Filomat 33:1 (2019), 177–192
https://doi.org/10.2298/FIL1901177W

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

The Signless Laplacian Coefficients and the Incidence Energy of Unicyclic Graphs with given Pendent Vertices

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Abstract. Let $\mathcal{U}_n^r$ be the set of unicyclic graphs with n vertices and r pendent vertices (namely, r leaves), where $n \geq 4$ and $r \geq 1$. We consider the signless Laplacian coefficients (SLCs) and the incidence energy (IE) in $\mathcal{U}_n^r$. Firstly, among a subset of $\mathcal{U}_n^r$ in which each graph has a fixed odd girth $g \geq 3$, where $n \geq g+1$ and $r \geq 1$, we characterize a unique extremal graph which has the minimum SLCs and the minimum IE. Secondly, if $G \in \mathcal{U}_n^r$ and G has odd girth $g \geq 5$, where $n \geq 7$ and $r \geq 1$, then we prove that a unique extremal graph $L_n \in \mathcal{U}_n^r$ with girth 4 satisfies that both the SLCs and the IE of G are more than the counterparts of L_n.

1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with a vertex set $V(G) = \{v_1, \ldots, v_n\}$ and an edge set $E(G) = \{e_1, \ldots, e_m\}$. The vertex-edge incidence matrix of G is denoted by $\boldsymbol{I}(G)$, where $\boldsymbol{I}(G)$ 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. Let $d_G(v_i)$ be the degree of the vertex v_i with $1 \leq i \leq n$. The adjacency matrix, Laplacian matrix and signless Laplacian matrix of G are denoted by $\boldsymbol{A}(G)$, $\boldsymbol{L}(G) = \boldsymbol{D}(G) - \boldsymbol{A}(G)$, and $\boldsymbol{Q}(G) = \boldsymbol{D}(G) + \boldsymbol{A}(G)$, respectively. It is well known that $\boldsymbol{A}(G)$ is a symmetric matrix and $\boldsymbol{L}(G)$ and $\boldsymbol{Q}(G)$ are positive semi-definite matrices.

The characteristic polynomial of G is defined as

$$\phi(G; x) = \det(x\boldsymbol{I} - \boldsymbol{A}(G)) = \sum_{i=0}^{n} a_i(G)x^{n-i}, \tag{1}$$

where $\boldsymbol{I}$ is the identity matrix of order n and $a_i(G)$ are coefficients of characteristic polynomial with $0 \leq i \leq n$.

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

$$L(G; x) = \det(x\boldsymbol{I} - \boldsymbol{L}(G)) = \sum_{i=0}^{n} (-1)^i c_i(G)x^{n-i}, \tag{2}$$

2010 *Mathematics Subject Classification*. Primary 05C50; Secondary 92E10
Keywords. Signless Laplacian coefficient, incidence energy, unicyclic graph, pendent vertex
Received: 26 January 2018; Accepted: 13 February 2019
Communicated by Francesco Belardo
Research supported by the National Natural Science Foundation of China under Grant No. 11001166 and the Shanghai Leading Academic Discipline Project under Project No. S30104.
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$$Q(G;x) = \det(x\boldsymbol{I} - \boldsymbol{Q}(G)) = \sum_{i=0}^{n}(-1)^i p_i(G)x^{n-i}, \tag{3}$$

where $c_i(G)$ and $p_i(G)$ are coefficients of corresponding characteristic polynomials.

The energy of G was defined by Gutman [1] in 1978 as the sum of the absolute values of the eigenvalues of $\boldsymbol{A}(G)$. It has many chemical applications and stimulated interests among mathematician. For more details on the energy of G, one can refer to books [2, 3]. By extending the concept of graph energy, Nikiforov [4] defined the energy of a matrix as the sum of the singular values of the matrix.

Let $\sigma_1, \sigma_2, \ldots, \sigma_n$ be the singular values of $\boldsymbol{I}(G)$. The authors in [5, 6] defined the incidence energy (IE), denoted by $IE(G)$, of a graph G as

$$IE(G) = \sum_{i=1}^{n} \sigma_i. \tag{4}$$

It is known that [5]

$$\boldsymbol{I}(G)\boldsymbol{I}^{\mathrm{t}}(G) = \boldsymbol{D}(G) + \boldsymbol{A}(G) = \boldsymbol{Q}(G). \tag{5}$$

Recalled that for a matrix $\boldsymbol{B}$ with real entries, the singular values of the matrix $\boldsymbol{B}$ are the square roots of the eigenvalues of $\boldsymbol{B}\boldsymbol{B}^{\mathrm{t}}$, where $\boldsymbol{B}^{\mathrm{t}}$ is the transpose of $\boldsymbol{B}$. Denote by $\mu_1^+(G) \geq \mu_2^+(G) \geq \ldots \geq \mu_n^+(G)$ the eigenvalues of the signless Laplacian characteristic polynomial $Q(G;x)$. Then $\mu_1^+(G), \mu_2^+(G), \ldots, \mu_n^+(G)$ are real and non-negative. Thus, from (4) and (5), we have

$$IE(G) = \sum_{i=1}^{n} \sqrt{\mu_i^+(G)}. \tag{6}$$

We denote by $S(G)$ the subdivision graph of G, where $S(G)$ is the graph obtained from G by inserting an additional vertex into each edge of G. Obviously, $S(G)$ is a bipartite graph with $n + m$ vertices and $2m$ edges. The characteristic polynomial of $S(G)$ is

$$\phi(S(G);x) = \det(x\boldsymbol{I} - \boldsymbol{A}(S(G))) = \sum_{i=0}^{\lfloor \frac{n+m}{2} \rfloor} a_{2i}(S(G))x^{n+m-2i}, \tag{7}$$

where $a_{2i}(S(G))$ are coefficients of characteristic polynomial $\phi(S(G);x)$ with $0 \leq i \leq \lfloor \frac{n+m}{2} \rfloor$. Let $b_{2i}(S(G)) = |a_{2i}(S(G))|$, where $0 \leq i \leq \lfloor \frac{n+m}{2} \rfloor$. Specially, $b_0(S(G)) = 1$ and $b_2(S(G)) = n + m$. If G is a tree, then $b_{2i}(S(G)) = m_i(S(G))$, where $m_i(S(G))$ is the number of i–matchings in $S(G)$. It is convenient to define $m(G, 0) = 1$.

It has been obtained in [7] that

$$\phi(S(G);x) = x^{m-n}Q(G;x^2). \tag{8}$$

Therefore, we have [7]

$$b_{2i}(S(G)) = \begin{cases} p_i(G), & 0 \leq i \leq n; \\ 0, & n < i \leq \lfloor \frac{n+m}{2} \rfloor. \end{cases} \tag{9}$$

The authors in [8] and [9] independently obtained

$$p_i(G_1) \leq p_i(G_2) \Longrightarrow IE(G_1) \leq IE(G_2). \tag{10}$$

Moreover, if there exists a positive integer i_0 such that $p_{i_0}(G_1) < p_{i_0}(G_2)$, then $IE(G_1) < IE(G_2)$.

In 2007, among classes of Laplacian-cospectral trees of the same order n, Mohar [10] defined a new partial ordering, namely $T \preceq T'$ if $c_i(T) \leq c_i(T')$ for $i = 1, \ldots, n$, and he [10] also showed that this poset has a unique minimum and has a unique maximum element. Later, many interesting results have been obtained about the poset among many classes of graphs. For example, the trees with a fixed matching number [11], the unicyclic graphs [12, 13], the bicyclic graphs [14], etc.

Recently, the signless Laplacian matrix has attracted more and more attention [15], which may have more properties than the adjacency and Laplacian matrices, and can be used to discover more structural characterization of graphs. It is known that $\boldsymbol{L}(G)$ and $\boldsymbol{Q}(G)$ are similar if and only if (iff) G is bipartite. So the Laplacian coefficients are the same as the signless Laplacian coefficients (SLCs) iff G is bipartite.

We write $G \preceq' H$ if $p_i(G) \leq p_i(H)$ for $0 \leq i \leq n$. We write $G \prec' H$ if $G \preceq' H$ with a k in such a way that $p_k(G) < p_k(H)$. Recently, some results have been obtained in terms of the ordering $\preceq'$. For example, Li et al. [16] determined two maximum elements and two minimum elements among the set of unicyclic graphs, Zhang and Zhang [15] got two minimum elements among the set of bicyclic graphs, Zhang and Zhang [17] characterized all the minimum elements among the set of unicyclic graphs having a fixed matching number. Mirzakhah and Kiani [9] studied the coefficients of the signless Laplacian matrix of unicyclic graphs. For further information on the signless Laplacian matrix, one can refer to three surveys [18–20].

The IE of G can help explain some phenomena of chemical molecule. By using (10) and other methods, the graphs with the extremal IE have been characterized among some classes of graphs. Among all the trees, Gutman et al. [5] got the graphs with the smallest and the largest IE and Tang and Hou [21] got the the trees with the second smallest, the third smallest, the second largest, and the third largest IE. Among all the trees with a given matching number, Ilić [22] obtained the graph with the minimum IE. Among all the trees with a described maximum degree, Jin et al. [23] characterized the trees with the minimum IE. Among all the trees with a given pendent vertex number, Zhang et al. [24] got the one with the minimum IE. Among all the unicyclic graphs and bicyclic graphs, Zhang and Li [8] determined the graphs having the minimum and the maximum IE, respectively.

