted by R'_1) containing v and w and R'_u containing u in H, respectively. Obviously, we have

$$|V(R'_1)| = h + 2, \ |V(R'_n)| = c + 1.$$
(30)

Thus, by Fact 3.6, (7), (29), and (30), we have

$$W(f_2(H^*)) - W(H^*) = (h+2)(c+1)N - (h+c+2)N = N(h+1)c \ge 0,$$
(31)

with the third equality iff c = 0.

Case (II) $uv \in E(H^*)$ and $vw \notin E(H^*)$.

Two subcases are considered as follows.

Subcase (II.i) v and w of H^* are not contained in a SC.

Since $uv \in E(H^*)$ and $vw \notin E(H^*)$, by the bijection f_2 , we obtain that a TC (denoted by $R_{u,v}$) of order a + 2 containing u and v and \tilde{R}_w containing w in H^* correspond respectively to a TC (denoted by $R'_{u,v}$) of order a + c + 2 containing u and v and R'_w containing w in H, where $\tilde{R}_{u,v} = \tilde{R}_u + uv + \tilde{R}_v$ and $R'_{u,v} = R'_u + uv + R'_v$. Thus, by Fact 3.6, (7), (26), and (27), we have

$$W(f_2(H^*)) - W(H^*) = (a + c + 2)(b + 1)N - (a + 2)(b + c + 1)N$$

= Nc(b - a - 1). (32)

We denote

$$\mathcal{H}_{3}^{*} = \{H^{*} \in \mathcal{H}^{*} \mid uv \in E(H^{*}), vw \notin E(H^{*}), v \text{ and } w \text{ of } H^{*} \text{ are not contained in a SC} \}.$$

Subcase (II.ii) v and w of H^* are contained in a SC.

In this subcase, u, v and w of H^* are contained in a TC of order h + c + 3, which corresponds to a TC of order h + c + 3 containing u, v and w in H (by the bijection f_2). Thus, by Fact 3.6 and (7), we obtain

$$W(f_2(H^*)) - W(H^*) = 0.$$
(33)

Case (III) $uv \notin E(H^*)$ and $vw \in E(H^*)$.

Subcase (III.i) v and w of H^* are contained in a TC (namely, $\overline{R}_{v,w} = \overline{R}_v + vw + \overline{R}_w$) of H^* .

By the bijection f_2 , we obtain that $\widetilde{R}_{v,w}$ of order a + b + c + 2 containing v and w and $\widetilde{R}_u = \{u\}$ in H^* correspond respectively to a TC (namely, $R'_{v,w} = R'_v + vw + R'_w$) of order a + b + 2 containing v and w and R'_u in H. Thus, by Fact 3.6, (7) and (27), we have

$$W(f_2(H^*)) - W(H^*) = (a+b+2)(c+1)N - (a+b+c+2)N$$

= Nc(a+b+1) \ge 0, (34)

with the third equality iff c = 0.

We denote

 $\mathcal{H}_4^* = \{H^* \in \mathcal{H}^* \mid uv \notin E(H^*), vw \in E(H^*), v \text{ and } w \text{ of } H^* \text{ are contained in a TC of } H^*\}.$

We construct a mapping ξ_2 from \mathcal{H}_3^* to \mathcal{H}_4^* as follows. For $H^* \in \mathcal{H}_{3'}^*$ let

$$\xi_2: H^* \to \xi_2(H^*) = H^* - uv + vw. \tag{35}$$

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Obviously, ξ_2 is bijective. Therefore, there exists a one-to-one relationship between \mathcal{H}_3^* and \mathcal{H}_4^* . Namely, for an arbitrary $H^* \in \mathcal{H}_3^*$, we can find, by ξ_2 , a unique element $\xi_2(H^*) \in \mathcal{H}_4^*$ corresponding to it, and vice versa. For $H^* \in \mathcal{H}_3^*$, by (32) and (34), we obtain

$$[W(f_2(H^*)) - W(H^*)] + [W(f_2(\xi_2(H^*))) - W(\xi_2(H^*))] = 2Nbc \ge 0,$$
(36)

with the second equality iff b = 0 or c = 0. Therefore, by (36), we get

$$\sum_{H^{*} \in \mathcal{H}_{3}^{*}} [W(f_{2}(H^{*})) - W(H^{*})] + \sum_{H^{*} \in \mathcal{H}_{4}^{*}} [W(f_{2}(H^{*})) - W(H^{*})]$$

$$= \sum_{H^{*} \in \mathcal{H}_{3}^{*}} [W(f_{2}(H^{*})) - W(H^{*}) + W(f_{2}(\xi_{2}(H^{*}))) - W(\xi_{2}(H^{*}))] \ge 0.$$
(37)

Subcase (III.ii) *v* and *w* of H^* are contained in an OUC (namely $\tilde{R}_1 + vw$).

By the bijection f_2 , we obtain that $\overline{R}_1 + vw$ and $\overline{R}_u = \{u\}$ in H^* correspond respectively to an OUC (namely $R'_1 + vw$) containing v and w and R'_u in H. Thus, by Fact 3.6, (7) and (30), we have

$$W(f_2(H^*)) - W(H^*) = 4(c+1)N - 4N = 4Nc \ge 0,$$
(38)

with the third equality iff c = 0.

Case (IV) $uv, vw \in E(H^*)$.

