

New Results on the Incidence Energy of Graphs¹

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Abstract

For a simple graph G , the incidence energy $IE(G)$ is defined as the sum of all singular values of its incidence matrix. In this paper, we determine the unique graph with minimal incidence energy among all connected unicyclic graphs and bicyclic graphs of order n , respectively. We also determine the unique graph with maximal incidence energy in the two graph classes, respectively.

1 Introduction

Given a simple graph G with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$, the incidence matrix $X(G) = (x_{ij})$ of G is an $n \times m$ (vertex-edge) matrix with $x_{ij} = 1$ if v_i is incident to e_j , and $x_{ij} = 0$ otherwise; the adjacency matrix $A(G) = (a_{ij})$ of G is an $n \times n$ (vertex-vertex) symmetric matrix with $a_{ij} = 1$ if v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. Denote the degree of vertex v_i by $d(v_i)$, the signless Laplacian matrix $Q(G)$ of G is defined as $Q(G) = D(G) + A(G)$, where $D(G) = \text{diag}(d(v_1), d(v_2), \dots, d(v_n))$ is the diagonal matrix of the degrees of G .

Let $\sigma_1, \sigma_2, \dots, \sigma_n$ be the singular values of $X(G)$, i. e., the square roots of the eigenvalues of $X(G)X^T(G)$, where $X^T(G)$ is the transpose of $X(G)$. Denote by $q_1(G), q_2(G), \dots, q_n(G)$ the eigenvalues of $Q(G)$. Then the incidence energy of the

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graph G is defined as [14]

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

Since the equality $X(G)X^T(G) = D(G) + A(G) = Q(G)$ always holds for a simple graph G , the incidence energy of a graph G is also defined as [6]

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

Let $\mu_1, \mu_2, \dots, \mu_n$ be the eigenvalues of the laplacian matrix $L(G) = D(G) - A(G)$. The Laplacian-like energy of G proposed by Liu and Liu [17] is defined as $LEL(G) = \sum_{i=1}^n \sqrt{\mu_i}$. If G is a bipartite graph, then the spectra of $L(G)$ and $Q(G)$ coincide. Thus $IE(G) = LEL(G)$ for a bipartite graph G .

Let G be a connected graph with n vertices and m edges. Let $S(G)$ be the subdivision graph of G , that is, $S(G)$ is obtained from G by inserting a new vertex in each edge. Clearly, $S(G)$ is a bipartite graph with $n + m$ vertices and $2m$ edges. Let

$$Q_G(x) = \sum_{j=0}^n p_j(G) x^{n-j} \quad \text{and} \quad P_{S(G)}(x) = \sum_{j=0}^{\lfloor \frac{n+m}{2} \rfloor} a_{2j}(S(G)) x^{n+m-2j}$$

be the Q -polynomial of G and characteristic polynomial of $S(G)$, respectively. It was proved in [19] that

$$P_{S(G)}(x) = x^{m-n} Q_G(x^2) . \tag{3}$$

From Eq.(3) we know that $a_{2j}(S(G)) = p_j(G)$ for $0 \leq j \leq n$, $a_{2j}(G) = 0$ for $n < j \leq \lfloor \frac{n+m}{2} \rfloor$, and $\pm\sqrt{q_1(G)}, \pm\sqrt{q_2(G)}, \dots, \pm\sqrt{q_n(G)}$ and 0^{m-n} are the eigenvalues of $S(G)$. Thus the incidence energy of G is also equal to [14]

$$IE(G) = \frac{1}{2} E(S(G)) \tag{4}$$

where $E(G)$ denotes the energy of G is defined as the sum of the absolute values of all the eigenvalues of G . Details on $E(G)$ can be found in [5, 8, 9, 15].

Let $b_{2i}(S(G)) = (-1)^i a_{2i}(S(G))$. Then [2] $b_{2i}(S(G)) \geq 0$ for all $i = 1, \dots, \lfloor \frac{n+m}{2} \rfloor$. Further, $b_0(S(G)) = 1$ and $b_2(S(G))$ equals the number of edges of $S(G)$. If G is an acyclic graph, then $b_{2i}(G) = m(G, i)$, where $m(G, i)$ denotes the number of i independent edges in G .

It is known [4,9] that for the bipartite graph $S(G)$, $E(S(G))$ can be also expressed as the Coulson integral formula

$$E(S(G)) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{i=1}^{\lfloor (n+m)/2 \rfloor} b_{2i}(S(G)) x^{2i} \right] dx . \quad (5)$$

Thus for $m \geq n$, we have [6]

$$IE(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{i=1}^n (-1)^i p_i(G) x^{2i} \right] dx . \quad (6)$$

If for two bipartite graphs G_1 and G_2 , the inequalities $b_{2i}(G_1) \leq b_{2i}(G_2)$ hold for all $i = 1, 2, \dots, \lfloor n/2 \rfloor$, then we say that G_1 is smaller than G_2 , and write $G_1 \preceq G_2$ or $G_2 \succeq G_1$. Moreover, if $b_{2i}(G_1) < b_{2i}(G_2)$ holds for some i , we write $G_1 \prec G_2$ or $G_2 \succ G_1$. From Eq.(5) and Eq.(6) we know that for two bipartite graphs $S(G_1)$ and $S(G_2)$,

$$\begin{aligned} S(G_1) \preceq S(G_2) &\Rightarrow IE(G_1) \leq IE(G_2) \\ S(G_1) \prec S(G_2) &\Rightarrow IE(G_1) < IE(G_2) . \end{aligned}$$

A spanning subgraph of G whose components are trees or unicyclic graphs is called a TU-subgraph of G . Suppose that a TU-subgraph H of G contains $c(H)$ unicyclic graphs and s trees T_1, T_2, \dots, T_s . Then the weight $W(H)$ of H is defined by $W(H) = 4^{c(H)} \prod_{i=1}^s (1 + |E(T_i)|)$. Clearly, the isolated vertices in H do not contribute to $W(H)$. It is known that [3]

$$(-1)^i p_i(G) = \sum_{H_i} W(H_i)$$

where the summation runs over all TU-subgraphs H_i of G with i edges. The Sachs theorem [2, 9] states that for $i \geq 1$,

$$a_{2i}(S(G)) = \sum_{F \in L_{2i}} (-1)^{p(F)} 2^{c(F)}$$

where L_{2i} denotes the set of Sachs graphs of $S(G)$ with $2i$ vertices, that is, the graphs in which every component is either a K_2 or a cycle, $p(F)$ is the number of components of F and $c(F)$ is the number of cycles contained in F . Thus we have

$$b_{2i}(S(G)) = \sum_{H_i} W(H_i) = (-1)^i \sum_{F \in L_{2i}} (-1)^{p(F)} 2^{c(F)}$$

where H_i is the TU-subgraph of G with i edges and L_{2i} is the set of the Sachs graph of $S(G)$ with $2i$ vertices.

Lemma 1. *Let G be a simple graph, T be a tree with t edges, and $u \in V(G), v \in V(T)$. Let G_1 be the graph obtained from G and T by identifying the vertices u of G and v of T , G_2 be the graph obtained from G and the star S_{t+1} by identifying the vertex u of G and the unique central vertex of S_{t+1} . Then*

$$IE(G_1) \geq IE(G_2)$$

with equality if and only if $T \cong S_{t+1}$ and v is its central vertex.

Proof. We label the edges of G_1 and G_2 such that the edges in G have the same labels in the two graphs and $E(T) = E(S_{t+1})$. Set $E(G) = \{e_{t+1}, e_{t+2}, \dots, e_m\}$ and $E(T) = \{e_1, e_2, \dots, e_t\} = E(S_{t+1})$. Let H_i be an any TU-subgraph of G_1 , then we can find a unique TU-subgraph H'_i of G_2 such that $E(H_i) = E(H'_i)$. Clearly, $c(H_i) = c(H'_i)$. Let e_i and e_j be any two edges of $E(H_i)$ (or $E(H'_i)$). If e_i and e_j are adjacent in H_i , then they must be adjacent in H'_i , and the inverse assertion is not true. It thus follows that

Claim 1: *the edge set of each component of H'_i must be the union of the edge set of some components of H_i .*

Here we denote by U the unicyclic graph, by T the tree. Let $U'_1, U'_2, \dots, U'_t, T'_1, T'_2, \dots, T'_x$ be the nontrivial components of H'_i , then by Claim 1 we can suppose that

$$U_1, U_2, \dots, U_t, T^{11}, T^{12}, \dots, T^{1i_1}, T^{21}, T^{22}, \dots, T^{2i_2}, \dots, T^{t1}, T^{t2}, \dots, T^{ti_t}, \\ T_{11}, T_{12}, \dots, T_{1j_1}, T_{21}, T_{22}, \dots, T_{2j_2}, \dots, T_{x1}, T_{x2}, \dots, T_{xj_x}$$

are the components of H_i such that $E(U'_s) = E(U_s) \bigcup_{l=1}^{i_s} E(T^{sl}) (1 \leq s \leq t), E(T'_k) = \bigcup_{y=1}^{j_k} E(T_{ky}) (1 \leq k \leq x)$, where U_i, U'_i contain the same edge set in G . Thus we have

$$W(H'_i) = 4^t \prod_{i=1}^x (1 + |E(T'_i)|) \leq 4^t \prod_{i=1}^x \left(\prod_{l=1}^{j_i} (1 + |E(T_{il})|) \right) = W(H_i)$$

with equality if and only if $E(U'_i) = E(U_i) (1 \leq i \leq t)$, and $j_1 = j_2 = \dots = j_x = 1$. Thus $b_{2i}(S(G_1)) \geq b_{2i}(S(G_2))$ for $0 \leq i \leq n$, with equalities if and only if $G_1 \cong G_2$.