Let $\mathcal{U}_n^r$ be the set of unicyclic graphs with $n \geq 4$ vertices and $r \geq 1$ pendent vertices. Let $\mathcal{U}_{n,g}^r$ be the subset of $\mathcal{U}_n^r$ in which every graph has a cycle with girth $g \geq 3$, where $n \geq g+1$ and $r \geq 1$. Motivated by all the above-mentioned work, we will deduce, in the present study, the graph having the minimum SLCs according to the ordering of $\preceq'$ (namely, the graph with the minimum IE) in $\mathcal{U}_{n,g}^r$ and $\mathcal{U}_n^r$.

The rest of this paper is organized as follows. Firstly, for two graphs in $\mathcal{U}_{n,g}^r$, we introduce two new graph transformations (see Lemmas 3.1 and 3.2) that preserve order, size and the number of the pendent vertices, but decrease the matching number of the subdivision graphs and the SLCs of the graphs under consideration. Then, we characterize a unique extremal graph which has the minimum SLCs and the minimum IE among $\mathcal{U}_{n,g}^r$, where $r \geq 1$, $n > g \geq 3$ and g is odd (see Theorems 3.8 and 3.9). Secondly, if $G \in \mathcal{U}_n^r$ and G has odd girth $g \geq 5$, where $n \geq 7$ and $r \geq 2$, then we prove that a unique extremal graph $L_n \in \mathcal{U}_n^r$ with girth 4 satisfies that both the SLCs and the IE of G are more than the counterparts of L_n (see Theorems 3.17 and 3.18). Thirdly, in $\mathcal{U}_n^1$ with $n \geq 5$, a graph with the minimum SLCs and the minimum IE is obtained (see Theorem 3.19).

2. Preliminaries

To obtain the main results of this paper, some necessary definitions and lemmas are introduced.

Lemma 2.1. *[25] Let G be a graph with characteristic polynomial $\phi(G;x) = \sum_{k=0}^{n} a_k x^{n-k}$. Then for $k \geq 1$,*

$$a_k = \sum_{S \in L_k} (-1)^{\omega(S)} 2^{c(S)},$$

where L_k denotes the set of Sachs subgraphs of G with k vertices, that is, the subgraphs in which every component is either a K_2 or a cycle; $\omega(S)$ is the number of connected components of S, and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$.

Let $b_i(G) = |a_i(G)|$ with $0 \leq i \leq n$. Then by Lemma 2.1, we get $b_0(G) = 1$, $b_1(G) = 0$, and $b_2(G)$ equals to the number of edges of G.

For a given graph G and $e \in E(G)$ (respectively, $e \notin E(G)$), let $G - e$ (respectively, $G + e$) be the graph obtained from G by deleting (respectively, adding) the edge e. For $v \in V(G)$, let $G - v$ be the graph obtained from G by deleting the vertex v together with its incident edges. Let $G - H$ be the graph obtained from G by deleting all the vertices of H and all the edges which are incident with the vertices of H.

Lemma 2.2. *[26] Let G be a graph with n vertices.*
(a) If G contains exactly one cycle C_g and uv is an edge on C_g, then

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-g}(G - C_g) \quad if \;\; g = 0 \; (mod\; 4)$$
$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-g}(G - C_g) \quad if \;\; g \neq 0 \; (mod\; 4).$$

(b) If uv is a cut edge, then $b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v)$.

Lemma 2.3. *[27] Let G be a unicyclic graph and G′ a graph obtained from G by deleting at least one edge outside its unique cycle. Then $b_i(G_1) \geq b_i(G_2)$ for all $i \geq 0$. Moreover, there exists at least one i_0 such that $b_{i_0}(G_1) > b_{i_0}(G_2)$.*

Lemma 2.4. *[7][28] Let $G \cup H$ denote the graph whose components are G and H. Then, we have $m_k(G \cup H) = \sum_{h=0}^{k} m_h(G)m_{k-h}(H)$.*

Lemma 2.5. *[28] If uv is an edge of G, then for all $k \geq 1$, $m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v)$.*

We denote by P_n a path with n vertices. The vertices of P_n are labeled by $u_0, u_1, \ldots, u_{n-1}$. Denote $P_{n_1} \cup P_{n_2}$ by U_{n_1,n_2}.

Lemma 2.6. *[29] If $n = 4h + i$ with $h \geq 1$ and $i \in \{0, 1, 2, 3\}$, then for $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$, $m_k(P_n) \geq m_k(U_{2,n-2}) \geq \ldots \geq m_k(U_{2h,n-2h}) \geq m_k(U_{2h+1,n-2h-1}) \geq m_k(U_{2h-1,n-2h+1}) \geq \ldots \geq m_k(U_{1,n-1})$.*

Let F and H be two disjoint graphs. Let u be a vertex of F and v a vertex of H. The graph obtained from F and H by identifying u of F and v of H is denoted by $F(u, v)H$.

Lemma 2.7. *[29] Let v be an arbitrary vertex of G. If $n = 4h+i$ with $h \geq 1$ and $i \in \{-1, 0, 1, 2\}$, then $m_k(P_n(u_0, v)G) \geq m_k(P_n(u_2, v)G) \geq \ldots \geq m_k(P_n(u_{2h}, v)G) \geq m_k(P_n(u_{2h-1}, v)G) \geq m_k(P_n(u_{2h-3}, v)G) \geq \ldots \geq m_k(P_n(u_1, v)G)$.*

Lemma 2.8. *[16] Let G be a unicyclic graph with n vertices and the girth of cycle contained in G be g. When $0 \leq k \leq n$ and $3 \leq g \leq n$, we have*

$$p_k(G) = m_k(S(G)) + (-1)^{g+1} 2m_{k-g}(S(G) - C_{2g}).$$

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

Lemma 2.9. *Let F and T be disjoint graphs, where F is a connected graph with $u \in V(F)$ and T is a tree with $v \in V(T)$. Let $N_T(v) = \{w_1, \ldots, w_{|N_T(v)|}\}$. For $2 \leq i \leq |V(F)| + |V(T)|$, we have*

$$b_i(F(u, v)T) = b_i\Big(F \cup (T - v)\Big) + \sum_{k=1}^{|N_T(v)|} b_{i-2}\Big((F - u) \cup (T - v - w_k)\Big).$$

Proof. Let $\widetilde{Q} = F(u, v)T$. Let G and uv in Lemma 2.2 be $\widetilde{Q}$ and vw_1, respectively. Let i be a fixed integer with $2 \leq i \leq |V(F)| + |V(T)|$. By Lemma 2.2(b), we have

$$b_i(\widetilde{Q}) = b_i(\widetilde{Q} - vw_1) + b_{i-2}\Big((F - u) \cup (T - v - w_1)\Big). \tag{11}$$

Again, let G and uv in Lemma 2.2 be $\widetilde{Q} - vw_1$ and vw_2, respectively. By Lemma 2.2(b) and (11), we obtain

$$b_i(\widetilde{Q}) = b_i(\widetilde{Q} - vw_1 - vw_2) + \sum_{k=1}^{2} b_{i-2}\Big((F - u) \cup (T - v - w_k)\Big). \tag{12}$$

Furthermore, by the same procedure and by using Lemma 2.2(b) $|N_T(v)| - 2$ times, we can get Lemma 2.9. □

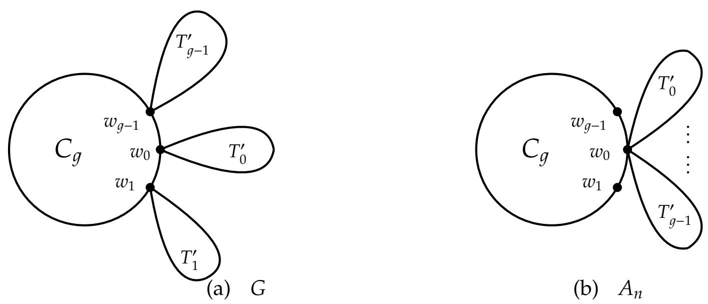


Figure 1: α–transformation from G to A_n

3. Main Results

3.1. *The graph with the minimum SLCs and the minimum IE in $\mathcal{U}^r_{n,g}$*

In this subsection, we will deduce the unique graph with the minimum SLCs and the minimum IE in $\mathcal{U}^r_{n,g}$, where $r \geq 1$, $n > g \geq 3$ and g is odd. Two new transformations (see Lemmas 3.1 and 3.2) will be introduced. These two new transformations preserve order, size and the number of the pendent vertices, but decrease the matching number of the subdivision graphs and the SLCs of the graphs under consideration.

We denote by C_n a cycle with $n \geq 3$ vertices. The vertices of C_n are clockwise labeled by $w_0, w_1, \ldots, w_{n-1}$. Obviously, for $G \in \mathcal{U}^r_{n,g}$, the vertex w_i on C_g of G maybe (or maybe not) be attached by a tree (denoted by T'_i), where $0 \leq i \leq g-1$. For $G \in \mathcal{U}^r_{n,g}$, let A_n be the graph obtained from G by transplanting all the trees attached at w_i on C_g of G to the vertex w_0 of C_g, where $1 \leq i \leq g-1$. In other words, for $G \in \mathcal{U}^r_{n,g}$,

$$A_n = G - \bigcup_{i=1}^{g-1}\Big\{w_iv|v \in N_{T'_i}(w_i)\Big\} + \bigcup_{i=1}^{g-1}\Big\{w_0v|v \in N_{T'_i}(w_i)\Big\}.$$

G and A_n are shown in Fig. 1(a) and Fig. 1(b), respectively. The transformation from G to A_n is hereinafter called α–transformation, where $G \in \mathcal{U}^r_{n,g}$. Obviously, $A_n \in \mathcal{U}^r_{n,g}$.