We have three facts: (i) u, v and w of H^* are contained in a component of H^* (denoted by $\overline{R}_{u,v,w}$); (ii) $\overline{R}_{u,v,w}$ corresponds to a component (denoted by $f_2(\widetilde{R}_{u,v,w})$) of H containing u, v and w; and (iii) $\widetilde{R}_{u,v,w}$ and $f_2(\widetilde{R}_{u,v,w})$ are TCs or OUCs simultaneously and have the same order. Therefore, by Fact 3.6 and (7), we obtain

$$W(f_2(H^*) = W(H^*).$$
 (39)

By (28), (31), (33), and (37)–(39), for a fixed $i (2 \le i \le n)$, we finally get

$$\sum_{H^* \in \mathcal{H}^*} W(f_2(H^*)) \ge \sum_{H^* \in \mathcal{H}^*} W(H^*).$$

$$\tag{40}$$

The inequality in (40) holds when at least one of the inequalities in (31) and (38) holds for $c \ge 1$. By Lemma 2.1, we get $\varphi_i(B_n) \ge \varphi_i(B_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all *i*. Therefore, we obtain Lemma 3.5. \Box

Remark 3.7. If B_n is a bipartite unicyclic graph, then after performing the β -transformation once from B_n to B_n^* in Lemma 3.5, we have three properties: (i) B_n and B_n^* have the same girth; (ii) B_n and B_n^* have the same bipartition; and (iii) the number of pendent vertices of B_n^* is one more than that of B_n .

Let F_n be the graph obtained from $C_l = w_1 w_2 \dots w_l$ by identifying w_i of C_l with w'_i of T_i , where T_i is a tree, w'_i is a vertex of T_i and $1 \le i \le l$. It is noted that T_i may be an empty graph, where $1 \le i \le l$. F_n is shown in Fig. 3(a). Let F_n^* be the graph obtained from F_n through the following steps: (i) Replanting the tree T_2 from w_2 to w_4 ; (ii) Replanting the tree T_3 from w_3 to w_1 ; (iii) deleting the edge $w_2 w_3$; and (iv) adding a new edge $w_1 w_4$. F_n^* is shown in Fig. 3(b). In other words, we have

$$F_n^* = F_n - \{w_2 y \mid y \in N_{T_2}(w_2')\} - \{w_3 y \mid y \in N_{T_3}(w_3')\} - \{w_2 w_3\} + \{w_4 y \mid y \in N_{T_2}(w_2')\} + \{w_1 y \mid y \in N_{T_3}(w_3')\} + \{w_1 w_4\}.$$
(41)

The transformation from F_n to F_n^* in (41) is called γ -transformation.



Figure 3: γ -transformation from F_n to F_n^*

Lemma 3.8. We have $\varphi_i(F_n) \ge \varphi_i(F_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all *i*.

Proof. It follows from Lemma 2.1 that $\varphi_i(F_n) = \varphi_i(F_n^*)$ when i = 0, 1. Next, let $2 \le i \le n$.

For a fixed *i*, let \mathcal{H}^* and \mathcal{H} be the sets of all the TU-subgraphs of F_n^* and of F_n with exactly *i* edges, respectively. For an arbitrary TU-subgraph $H^* \in \mathcal{H}^*$, let

$$f_3: \mathcal{H}^* \to \mathcal{H}, H^* \to H = f_3(H^*), \tag{42}$$

with $V(H) = V(H^*)$ and

$$E(H) = E(H^*) - \{w_4 y \mid y \in A\} - \{w_1 y \mid y \in B\} - \{w_1 w_4\} + \{w_2 y \mid y \in A\} + \{w_3 y \mid y \in B\} + \{w_2 w_3\},\$$

where $A = N_{T_2}(w'_2) \cap V(H^*)$ and $B = N_{T_3}(w'_3) \cap V(H^*)$. Obviously, f_3 is injective from \mathcal{H}^* to \mathcal{H} .

Let *N* be the weight of all the components of H^* not containing w_1, w_2, w_3 or w_4 .

If all of w_1w_2 , w_1w_4 and w_3w_4 are contained in $E(H^*)$, then we have three facts: (i) w_1 , w_2 , w_3 and w_4 are contained in a component of H^* (denoted by $R^*_{1,2,3,4}$); (ii) $R^*_{1,2,3,4}$ corresponds to a component $f_3(R^*_{1,2,3,4})$ of H containing w_1 , w_2 , w_3 , and w_4 ; and (iii) $R^*_{1,2,3,4}$ and $f_3(R^*_{1,2,3,4})$ are TCs or OUCs simultaneously and have the same order. Furthermore, we have the following statement.

Fact 3.9. Except for the component(s) containing w_1 , w_2 , w_3 , and w_4 in H^* , an AC of H^* corresponds to the SC of H.

Therefore, by Fact 3.9 and (7), we obtain

$$W(f_3(H^*)) = W(H^*).$$

Next, we assume that at least one of w_1w_2 , w_1w_4 and w_3w_4 does not belong to $E(H^*)$. Seven cases are considered as follows.

Case (I) $w_1w_2, w_1w_4, w_3w_4 \notin E(H^*)$.

Two subcases are considered as follows.

Subcase (I.i) w_1 and w_4 of H^* are not contained in a SC.

In this subcase, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by R_1^* , R_2^* , R_3^* , and R_4^* the connected components of H^* containing w_1 , w_2 , w_3 , and w_4 , respectively. Obviously, $R_2^* = \{w_2\}$ and $R_3^* = \{w_3\}$. It is noted that R_1^* , R_2^* , R_3^* , and R_4^* are mutually disjoint and they are TCs since w_1w_2 , w_1w_4 , $w_3w_4 \notin E(H^*)$. Let $|V(R_1^* - T_3 - w_1)| = a$, $|V(T_2) \cap V(R_4^*) \setminus \{w_4\}| = b$, $|V(T_3) \cap V(R_1^*) \setminus \{w_1\}| = c$, and $|V(R_4^* - T_2 - w_4)| = d$. Thus, we get

$$|V(R_1^*)| = a + c + 1, \quad |V(R_2^*)| = 1, \quad |V(R_3^*)| = 1, \quad |V(R_4^*)| = b + d + 1.$$
(44)