That is, $S(G_1) \succeq S(G_2)$ with equality if and only if $T \cong S_{t+1}$ and v is its central vertex. □

By Lemma 1 it is easy to prove that the star S_n is the unique tree on n vertices with minimum incidence energy. Note that [4, 8] P_n is the unique tree on n vertices with maximum energy and the subdivision of a tree is still a tree. Thus, for any tree T on n vertices, we have [6, 7, 14, 18]

$$IE(S_n) \leq IE(T) \leq IE(P_n)$$

with left (right, respectively) equality if and only if $G \cong S_n$ ($T \cong P_n$, respectively).

If G_1 is a subgraph of G_2 , then the TU-subgraph H of G_1 is also that of G_2 . Thus $S(G_1) \preceq S(G_2)$. Thus, for any simple connected graph G with n vertices, we have [14]

$$IE(S_n) \leq IE(G) \leq IE(K_n)$$

with left (right, respectively) equality if and only if $G \cong S_n$ ($G \cong K_n$, respectively).

In order to obtain our main results we need the following lemmas.

Lemma 2. [16] *Let uv be an edge of a bipartite graph G , then*

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) + 2 \sum_{C_i \in \mathcal{C}(uv)} (-1)^{1+\frac{i}{2}} b_{2i-i}(G - C_i)$$

where $\mathcal{C}(uv)$ is the set of cycles containing uv . In particular, if uv is a pendant edge of G with the pendent vertex v , then

$$b_{2i}(G) = b_{2i}(G - v) + b_{2i-2}(G - u - v) .$$

By means of Lemma 2 it is easy to prove:

Lemma 3. [10] *Let $X_{n,i}$ be the graph obtained from the bipartite graph X and the path $P_n = v_1v_2 \dots v_n$ by identifying the vertex u of X and v_i of P_n . Then*

$$X_{n,1} \succ X_{n,3} \succeq X_{n,5} \succeq \dots \succeq X_{n,4} \succeq X_{n,2} .$$

2 The incidence energy of a unicyclic graph

Let G be a unicyclic graph on n vertices, $S(G)$ the subdivision graph of G . It is easy to prove that $S(G)$ contains a perfect matching. Let P_n^l be the unicyclic graph obtained by connecting a vertex of C_l with a pendent vertex of P_{n-l} . Hou et al. [11] proved that P_n^6 has the largest energy among all unicyclic bipartite n -vertex graphs except possibly the cycle C_n . Huo et al. [13] and Andriantiana [1] showed independently that the energy of P_n^6 is greater than that of C_n for even number $n \geq 16$. Since $S(G)$ is a bipartite graph and $S(P_n^3) \cong P_{2n}^6$, combining the above results and Eq.(4), we get:

Theorem 1. *Let G be a unicyclic graph with n vertices, $n \geq 8$. Then $IE(G) \leq IE(P_n^3)$ with equality if and only if $G \cong P_n^3$.*

Let $U_k^s(l_1, l_2, \dots, l_k)$ be the graph obtained from C_s by attaching k pendent paths of respectively lengths l_1, l_2, \dots, l_k at a vertex of C_s . Let U_n^s be the graph obtained from C_s by adding $n - s$ pendent vertices adjacent to a vertex of C_s . Clearly, $U_n^s \cong U_{n-s}^s(\overbrace{1, \dots, 1}^{n-s})$ and $U_1^l(n - l) \cong P_n^l$. Let $T_k(l_1, l_2, \dots, l_k)$ be the star-like tree with k pendent paths of respectively lengths l_1, l_2, \dots, l_k . Clearly, $T_{n-1}(\overbrace{1, \dots, 1}^{n-1}) \cong S_n$.

Lemma 4. *Let G be a unicyclic graph on n vertices with girth $g \geq 4$. Then $IE(G) \geq IE(U_n^4)$ with equality if and only if $G \cong U_n^4$.*

Proof. It suffices to prove that $b_{2k}(S(G)) \geq b_{2k}(S(U_n^4))$ for any positive integer k , and the equalities always hold if and only if $G \cong U_n^4$. We use induction on n to prove it. If $n = g$, then $G \cong C_g$, and by Lemma 2 it follows that $b_{2g}(C_{2g}) = 2 + (-1)^{g+1} \cdot 2 \geq 0 = b_{2g}(S(U_n^4))$. Suppose now $1 \leq k \leq g - 1$. Then by Lemma 2, we have

$$\begin{aligned} b_{2k}(C_{2g}) &= m(P_{2g}, k) + m(P_{2g-2}, k - 1), \\ b_{2k}(S(U_n^4)) &= m(T_{n-2}(4, 3, \overbrace{2, \dots, 2}^{n-4}), k) + m(T_{n-2}(3, \overbrace{2, \dots, 2}^{n-3}), k - 1) - 2 \binom{n-4}{k-4}. \end{aligned}$$

In [4] it was shown that $m(P_n, k) \geq m(T, k)$ for any tree T on n vertices, and these equalities hold if and only if $T \cong P_n$. Thus $b_{2k}(S(C_g)) > b_{2k}(S(U_n^4))$ for all $1 \leq k \leq g - 1$. Hence the result is true for $n = g$. Suppose now $n \geq g + 1$. Then

$G \not\cong C_n$ and G contains many pendent vertices. By Lemma 1 we can assume that all vertices of G except those in C_g are pendent vertices, each of which is adjacent to some vertex of C_g . Let uv be a pendent edge with pendent vertex u , and u' be the new vertex of $S(G)$ inserted in uv . From the fact that $S(G) - v - u'$ is a forest and Lemma 2, we have

$$\begin{aligned} b_{2k}(S(G)) &= b_{2k}(S(G) - vu') + b_{2k-2}(S(G) - v - u', k - 1) \\ &= b_{2k}(S(G) - vu') + m(S(G) - v - u', k - 1) \\ &= b_{2k}(S(G - u) \cup P_2) + m(S(G) - v - u', k - 1) \\ b_{2k}(S(U_n^4)) &= b_{2k}(S(U_{n-1}^4) \cup P_2) + m(P_1 \cup (n - 5)P_2 \cup P_7, k - 1) . \end{aligned}$$

By the induction hypothesis, $b_{2k}(S(G - u) \cup P_2) \geq b_{2k}(S(U_{n-1}^4) \cup P_2)$. Therefore,

$$\begin{aligned} &b_{2k}(S(G)) - b_{2k}(S(U_n^4)) \\ &\geq m(S(G) - v - u', k - 1) - m(P_1 \cup (n - 5)P_2 \cup P_7, k - 1) . \end{aligned}$$

Let M be a perfect matching of $S(G)$, and $e_1, e_2 \in M$, where $e_1(e_2)$ is incident with $v(u')$. Then $M - e_1 - e_2$ is a maximal matching of $S(G) - v - u'$. It saturates all vertices of $S(G) - \{V(C_{2g})\} - u' - u$. Since $g \geq 4$, $P_1 \cup (n - 5)P_2 \cup P_7$ is a spanning subgraph of $S(G) - v - u'$. So $m(S(G) - v - u', k - 1) \geq m(P_1 \cup (n - 5)P_2 \cup P_7, k - 1)$, i. e., $b_{2k}(S(G)) \geq b_{2k}(S(U_n^4))$. These equalities hold if and only if $G - u \cong U_{n-1}^4$ and $S(G) - v - u' \cong P_1 \cup (n - 5)P_2 \cup P_7$, i. e., $G \cong U_n^4$. \square

Lemma 5. *Let G be a unicyclic graph on n vertices with girth 3. Then $IE(G) \geq IE(U_n^3)$ with equality if and only if $G \cong U_n^3$.*