Lemma 3.1. *If $G \in \mathcal{U}^r_{n,g} \setminus \{A_n\}$ with $r \geq 2$ and $n > g \geq 3$, then after performing the α–transformation, we have $p_i(G) \geq p_i(A_n)$ for $0 \leq i \leq n$, and at least one inequality holds within $0 \leq i \leq n$.*

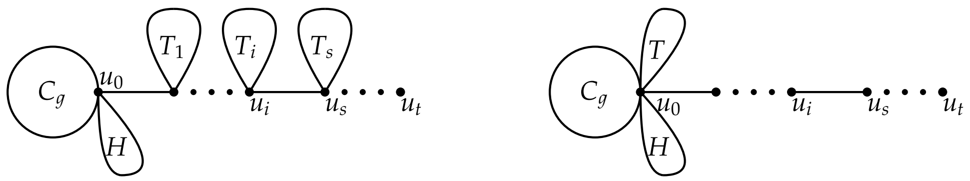
Proof. By (9), to obtain $p_i(G) \geq p_i(A_n)$ for $0 \leq i \leq n$, we only need to prove $b_{2i}\big(S(G)\big) \geq b_{2i}\big(S(A_n)\big)$ for $0 \leq i \leq n$. Since $S(G)$ is a bipartite graph, by Lemma 2.1, $b_{2i+1}\big(S(G)\big) = 0$ for $0 \leq i \leq n$. By Lemma 2.1, we have $b_0\big(S(G)\big) = b_0\big(S(A_n)\big) = 1$ and $b_2\big(S(G)\big) = b_2\big(S(A_n)\big) = 2n$. Next, let $2 \leq i \leq n$.

In $S(A_n)$, we denote $S(T'_j) - w_0$ by Q_j, where $0 \leq j \leq g-1$. Denote $Q_0 \cup \ldots \cup Q_{g-1}$ by Q. Let $G \setminus H$ (respectively $G \setminus \{H, F\}$) be the graph obtained from G by deleting all the edges of H (respectively all the edges of H and F).

In Lemma 2.9, let $F(u,v)T = S(A_n)$, where $F = C_{2g}$, $T = S(A_n) \setminus C_{2g}$, and $u = v = w_0$. By Lemma 2.9, we get

$$b_{2i}\big(S(A_n)\big) = b_{2i}(C_{2g} \cup Q) + \sum_{j=0}^{g-1} \sum_{w \in N_{S(T'_j)}(w_0)} b_{2i-2}\Big(P_{2g-1} \cup (Q_j - w) \cup (Q \setminus Q_j)\Big). \tag{13}$$

Let $G \in \mathcal{U}^r_{n,g} \setminus \{A_n\}$. In Lemma 2.9, let $F(u,v)T = S(G)$, where $F = S(G) \setminus S(T'_0)$, $T = S(T'_0)$, and $u = v = w_0$. Then, we have $F - u = \big(S(G) \setminus S(T'_0)\big) - w_0$ and $T - v = Q_0$. For a fixed $w'_a \in N_{S(T'_0)}(w_0)$, $(F-u) \cup (T - v - w'_a)$



(a) A_n (b) A_n^*

Figure 2: β–transformation from A_n to A_n^*

contains $P_{2g-1} \cup (Q_0 - w_a') \cup (Q \setminus Q_0)$ as its proper subgraph. By Lemma 2.3, we get

$$b_{2i-2}\Big((F-u) \cup (T - v - w_a')\Big) \geq b_{2i-2}\Big(P_{2g-1} \cup (Q_0 - w_a') \cup (Q \setminus Q_0)\Big). \tag{14}$$

Moreover, there exists one $i = 2$ such that the inequality in (14) holds.

By Lemma 2.9 and (14), we get

$$b_{2i}\Big(S(G)\Big) \geq b_{2i}\Big(S(G) \setminus S(T_0') \cup Q_0\Big) + \sum_{a=1}^{|N_{S(T_0')}(w_0)|} b_{2i-2}\Big(P_{2g-1} \cup (Q_0 - w_a') \cup (Q \backslash Q_0)\Big). \tag{15}$$

Moreover, there exists one $i = 2$ such that the inequality in (15) holds.

Next, for the first term in the right-hand side of (15), we will prove that (16) holds.

In Lemma 2.9, let $F(u,v)T = S(G) \setminus S(T_0')$, where $F = S(G) \setminus \{S(T_0'), S(T_1')\}$, $T = S(T_1')$ and $u = v = w_1$. For a fixed vertex $w_b' \in N_{S(T_1')}(w_1)$, $(F - w_1) \cup (T - w_1 - w_b') \cup Q_0$ contains $P_{2g-1} \cup (Q_1 - w_b') \cup (Q \setminus Q_1)$ as its subgraph. By Lemma 2.3, we get

$$b_{2i-2}\Big((F - w_1) \cup (T - w_1 - w_b') \cup Q_0\Big) \geq b_{2i-2}\Big(P_{2g-1} \cup (Q_1 - w_b') \cup (Q \setminus Q_1)\Big).$$

Furthermore, by Lemma 2.9, we obtain

$$\begin{aligned} b_{2i}\Big((S(G) \setminus S(T_0') \cup Q_0\Big) &\geq b_{2i}\Big((S(G) \setminus \{S(T_0'), S(T_1')\} \cup Q_0 \cup Q_1\Big) \\ &+ \sum_{b=1}^{|N_{S(T_1')}(w_1)|} b_{2i-2}\Big(P_{2g-1} \cup (Q_1 - w_b') \cup (Q \setminus Q_1)\Big). \end{aligned} \tag{16}$$

By using Lemma 2.9 $(g-1)$ times and by the same procedure, we finally get

$$b_{2i}\Big(S(G)\Big) \geq b_{2i}(C_{2g} \cup Q) + \sum_{j=0}^{g-1} \sum_{w \in N_{S(T_j')}(w_j)} b_{2i-2}\Big(P_{2g-1} \cup (Q_j - w) \cup (Q \setminus Q_j)\Big). \tag{17}$$

By comparing (13) and (17), we obtain $b_{2i}(S(G)) \geq b_{2i}(S(A_n))$ for $2 \leq i \leq n$. Thus, we get Lemma 3.1. □

In Lemma 3.1, A_n can be viewed as the graph obtained from C_g by first attaching a tree H at w_0 of C_g, and then attaching a path $P_{t+1} = u_0u_1 \dots u_t$ at w_0 of C_g, where the vertex u_i $(1 \leq i \leq t-1)$ of P_{t+1} maybe (maybe not) be attached by a tree (denoted by T_i). A_n is shown in Fig. 2(a). Let A_n^* be the graph obtained from A_n by transplanting all the trees T_i attached at u_i of P_{t+1} to u_0, where $1 \leq i \leq t-1$. A_n^* is shown in Fig. 2(b). In other words,

$$A_n^* = A_n - \bigcup_{i=1}^{t-1} \Big\{u_i v | v \in N_{T_i}(u_i)\Big\} + \bigcup_{i=1}^{t-1} \Big\{u_0 v | v \in N_{T_i}(u_i)\Big\}.$$

The transformation from A_n to A_n^* is hereinafter called β–transformation. Obviously, if $A_n \in \mathcal{U}_{n,g}^r$, then after performing the β–transformation, $A_n^* \in \mathcal{U}_{n,g}^r$.

Lemma 3.2. *Let A_n and A_n^* be the graphs as shown in Fig. 2. If $n > g \geq 3$, then we have $m_k\Big(S(A_n)\Big) \geq m_k\Big(S(A_n^*)\Big)$, where $0 \leq k \leq n$.*

Proof. We have $m_0\Big(S(A_n^*)\Big) = m_0\Big(S(A_n)\Big) = 1$ and $m_1\Big(S(A_n^*)\Big) = m_1\Big(S(A_n)\Big) = 2n$. Next, we consider the cases with $2 \leq k \leq n$.

Let k be a fixed integer, where $2 \leq k \leq n$. The k-matchings of $S(A_n)$ and $S(A_n^*)$ are denoted by M and M^*, respectively. The sets of M and M^* are denoted by $\mathcal{M}$ and $\mathcal{M}^*$, respectively.

In $S(A_n)$ and $S(A_n^*)$, the original vertex u_i $(0 \leq i \leq t)$ of P_t of A_n and of A_n^* is relabeled by u_{2i} $(0 \leq i \leq t)$. Namely, the vertices of P_{2t+1} of $S(A_n)$ and of $S(A_n^*)$ are labeled by $u_0, u_1, \ldots, u_{2t}$. Similarly, in $S(A_n)$ and $S(A_n^*)$, the original vertex w_i $(0 \leq i \leq g-1)$ on C_g of A_n and of A_n^* is relabeled by w_{2i} $(0 \leq i \leq g-1)$. Namely, the vertices of C_{2g} of $S(A_n)$ and of $S(A_n^*)$ are labeled by $w_0, w_1, \ldots, w_{2g-1}$.

We construct a mapping ξ as follows:

$$E(S(A_n)) = E(S(A_n^*)) - \bigcup_{i=1}^{t-1}\Big\{u_0v|v \in N_{S(T_i)}(u_0)\Big\} + \bigcup_{i=1}^{t-1}\Big\{u_{2i}v|v \in N_{S(T_i)}(u_{2i})\Big\}. \tag{18}$$

Obviously, ξ is a bijection.