By the bijection f_3 , in H, there exist four components, denoted by R_1 , R_2 , R_3 , and R_4 , which correspond to R_1^* , R_2^* , R_3^* , and R_4^* , respectively. It is noted that R_1 , R_2 , R_3 , and R_4 contain respectively w_1 , w_2 , w_3 , and w_4 in

(43)

H and they are mutually disjoint. Obviously, R_1 , R_2 , R_3 , and R_4 are all TCs since w_1w_2 , w_1w_4 , $w_3w_4 \notin E(H)$. We have

$$|V(R_1)| = a + 1, \quad |V(R_2)| = b + 1, \quad |V(R_3)| = c + 1, \quad |V(R_4)| = d + 1.$$
(45)

Therefore, by Fact 3.9, (7), (44), and (45), we obtain

$$W(f_{3}(H^{*})) - W(H^{*}) = (a+1)(b+1)(c+1)(d+1)N - (a+c+1)(b+d+1)N$$

= N[abcd + ac(b+d+1) + bd(a+c+1)] ≥ 0. (46)

Subcase (I.ii) w_1 and w_4 of H^* are contained in a SC.

In this subcase, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by R_5^* the connected component of H^* containing w_1 and w_4 . Since $w_1w_4 \notin E(H^*)$, R_5^* is a TC. Obviously, $R_2^* = \{w_2\}$ and $R_3^* = \{w_3\}$ are the components containing w_2 and w_3 in \mathcal{H}^* , respectively. Let $|V(R_5^* - T_2 - T_3 - w_1 - w_4)| = h$, $|V(T_2) \cap V(R_5^*) \setminus \{w_4\}| = b$ and $|V(T_3) \cap V(R_5^*) \setminus \{w_1\}| = c$. Thus, we get

$$|V(R_5^*)| = h + b + c + 2, \quad |V(R_2^*)| = 1, \quad |V(R_3^*)| = 1.$$
(47)

By the bijection f_3 , we obtain that R_5^* , R_2^* and R_3^* in H^* correspond respectively to a TC (denoted by R_5) containing w_1 and w_4 , R_2 containing w_2 and R_3 containing w_3 in H. It is noted that R_5 , R_2 and R_3 are mutually disjoint. Obviously, we have

$$|V(R_5)| = h + 2, \quad |V(R_2)| = b + 1, \quad |V(R_3)| = c + 1.$$
(48)

Thus, by Fact 3.9, (7), (47), and (48), we get

$$W(f_{3}(H^{*})) - W(H^{*}) = (h+2)(b+1)(c+1)N - (h+b+c+2)N$$

= $N[(h+2)bc + (h+1)(b+c)] \ge 0.$ (49)

Case (II) $w_1w_2, w_1w_4 \in E(H^*)$ and $w_3w_4 \notin E(H^*)$.

In this case, w_3 of H^* is contained in $R_3^* = \{w_3\}$ and w_1 , w_2 and w_4 of H^* are contained in a component denoted by $R_{2,1,4}^*$. Here $R_{i,j,k}^* = R_i^* + w_i w_j + R_j^* + w_j w_k + R_k^*$ with $1 \le i, j, k \le 4$. Obviously, $|V(R_{i,j,k}^*)| = |V(R_i^*)| + |V(R_j^*)| + |V(R_k^*)|$ and $R_{i,j,k}^*$ contains w_i , w_j and w_k of H^* . Let $R_{i,j,k} = R_i + w_i w_j + R_j + w_j w_k + R_k$ with $1 \le i, j, k \le 4$. Obviously, $|V(R_{i,j,k})| = |V(R_i)| + |V(R_j)| + |V(R_k)|$ and $R_{i,j,k}$ contains w_i , w_j and w_k of H^* . Let $R_{i,j,k}$ contains w_i , w_j and w_k of H. Two subcases are considered as follows.

Subcase (II.i) $R_{2.1.4}^*$ is a TC.

By the bijection f_3 , we obtain that $R_{2,1,4}^*$ of order a+b+c+d+3 and $R_3^* = \{w_3\}$ in H^* correspond respectively to a TC (namely $R_{1,2,3}$) of order a + b + c + 3 and R_4 of order d + 1 in H. Thus, by Fact 3.9 and (7), we get

$$W(f_3(H^*)) - W(H^*) = (a + b + c + 3)(d + 1)N - (a + b + c + d + 3)N$$

= Nd(a + b + c + 2) \ge 0. (50)

We denote

 $\mathcal{H}_5^* = \{H^* \in \mathcal{H}^* \mid w_1 w_2, w_1 w_4 \in E(H^*), w_3 w_4 \notin E(H^*), \text{ and } R_{2,1,4}^* \text{ is a TC} \}.$

Subcase (II.ii) $R_{2,1,4}^*$ is an OUC.

By the bijection f_3 , we obtain that $R_{2,1,4}^*$ and $R_3^* = \{w_3\}$ in H^* correspond to a TC (namely, $R_5 + w_1w_2 + R_2 + w_2w_3 + R_3$) of order h + b + c + 4 containing w_1, w_2, w_3 , and w_4 in H. Thus, by Fact 3.9 and (7), we have

$$W(f_3(H^*)) - W(H^*) = (h+b+c+4)N - 4N = N(h+b+c) \ge 0.$$
(51)

Case (III) $w_1w_2 \notin E(H^*)$ and $w_1w_4, w_3w_4 \in E(H^*)$.

In this case, w_1 , w_3 and w_4 of H^* are contained in a component denoted by $R^*_{1,4,3}$. Two subcases are considered as follows.

Subcase (III.i) $R^*_{1,4,3}$ is a TC.