Proof. Similarly, we can assume that all vertices of G except these in C_3 are all pendent vertices. We prove it by induction on n . The case $n = 3$ or 4 is obvious since in these cases $G \cong U_n^3$. Suppose, now $n \geq 5$. Using the Sachs theorem we obtain

$$b_{2k}(S(G)) = m(S(G), k) + 2m(S(G) - C_6, k - 3)$$

and

$$b_{2k}(S(U_n^3)) = m(U_n^3, k) + 2\binom{n-3}{k-3}.$$

Note that $S(G) - V(C_6) \cong (n - 3)P_2$. Then we have

$$b_{2k}(S(G)) - b_{2k}(S(U_n^3)) = m(S(G), k) - m(U_n^3, k) .$$

Suppose u, v, u' are the same vertices as the proof of Lemma 4. Then

$$m(S(G), k) = m(S(G - u) \cup uu', k) + m(S(G) - v - u', k - 1)$$

and

$$m(U_n^3, k) = m(S(U_{n-1}^3) \cup P_2, k) + m(P_5 \cup (n - 3)P_2, k - 1) .$$

Combining the induction hypothesis and the fact the matching number of $S(G) - v - u'$ is $n - 2$ and $P_5 \cup (n - 3)P_2$ is its subgraph of $S(G) - v - u'$, it follows that $m(S(G), k) \geq m(S(U_n^3), k)$ for any positive integer k . If $b_{2k}(S(G)) = b_{2k}(S(U_n^3))$ for any positive integer k , then $P_5 \cup (n - 3)P_2 \cong S(G) - v - u'$, which implies that G has $n - 3$ pendent vertices adjacent to v of C_3 , i. e., $G \cong U_n^3$. □

Theorem 2. (i) Let G be a unicyclic graph with n vertices, $6 \leq n \leq 27$. Then $IE(G) \geq IE(U_n^4)$ with equality if and only if $G \cong U_n^4$.

(ii) Let G be a unicyclic graph with $n \geq 28$ vertices. Then $IE(G) \geq IE(U_n^3)$ with equality if and only if $G \cong U_n^3$.

Proof. By Lemmas 4 and 5 we only need to compare the energies of $S(U_n^3)$ and $S(U_n^4)$. By simple computation it follows that the characteristic polynomials of $S(U_n^3)$ and $S(U_n^4)$ are

$$\begin{aligned} P_{S(U_n^3)}(x) &= (x^2 - 1)^{n-3}[x^6 - (n + 3)x^4 + 3nx^2 - 4] \\ P_{S(U_n^4)}(x) &= x^2(x^2 - 2)(x^2 - 1)^{n-5}[x^6 - (n + 3)x^4 + (4n - 2)x^2 - 2n] . \end{aligned}$$

Let $x_1, x_2, x_3 (x_1 \geq x_2 \geq x_3)$ be the three positive roots of $f(x) = x^6 - (n + 3)x^4 + 3nx^2 - 4$, and $y_1, y_2, y_3 (y_1 \geq y_2 \geq y_3)$ be the three positive roots of $g(x) = x^6 - (n + 3)x^4 + (4n - 2)x^2 - 2n$. Then we get

$$\begin{aligned} \frac{1}{2}E(S(U_n^3)) &= n - 3 + x_1 + x_2 + x_3 \\ \frac{1}{2}E(S(U_n^4)) &= \sqrt{2} + n - 5 + y_1 + y_2 + y_3 . \end{aligned}$$

By using Maple we can easily obtain the result for $6 \leq n < 200$. Assume that $n \geq 200$.

By direct calculation we have that for $n \geq 200$,

$$\begin{aligned} f(0) &= -4 < 0, f(0.085) = -4.000156225 + 0.02162279938n > 0 \\ f(1.73) &= -4.06359790 + 0.02124959n > 0, f(\sqrt{3}) = -4 < 0 \\ f(\sqrt{n}) &= -4 < 0 \\ f(\sqrt{n-1} + 0.2) &= 3.3424n + 3.34592\sqrt{n-1} - 0.64n^2 - 3.3872n\sqrt{n-1} \\ &\quad + 0.4n^2\sqrt{n-1} - 4.708736 \\ &> (0.4n - 3.872)n\sqrt{n-1} - 0.64n^2 \\ &> (0.3\sqrt{n-1} - 0.64)n^2 > 0. \end{aligned}$$

These inequalities imply that $x_1 < \sqrt{n-1} + 0.2$, $x_2 < \sqrt{3}$ and $x_3 < 0.085$ for $n \geq 200$.

Similarly, we have that $g(0.76) = -1.963365351 - 0.02322176n < 0$, $g(0.8) = -2.246656 + 0.1504n > 0$, $g(1.845) = -2.12645629 + 0.0287138n > 0$, $g(1.9) = 0.729381 - 0.5921n < 0$, $g(\sqrt{n-1}) < 0$, $g(\sqrt{n}) > 0$. So we have $y_1 > \sqrt{n-1}$, $y_2 > 1.845$, $y_3 > 0.76$. Thus it follows that

$$\begin{aligned} \frac{1}{2}E(S(U_n^4)) &= \sqrt{2} + n - 5 + y_1 + y_2 + y_3 \\ &> \sqrt{2} + n - 5 + 2.605 + \sqrt{n-1} \\ &> n - 3 + \sqrt{3} + 0.085 + 0.2 + \sqrt{n-1} \\ &> \frac{1}{2}E(S(U_n^3)) \end{aligned}$$

as desired. □

3 The incidence energies of bicyclic graphs

Let $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path P_{n-10} , and $P_n^{3,3}$ be the graph obtained from two copies of C_3 joined by a path P_{n-4} . Clearly, $S(P_n^{3,3}) \cong P_{2n+1}^{6,6}$. Let \mathcal{B}_n denote the class of all bipartite bicyclic graphs but not the graph $R_{a,b}$, which is obtained from joining two cycles C_a and C_b ($a, b \leq 10$ and $a \equiv b \equiv 2 \pmod{4}$) by an edge. Li et al. [16] proved that $P_n^{6,6}$ is the unique graph on n vertices with maximal energy in \mathcal{B}_n . Huo et al. [12] proved that $E(P_n^{6,6}) > E(R_{a,b})$. Thus we get:

Theorem 3. *Let G be a bicyclic graph with n vertices, where $n \geq 6$. Then $IE(G) \leq IE(P_n^{3,3})$ with equality if and only if $G \cong P_n^{3,3}$.*

Let $\theta(a, b, c)$ be the graph obtained by connecting isolated vertices u and v by three paths of respectively lengths a, b, c . Let $\theta_n^*(a, b, c)$ be the graph obtained from $\theta(a, b, c)$ by adding $n - (a + b + c) + 1$ pendent vertices adjacent to v .

Lemma 6. *Let G be a bicyclic graph on n vertices, which has a subgraph isomorphic to $\theta(a, b, c)$. Then $S(G) \succeq S(\theta_n^*(a, b, c))$ with equality if and only if $G \cong \theta_n^*(a, b, c)$.*

Proof. The proof is by induction on n . The case $n = a + b + c - 1$ is obvious since in this case $G \cong \theta_n^*(a, b, c)$. Thus, assume $n \geq a + b + c$. By Lemma 1 we can suppose that all vertices of G except the vertices in $\theta(a, b, c)$ are all pendent vertices. Let wr be a pendent edge, where w be a vertex of $\theta(a, b, c)$. Let w' be the vertex of $S(G)$ adjacent to w and r . Using Lemma 2 we get

$$\begin{aligned} b_{2k}(S(G)) &= b_{2k}(S(G) - ww') + b_{2k-2}(S(G) - w - w') \\ &= b_{2k}(S(G - r) \cup w'r) + b_{2k-2}(S(G) - w - w') \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(\theta_n^*(a, b, c))) &= b_{2k}(S(\theta_{n-1}^*(a, b, c) \cup P_2)) \\ &+ m(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1, k - 1) \end{aligned}$$

Clearly, $G - r$ satisfies the inductive hypothesis, and so

$$\begin{aligned} b_{2k}(S(G)) - b_{2k}(S(\theta_n^*(a, b, c))) &\geq b_{2k-2}(S(G) - w - w') \\ &- m(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1, k - 1) . \end{aligned}$$

If w is the vertex of degree 3 in $\theta(a, b, c)$, then $T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1$ is a spanning subgraph of $S(G) - w - w'$, and $b_{2k-2}(S(G) - w - w') \geq m(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1, k - 1)$. Equalities always hold if and only if $T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1 \cong S(G) - w - w'$, that is, $G \cong \theta_n^*(a, b, c)$. Hence $S(G) \succeq S(\theta_n^*(a, b, c))$ with equality if and only if $G \cong \theta_n^*(a, b, c)$.