Next, two cases are considered according to whether M^* of $S(A_n^*)$ contains u_0v or not, where $v \in N_{S(T)}(u_0)$ and T is shown in Fig. 2(b).

Case (i). M^* of $S(A_n^*)$ does not contain u_0v, where $v \in N_{S(T)}(u_0)$.

In this case, the set of M^* of $S(A_n^*)$ is denoted by $\mathcal{M}_1^*$. By the mapping ξ, there is one-to-one correspondence between a matching M^* of $S(A_n^*)$ and a matching M of $S(A_n)$. We denote the set of this kind of M of $S(A_n)$ by $\mathcal{M}_1$. Obviously, $|\mathcal{M}_1^*| = |\mathcal{M}_1|$.

Case (ii). M^* of $S(A_n^*)$ contains u_0v, where v is a vertex of $S(T_s)$ of $S(A_n^*)$ with $1 \leq s \leq t-1$.

In this case, there subcases are considered as follows according to whether M^* of $S(A_n^*)$ contains the edge which is incident with u_{2s} or not, where $1 \leq s \leq t-1$.

Subcase (ii.i). $u_{2s-1}u_{2s}, u_{2s}u_{2s+1} \notin M^*$.

In this subcase, the set of M^* of $S(A_n^*)$ is denoted by $\mathcal{M}_2^*$. By the mapping ξ, there is one-to-one correspondence between a matching M^* of $S(A_n^*)$ and a matching M of $S(A_n)$. We denote the set of this kind of M of $S(A_n)$ by $\mathcal{M}_2$. We have $|\mathcal{M}_2^*| = |\mathcal{M}_2|$.

Subcase (ii.ii). $u_{2s-1}u_{2s} \in M^*$, $u_{2s}u_{2s+1} \notin M^*$.

In this subcase, the set of M^* of $S(A_n^*)$ is denoted by $\mathcal{M}_3^*$.

For a matching M^* of $\mathcal{M}_3^*$, by the mapping ξ, we get an edge set of $S(A_n)$ with k edges. We denote the edge set by $\widetilde{E}$. Obviously, $\widetilde{E}$ has three properties. (i) $\widetilde{E}$ does not contain the edges which are incident with u_0 of $S(A_n)$. (ii) $\widetilde{E}$ contains $u_{2s}v$ and $u_{2s-1}u_{2s}$, where v is a vertex of $S(T_s)$ of $S(A_n)$. (iii) Except for $u_{2s}v$ and $u_{2s-1}u_{2s}$, all the edges in $\widetilde{E}$ are disjoint mutually. Therefore, $\widetilde{E}$ of $S(A_n)$ is not a k-matching since $u_{2s}v$ and $u_{2s-1}u_{2s}$ are adjacent.

We construct a mapping ζ as follows. For $e \in \widetilde{E}$, if e is an edge of $P_{2s+1} = u_0u_1 \ldots u_{2s}$ of $S(A_n)$, then denote e by u_iu_{i+1} with $0 \leq i \leq 2s-1$. Let $\zeta(u_iu_{i+1}) = u_{2s-i-1}u_{2s-i}$, where $0 \leq i \leq 2s-1$. For example, $\zeta(u_{2s-1}u_{2s}) = u_0u_1$. Otherwise, for each edge (denoted by e) of the other edges in $\widetilde{E}$, let $\zeta(e) = e$. Obviously, ζ is a bijection. Therefore, we get a new edge set (denoted by M) of $S(A_n)$ with k edges. Obviously, M is a k-matching of $S(A_n)$ since any two edges in M are disjoint. We denote the set of this kind of M of $S(A_n)$ by $\mathcal{M}_3$. Therefore, we obtain $|\mathcal{M}_3^*| = |\mathcal{M}_3|$.

Subcase (ii.iii). $u_{2s-1}u_{2s} \notin M^*$, $u_{2s}u_{2s+1} \in M^*$.

In this subcase, the set of M^* of $S(A_n^*)$ is denoted by $\mathcal{M}_4^*$. In $S(A_n)$, we can choose a set of k-matching (denoted by $\mathcal{M}_4$) satisfying that for any $M \in \mathcal{M}_4$, there exists exactly one s with $1 \leq s \leq t-1$ such that $u_{2s}v, u_0w_1 \in M$ or $u_{2s}v, u_0w_{2g-1} \in M$, where $v \in N_{S(T_s)}(u_{2s})$, and w_1 and w_{2g-1} are the vertices of C_{2g} of $S(A_n)$.

By the definition of $\mathcal{M}_4^*$, for any $M^* \in \mathcal{M}_4^*$, $u_0v, u_{2s}u_{2s+1} \in M^*$, where $1 \le s \le t-1$ and $v \in N_{S(T_s)}(u_0)$. Therefore, for fixed s and v, we denote the subsets of $\mathcal{M}_4$ and $\mathcal{M}_4^*$ by $\mathcal{M}_{s,v}$ and $\mathcal{M}_{s,v}^*$, respectively. Then, we have

$$|\mathcal{M}_4| = \sum_{1\le s\le t-1} \sum_{v\in N_{S(T_s)}(u_{2s})} |\mathcal{M}_{s,v}|, \tag{19}$$

$$|\mathcal{M}_4^*| = \sum_{1\le s\le t-1} \sum_{v\in N_{S(T_s)}(u_0)} |\mathcal{M}_{s,v}^*|. \tag{20}$$

Since the k-matching in $\mathcal{M}_{s,v}$ (respectively $\mathcal{M}_{s,v}^*$) contains $u_{2s}v$ and u_0w_1 or contains $u_{2s}v$ and u_0w_{2g-1} (respectively u_0v and $u_{2s}u_{2s+1}$), and $S(A_n) - u_0 - w_1 - u_{2s} - v = S(A_n) - u_0 - w_{2g-1} - u_{2s} - v$, we obtain

$$|\mathcal{M}_{s,v}| = 2m_{k-2}\Big(S(A_n) - u_0 - w_1 - u_{2s} - v\Big), \tag{21}$$

$$|\mathcal{M}_{s,v}^*| = m_{k-2}\Big(S(A_n^*) - u_{2s} - u_{2s+1} - u_0 - v\Big). \tag{22}$$

Let $S(A_n^*) - u_{2s} - u_{2s+1} - u_0 - v = F \cup U_{2g-1,2t-2s-1}$ with $F = \Big(S(H) - x\Big) \cup \Big(S(T_s) - u_{2s} - v\Big) \cup P_{2s-1} \cup B$, where x is the rooted vertex of $S(H)$ which identifies with w_0 of C_{2g}, and $B = \bigcup_{1\le i\le t-1, i\ne s}\Big(S(T_i) - u_{2i}\Big)$. We can check that $S(A_n) - u_0 - w_1 - u_{2s} - v$ contains $F \cup U_{2g-2,2t-2s}$ as its proper subgraph. Therefore, by (21) and (22), we obtain

$$|\mathcal{M}_{s,v}| \ge 2m_{k-2}(F \cup U_{2g-2,2t-2s}) = 2\sum_{i+j=k-2} m_i(F)m_j(U_{2g-2,2t-2s}), \tag{23}$$

$$|\mathcal{M}_{s,v}^*| = m_{k-2}(F \cup U_{2g-1,2t-2s-1}) = \sum_{i+j=k-2} m_i(F)m_j(U_{2g-1,2t-2s-1}). \tag{24}$$

By Lemma 2.6, $m_j(U_{2g-2,2t-2s}) \ge m_j(U_{2g-1,2t-2s-1})$, where $0 \le j \le k-2$. Therefore, by (23) and (24), we obtain

$$|\mathcal{M}_{s,v}| \ge |\mathcal{M}_{s,v}^*|. \tag{25}$$

Furthermore, by (19) and (20), we obtain $|\mathcal{M}_4| \ge |\mathcal{M}_4^*|$.

By the definitions of $\mathcal{M}_i^*$ and $\mathcal{M}_i$ $(1 \le i \le 4)$, we have $\mathcal{M}^* = \mathcal{M}_1^* \cup \mathcal{M}_2^* \cup \mathcal{M}_3^* \cup \mathcal{M}_4^*$ and $\mathcal{M}_1 \cup \mathcal{M}_2 \cup \mathcal{M}_3 \cup \mathcal{M}_4 \subseteq \mathcal{M}$, where $\mathcal{M}_i^* \cap \mathcal{M}_j^* = \emptyset$ and $\mathcal{M}_i \cap \mathcal{M}_j = \emptyset$ with $1 \le i, j \le 4$. Therefore, for $2 \le k \le n$, we obtain

$$m_k\Big(S(A_n)\Big) - m_k\Big(S(A_n^*)\Big) = |\mathcal{M}| - |\mathcal{M}^*| \ge \sum_{i=1}^{4} |\mathcal{M}_i| - \sum_{i=1}^{4} |\mathcal{M}_i^*|. \tag{26}$$

By the proofs of Cases (i) and (ii), we have $|\mathcal{M}_i| = |\mathcal{M}_i|$ for $i = 1, 2, 3$ and $|\mathcal{M}_4| \ge |\mathcal{M}_4^*|$. Therefore, by (26), we get $m_k\Big(S(A_n)\Big) \ge m_k\Big(S(A_n^*)\Big)$ for $0 \le k \le n$. Lemma 3.2 is thus proved. □

Let n, g and r be fixed. Let $H(l_1, l_2, \ldots, l_r)$ be the tree obtained from a common vertex v by attaching r paths of length l_1, l_2, …, l_r at v, where l_i $(1 \le i \le r)$ is a positive integer and $l_1 + l_2 + \ldots + l_r = n - g$. For simplicity, we denote $C_g(w_0, v)H(l_1, l_2, \ldots, l_r)$ by B_n^*.