By the bijection f_3 , we obtain that $R_{1,4,3}^*$ of order a+b+c+d+3 and $R_2^* = \{w_2\}$ in H^* correspond respectively to a TC (namely, $R_{2,3,4}$) of order b+c+d+3 and R_1 of order a+1 in H. Thus, by Fact 3.9 and (7), we get

$$W(f_{3}(H^{*})) - W(H^{*}) = (a+1)(b+c+d+3)N - (a+b+c+d+3)N$$
$$= Na(b+c+d+2) \ge 0.$$
(52)

We denote

$$\mathcal{H}_{6}^{*} = \{H^{*} \in \mathcal{H}^{*} \mid w_{1}w_{2} \notin E(H^{*}), w_{1}w_{4}, w_{3}w_{4} \in E(H^{*}), \text{ and } R_{143}^{*} \text{ is a TC}\}.$$

Subcase (III.ii) $R_{1,4,3}^*$ is an OUC.

By the bijection f_3 , we obtain that $R_{1,4,3}^*$ and $R_2^* = \{w_2\}$ in H^* correspond to a TC (namely, $R_2 + w_2w_3 + R_3 + w_3w_4 + R_5$) of order h + b + c + 4 containing w_1, w_2, w_3 , and w_4 in H. Thus, by Fact 3.9 and (7), we get

$$W(f_3(H^*)) - W(H^*) = (h+b+c+4)N - 4N = N(h+b+c) \ge 0.$$
(53)

Case (IV) $w_1w_2, w_3w_4 \in E(H^*)$ and $w_1w_4 \notin E(H^*)$.

Two subcases are considered as follows.

Subcase (IV.i) w_1 and w_4 of H^* are not contained in a SC.

In this subcase, w_1 and w_2 of H^* are contained in $R_{1,2}^*$ and w_3 and w_4 of H^* are contained in $R_{3,4}^*$, where $R_{1,2}^* = R_1^* + w_1w_2 + R_2^*$ and $R_{3,4}^* = R_3^* + w_3w_4 + R_4^*$. By the bijection f_3 , $R_{1,2}^*$ of order a + c + 2 and $R_{3,4}^*$ of order b + d + 2 correspond respectively to a TC (namely, $R_{1,2}$) of order a + b + 2 containing w_1 and w_2 and a TC (namely, $R_{3,4}$) of order c + d + 2 containing w_3 and w_4 in H, where $R_{1,2} = R_1 + w_1w_2 + R_2$ and $R_{3,4} = R_3 + w_3w_4 + R_4$. Thus, by Fact 3.9 and (7), we get

$$W(f_3(H^*)) - W(H^*) = (a+b+2)(c+d+2)N - (a+c+2)(b+d+2)N$$

= N(b-c)(d-a). (54)

We denote

 $\mathcal{H}_7^* = \{H^* \in \mathcal{H}^* \mid w_1w_2, w_3w_4 \in E(H^*), w_1w_4 \notin E(H^*), w_1 \text{ and } w_4 \text{ are not contained in a SC}\}.$

We construct a mapping ξ_3 from \mathcal{H}_7^* to \mathcal{H}_5^* and a mapping ξ_4 from \mathcal{H}_7^* to \mathcal{H}_6^* as follow. For $H \in \mathcal{H}_7^*$, let

 $\xi_3: H^* \to \xi_3(H^*) = H^* + w_1 w_4 - w_3 w_4,$ $\xi_4: H^* \to \xi_4(H^*) = H^* + w_1 w_4 - w_1 w_2.$

For an arbitrary $H^* \in \mathcal{H}_{7'}^*$, we can find, by ξ_3 and ξ_4 , a unique $\xi_3(H^*) \in \mathcal{H}_5^*$ and a unique $\xi_4(H^*) \in \mathcal{H}_6^*$ corresponding to it, respectively. For $H \in \mathcal{H}_7^*$, by (54), (50) and (52), we get

$$[W(f_{3}(H^{*})) - W(H^{*})] + [W(f_{3}(\xi_{3}(H^{*}))) - W(\xi_{3}(H^{*}))] + [W(f_{3}(\xi_{4}(H^{*}))) - W(\xi_{4}(H^{*}))] = N[d(a + 2b + 2) + a(2c + d + 2)] \ge 0.$$
(55)

Since ξ_3 and ξ_4 are bijective, by (55), we have

$$\sum_{\substack{H^* \in \mathcal{H}_5^* \ \cup \ \mathcal{H}_6^* \ \cup \ \mathcal{H}_7^*}} [W(f(H^*)) - W(H^*)] = \sum_{\substack{H^* \in \mathcal{H}_7^* \ \to \ \mathcal{H}_7^*}} [W(f_3(H^*)) - W(H^*) + W(f_3(\xi_3(H^*))) - W(\xi_3(H^*))) + W(f_3(\xi_4(H^*))) - W(\xi_4(H^*))] \ge 0.$$
(56)

Subcase (IV.ii) w_1 and w_4 are contained in a SC.

In this subcase, w_1 , w_2 , w_3 , and w_4 of H^* are contained in a TC of order h + b + c + 4, which corresponds to a TC of order h + b + c + 4 containing w_1 , w_2 , w_3 , and w_4 in H (by the bijection f_3). Thus, by Fact 3.9 and (7), we get

$$W(f_3(H^*)) - W(H^*) = 0.$$
(57)

Case (V) $w_1w_2, w_1w_4 \notin E(H^*)$ and $w_3w_4 \in E(H^*)$.

Two subcases are considered as follows.

Subcase (V.i) w_1 and w_4 of H^* are not contained in a SC.