Otherwise, without loss of generality we suppose w is an inner vertex of P_{a+1} in $\theta(a, b, c)$. Let $C_{2b+2c}(x, y)$ be the graph obtained by connecting isolated vertices u and v by two paths of lengths $2b, 2c$, respectively, and by identifying a pendent vertex of the path P_{x+1} and u , and a pendent vertex of the path P_{y+1} and v , respectively. Let G be a graph with unique cycle C_{2l} , and $m^*(G, k)$ denote the number of k -matching in G , each of which contains at most $l - 1$ edges of C_{2l} . Then

$$\begin{aligned} b_{2k-2}(S(G) - w - w') &\geq m^*(S(G) - w - w', k - 1) \\ &\geq m^*(C_{2b+2c}(x, y) \cup (n - a - b - c)P_2 \cup P_1, k - 1) \end{aligned}$$

where $x, y \geq 1, x \equiv y \equiv 1 \pmod{2}$ and $x + y = 2a - 2$. Note that for all positive s ,

$$\begin{aligned} m^*(C_{2b+2c}(x, y), s) &= m^*(U_1^{2b+2c}(y), s) + m(T_3(y, 2b - 1, 2c - 1) \cup P_{x-1}, s - 1) \\ &= m^*(C_{2b+2c} \cup P_y \cup P_x, s) + m(P_{2b+2c-1} \cup P_{y-1} \cup P_x, s - 1) \\ &\quad + m(T_3(y, 2b - 1, 2c - 1) \cup P_{x-1}, s - 1) \end{aligned}$$

and

$$\begin{aligned} &m(T_3(2a - 1, 2b - 1, 2c - 1), s) \\ &= m(T_3(y + 1, 2b - 1, 2c - 1) \cup P_x, s) + m(T_3(y, 2b - 1, 2c - 1) \cup P_{x-1}, s - 1) \\ &= m(T_3(1, 2b - 1, 2c - 1) \cup P_y \cup P_x, s) + m(P_{2b+2c-1} \cup P_{y-1} \cup P_x, s - 1) \\ &\quad + m(T_3(y, 2b - 1, 2c - 1) \cup P_{x-1}, s - 1). \end{aligned}$$

Further, $m^*(C_{2b+2c}, t) \geq m(P_{2b+2c}, t) \geq m(T_3(1, 2b - 1, 2c - 1), t)$ for $2 \leq t \leq b + c - 1$, $m^*(C_{2b+2c}, b + c) = m(T_3(1, 2b - 1, 2c - 1), b + c) = 0$ and $m^*(C_{2b+2c}, 1) = 2b + 2c > m(T_3(1, 2b - 1, 2c - 1), 1) = 2b + 2c - 1$. So we have

$$\begin{aligned} &b_{2k-2}(S(G) - w - w') \\ &\geq m^*(C_{2b+2c}(x, y) \cup (n - a - b - c)P_2 \cup P_1, k - 1) \\ &\geq m(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1, k - 1). \end{aligned}$$

The last inequality is strict for $k = 2$. Hence the result follows. □

Lemma 7. *Let G be a bicyclic graph on n vertices with girth $g \geq 4$ and containing θ -subgraph. Then $IE(G) \geq IE(\theta_n^*(2, 2, 2))$ with equality if and only if $G \cong \theta_n^*(2, 2, 2)$.*

Proof. Let G be a bicyclic graph with n vertices, and $\theta(a, b, c)$ be its induced subgraph. By Lemma 6, it suffices to prove to $S(\theta_n^*(a, b, c)) \succeq S(\theta_n^*(2, 2, 2))$, where $n \geq a+b+c-1$ and $g(\theta_n^*(a, b, c)) \geq 4$. By induction on n to prove it. We first suppose that $n = a + b + c - 1$ i. e., $G \cong \theta(a, b, c)$. Then $S(\theta(a, b, c)) = \theta(2a, 2b, 2c)$. We will consider the following three cases.

Case 1: $c + a \equiv c + b \equiv 1 \pmod{2}$.

Subcase 1: $c = 1$. Then a, b are two even number of greater than 3. Using Lemma 2 we get

$$\begin{aligned} b_{2k}(\theta(2a, 2b, 2)) &= b_{2k}(U_1^{2b+2}(2a-1)) + m(T_3(2a-2, 2b-1, 1), k-1) \\ &\quad - 2m(P_1, k-a-b) + 2m(P_{2b-1}, k-a-1) \\ &\geq b_{2k}(U_1^{2b+2}(2a-1)) + m(T_3(2a-2, 2b-1, 1), k-1) \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(\theta_n^*(2, 2, 2))) &= b_{2k}(U_{n-4}^8(\overbrace{3, 2, \dots, 2}^{n-5})) + m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1) \\ &\quad - 4m(P_3 \cup (n-5)P_2, k-4). \end{aligned}$$

So we have

$$\begin{aligned} &b_{2k}(\theta(2a, 2b, 2)) - b_{2k}(S(\theta_n^*(2, 2, 2))) \\ &\geq b_{2k}(U_1^{2b+2}(2a-1)) + m(T_3(2a-2, 2b-1, 1), k-1) \\ &\quad - [b_{2k}(U_{n-4}^8(\overbrace{3, 2, \dots, 2}^{n-5})) + m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1)] \\ &= b_{2k}(U_1^{2b+2}(2a-1)) - b_{2k}(U_{n-4}^8(\overbrace{3, 2, \dots, 2}^{n-5})) \\ &\quad + \left[m(T_3(2a-2, 2b-1, 1), k-1) - m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1) \right]. \end{aligned}$$

We look at the last two parts separately. The first part is

$$\begin{aligned} &b_{2k}(U_1^{2b+2}(2a-1)) - b_{2k}(U_{n-4}^8(\overbrace{3, 2, \dots, 2}^{n-5})) \\ &= [b_{2k}(U_1^{2b+2}(2a-4) \cup P_3) + b_{2k-2}(U_1^{2b+2}(2a-5) \cup P_2)] \\ &\quad - [b_{2k}(S(U_{n-1}^4) \cup P_3) + m(P_7 \cup (n-4)P_2, k-1)] \\ &\geq b_{2k-2}(U_1^{2b+2}(2a-5) \cup P_2) - m(P_7 \cup (n-4)P_2, k-1) \quad (\text{from Lemma 4}) \end{aligned}$$

$$\begin{aligned} &\geq m(P_{2n-3} \cup P_2, k-1) - m(P_7 \cup (n-4)P_2, k-1) \text{ (since } b+1 \equiv 1 \pmod{2}\text{)} \\ &\geq 0, \end{aligned}$$

the second inequality is strict for $k = 2$. The second part is

$$\begin{aligned} &m(T_3(2a-2, 2b-1, 1), k-1) - m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1) \\ &\geq m(T_3(2a+2b-8, 5, 1), k-1) - m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1) \text{ (by Lemma 3)} \\ &= m(T_3(2n-8, 5, 1), k-1) - m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1) \text{ (since } a+b=n\text{)}. \end{aligned}$$

Claim 2: For $n \geq 6$, $T_3(2n-8, 5, 1), s \succ T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4})$.

Proof. The proof is by induction on n . Suppose that $n = 6$, we can compute that

$$\begin{aligned} P_{T_3(4,5,1)}(x) &= x^{11} - 10x^9 + 35x^7 - 51x^5 + 28x^3 - 4x \\ P_{T_4(3,3,2,2)}(x) &= x^{11} - 10x^9 + 33x^7 - 46x^5 + 26x^3 - 4x. \end{aligned}$$

Comparing their coefficients the claim follows. Suppose that $n \geq 7$ and the result is true for less than n . By Lemma 2 it follows that

$$m(T_3(2n-8, 5, 1), s) = m(T_3(2n-10, 5, 1) \cup P_2, s) + m(T_3(2n-11, 5, 1) \cup P_1, s-1)$$

and

$$\begin{aligned} m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), s) &= m(T_{n-3}(3, 3, \overbrace{2, \dots, 2}^{n-5}) \cup P_2, s) \\ &\quad + m(2P_3 \cup (n-5)P_2 \cup P_1, s-1). \end{aligned}$$

Note that $2P_3 \cup (n-5)P_2 \cup P_1$ is a proper subgraph of $T_3(2n-11, 5, 1) \cup P_1$ and by the induction hypothesis the inequality

$$m(T_3(2n-10, 5, 1) \cup P_2, s) \geq m(T_{n-3}(3, 3, \overbrace{2, \dots, 2}^{n-5}) \cup P_2, s)$$

holds. So the Claim follows. □

From Claim 2, $T_3(2a-2, 2b-1, 1) \succ T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1$ for $n \geq 6$. Therefore, for $c = 1$, we can get that $\theta(2a, 2b, 2) \succ S(\theta_n^*(2, 2, 2))$, i. e., $IE(\theta(a, b, 1)) > IE(\theta_n^*(2, 2, 2))$.