Lemma 3.3. *Let A_n^* be the graph as shown in Fig. 2(b). If $n > g \ge 3$, then we have $m_k\Big(S(A_n^*)\Big) \ge m_k\Big(S(B_n^*)\Big)$, where $0 \le k \le n$.*

Proof. By repeatedly performing the β–transformation on A_n^*, we can finally get a graph $C_g(w_0, v)H(l_1, l_2, \ldots, l_r) = B_n^*$. By repeatedly using Lemma 3.2, we obtain Lemma 3.3. □

Lemma 3.4. *In A_n and B_n^*, if $n > g \geq 3$ and g is odd, then we have $p_k(A_n) \geq p_k(B_n^*)$ for $0 \leq k \leq n$, and at least one of inequalities holds within $0 \leq k \leq n$.*

Proof. By Lemma 2.8, we get $p_0(A_n) = p_0(B_n^*) = 1$ and $p_1(A_n) = p_1(B_n^*) = n$. Let $2 \leq k \leq n$. By Lemma 2.8, we obtain

$$p_k(A_n) = m_k\Big(S(A_n)\Big) + (-1)^{g+1} 2 m_{k-g}\Big(S(A_n) - C_{2g}\Big), \tag{27}$$

$$p_k(B_n^*) = m_k\Big(S(B_n^*)\Big) + (-1)^{g+1} 2 m_{k-g}\Big(S(B_n^*) - C_{2g}\Big). \tag{28}$$

By Lemmas 3.2 and 3.3, we have $m_k(S(A_n)) \geq m_k(S(B_n^*))$ for $0 \leq k \leq n$. When $A_n \neq B_n^*$, $S(A_n) - C_{2g}$ contains $S(B_n^*) - C_{2g}$ as its proper subgraph. We have $m_{k-g}(S(A_n) - C_{2g}) \geq m_{k-g}(S(B_n^*) - C_{2g})$. Furthermore, we have $m_1(S(A_n) - C_{2g}) > m_1(S(B_n^*) - C_{2g})$. Thus, by (27) and (28), when g is odd, we get $p_k(A_n) \geq p_k(B_n^*)$ and there exists a $k = g + 1$ such that $p_k(A_n) > p_k(B_n^*)$. Therefore, we obtain Lemma 3.4. □

Remark. In A_n and B_n^*, if g is even, then $(-1)^{g+1} = -1$ in (27) and (28). Thus, the methods used to prove $p_k(A_n) \geq p_k(B_n^*)$ in Lemma 3.4 for odd $g \geq 3$ can not be applied to compare $p_k(A_n)$ and $p_k(B_n^*)$ for even g, where $0 \leq k \leq n$.

In $H(l_1, l_2, \ldots, l_r)$, specially, for any two $1 \leq i, j \leq k$, if $|l_i - l_j| \leq 1$, then we denote $H(l_1, l_2, \ldots, l_r)$ by $H_{n-g+1,r}$. Let $p = \lfloor \frac{n-g}{r} \rfloor + 1$ and $s = (n - g) - r\lfloor \frac{n-g}{r} \rfloor$. Obviously, $H_{n-g+1,r}$ is the tree obtained from a common vertex v by attaching s paths of length p and $(r - s)$ paths of length $p - 1$. Let $M_n = C_g(w_0, v)H_{n-g+1,r}$, where M_n is shown in Fig. 3(a). Obviously, $M_n \in \mathcal{U}_{n,g}^r$.

To obtain Lemma 3.7, we introduce Lemmas 3.5 and 3.6 as follows.

Lemma 3.5. *If $G = C_g(w_0, v)H(l_1', l_2, \ldots, l_r')$ with $g \geq 3$, then we have $m_k\Big(S(G)\Big) \geq m_k\Big(S(M_n)\Big)$, where $k \geq 0$.*

Proof. By contradiction. We suppose that there exists a graph $Q_n = C_g(w_0, v)H(l_1, l_2, \ldots, l_r)$ such that $m_k\Big(S(G)\Big) \geq m_k\Big(S(Q_n)\Big)$, where $Q_n \neq M_n$. Since $Q_n \neq M_n$, there exist at least two numbers l_i and l_j such that $|l_i - l_j| \geq 2$, where $1 \leq i, j \leq r$. Without loss of generality, we suppose $l_2 - l_1 \geq 2$. We rewrite $S(Q_n)$ by $P_{2l_1+2l_2+1}(u_{2l_1}, v)\widehat{L}$, where $\widehat{L} = S(Q_n) \setminus P_{2l_1+2l_2+1}$. Since $2l_1 \leq l_1 + l_2 - 2$, by Lemma 2.7, we have $m_k(S(Q_n)) \geq m_k(P_{2l_1+2l_2+1}(u_{l_1+l_2}, v)\widehat{L}) = m_k\Big(S(C_g(w_0, v)H(\frac{l_1+l_2}{2}, \frac{l_1+l_2}{2}, l_3 \ldots, l_r))\Big)$ when $l_1 + l_2$ is even or $m_k(S(Q_n)) \geq m_k(P_{2l_1+2l_2+1}(u_{l_1+l_2-1}, v)\widehat{L}) = m_k\Big(S(C_g(w_0, v)H(\frac{l_1+l_2-1}{2}, \frac{l_1+l_2+1}{2}, l_3 \ldots, l_r))\Big)$ when $l_1 + l_2$ is odd. This contradicts the minimality of $S(Q_n)$. Therefore, we get $Q_n = M_n$. Thus, we obtain Lemma 3.5. □

For fixed n, g and r, let $P_{2n-2g,r}$ be the set of $P_{2l_1} \cup P_{2l_2} \cup \ldots \cup P_{2l_r}$, where $2l_1 + \ldots + 2l_r = 2n - 2g$ and l_i is a positive integer for $1 \leq i \leq r$. Let aP_h be the union graph with a paths of length $h - 1$, where a and h are positive integers with $a \geq 2$ and $h \geq 2$.

Lemma 3.6. *If $G \in P_{2n-2g,r}$, then we have $m_k(G) \geq m_k\Big(sP_{2p} \cup (r-s)P_{2p-2}\Big)$ for $0 \leq k \leq n-g$, where $2ps + (r-s)(2p-2) = 2n - 2g$.*

Proof. For any $G \in P_{2n-2g,r}$, we suppose that there exists a $\overline{G} \in P_{2n-2g,r}$ such that $m_k(G) \geq m_k(\overline{G})$ for $0 \leq k \leq n - g$. We denote $\overline{G}$ by $P_{2l_1} \cup P_{2l_2} \cup \ldots \cup P_{2l_r}$ and suppose $\overline{G} \neq sP_{2p} \cup (r - s)P_{2p-2}$. Thus, among $\{2l_1, \ldots, 2l_r\}$, there exist $2l_i$ and $2l_j$ such that $|l_i - l_j| \geq 2$, where $1 \leq i, j \leq r$. Without loss of generality, we suppose $l_1 - l_2 \geq 2$. By Lemma 2.6, we have $m_i(U_{2l_1,2l_2}) \geq m_i(U_{2l_1-2,2l_2+2})$ for $0 \leq i \leq l_1 + l_2$. Let $\widetilde{G} = P_{2l_1-2} \cup P_{2l_2+2} \cup P_{2l_3} \cup \ldots \cup P_{2l_r}$. Obviously, $\widetilde{G} \in P_{2n-2g,r}$. By Lemma 2.4, we get

$$m_k(\overline{G}) = \sum_{i=0}^{k} m_i(U_{2l_1,2l_2}) m_{k-i}(\overline{G} \setminus \{U_{2l_1,2l_2}\}) \geq \sum_{i=0}^{k} m_i(U_{2l_1-2,2l_2+2}) m_{k-i}(\overline{G} \setminus \{U_{2l_1,2l_2}\}) = m_k(\widetilde{G}). \tag{29}$$

This contradicts the minimality of $\overline{G}$. Therefore, for any two $2l_i$ and $2l_j$ with $1 \leq i, j \leq r$, we have $|l_i - l_j| \leq 1$. Therefore, $\overline{G} = sP_{2p} \cup (r - s)P_{2p-2}$. Lemma 3.6 is thus proved. □

Lemma 3.7. *In B_n^* and M_n, if $n > g \geq 3$ and g is odd, then we have $p_k(B_n^*) \geq p_k(M_n)$, where $0 \leq k \leq n$.*

Proof. If the girth g of B_n^* and of M_n is odd, then by Lemma 2.8, we obtain

$$p_k(B_n^*) = m_k\Big(S(B_n^*)\Big) + 2m_{k-g}\Big(S(B_n^*) - C_{2g}\Big), \tag{30}$$

$$p_k(M_n) = m_k\Big(S(M_n)\Big) + 2m_{k-g}\Big(S(M_n) - C_{2g}\Big). \tag{31}$$

Bearing in mind that $B_n^* = C_g(w_0, v)H(l_1, l_2, \ldots, l_r)$, therefore, by Lemma 3.5, we have $m_k\Big(S(B_n^*)\Big) \geq m_k\Big(S(M_n)\Big)$. Since $S(B_n^*) - C_{2g} = P_{2l_1} \cup P_{2l_2} \cup \ldots \cup P_{2l_r}$ and $S(M_n) - C_{2g} = sP_{2p} \cup (r - s)P_{2p-2}$, by Lemma 3.6, we get $m_{k-g}\Big(S(B_n^*) - C_{2g}\Big) \geq m_{k-g}\Big(S(M_n) - C_{2g}\Big)$. Thus, Lemma 3.7 follows from (30) and (31). □

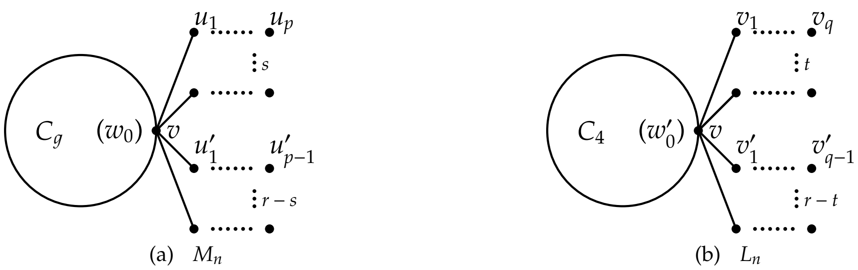


Figure 3: The graphs M_n and L_n

In $\mathcal{U}_{n,g}^r$, we will characterize the minimum graph in terms of $\preceq'$ according to their SLCs and then deduce the graph with the minimum IE.