By the bijection f_3 , we obtain that $R_1^*, R_2^* = \{w_2\}$ and $R_{3,4}^*$ with order b + d + 2 in H^* correspond respectively to R_1, R_2 and $R_{3,4}$ with order c + d + 2 in H. Therefore, by Fact 3.9, (7), (44), and (45), we get

$$W(f_{3}(H^{*})) - W(H^{*}) = (a+1)(b+1)(c+d+2)N - (a+c+1)(b+d+2)N$$

= N[ab(c+d+1) + b(d+1) + ac - c(d+1)]. (58)

We denote

 $\mathcal{H}_8^* = \{H^* \in \mathcal{H}^* \mid w_1 w_2, w_2 w_4 \notin E(H^*), w_3 w_4 \in E(H^*), w_1 \text{ and } w_4 \text{ of } H^* \text{ are not contained in a SC} \}.$

Subcase (V.ii) w_1 and w_4 of H^* are contained in SC.

By the bijection f_3 , a TC (namely, $R_3^* + w_3w_4 + R_5^*$) with order h + b + c + 3 containing w_1 , w_3 and w_4 and $R_2^* = \{w_2\}$ in H^* correspond respectively to a TC (namely, $R_3 + w_3w_4 + R_5$) with order h + c + 3 containing w_1 , w_3 and w_4 and R_2 of order b + 1 in H. Therefore, by Fact 3.9 and (7), we get

$$W(f_3(H^*)) - W(H^*) = (b+1)(h+c+3)N - (h+b+c+3)N$$

= Nb(h+c+2) \ge 0. (59)

Case (VI) $w_1w_2 \in E(H^*)$ and $w_1w_4, w_3w_4 \notin E(H^*)$.

Two subcases are considered as follows.

Subcase (VI.i) w_1 and w_4 of H^* are not contained in SC.

By the bijection f_3 , we obtain that $R_{1,2}^*$ of order a + c + 2, $R_3^* = \{w_3\}$ and R_4^* in H^* correspond respectively to a TC (namely, $R_{1,2}$) of order a + b + 2, R_3 and R_4 in H. Therefore, by Fact 3.9, (7), (44), and (45), we obtain

$$W(f_{3}(H^{*})) - W(H^{*}) = (a + b + 2)(c + 1)(d + 1)N - (a + c + 2)(b + d + 1)N$$

= N[cd(a + b + 1) + bd + c(a + 1) - b(a + 1)]. (60)

We denote

$$\mathcal{H}_{9}^{*} = \{H^{*} \in \mathcal{H}^{*} \mid w_{1}w_{2} \in E(H^{*}), w_{1}w_{4}, w_{3}w_{4} \notin E(H^{*}), w_{1} \text{ and } w_{4} \text{ of } H^{*} \text{are not contained in SC} \}$$

We construct a mapping ξ_5 from \mathcal{H}_8^* to \mathcal{H}_9^* as follows. For $H \in \mathcal{H}_{8'}^*$ let

 $\xi_5: H^* \to \xi_5(H^*) = H^* + w_1 w_2 - w_3 w_4.$

Obviously, ξ_5 is bijective. Thus, there exists a one-to-one relationship between \mathcal{H}_8^* and \mathcal{H}_9^* . By (58) and (60), we have

$$\sum_{H^* \in \mathcal{H}_8^* \cup \mathcal{H}_9^*} [W(f_3(H^*)) - W(H^*)] = \sum_{H^* \in \mathcal{H}_8^*} [W(f_3(H^*)) - W(H^*) + W(f_3(\xi_5(H^*))) - W(\xi_5(H^*))] \ge 0.$$
(61)

Subcase (VI.ii) w_1 and w_4 of H^* are contained in SC.

By the bijection f_3 , we obtain that a TC (namely, $R_2^* + w_2w_1 + R_5^*$) of order h + b + c + 3 containing w_1 , w_2 and w_4 and $R_3^* = \{w_3\}$ in H^* correspond respectively to a TC (namely, $R_2 + w_2w_1 + R_5$) of order h + b + 3 containing w_1 , w_2 and w_4 and R_3 of order c + 1 in H. Therefore, by Fact 3.9 and (7), we obtain

$$W(f_3(H^*)) - W(H^*) = (c+1)(h+b+3)N - (h+b+c+3)N$$

= Nc(h+b+2) \ge 0. (62)

Case (VII) $w_1w_2, w_3w_4 \notin E(H^*)$ and $w_1w_4 \in E(H^*)$.

In this case, w_1 and w_4 of H^* are contained in a SC. Two subcases are considered as follows.

Subcase (VII.i) w_1 and w_4 of H^* are contained in a TC (namely $R_{1,4}^* = R_1^* + w_1w_4 + R_4^*$).

By the bijection f_3 , we get that $R_{1,4}^*$ with order a + b + c + d + 2, $R_2^* = \{w_2\}$ and $R_3^* = \{w_3\}$ in H^* correspond respectively to a TC (namely, $R_{2,3} = R_2 + w_2w_3 + R_3$) of order b + c + 2 containing w_2 and w_3 , R_1 and R_4 in H. Therefore, by Fact 3.9, (7) and (45), we get

$$W(f_3(H^*)) - W(H^*) = (a+1)(b+c+2)(d+1)N - (a+b+c+d+2)N$$

= N[(ad+a+d)(b+c+1)+ad] \ge 0. (63)

Subcase (VII.ii) w_1 and w_4 of H^* are contained in an OUC (namely $R_5^* + w_1w_4$).