Subcase 2: $c \geq 2$. Then

$$\begin{aligned} b_{2k}(\theta(2a, 2b, 2c)) &= b_{2k}(U_1^{2a+2b}(2c-1)) + m(T_3(2a-1, 2b-1, 2c-2), k-1) \\ &\quad + 2b_{2k-2a-2c}(P_{2b-1}) + 2b_{2k-2b-2c}(P_{2a-1}) \\ &\geq b_{2k}(U_1^{2a+2b}(2c-1)) + m(T_3(2a-1, 2b-1, 2c-2), k-1). \end{aligned}$$

Similarly, we have that

$$\begin{aligned} &b_{2k}(\theta(2a, 2b, 2c)) - b_{2k}(S(\theta_n^*(2, 2, 2))) \\ &\geq [b_{2k}(U_1^{2a+2b}(2c-1)) - b_{2k}(U_{n-4}^8(3, \overbrace{2, \dots, 2}^{n-5}))] \\ &\quad + [m(T_3(2a-1, 2b-1, 2c-2), k-1) - m(T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}), k-1)]. \end{aligned}$$

By a similar argument as above, we can prove that for $n \geq 6$ $U_1^{2a+2b}(2c-1) \succ U_{n-4}^8(3, \overbrace{2, \dots, 2}^{n-5})$ and $T_3(2a-1, 2b-1, 2c-2) \succ T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4})$ for $a = 1$ or $b = 1$. Hence $\theta(2a, 2b, 2c) \succ S(\theta_n^*(2, 2, 2))$ for $n \geq 6$ and $a = 1$ or $b = 1$. Suppose now $a, b \geq 2$, and by Lemma 3 it follows that for $n \geq 6$

$$T_3(2a-1, 2b-1, 2c-2) \succ T_4(2a-3, 2b-1, 2c-2, 2) \succ \dots \succ T_{n-2}(3, 3, \overbrace{2, \dots, 2}^{n-4}).$$

So $\theta(2a, 2b, 2c) \succ S(\theta_n^*(2, 2, 2))$ for $a, b \geq 2$ and completes the proof of this subcase.

Case 2: $c+a \equiv 0, c+b \equiv 1 \pmod{2}$. Then $b+a \equiv 1, c+b \equiv 1 \pmod{2}$. This case is reduced to above case.

Case 3: $c+a \equiv 0, c+b \equiv 0 \pmod{2}$, then $a \equiv b \equiv c \pmod{2}$. Assume that $c \geq b \geq a$.

Using Lemma 2 we obtain

$$\begin{aligned} &b_{2k}(S(\theta(a, b, c))) = b_{2k}(\theta(2a, 2b, 2c)) \\ &= b_{2k}(U_1^{2a+2b}(2c-1)) + m(T_3(2c-2, 2a-1, 2b-1), k-1) \\ &\quad - 2m(P_{2b-1}, k-a-c) - 2m(P_{2a-1}, k-b-c) \end{aligned}$$

and

$$\begin{aligned} &b_{2k}(\theta_{a+b+c-1}^*(a, b, c-2)) \\ &= b_{2k}(U_3^{2a+2b}(2c-5, 2, 2)) + m(T_5(2c-6, 2a-1, 2b-1, 2, 2), k-1) \end{aligned}$$

$$- 2m(P_{2b-1} \cup 2P_2, k - a - c + 2) - 2m(P_{2a-1} \cup 2P_2, k - b - c + 2) .$$

Clearly, $-2m(P_{2b-1}, k - a - c) - 2m(P_{2a-1}, k - b - c) \geq -2m(P_{2b-1} \cup 2P_2, k - a - c + 2) - 2m(P_{2a-1} \cup 2P_2, k - b - c + 2)$. And by Lemma 3, it follows that $b_{2k}(U_1^{2a+2b}(2c - 1)) \geq b_{2k}(U_3^{2a+2b}(2c - 5, 2, 2))$ and $b_{2k-2}(T_3(2c - 2, 2a - 1, 2b - 1)) \geq b_{2k-2}(T_5(2c - 6, 2a - 1, 2b - 1, 2, 2))$. Each of the two inequalities is strict for some k . Hence $S(\theta(a, b, c)) \succ S(\theta_{a+b+c-1}^*(a, b, c-2))$. Similarly, we can prove that $S(\theta_{a+b+c-1}^*(a, b, c-2)) \succeq S(\theta_{a+b+c-1}^*(a, b, c-4))$. Thus we have that $S(\theta(a, b, c)) \succ S(\theta_{a+b+c-1}^*(1, 3, 3))$ for odd numbers a, b, c , and $S(\theta(a, b, c)) \succ S(\theta_{a+b+c-1}^*(2, 2, 2))$ for even numbers a, b, c . So we only need to prove that $S(\theta_{a+b+c-1}^*(1, 3, 3)) \succ S(\theta_{a+b+c-1}^*(2, 2, 2))$. By direct computation we can prove $S(\theta(1, 3, 3)) \succ S(\theta_6^*(2, 2, 2))$, the remain proof is reduce to following proof for the graph with at least one pendent vertex. So the result is true for $n = a + b + c - 1$. We suppose that $n \geq a + b + c$.

If $a, b, c \geq 2$, then by Lemma 2 it follows that

$$\begin{aligned} b_{2k}(S(\theta_n^*(a, b, c))) &= b_{2k}(S(\theta_{n-1}^*(a, b, c)) \cup P_2) \\ &+ m(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1, k - 1) \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(\theta_n^*(2, 2, 2))) &= b_{2k}(S(\theta_{n-1}^*(2, 2, 2)) \cup P_2) \\ &+ m(T_3(3, 3, 3) \cup (n - 6)P_2 \cup P_1, k - 1) . \end{aligned}$$

From the induction hypothesis and the fact that $T_3(3, 3, 3) \cup (n - 6)P_2 \cup P_1$ is the spanning subgraph of $T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1$, it follows that $b_{2k}(S(\theta_{n-1}^*(a, b, c)) \cup P_2) \geq b_{2k}(S(\theta_{n-1}^*(2, 2, 2)) \cup P_2)$ and $b_{2k-2}(T_3(2a - 1, 2b - 1, 2c - 1) \cup (n - a - b - c)P_2 \cup P_1) \geq b_{2k-2}(T_3(3, 3, 3) \cup (n - 6)P_2 \cup P_1)$. Hence $b_{2k}(S(\theta_n^*(a, b, c))) \geq b_{2k}(S(\theta_n^*(2, 2, 2)))$. The second equality for $k = 2$ holds if and only if $a = 2, b = 2, c = 2$, that is, $G \cong \theta_n^*(2, 2, 2)$.

If $a = 1$, then $b, c \geq 3$. By Lemma 2 we have

$$\begin{aligned} b_{2k}(S(\theta_n^*(1, b, c))) &= b_{2k}(S(\theta_{n-1}^*(1, b, c)) \cup P_2) \\ &+ m(T_3(2b - 1, 2c - 1, 1) \cup (n - b - c - 1)P_2 \cup P_1, k - 1) \\ &\geq b_{2k}(S(\theta_{n-1}^*(1, b, c)) \cup P_2) \end{aligned}$$

$$+ m(T_3(5, 5, 1) \cup (n - 7)P_2 \cup P_1, k - 1) .$$

The last inequality holds since $T_3(5, 5, 1) \cup (n - 7)P_2 \cup P_1$ is a subgraph of $T_3(2b - 1, 2c - 1, 1) \cup (n - b - c - 1)P_2 \cup P_1$. By the induction hypothesis, it suffices to prove that $m(T_3(5, 5, 1) \cup (n - 7)P_2 \cup P_1, k - 1) \geq m(T_3(3, 3, 3) \cup (n - 6)P_2 \cup P_1, k - 1)$, that is, $T_3(5, 5, 1) \succeq T_3(3, 3, 3) \cup P_2$. By direct computation it follows that

$$\begin{aligned} P_{T_3(5,5,1)}(x) &= x^{12} - 11x^{10} + 44x^8 - 78x^6 + 59x^4 - 15x^2 \\ P_{T_3(3,3,3) \cup P_2}(x) &= x^{12} - 10x^{10} + 36x^8 - 59x^6 + 44x^4 - 12x^2 . \end{aligned}$$

Comparing the coefficients we can obtain $T_3(5, 5, 1) \succ T_3(3, 3, 3) \cup P_2$, i. e., $T_3(5, 5, 1) \cup (n - 7)P_2 \cup P_1 \succ T_3(3, 3, 3) \cup (n - 6)P_2 \cup P_1$. So $S(\theta_n^*(a, b, c)) \succ S(\theta_n^*(2, 2, 2))$. \square