Theorem 3.8. *If $G \in \mathcal{U}_{n,g}^r$, where $r \geq 1$, $n > g \geq 3$ and g is odd, then for $0 \leq k \leq n$, we have $p_k(G) \geq p_k(M_n)$ and at least one of inequalities holds within $0 \leq k \leq n$.*

Proof. Let $G \in \mathcal{U}_{n,g}^r$. Let $0 \leq k \leq n$. By Lemma 3.1, we have $p_k(G) \geq p_k(A_n)$. By Lemma 3.4, we get $p_k(A_n) \geq p_k(B_n^*)$, and at least one inequality holds within $0 \leq k \leq n$. Furthermore, by Lemma 3.7, we have $p_k(B_n^*) \geq p_k(M_n)$. Thus, we obtain Theorem 3.8. □

Theorem 3.9. *If $G \in \mathcal{U}_{n,g}^r$, where $r \geq 1$, $n > g \geq 3$ and g is odd, then we have $IE(G) \geq IE(M_n)$, with the equality iff $G = M_n$.*

Proof. By (9) and Theorem 3.8, we have Theorem 3.9. □

3.2. The graph with the minimum SLCs and the minimum IE in $\mathcal{U}_n^r$

In this subsection, we will consider the graph with the minimum SLCs and the minimum IE in $\mathcal{U}_n^r$. A graph L_n with girth 4 having the minimum SLCs and the minimum IE in $\mathcal{U}_n^r$ is introduced.

Let n and $r \geq 2$ be fixed. Let L_n be the graph obtained from C_4 by attaching t paths of length q and $r - t$ paths of length $q - 1$ at w_0 of C_4, where $q = \lfloor \frac{n-4}{r} \rfloor + 1$ and $t = (n - 4) - r\lfloor \frac{n-4}{r} \rfloor$. L_n is shown in Fig. 3(b). Obviously, $L_n \in \mathcal{U}_n^r$. When n and r are fixed, L_n is unique.

Lemmas 3.10–3.16 are introduced to obtain our results.

Lemma 3.10. *Let H be a simple graph with n vertices. Let $b > 2a$, where a and b are positive integers. We have $m_k(P_b \cup H) \geq m_{k-a}(P_{b-2a} \cup H)$ for $a \leq k \leq \lfloor \frac{n+b}{2} \rfloor$.*

Proof. By Lemma 2.5, we have $m_k(P_b) \geq m_k(P_{2a} \cup P_{b-2a})$. Therefore, we get

$$m_k(P_b \cup H) \geq m_k(P_{2a} \cup P_{b-2a} \cup H). \tag{32}$$

From Lemma 2.4 and $m_a(P_{2a}) = 1$, we obtain

$$m_k(P_{2a} \cup P_{b-2a} \cup H) = \sum_{k_1+k_2=k} m_{k_1}(P_{2a}) m_{k_2}(P_{b-2a} \cup H) \geq m_a(P_{2a}) m_{k-a}(P_{b-2a} \cup H) = m_{k-a}(P_{b-2a} \cup H). \tag{33}$$

Therefore, Lemma 3.10 follows from (32) and (33). □

Let $\widehat{H} = S(M_n) - C_{2g} = sP_{2p} \cup (r-s)P_{2p-2}$, where $|V(\widehat{H})| = 2n - 2g$ and $g \geq 4$. Let $\widetilde{H} = S(L_n) - C_8 = tP_{2q} \cup (r-t)P_{2q-2}$, where $|V(\widetilde{H})| = 2n - 8$.

Lemma 3.11. *Let $\widehat{H}$ and $\widetilde{H}$ be the graphs as defined as above. We have*
(i) $p \leq q$.
(ii) If $p = q$, then $s \leq t$.

Proof. (i) The proof of Lemma 3.11(i).

Otherwise, we suppose $p \geq q + 1$. Then we have $2p > 2p - 2 \geq 2q > 2q - 2$. Since both $\widehat{H}$ and $\widetilde{H}$ have r paths, we have $|V(\widehat{H})| > |V(\widetilde{H})|$. This contradicts the fact $|V(\widehat{H})| = 2n - 2g \leq 2n - 8 = |V(\widetilde{H})|$ when $g \geq 4$.

(ii) The proof of Lemma 3.11(ii).

By the definitions of $\widehat{H}$ and $\widetilde{H}$, we have $2ps + (2p-2)(r-s) = 2n - 2g$ and $2qt + (2q-2)(r-t) = 2n - 8$. Since $g \geq 4$, we have $2n - 8 \geq 2n - 2g$. It follows from $p = q$ that $s \leq t$. □

Lemma 3.12. *Let $\widehat{H}$ and $\widetilde{H}$ be the graphs as defined as above. Let $g \geq 5$. We have*
(i) $m_{k-1}(P_{2g-3} \cup \widehat{H}) \geq m_{k-1}(P_5 \cup \widetilde{H})$ for $k \geq 1$;
(ii) $m_{k-2}(P_{2g-5} \cup \widehat{H}) \geq m_{k-2}(P_3 \cup \widetilde{H})$ for $k \geq 2$;
(iii) $m_{k-3}(P_{2g-7} \cup \widehat{H}) \geq m_{k-3}(\widetilde{H})$ for $k \geq 3$.

Proof. (i) The proof of Lemma 3.12(i).

Obviously, when $r = 1$, Lemma 3.12(i) holds. Let $r \geq 2$. We get that at least one of s and $r - s$ is not less than 1. Next, we suppose $s \geq 1$. When $g \geq 5$, by Lemma 2.6, we have $m_i(U_{2g-3,2p}) \geq m_i(U_{5,2g+2p-8})$ for $i \geq 0$. Therefore, we get

$$m_{k-1}\Big(P_{2g-3} \cup \widehat{H}\Big) \geq m_{k-1}\Big(P_5 \cup P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}\Big). \tag{34}$$

We can easily check that both $P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}$ and $\widetilde{H}$ have $2n - 8$ vertices, r disjoint paths, and the number of vertices of each path in the two graphs is even. Furthermore, for any two disjoint paths in $\widetilde{H}$, their length difference does not exceed 2. Therefore, by Lemmas 2.4 and 3.6, for $k \geq 1$, we get

$$m_{k-1}\Big(P_5 \cup P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}\Big) \geq m_{k-1}(P_5 \cup \widetilde{H}). \tag{35}$$

It follows from (34) and (35) that Lemma 3.12(i) holds.

Similarly, if $r - s \geq 1$, then by the same analysis as that for $s \geq 1$, we get (35).

(ii) The proof of Lemma 3.12(ii)–(iii).

By the methods similar to those for Lemma 3.12(i), we have Lemma 3.12(ii)–(iii). □

Lemma 3.13. *Let $\widehat{H}$ and $\widetilde{H}$ be the graphs as defined as above. For $5 \leq g \leq k$, we have $m_{k-4}(\widetilde{H}) \geq m_{k-g}(\widehat{H})$.*

Proof. By Lemma 3.11(i), we have $p \le q$. Two cases are considered as follows.

Case (i) $p < q$.

In this case, we have $2p - 2 < 2p \le 2q - 2 < 2q$. Bearing in mind that $\widehat{H} = sP_{2p} \cup (r - s)P_{2p-2}$ and $\widetilde{H} = tP_{2q} \cup (r - t)P_{2q-2}$. It is noted that $\widehat{H}$ and $\widetilde{H}$ are written according to the decreasing order of the lengths of their paths. So we get that the length of the i-th path in $\widetilde{H}$ is not less than that of $\widehat{H}$.

For $1 \le i \le r$, let j_i and h_i be respectively the number of the vertices of the i-th path of $\widetilde{H}$ and $\widehat{H}$. Obviously, j_i and h_i are even for $1 \le i \le r$. Let $j_i - h_i = 2\Delta_i$, where $\Delta_i \ge 0$ and $\sum_{i=1}^{r} \Delta_i = \frac{(2n-8)-(2n-2g)}{2} = g - 4$. By using Lemma 3.10 one time, we get

$$m_{k-4}(\widetilde{H}) = m_{k-4}\Big(tP_{2q} \cup (r-t)P_{2q-2}\Big) \ge m_{k-4-\Delta_1}\Big(P_{2p} \cup (t-1)P_{2q} \cup (r-t)P_{2q-2}\Big).$$

Furthermore, by using Lemma 3.10 $(r - 1)$ times, we finally obtain

$$m_{k-4}(\widetilde{H}) \ge m_{k-4-\sum_{i=1}^{r}\Delta_i}(sP_{2p} \cup (r-s)P_{2p-2}) = m_{k-g}(\widehat{H}).$$

Case (ii) $p = q$.