By the bijection f_3 , we get that $R_5^* + w_1w_4$ in H^* corresponds to R_5 of order h + 2 containing w_1 and w_4 in H, and $R_2^* = \{w_2\}$ and $R_3^* = \{w_3\}$ in H^* correspond to a TC (namely, $R_{2,3}$) of order b + c + 2 containing w_2 and w_3 in H. Therefore, by Fact 3.9 and (7), we have

$$W(f_3(H^*)) - W(H^*) = (h+2)(b+c+2)N - 4N$$

= N[h(b+c) + 2(b+c+f)] \ge 0. (64)

By combining the proofs of Cases (I)–(VII), for a fixed $i (2 \le i \le n)$, it follows from (43), (46), (49), (51), (53), (56), (57), (59), and (61)–(64) that

$$\sum_{H^* \in \mathcal{H}^*} W(f_3(H^*)) \ge \sum_{H^* \in \mathcal{H}^*} W(H^*).$$
(65)

The inequality in (65) holds when the inequalities in (51) and (53) hold for $b \ge 1$ or $c \ge 1$ or $h \ge 1$. Furthermore, by Lemma 2.1, we have $\varphi_i(F_n) \ge \varphi_i(F_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all *i*. Thus, we get Lemma 3.8. \Box

Remark 3.10. After performing the γ -transformation once from F_n to F_n^* in Lemma 3.8, we have three facts: (i) The girth of F_n^* is two smaller than that of F_n ; (ii) F_n and F_n^* have the same bipartition; and (iii) The number of pendent vertices of F_n^* is two more than that of F_n .

Let X_{n+1} be a star with n + 1 vertices and w_0 the center vertex of X_{n+1} . Let $n'_1 + n'_2 + n'_3 + n'_4 = n - 4$, $n'_1 + n'_3 + 2 = n_1$ and $n'_2 + n'_4 + 2 = n_2$, where $0 \le n'_i \le n - 4$ for $1 \le i \le 4$. Let D_n be the graph obtained from $C_4 = w_1 w_2 w_3 w_4$ by identifying w_i with the center vertex of $X_{n'_i+1}$, where $1 \le i \le 4$. Let M_n be the graph obtained from $C_4 = w_1 w_2 w_3 w_4$ by identifying w_1 with the center vertex of $X_{n'_1+1}$, where $1 \le i \le 4$. Let M_n be the graph obtained from $C_4 = w_1 w_2 w_3 w_4$ by identifying w_1 with the center vertex of $X_{n'_1+n'_3+1}$ and by identifying w_2 with the center vertex of $X_{n'_2+n'_3+1}$. In other words,

$$M_n = D_n - \{w_3 y \mid y \in A\} - \{w_4 y \mid y \in B\} + \{w_1 y \mid y \in A\} + \{w_2 y \mid y \in B\},$$
(66)

where $A = N_{X_{n'_{4}+1}}(w_0)$ and $B = N_{X_{n'_{4}+1}}(w_0)$. The transformation from D_n to M_n in (66) is called ξ -transformation. D_n and M_n are shown in Figs. 4(a) and 4(b), respectively. Obviously, $D_n, M_n \in \mathcal{U}_{n_1,n_2}$.

Lemma 3.11. For $0 \le i \le n$, we have $\varphi_i(D_n) \ge \varphi_i(M_n)$ and the equalities do not hold for all *i*.



Figure 4: ξ -transformation from D_n to M_n

Proof. By Lemma 2.1, $\varphi_i(D_n) = \varphi_i(D_n^*)$ for i = 0, 1. Next, we assume $2 \le i \le n$.

For a fixed *i*, we denote by \mathcal{H}^* and \mathcal{H} the sets of all the TU-subgraphs of M_n and of D_n with exactly *i* edges, respectively. For an arbitrary TU-subgraph $H^* \in \mathcal{H}^*$, let

$$f_4: \mathcal{H}^* \to \mathcal{H}, H^* \to H = f_4(H^*), \tag{67}$$

with $V(H) = V(H^*)$ and

$$E(H) = E(H^*) - \{w_1 y \mid y \in A \cap V(H^*)\} - \{w_2 y \mid y \in B \cap V(H^*)\} + \{w_3 y \mid y \in A \cap V(H^*)\} + \{w_4 y \mid y \in B \cap V(H^*)\},$$

where $A = N_{X_{n'_2+1}}(w_0)$ and $B = N_{X_{n'_4+1}}(w_0)$. Obviously, f_4 is a bijection from \mathcal{H}^* to \mathcal{H} .

Let *N* be the weight of all the components of H^* not containing w_1 , w_2 , w_3 , or w_4 . In M_n , let $w_1w_2 = e_1$, $w_2w_3 = e_2$, $w_3w_4 = e_3$, and $w_1w_4 = e_4$.

If all of e_1 , e_2 , e_3 , and e_4 are contained in $E(H^*)$, then the component containing w_1 , w_2 , w_3 , and w_4 in M_n has a cycle with even girth. This is contrary to the definition of TU-subgraph. Therefore, we get that at most three of e_1 , e_2 , e_3 , and e_4 are contained in $E(H^*)$. Three cases are considered as follows.

Case (i) None of e_1 , e_2 , e_3 , and e_4 is contained in $E(H^*)$.

In this case, for an arbitrary TU-subgraph H^* in \mathcal{H}^* , we denote by $R^*_{w_1}$, $R^*_{w_2}$, $R^*_{w_3}$, and $R^*_{w_4}$ the connected components of H^* containing w_1 , w_2 , w_3 , and w_4 , respectively. Obviously, $R^*_{w_3} = \{w_3\}$ and $R^*_{w_4} = \{w_4\}$. It is noted that $R^*_{w_1}$, $R^*_{w_2}$, $R^*_{w_3}$, and $R^*_{w_4}$ are mutually disjoint and they are TCs. Let $|V(R^*_{w_1}) \cap V(X_{n'_1+1}) \setminus \{w_1\}| = s$, $|V(R^*_{w_1}) \cap V(X_{n'_2+1}) \setminus \{w_1\}| = q$, $|V(R^*_{w_2}) \cap V(X_{n'_2+1}) \setminus \{w_2\}| = t$, and $|V(R^*_{w_2}) \cap V(X_{n'_4+1}) \setminus \{w_2\}| = p$. Thus, we get

$$|V(R_{w_1}^*)| = s + q + 1, \ |V(R_{w_2}^*)| = t + p + 1, \ |V(R_{w_2}^*)| = 1, \ V(R_{w_4}^*)| = 1.$$
(68)