Lemma 8. *Let $a \geq 3$ be an odd number. Then $S(U_n^{a+2}) \succ S(U_n^a)$.*

Proof. The proof is by induction on n . If $n = a + 2$, then $U_n^{a+2} = C_{a+2}$. Using Lemma 2 we get

$$b_{2k}(S(U_n^{a+2})) = m(P_{2a+4}, k) + m(P_{2a+2}, k - 1) + 2A_k$$

where

$$A_k = \begin{cases} 1 & \text{if } k = a + 2 \\ 0 & \text{otherwise} \end{cases}$$

and

$$b_{2k}(S(U_n^a)) = m(T_3(2a - 1, 2, 2), k) + m(P_{2a-2} \cup 2P_2, k - 1) + 2m(2P_2, k - a)$$

where

$$m(2P_2, k - a) = \begin{cases} 1 & \text{if } k = a \text{ or } k = a + 2 \\ 2 & \text{if } k = a + 1 \\ 0 & \text{otherwise.} \end{cases}$$

Note that $m(P_{2a+4}, k) \geq m(T_3(2a - 1, 2, 2), k)$. Then

$$\begin{aligned} b_{2k}(S(U_n^{a+2})) - b_{2k}(S(U_n^a)) &\geq m(P_{2a+2}, k - 1) \\ &+ 2A_k - m(P_{2a-2} \cup 2P_2, k - 1) - 2m(2P_2, k - a) \end{aligned}$$

If $k \leq a - 1$ or $k = a + 2$, then $m(P_{2a+2}, k - 1) \geq m(T_3(2a - 2, 2, 2), k - 1)$, and $2A_k = 2m(2P_2, k - a)$. And so $b_{2k}(S(U_n^{a+2})) - b_{2k}(S(U_n^a)) \geq 0$.

If $k = a$, then

$$m(P_{2a+2}, k - 1) + 2A_k - (m(P_{2a-2} \cup 2P_2, k - 1) + 2m(2P_2, k - a))$$

$$\begin{aligned}
 &= m(P_{2a+2}, k-1) - [m(P_{2a-2} \cup 2P_2, k-1) + 2] \\
 &= \binom{a+3}{a-1} - \left[\binom{a-1}{a-1} + 2\binom{a}{a-2} + \binom{a+1}{a-3} + 2 \right] \\
 &= \frac{2a^3 - 3a^2 + 7a - 18}{6} > 0 \text{ (for } a \geq 3 \text{)}.
 \end{aligned}$$

If $k = a + 1$, then

$$\begin{aligned}
 &m(P_{2a+2}, k-1) + 2A_k - (m(P_{2a-2} \cup 2P_2, k-1) + 2m(2P_2, k-a)) \\
 &= m(P_{2a+2}, k-1) - [m(P_{2a-2} \cup 2P_2, k-1) + 4] \\
 &= \binom{a+2}{a} - \left[\binom{a-2}{a} + 2\binom{a-1}{a-1} + \binom{a}{a-2} + 4 \right] \\
 &= \frac{4a - 10}{2} > 0 \text{ (for } a \geq 3 \text{)}.
 \end{aligned}$$

So the result is true for $n = a + 2$.

Suppose now $n > a + 2$. Then by Lemma 2 we have

$$b_{2k}(S(U_n^{a+2})) = b_{2k}(S(U_{n-1}^{a+2}) \cup P_2) + m(P_{2a+3} \cup (n-a-3)P_2 \cup P_1, k-1)$$

and

$$b_{2k}(S(U_n^a)) = b_{2k}(S(U_{n-1}^a) \cup P_2) + m(P_{2a-1} \cup (n-a-1)P_2 \cup P_1, k-1).$$

Note that $P_{2a+3} \cup (n-a-3)P_2 \cup P_1$ is a proper subgraph of $P_{2a-1} \cup (n-a-1)P_2 \cup P_1$.

Then $m(P_{2a+3} \cup (n-a-3)P_2 \cup P_1, k-1) \geq m(P_{2a-1} \cup (n-a-1)P_2 \cup P_1, k-1)$, which is strict for $k = 2$. By the induction hypothesis, it follows that $S(U_n^{a+2}) \succ S(U_n^a)$. \square

Lemma 9. *Let G be a bicyclic graph with n vertices containing $\theta(1, 2, a)$ -subgraph, where a is an even number of greater than 2. Then $IE(G) > IE(\theta_n^*(1, 2, 2))$.*

Proof. By Lemma 6, we only need to prove that $IE(\theta_n^*(1, 2, a)) > IE(\theta_n^*(1, 2, 2))$ for even number $a > 2$. Using Lemma 2 we have

$$\begin{aligned}
 &b_{2k}(S(\theta_n^*(1, 2, a+2))) \\
 &= b_{2k}(U_{n-a-3}^{2a+6}(\underbrace{3, 2, \dots, 2}_{n-a-4})) + m(T_{n-a-1}(2a+3, \underbrace{2, \dots, 2}_{n-a-3}, 1), k-1)
 \end{aligned}$$

$$+ 2m(P_{2a+3} \cup (n-a-4)P_2, k-3) - 2m(P_1 \cup (n-a-4)P_2, k-a-4)$$

and

$$\begin{aligned} & b_{2k}(S(\theta_n^*(1, 2, a))) \\ &= b_{2k}(U_{n-a-1}^{2a+2}(3, \overbrace{2, \dots, 2}^{n-a-2})) + m(T_{n-a+1}(2a-1, \overbrace{2, \dots, 2}^{n-a-1}, 1), k-1) \\ &+ 2m(P_{2a-1} \cup (n-a-2)P_2, k-3) - 2m(P_1 \cup (n-a-2)P_2, k-a-2) . \end{aligned}$$

Clearly, $m(P_{2a+3} \cup (n-a-4)P_2, k-3) \geq m(P_{2a-1} \cup (n-a-2)P_2, k-3)$ and $m(P_1 \cup (n-a-4)P_2, k-a-4) < m(P_1 \cup (n-a-2)P_2, k-a-2)$. From Lemma 2 we have $m(T_{n-a-1}(2a+3, \overbrace{2, \dots, 2}^{n-a-3}, 1), k-1) \geq m(T_{n-a+1}(2a-1, \overbrace{2, \dots, 2}^{n-a-1}, 1), k-1)$. So we can get that

$$\begin{aligned} & b_{2k}(S(\theta_n^*(1, 2, a+2))) - b_{2k}(S(\theta_n^*(1, 2, a))) \\ &\geq b_{2k}(U_{n-a-3}^{2a+4}(3, \overbrace{2, \dots, 2}^{n-a-4})) - b_{2k}(U_{n-a-1}^{2a}(3, \overbrace{2, \dots, 2}^{n-a-2})) \\ &= [b_{2k}(S(U_{n-2}^{a+3}) \cup P_2) + m(P_{2a+3} \cup (n-a-4)P_2 \cup P_1, k-1)] \\ &- [b_{2k}(S(U_{n-2}^{a+1}) \cup P_2) + m(P_{2a-1} \cup (n-a-2)P_2 \cup P_1, k-1)] \text{ (from Lemma 2)} \\ &\geq m(P_{2a+3} \cup (n-a-4)P_2 \cup P_1, k-1) - m(P_{2a-1} \cup (n-a-2)P_2 \cup P_1, k-1) \\ &\text{(from Lemma 8)} \\ &\geq 0 \text{ (it is strict for } k=2\text{)}. \end{aligned}$$

It follows that $S(\theta_n^*(1, 2, a+2)) \succ S(\theta_n^*(1, 2, a))$, and hence $IE(G) > IE(\theta_n^*(1, 2, 2))$. □

Lemma 10. *Let G be a bicyclic graph with n vertices containing $\theta(1, 2, a)$ -subgraph, where a is an odd number of greater than 3, then $IE(G) > IE(\theta_n^*(1, 2, 3))$.*

Proof. By Lemma 6, we only need to prove that $IE(\theta_n^*(1, 2, a)) > IE(\theta_n^*(1, 2, 3))$ holds for odd number $a > 3$. Note that by the Sachs theorem, $b_0(S_n^*(1, 2, a)) = b_0(S_n^*(1, 2, 3)) = 1$ and $b_{2n}(S(\theta_n^*(1, 2, a))) = 0 = b_{2n}(S(\theta_n^*(1, 2, 3)))$. Now, we assume that $1 \leq k < n$. By Lemma 2 we have

$$\begin{aligned} & b_{2k}(S(\theta_n^*(1, 2, a))) \\ &= b_{2k}(U_{n-a-1}^6(2a-1, \overbrace{2, \dots, 2}^{n-a-2})) + m(T_{n-a+1}(2a-2, 3, \overbrace{2, \dots, 2}^{n-a-2}, 1), k-1) \end{aligned}$$

$$- 2m(P_3 \cup (n - a - 2)P_2, k - a - 1) + 2m(P_1 \cup (n - a - 2)P_2, k - a - 2)$$

and

$$\begin{aligned} b_{2k}(S(\theta_n^*(1, 2, 3))) &= b_{2k}(U_{n-4}^6(\overbrace{5, 2, \dots, 2}^{n-5})) + m(T_{n-2}(4, 3, \overbrace{2, \dots, 2}^{n-5}, 1), k - 1) \\ &- 2m(P_3 \cup (n - 5)P_2, k - 4) + 2m(P_1 \cup (n - 5)P_2, k - 5) . \end{aligned}$$