In this case, by Lemma 3.11(ii), we have $s \le t$. Thus, $\widehat{H}$ and $\widetilde{H}$ can be rewritten as $\widehat{H} = sP_{2p} \cup (t-s)P_{2p-2} \cup (r-t)P_{2p-2}$ and $\widetilde{H} = sP_{2q} \cup (t-s)P_{2q} \cup (r-t)P_{2q-2}$. So we get that the length of the i-th path in $\widetilde{H}$ is not less than that of $\widehat{H}$. By the methods similar to those for Case (i), we obtain $m_{k-4}(\widetilde{H}) \ge m_{k-g}(\widehat{H})$. □

In $S(M_n)$, the vertices on C_{2g} of $S(M_n)$ are labeled by $w_0, \dots, w_{2g-1}$. In $S(L_n)$, the vertices on C_8 of $S(L_n)$ are labeled by $w'_0, \dots, w'_7$.

Lemma 3.14. *Let M_n and L_n be the graphs as shown in Fig 3, where $g \ge 5$ in M_n. We have $m_k(S(M_n) - w_0w_{2g-1}) \ge m_k(S(L_n) - w'_0w'_7)$, where $k \ge 0$.*

Proof. Obviously, $S(M_n) - w_0w_{2g-1}$ is the tree obtained from a common vertex v by attaching a path of length $2g - 1$, s paths of length $2p$ and $r - s$ paths of length $2p - 2$. We denote this kind of tree by $T(2g-1, (2p)^s, (2p-2)^{r-s})$.

Similarly, we have $S(L_n) - w'_0w'_7 = T(7, (2q)^t, (2q-2)^{r-t})$.

By Lemma 2.5, we get

$$m_k\Big(T(7, (2q)^t, (2q-2)^{r-t})\Big) = m_k\Big(P_7 \cup T((2q)^t, (2q-2)^{r-t})\Big) + m_{k-1}\Big(P_6 \cup tP_{2q} \cup (r-t)P_{2q-2}\Big). \tag{36}$$

Similarly, by Lemma 2.5, we obtain

$$\begin{aligned} &m_k\Big(T(7, 2g+2p-8, (2p)^{s-1}, (2p-2)^{r-s})\Big) \\ &= m_k\Big(P_7 \cup T(2g+2p-8, (2p)^{s-1}, (2p-2)^{r-s})\Big) + m_{k-1}\Big(P_6 \cup P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}\Big). \end{aligned} \tag{37}$$

By the methods similar to those for Lemma 3.5, we have

$$m_k\Big(T(2g+2p-8, (2p)^{s-1}, (2p-2)^{r-s})\Big) \ge m_k\Big(T((2q)^t, (2q-2)^{r-t})\Big). \tag{38}$$

Furthermore, $P_6 \cup tP_{2q} \cup (r-t)P_{2q-2}$ and $P_6 \cup P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}$ are graphs in $P_{2n-6,r+1}$. By Lemma 3.6, we have

$$m_{k-1}\Big(P_6 \cup P_{2g+2p-8} \cup (s-1)P_{2p} \cup (r-s)P_{2p-2}\Big) \ge m_{k-1}\Big(P_6 \cup tP_{2q} \cup (r-t)P_{2q-2}\Big). \tag{39}$$

By substitution (38) and (39) into (36) and (37), we finally deduce

$$m_k\Big(T(7, 2g+2p-8, (2p)^{s-1}, (2p-2)^{r-s})\Big) \ge m_k\Big(T(7, (2q)^t, (2q-2)^{r-t})\Big). \tag{40}$$

By the methods similar to those for Lemma 3.12, we have $p \leq q$ and at least one of s and $r-s$ is positive when $r \geq 2$. Next, we suppose $s \geq 1$. Note that $T(2g-1,(2p)^s,(2p-2)^{r-s}) = P_{2g+2p}(u_{2g-1},v)T((2p)^{s-1},(2p-2)^{r-s})$ and $T(7,2g+2p-8,(2p)^{s-1},(2p-2)^{r-s}) = P_{2g+2p}(u_7,v)T((2p)^{s-1},(2p-2)^{r-s})$. By Lemma 2.6, when $g \geq 5$, we have

$$m_k\Big(T(2g-1,(2p)^s,(2p-2)^{r-s})\Big) \geq m_k\Big(T(7,2g+2p-8,(2p)^{s-1},(2p-2)^{r-s})\Big). \tag{41}$$

Similarly, if $r-s \geq 1$, then by the same analysis as that for $s \geq 1$, we get (41).

Therefore, by (40) and (41), we have

$$m_k\Big(T(2g-1,(2p)^s,(2p-2)^{r-s})\Big) \geq m_k\Big(T(7,(2q)^t,(2q-2)^{r-t})\Big). \tag{42}$$

Note that $S(M_n) - w_0w_{2g-1} = T(2g-1,(2p)^s,(2p-2)^{r-s})$ and $S(L_n) - w_0'w_7' = T(7,(2q)^t,(2q-2)^{r-t})$. Thus, by (42), we get Lemma 3.14. □

Since Lemma 3.15 can be obtained by using Lemma 2.5 three times, the proof of Lemma 3.15 is omitted.

Lemma 3.15. *Let $G = P_h \cup Q$ with $h \geq 6$, where Q is a simple graph. Then we have $m_k(G) = m_k(P_{h-1} \cup Q) + m_{k-1}(P_{h-3} \cup Q) + m_{k-2}(P_{h-5} \cup Q) + m_{k-3}(P_{h-6} \cup Q)$ for $k \geq 0$.*

Lemma 3.16. *We have $p_k(M_n) \geq p_k(L_n)$ for $0 \leq k \leq n$, where g in M_n is odd with $g \geq 5$ and $n \geq g+1$.*

Proof. Case (i) g is even.

Obviously, $S(M_n) - C_{2g} = \widehat{H}$ and $S(L_n) - C_8 = \widetilde{H}$. By Lemma 2.8, we get

$$p_k(M_n) = m_k\Big(S(M_n)\Big) - 2m_{k-g}(\widehat{H}), \tag{43}$$

$$p_k(L_n) = m_k\Big(S(L_n)\Big) - 2m_{k-4}(\widetilde{H}). \tag{44}$$

Let G in Lemma 2.5 be $S(M_n)$ (respectively $S(L_n)$) and uv in Lemma 2.5 be w_0w_{2g-1} (respectively $w_0'w_7'$). By Lemma 2.5, we obtain

$$m_k\Big(S(M_n)\Big) = m_k\Big(S(M_n) - w_0w_{2g-1}\Big) + m_{k-1}\Big(P_{2g-2} \cup \widehat{H}\Big), \tag{45}$$

$$m_k\Big(S(L_n)\Big) = m_k\Big(S(L_n) - w_0'w_7'\Big) + m_{k-1}\Big(P_6 \cup \widetilde{H}\Big). \tag{46}$$

By (43)–(46) and Lemma 3.14, we obtain

$$p_k(M_n) - p_k(L_n) \geq m_{k-1}(P_{2g-2} \cup \widehat{H}) - m_{k-1}(P_6 \cup \widetilde{H}) - 2m_{k-g}(\widehat{H}) + 2m_{k-4}(\widetilde{H}). \tag{47}$$

By Lemma 3.15, we have

$$m_{k-1}(P_{2g-2} \cup \widehat{H}) = m_{k-1}(P_{2g-3} \cup \widehat{H}) + m_{k-2}(P_{2g-5} \cup \widehat{H}) + m_{k-3}(P_{2g-7} \cup \widehat{H}) + m_{k-4}(P_{2g-8} \cup \widehat{H}), \tag{48}$$

$$m_{k-1}(P_6 \cup \widetilde{H}) = m_{k-1}(P_5 \cup \widetilde{H}) + m_{k-2}(P_3 \cup \widetilde{H}) + m_{k-3}(\widetilde{H}) + m_{k-4}(\widetilde{H}). \tag{49}$$

By (48), (49) and Lemma 3.12(i)–(iii), we obtain

$$m_{k-1}(P_{2g-2} \cup \widehat{H}) - m_{k-1}(P_6 \cup \widetilde{H}) \geq m_{k-4}(P_{2g-8} \cup \widehat{H}) - m_{k-4}(\widetilde{H}). \tag{50}$$

Therefore, by (50), (47) can be translated into

$$p_k(M_n) - p_k(L_n) \geq m_{k-4}(P_{2g-8} \cup \widehat{H}) + m_{k-4}(\widetilde{H}) - 2m_{k-g}(\widehat{H}). \tag{51}$$

By Lemma 2.4, when $g \geq 5$, we have

$$m_{k-4}(P_{2g-8} \cup \widehat{H}) \geq m_{g-4}(P_{2g-8}) m_{k-g}(\widehat{H}) \geq m_{k-g}(\widehat{H}). \tag{52}$$

Furthermore, by Lemma 3.13, we have $m_{k-4}(\widetilde{H}) \geq m_{k-g}(\widehat{H})$. Therefore, from (51) and (52), we get $p_k(M_n) \geq p_k(L_n)$ for $k \geq 0$.