By the bijection f_4 , in H, there exist four components, denoted by R'_{w_1} , R'_{w_2} , R'_{w_3} , and R'_{w_4} , which correspond to $R^*_{w_1}$, $R^*_{w_2}$, $R^*_{w_3}$, and $R^*_{w_4}$, respectively. It is noted that R'_{w_1} , R'_{w_2} , R'_{w_3} , and R'_{w_4} contain respectively w_1 , w_2 , w_3 , and w_4 in H and they are mutually disjoint. Obviously, R'_{w_1} , R'_{w_2} , R'_{w_3} , and R'_{w_4} are TCs since $e_1, e_2, e_3, e_4 \notin E(H)$. We have

$$|V(R'_{w_1})| = s + 1, \ |V(R'_{w_2})| = t + 1, \ |V(R'_{w_3})| = q + 1, \ |V(R'_{w_4})| = p + 1.$$
(69)

Furthermore, we have the following statement:

Fact 3.12. *Except for the component(s) containing* w_1 , w_2 , w_3 , and w_4 in H^* , an AC of H^* corresponds to the SC of *H*.

Therefore, by Fact 3.12, (7), (68), and (69), we get

$$W(f_4(H^*)) - W(H^*) = (s+1)(t+1)(p+1)(q+1) - (s+q+1)(t+p+1)$$

= $stpq + sq(t+p+1) + tp(s+q+1) \ge 0.$ (70)

Case (ii) Only one of e_1 , e_2 , e_3 , and e_4 is contained in $E(H^*)$.

If $e_1 \in E(H^*)$ and $e_2, e_3, e_4 \notin E(H^*)$, then by the bijection f_4 , we obtain that a TC (namely, $R_{w_1}^* + w_1w_2 + R_{w_2}^*)$ with order s + t + p + q + 2 containing w_1 and w_2 , $R_{w_3}^* = \{w_3\}$ and $R_{w_4}^* = \{w_4\}$ in H^* correspond to a TC (namely, $R_{w_1}' + w_1w_2 + R_{w_2}')$ of order s + t + 2 containing w_1 and w_2 , R_{w_3}' and R_{w_4}' in H, respectively. Therefore, by Fact 3.12, (7) and (69), we obtain

$$W(f_4(H^*)) - W(H^*) = (s+t+2)(p+1)(q+1) - (s+t+p+q+2).$$
(71)

By the methods similar to (71), we get (72)–(74) as follows. If $e_2 \in E(H^*)$ and $e_1, e_3, e_4 \notin E(H^*)$, then

$$W(f_4(H^*)) - W(H^*) = (s+1)(t+q+2)(p+1) - (s+q+1)(t+p+2).$$
(72)

If $e_3 \in E(H^*)$ and $e_1, e_2, e_4 \notin E(H^*)$, then

$$W(f_4(H^*)) - W(H^*) = (s+1)(t+1)(p+q+2) - 2(s+q+1)(t+p+1).$$
(73)

If $e_4 \in E(H^*)$ and $e_1, e_2, e_3 \notin E(H^*)$, then

$$W(f_4(H^*)) - W(H^*) = (s+p+2)(q+1)(t+1) - (s+q+2)(t+p+1).$$
(74)

Therefore, in Case (ii), after adding (71)–(74) together, we get

$$W(f_4(H^*)) - W(H^*) = 4p(t+s) + 2(pqs + pqt + pst + qst) \ge 0.$$
(75)

Case (iii) Two of e_1 , e_2 , e_3 , and e_4 are contained in $E(H^*)$.

In this case, there exist six kinds of classification. By the same analysis as those for (75), we get

$$W(f_4(H^*)) - W(H^*)$$

$$= [(s + t + p + 3)(q + 1) - (s + t + p + q + 3)] + [(s + t + q + 3)(p + 1) - (s + t + p + q + 3)] + [(s + t + 2)(p + q + 2) - 2(s + t + p + q + 2)] + [(s + p + 2)(t + q + 2) - (s + q + 2)(t + p + 2)] + [(s + p + q + 3)(t + 1) - (s + q + 3)(t + p + 1)] + [(s + 1)(t + p + q + 3) - (s + q + 1)(t + p + 3)]$$

$$= 4p(t + s) \ge 0.$$
(76)

Case (iv) Three of e_1 , e_2 , e_3 , and e_4 are contained in $E(H^*)$. In this case, there exist four kinds of classification. By the same analysis as those for (75), we obtain

$$W(f_4(H)) = W(H^*).$$
 (77)

By combining (70), (75)–(77), for a fixed $i (2 \le i \le n)$, we obtain

$$\sum_{H^* \in \mathcal{H}^*} W(f_4(H^*)) \ge \sum_{H^* \in \mathcal{H}^*} W(H^*).$$
(78)

The inequality in (78) holds when the inequalities in (75) and (76) hold for $p, s, t \ge 1$. Furthermore, by Lemma 2.1, we get $\varphi_i(D_n) \ge \varphi_i(M_n)$ for $0 \le i \le n$ and the equalities do not hold for all i. \Box

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3.2. The graphs with the minimal SLCs and the minimal IEs among \mathcal{T}_{n_1,n_2} and \mathcal{U}_{n_1,n_2}

In this subsection, we will use the α -transformation (presented in Lemma 3.3 in Subsection 3.1) to obtain the graph with the minimal SLCs among \mathcal{T}_{n_1,n_2} , which is shown in Theorem 3.13. The β -, γ - and ξ -transformations, as presented in Lemmas 3.5, 3.8 and 3.11 in Subsection 3.1, respectively, will be used to obtain the graph with the minimal SLCs among \mathcal{U}_{n_1,n_2} , which is shown in Theorem 3.17. Furthermore, by Theorems 3.13 and 3.17, we obtain the graphs with the minimal IEs among \mathcal{T}_{n_1,n_2} , respectively.