By Lemmas 3 and 5 it is easy to prove that

$$b_{2k}(U_{n-a-1}^6(2a - 1, \overbrace{2, \dots, 2}^{n-a-2})) \geq b_{2k}(U_{n-4}^6(\overbrace{5, 2, \dots, 2}^{n-5}))$$

and

$$m(T_{n-a+1}(2a - 2, 3, \overbrace{2, \dots, 2}^{n-a-2}, 1), k - 1) \geq m(T_{n-2}(4, 3, \overbrace{2, \dots, 2}^{n-5}, 1), k - 1) .$$

Let

$$A = -2m(P_3 \cup (n - a - 2)P_2, k - a - 1) + 2m(P_1 \cup (n - a - 2)P_2, k - a - 2),$$

$$B = -2m(P_3 \cup (n - 5)P_2, k - 4) + 2m(P_1 \cup (n - 5)P_2, k - 5) .$$

Then we have

$$\begin{aligned} &b_{2k}(S(\theta_n^*(1, 2, a)) - b_{2k}(S(\theta_n^*(1, 2, 3))) \geq A - B \\ &= -2 \left[\binom{n - a - 2}{k - a - 2} + \binom{n - a - 2}{k - a - 1} \right] + 2 \left[\binom{n - 5}{k - 5} + \binom{n - 5}{k - 4} \right] \\ &= 2 \left\{ \left[\binom{n - 5}{k - 5} - \binom{n - a - 2}{k - a - 2} \right] + \left[\binom{n - 5}{k - 4} - \binom{n - a - 2}{k - a - 1} \right] \right\} > 0 . \end{aligned}$$

The proof is thus complete. □

Let $B(a, b)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_a and C_b by identifying vertices u of C_a and v of C_b , and $B_n^*(a, b)$ be the graph obtained from $B(a, b)$ by adding $n - a - b + 1$ pendent vertices adjacent to the vertex of degree 4 in $B(a, b)$.

Lemma 11. *Let G be a bicyclic graph on n vertices containing exactly two cycles, say C_a and C_b . If $a \geq b \geq 4$, then $S(G) \succeq S(B_n^*(4, 4))$ with equality if and only if $G \cong B_n^*(4, 4)$.*

Proof. Let $w_1 \in V(C_a), w_2 \in V(C_b)$, if C_a and C_b are connected by a tree T with pendent vertices w_1 and w_2 in G . Let G' be the graph obtained from $G - \{V(T) \setminus \{w_1, w_2\}\}$ by identifying w_1 and w_2 (the new vertex is denoted by w), and adding $|V(T)| - 2$ pendent vertices adjacent to w . By a similar proof of Lemma 1, we can prove that $S(G) \succeq S(G')$. So, assume that the two cycles C_a and C_b of G have a common vertex w , and By Lemma 1 we also suppose that all vertices not in cycles are pendent vertices.

Claim 3: $S(G) \succeq S(B_n^*(a, b))$ for $a \geq b \geq 4$.

Proof. The proof is by induction on n . If $n = a + b - 1$, then the result is true since $G \cong B(a, b) \cong B_n^*(a, b)$. Suppose now $n > a + b - 1$. Then G has a pendent edge, denoted by ur , where r be a pendent vertex of G . Let u' be the vertex of $S(G)$ adjacent to u and r . From Lemma 3, we have

$$\begin{aligned} b_{2k}(S(G)) &= b_{2k}(S(G) - uu') + b_{2k-2}(S(G) - u - u') \\ &= b_{2k}(S(G - r) \cup u'r) + b_{2k-2}(S(G) - u - u') \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(B_n^*(a, b))) &= b_{2k}(S(B_{n-1}^*(a, b) \cup P_2)) \\ &+ m(P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1, k - 1) . \end{aligned}$$

By the induction hypothesis, $b_{2k}(S(G - r) \cup u'r) \geq b_{2k}(S(B_{n-1}^*(a, b) \cup P_2))$. Then

$$\begin{aligned} b_{2k}(S(G)) - b_{2k}(S(B_n^*(a, b))) &\geq b_{2k-2}(S(G) - u - u') \\ &- m(P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1, k - 1) . \end{aligned}$$

If $u = w$, then $P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1$ is a subgraph of $S(G) - u - u'$ and $S(G) - u - u'$ is a forest. And then $b_{2k-2}(S(G) - u - u') = m(S(G) - u - u', k - 1) \geq m(P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1, k - 1)$. If the equalities hold for all k if and only if $S(G) - u - u' \cong P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1$, that is, $G \cong B_n^*(a, b)$. Hence the result is true for $u = w$. Suppose now $u \neq w$. Without loss of generality, we suppose $u \in V(C_a)$, and $wa, wb \in C_b$ in $S(G) - u - u'$. Then $b_{2k-2}(S(G) - u - u') \geq m^*(S(G) - u - u', k - 1) \geq m((S(G) - u - u' - wa - wb, k - 1) \geq m(P_{2a-1} \cup P_{2b-1} \cup$

$(n - a - b)P_2 \cup P_1, k - 1)$. If $k = 2$, then $b_2(S(G) - u - u') = |E((S(G) - u - u'))| > |E(P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1)| = m(P_{2a-1} \cup P_{2b-1} \cup (n - a - b)P_2 \cup P_1, 1)$. Hence the result is also true for $u \neq w$. The proof of Claim 3 is complete. \square

Claim 4: $S(B_n^*(a, b)) \succeq S(B_n^*(4, 4))$ for $a \geq b \geq 4$, with equality if and only if $a = b = 4$.

Proof. We will consider the following two cases.

Case 1: $2a \equiv 2 \pmod{4}$ or $2b \equiv 2 \pmod{4}$. Without loss of generality, we suppose a is odd. For any positive integer k , from Lemma 2, we have

$$\begin{aligned} b_{2k}(S(B_n^*(a, b))) &= b_{2k}(U_{n-a-b+2}^{2b}(2a - 1, \overbrace{2, \dots, 2}^{n-a-b+1})) \\ &\quad + m(P_{2b-1} \cup P_{2a-2} \cup (n - a - b + 1)P_2, k - 1) \\ &\quad + 2m(P_{2b-1} \cup (n - a - b + 1)P_2, k - a) \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(B_n^*(4, 4))) &= b_{2k}(U_{n-6}^8(7, \overbrace{2, \dots, 2}^{n-7})) + m(P_7 \cup P_6 \cup (n - 7)P_2, k - 1) \\ &\quad - 2m(P_7 \cup (n - 7)P_2, k - 4). \end{aligned}$$

Using Lemma 2 again, we have

$$\begin{aligned} &b_{2k}(U_{n-a-b+2}^{2b}(2a - 1, \overbrace{2, \dots, 2}^{n-a-b+1})) \\ &= b_{2k}(U_{n-a-b+2}^{2b}(2a - 8, \overbrace{2, \dots, 2}^{n-a-b+1}) \cup P_7) + b_{2k-2}(U_{n-a-b+2}^{2b}(2a - 9, \overbrace{2, \dots, 2}^{n-a-b+1}) \cup P_6) \\ &= b_{2k}(S(U_{n-a-b+2}^b(a - 4, \overbrace{1, \dots, 1}^{n-a-b+1}) \cup P_7) + b_{2k-2}(U_{n-a-b+2}^{2b}(2a - 9, \overbrace{2, \dots, 2}^{n-a-b+1}) \cup P_6) \end{aligned}$$

and

$$b_{2k}(U_{n-6}^8(7, \overbrace{2, \dots, 2}^{n-7})) = b_{2k}(S(U_{n-3}^4) \cup P_7) + m(P_7 \cup P_6 \cup (n - 7)P_2, k - 1).$$

Note that the inequality $m(P_{2b-1} \cup P_{2a-2} \cup (n - a - b + 1)P_2, k - 1) \geq m(P_7 \cup P_6 \cup (n - 7)P_2, k - 1)$ holds for any k and by the induction hypothesis, we have

$b_{2k}(S(U_{n-a-b+2}^b(a - 4, \overbrace{1, \dots, 1}^{n-a-b+1}) \cup P_7) \geq b_{2k}(S(U_{n-3}^4) \cup P_7)$. Hence, we can get that

$$b_{2k}(S(B_n^*(a, b))) - b_{2k}(S(B_n^*(4, 4)))$$

$$\begin{aligned} &\geq b_{2k}(U_{n-a-b+2}^{2b}(2a-1, \overbrace{2, \dots, 2}^{n-a-b+1})) - b_{2k}(U_{n-6}^8(7, \overbrace{2, \dots, 2}^{n-7})) \\ &\geq m^*(U_{n-a-b+2}^{2b}(2a-9, \overbrace{2, \dots, 2}^{n-a-b+1}) \cup P_6, k) - m(P_7 \cup P_6 \cup (n-7)P_2, k-1) \geq 0. \end{aligned}$$

The last inequality is strict for $k = 2$. Thus we have $S(B_n^*(a, b)) \succ S(B_n^*(4, 4))$ for $a \geq b \geq 4$ and a is odd or b is odd.