Case (ii) g is odd with $g \geq 5$.

In this case, by Lemma 2.8, we have $p_k(M_n) = m_k\big(S(M_n)\big) + 2m_{k-g}\big(S(M_n) - C_{2g}\big)$. By the methods similar to those for even g, we get $p_k(M_n) \geq p_k(L_n)$ for $k \geq 0$. □

Theorem 3.17. *Let $G \in \mathcal{U}_n^r$ with $n \geq 7$ and $r \geq 2$. If G has odd girth $g \geq 5$, then we have $p_k(G) \geq p_k(L_n)$ for $0 \leq k \leq n$ and at least one of inequalities holds within $0 \leq k \leq n$.*

Proof. By Theorem 3.8 and Lemma 3.16, we obtain Theorem 3.17. □

Theorem 3.18. *Let $G \in \mathcal{U}_n^r$ with $n \geq 7$ and $r \geq 2$. If G has odd girth $g \geq 5$, then we have $IE(G) > IE(L_n)$.*

Proof. By (9) and Theorem 3.17, we get Theorem 3.18. □

In Theorems 3.17 and 3.18, if $G \in \mathcal{U}_n^r$ and G has odd girth $g \geq 5$, where $n \geq 7$ and $r \geq 2$, then we prove that there exists a graph $L_n \in \mathcal{U}_n^r$ with girth 4 such that both the SLCs and the IE of G are more than the counterparts of L_n. If $G \in \mathcal{U}_n^r$ with $r \geq 2$ and G has even girth $g \geq 4$, which graph has the minimum SLCs and the minimum IE? In $\mathcal{U}_n^r$ with $n \geq 5$ and $r \geq 2$, which graph has the minimum SLCs and the minimum IE? The two unsolved problems remain a task for the future.

For these graphs in $\mathcal{U}_n^r$ with $r \geq 2$, if their girth are even, then their Laplacian spectra and signless Laplacian spectra are the same, which implies the coefficients of both the Laplacian and signless Laplacian characteristic polynomials of the graphs in bipartite unicyclic graphs are the same. For the graphs with k leaves, Ilić and Ilić [30] characterized the trees with k leaves which simultaneously minimize all Laplacian coefficients and they posed a conjecture on the extremal unicyclic graphs with k leaves. Pai and Liu [31] completely solved the conjecture and they obtained the graph with the smallest Laplacian coefficients among unicyclic graphs with k leaves. Zhang and Zhang [32] investigated properties of the minimum elements in the partial ordering among the set of n-vertex unicyclic graphs with the number of leaves and girth. For the coefficients of the Laplacian characteristic polynomial of unicyclic graphs, one can refer to two references [12, 13].

Next, in $\mathcal{U}_n^r$ with $n \geq 5$ and $r = 1$, we will prove that E_n has the minimum SLCs and the minimum IE, where E_n is $C_4(w_0, u_0)P_{n-3}$ with $n \geq 5$. It is noted that E_n and L_n are the same graphs when $r = 1$ and $t = 0$ in L_n.

Theorem 3.19. *Let $G \in \mathcal{U}_n^r$ with $n \geq 5$ and $r = 1$. We have*
(i) $p_k(G) \geq p_k(E_n)$ for $0 \leq k \leq n$ and at least one of inequalities holds within $0 \leq k \leq n$.
(ii) $IE(G) > IE(E_n)$.

Proof. (i) $5 \leq n \leq 8$.

When $G \in \mathcal{U}_n^1$ with $5 \leq n \leq 8$, by direct calculation, we can easily verify that $p_k(G) \geq p_k(E_n)$ for $0 \leq k \leq n$, and the equalities hold for all $0 \leq k \leq n$ iff $G = E_n$. Thus, we obtain Theorem 3.19(i) when $5 \leq n \leq 8$. Furthermore, by Theorem 3.19(i) and (9), we get Theorem 3.19(ii) when $5 \leq n \leq 8$.

(ii) $n \geq 9$.

By Lemma 2.8, we can check that $p_0(G) = p_0(E_n) = 1$, $p_1(G) = p_1(E_n) = 2n$, $p_n(G) = p_n(E_n) = 0$ if the girth of the cycle contained in G is even, and $p_n(G) = 4 > 0 = p_n(E_n)$ if the girth of the cycle contained in G is odd. Next, we consider the cases with $2 \leq k \leq n-1$.

Obviously, $S(G) = C_{2g}(w_0, u_0)P_{2n-2g+1}$ and $S(E_n) = C_8(w_0, u_0)P_{2n-7}$. We get $S(G) - C_{2g} = P_{2n-2g}$ and $S(E_n) - C_8 = P_{2n-8}$. Let G in Lemma 2.5 be $S(G)$ (respectively $S(E_n)$) and uv in Lemma 2.5 be w_0w_1 (respectively $w_0'w_1'$). By Lemmas 2.5 and 2.8, we obtain

$$p_k(G) = m_k(P_{2n}) + m_{k-1}(U_{2g-2,2n-2g}) + 2(-1)^{g+1} m_{k-g}(P_{2n-2g}), \tag{53}$$

$$p_k(E_n) = m_k(P_{2n}) + m_{k-1}(U_{6,2n-8}) - 2m_{k-4}(P_{2n-8}). \tag{54}$$

Two cases are considered as follows.
Case (i) g is even.
From (53) and (54), we have

$$p_k(G) - p_k(E_n) = m_{k-1}(U_{2g-2,2n-2g}) - m_{k-1}(U_{6,2n-8}) - 2m_{k-g}(P_{2n-2g}) + 2m_{k-4}(P_{2n-8}). \tag{55}$$

By Lemma 3.15, we have

$$m_{k-1}(U_{2g-2,2n-2g}) = m_{k-1}(U_{2g-3,2n-2g}) + m_{k-2}(U_{2g-5,2n-2g}) + m_{k-3}(U_{2g-7,2n-2g}) + m_{k-4}(U_{2g-8,2n-2g}), \tag{56}$$

$$m_{k-1}(U_{6,2n-8}) = m_{k-1}(U_{5,2n-8}) + m_{k-2}(U_{3,2n-8}) + m_{k-3}(U_{1,2n-8}) + m_{k-4}(P_{2n-8}). \tag{57}$$

When $g \geq 4$, by Lemma 2.6, we get $m_{k-1}(U_{2g-3,2n-2g}) \geq m_{k-1}(U_{5,2n-8})$, $m_{k-2}(U_{2g-5,2n-2g}) \geq m_{k-2}(U_{3,2n-8})$, and $m_{k-3}(U_{2g-7,2n-2g}) \geq m_{k-3}(U_{1,2n-8})$. Thus, from (56) and (57),

$$m_{k-1}(U_{2g-2,2n-2g}) - m_{k-1}(U_{6,2n-8}) \geq m_{k-4}(U_{2g-8,2n-2g}) - m_{k-4}(P_{2n-8}). \tag{58}$$

By (58), (55) can be translated into

$$p_k(G) - p_k(E_n) \geq m_{k-4}(U_{2g-8,2n-2g}) + m_{k-4}(P_{2n-8}) - 2m_{k-g}(P_{2n-2g}). \tag{59}$$

When $g \geq 4$, by Lemmas 2.6 and 3.10, we have $m_{k-4}(P_{2n-8}) \geq m_{k-4}(U_{2g-8,2n-2g}) \geq m_{k-g}(P_{2n-2g})$. Furthermore, when $k = 5$, we have $m_{k-4}(P_{2n-8}) = 2n - 9 > 2n - 10 = m_{k-4}(U_{2g-8,2n-2g})$. Therefore, by (59), we obtain $p_k(G) \geq p_k(E_n)$ for $0 \leq k \leq n$ and there exists at least one $k_0 = 5$ such that $p_{k_0}(G) > p_{k_0}(E_n)$.
Case (ii) g is odd.
Two subcases are considered as follows.
Subcase (ii.i) $g = 3$.
When $g = 3$, $G = C_3(w_0, u_0)P_{n-2}$. By the same procedure as that for (55), we get

$$p_k(G) - p_k(E_n) = m_{k-1}(U_{4,2n-6}) - m_{k-1}(U_{6,2n-8}) + 2m_{k-3}(P_{2n-6}) + 2m_{k-4}(P_{2n-8}). \tag{60}$$

When $n > 9$, it follows from Lemma 2.6 that $m_{k-1}(U_{4,2n-6}) \geq m_{k-1}(U_{6,2n-8})$. Furthermore, when $k = 4$ and $n \geq 9$, we have $m_{k-3}(P_{2n-6}) = 2n - 7 > 1 = m_{k-4}(P_{2n-8})$. Thus, by (60), we get $p_k(G) \geq p_k(E_n)$ for $0 \leq k \leq n$ and there exists at least one $k_0 = 4$ such that $p_{k_0}(G) > p_{k_0}(E_n)$.
Subcase (ii.ii) $g \geq 5$.
When g is odd, by the same methods as those for even g in Case (i), we can get $p_k(G) \geq p_k(E_n)$ for $0 \leq k \leq n$ and there exists at least one k_0 such that $p_{k_0}(G) > p_{k_0}(E_n)$.
By combination of the proofs in Cases (i) and (ii), we obtain Theorem 3.19(i) when $n \geq 9$. Furthermore, by Theorem 3.19(i) and (9), we obtain Theorem 3.19(ii) when $n \geq 9$. □

Acknowledgments
The authors are grateful to the anonymous referee for his/her constructive comments.

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