Let $S(n_1, n_2)$ be a tree obtained from X_{n_1} and X_{n_2} by adding an edge between the center vertices of X_{n_1} and of X_{n_2} , where $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$.

Theorem 3.13. Let $T \in \mathcal{T}_{n_1,n_2}$ with $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$. For $0 \le i \le n$, we have $\varphi_i(T) \ge \varphi_i(S(n_1, n_2))$ with all the equalities iff $T = S(n_1, n_2)$.

Proof. Let T_0 be the graph with the minimal SLCs in \mathcal{T}_{n_1,n_2} , where $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$. Let dia (T_0) be the diameter of T_0 . We suppose dia $(T_0) \ge 4$. Thus, in T_0 , there exists a path P of length at least 4. Let u, v and w be three vertices lying on P in such a way that v is adjacent to both u and w and the vertex degrees of u and of w are greater than 1. Therefore, T_0 can be viewed as the graph A_n (as shown in Fig. 1(a)), where T_v in A_n may be an empty graph. By Lemma 3.3, we can find another graph A_n^* (as shown in Fig. 1(b)) satisfying $\varphi_i(T_0) \ge \varphi_i(A_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all i. This contradicts the minimality of T_0 . Therefore, we obtain dia $(T_0) = 3$ or dia $(T_0) = 2$. If dia $(T_0) = 2$, then $T_0 = X_{n+1}$. Since $X_{n+1} \notin \mathcal{T}_{n_1,n_2}$ as $n_1, n_2 \ge 2$, we get dia $(T_0) = 3$. As $T_0 \in \mathcal{T}_{n_1,n_2}$ and dia $(T_0) = 3, T_0$ must be $S(n_1, n_2)$. Theorem 3.13 is thus proved. \Box

From Theorem 3.13, we obtain the graph with the minimal IE in \mathcal{T}_{n_1,n_2} , as shown in Theorem 3.14.

Theorem 3.14. Let $T \in \mathcal{T}_{n_1,n_2}$ with $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$. We have $IE(T) \ge IE(S(n_1, n_2))$ with the equality iff $T = S(n_1, n_2)$.

By Lemmas 3.5–3.11, we get the graph with the minimal SLCs among \mathcal{U}_{n_1,n_2} , as shown in Theorem 3.17. To obtain Theorem 3.17, we introduce Lemmas 3.15 and 3.16 as follows.

Lemma 3.15. If G_0 has the minimum SLCs in \mathcal{U}_{n_1,n_2} , then a cut-edge of G_0 must be a pendent edge.

Proof. Suppose that G_0 has a cut-edge e = uv which is not a pendent edge. Hence u and v are two vertices of degree at least 2 with $N_{G_0}(v) \cap N_{G_0}(u) = \emptyset$. Without loss of generality, we assume that G_0 is B_n (as shown in Fig. 2(a)). By employing the β -transformation and by Lemma 3.5, there is a graph B_n^* (as shown in Fig. 2(b)) such that $\varphi_i(G_0) \ge \varphi_i(B_n^*)$ for $0 \le i \le n$, where B_n^* satisfies these three properties as shown in Remark 3.7. This contradicts the minimality of G_0 . Therefore, a cut-edge of G_0 must be a pendent edge. \Box

Lemma 3.16. If G_0 has the minimum SLCs in \mathcal{U}_{n_1,n_2} and C_l is the cycle of G_0 , then l = 4.

Proof. We assume that G_0 is F_n (as shown in Fig. 3(a)) and $l \ge 6$. By applying the γ -transformation and by Lemma 3.8, we obtain a new graph F_n^* (as shown in Fig. 3(b)) having a cycle C_{l-2} such that $\varphi_i(G_0) \ge \varphi_i(F_n^*)$ for $0 \le i \le n$ and the equalities do not hold for all *i*, where F_n^* satisfies these three properties as shown in Remark 3.10. This contradicts the minimality of G_0 . Therefore, l = 4. \Box

Theorem 3.17. Let $G \in \mathcal{U}_{n_1,n_2}$ with $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$. We have $\varphi_i(G) \ge \varphi_i(M_n)$ for $0 \le i \le n$ and the equalities do not hold for all *i*.

Proof. Let G_0 be the graph with the minimum SLCs in \mathcal{U}_{n_1,n_2} and C_l the cycle of G_0 . By Lemmas 3.15 and 3.16, we get that a cut-edge of G_0 must be a pendent edge and l = 4, respectively. Therefore, we suppose $G_0 = D_n$, where D_n is shown in Fig. 4(a). By applying the ξ -transformation and by Lemma 3.11, we have $\varphi_i(D_n) \ge \varphi_i(M_n)$ for $0 \le i \le n$ and the equalities do not hold for all *i*, where M_n is shown in Fig. 4(b) and $M_n \in \mathcal{U}_{n_1,n_2}$. This contradicts the minimality of G_0 . Therefore, we finally get $G_0 = M_n$. Theorem 3.17 is thus proved. \Box

By Theorem 3.17, we get the graph with the minimal IE among \mathcal{U}_{n_1,n_2} , which is shown in Theorem 3.18.

Theorem 3.18. Let $G \in \mathcal{U}_{n_1,n_2}$ with $n_1, n_2 \ge 2$ and $n_1 + n_2 = n$. We have $IE(G) \ge IE(M_n)$ with the equality iff $G = M_n$.

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