Case 2: $2a \equiv 2b \equiv 0 \pmod{4}$, i. e., a, b are even. From Lemma 3, it follows that

$$\begin{aligned} b_{2k}(S(B_n^*(a-2, b))) &= b_{2k}(U_{n-a-b+4}^{2b}(2a-5, \overbrace{2, \dots, 2}^{n-a-b+3})) \\ &\quad + m(P_{2b-1} \cup P_{2a-6} \cup (n-a-b+3)P_2, k-1) \\ &\quad - 2m(P_{2b-1} \cup (n-a-b+3)P_2, k-a+2). \end{aligned}$$

By a similar to the proof of Claim 2, we can prove $b_{2k}(S(B_n^*(a, b))) \geq b_{2k}(S(B_n^*(a-2, b)))$, and $S(B_n^*(a, b)) \succ S(B_n^*(a-2, b))$. Thus we have $S(B_n^*(a, b)) \succ S(B_n^*(a-2, b)) \succ \dots \succ S(B_n^*(4, 4))$ for $a \geq b > 4$ and a, b are even. □

Combining Claims 3 and 4, the result follows. □

Lemma 12. *Let G be a bicyclic graph on n vertices containing exactly two cycles C_a and C_3 . If $a \geq 4$, then $S(G) \succeq S(B_n^*(3, 4))$ with equality if and only if $G \cong B_n^*(3, 4)$.*

Proof. By a similar proof of Lemma 11, we can prove that $S(G) \succeq S(B_n^*(3, a))$ with equality if and only if $G \cong B_n^*(3, a)$. By Lemma 2 we have

$$\begin{aligned} b_{2k}(S(B_n^*(3, a))) &= b_{2k}(U_{n-a-1}^{2a}(5, \overbrace{2, \dots, 2}^{n-a-2})) + m(P_4 \cup P_{2a-1} \cup (n-a-2)P_2, k-1) \\ &\quad + 2m(P_{2a-1} \cup (n-a-2)P_2, k-3) \end{aligned}$$

and

$$\begin{aligned} b_{2k}(S(B_n^*(3, 4))) &= b_{2k}(U_{n-5}^8(5, \overbrace{2, \dots, 2}^{n-6})) \\ &\quad + m(P_4 \cup P_7 \cup (n-6)P_2, k-1) + 2m(P_7 \cup (n-6)P_2, k-3). \end{aligned}$$

So, we have

$$b_{2k}(S(B_n^*(3, a))) - b_{2k}(S(B_n^*(3, 4)))$$

$$\begin{aligned}
 &\geq b_{2k}(U_{n-a-1}^{2a}(\overbrace{5, 2, \dots, 2}^{n-a-2}) - b_{2k}(U_{n-5}^8(\overbrace{5, 2, \dots, 2}^{n-6})) \\
 &= [b_{2k}(U_{n-a-2}^{2a}(\overbrace{2, \dots, 2}^{n-a-2}) \cup P_5) + m(P_{2a-1} \cup P_4 \cup (n-a-2)P_2, k-1)] \\
 &\quad - [b_{2k}(U_{n-6}^8(\overbrace{2, \dots, 2}^{n-6}) \cup P_5) + m(P_7 \cup P_4 \cup (n-6)P_2, k-1)] \\
 &= [b_{2k}(S(U_{n-2}^a) \cup P_5) - b_{2k}(S(U_{n-2}^4) \cup P_5)] \\
 &\quad + [m(P_{2a-1} \cup P_4 \cup (n-a-2)P_2, k-1) - m(P_7 \cup P_4 \cup (n-6)P_2, k-1)] \\
 &\geq m(P_{2a-1} \cup P_4 \cup (n-a-2)P_2, k-1) - m(P_7 \cup P_4 \cup (n-6)P_2, k-1) \geq 0.
 \end{aligned}$$

The last inequality is strict for $k = 2$. Hence, the result follows. □

Lemma 13. *Let $n \geq 5$. Then $S(B_n^*(3, 3)) \succ S(\theta_n^*(1, 2, 2))$*

Proof. For $1 \leq k \leq n$, Using Lemma 2 we have

$$\begin{aligned}
 b_{2k}(S(B_n^*(3, 3))) &= b_{2k}(U_{n-3}^6(\overbrace{3, 2, \dots, 2}^{n-4})) \\
 &\quad + b_{2k-2}(U_{n-3}^6(\overbrace{2, \dots, 2, 1}^{n-4})) + 2m(P_5 \cup (n-5)P_2, k-3)
 \end{aligned}$$

and

$$\begin{aligned}
 b_{2k}(S(\theta_n^*(1, 2, 2))) &= b_{2k}(U_{n-3}^6(\overbrace{3, 2, \dots, 2}^{n-4})) + m(T_{n-1}(\overbrace{3, 2, \dots, 2, 1}^{n-3}), k-1) \\
 &\quad + 2m(P_3 \cup (n-4)P_2, k-3) + 2m(P_1 \cup (n-4)P_2, k-4).
 \end{aligned}$$

Note that

$$\begin{aligned}
 &b_{2k-2}(U_{n-3}^6(\overbrace{2, \dots, 2, 1}^{n-4})) \\
 &= m(T_{n-1}(\overbrace{3, 2, \dots, 2, 1}^{n-3}), k-1) + m(T_{n-1}(\overbrace{2, \dots, 2, 1, 1}^{n-3}), k-2) \\
 &\quad + 2m(P_1 \cup (n-4)P_2, k-4) > m(T_{n-1}(\overbrace{3, 2, \dots, 2, 1}^{n-3}), k-1)
 \end{aligned}$$

and

$$2m(P_5 \cup (n-5)P_2, k-3) = 2m(P_3 \cup (n-4)P_2, k-3) + 2m(P_1 \cup (n-4)P_2, k-4).$$

Then, for $1 \leq k \leq n$, we have

$$b_{2k}(S(B_n^*(3, 3))) > b_{2k}(S(\theta_n^*(1, 2, 2))) \quad \text{i. e.,} \quad S(B_n^*(3, 3)) \succ S(\theta_n^*(1, 2, 2)).$$

□

Lemma 14. *Let $n \geq 7$. Then $S(B_n^*(4, 4)) \succ S(\theta_n^*(2, 2, 2))$.*

Proof. By induction on n . Let $n = 7$. The Q-polynomial of $B_n^*(4, 4)$ and $\theta_n^*(2, 2, 2)$ are

$$Q_{B_7^*(4,4)}(x) = x^7 - 16x^6 + 100x^5 - 312x^4 + 508x^3 - 400x^2 + 112x$$

and

$$Q_{\theta_7^*(2,2,2)}(x) = x^7 - 16x^6 + 96x^5 - 278x^4 + 413x^3 - 300x^2 + 84x .$$

Comparing their coefficients the result follows for $n = 7$. So let $n \geq 8$ and the result holds for smaller values of n . By Lemma 2 we have

$$b_{2k}(S(B_n^*(4, 4))) = b_{2k}(S(B_{n-1}^*(4, 4)) \cup P_2) + m(2P_7 \cup (n-8)P_2 \cup P_1, k-1)$$

and

$$b_{2k}(S(\theta_n^*(2, 2, 2))) = b_{2k}(S(\theta_{n-1}^*(2, 2, 2)) \cup P_2) + m(T_3(3, 3, 3) \cup (n-6)P_2 \cup P_1, k-1) .$$

By the induction hypothesis, $b_{2k}(S(B_{n-1}^*(4, 4) \cup P_2)) \geq b_{2k}(S(\theta_{n-1}^*(2, 2, 2) \cup P_2))$. Therefore,

$$\begin{aligned} & b_{2k}(S(B_n^*(4, 4))) - b_{2k}(S(\theta_n^*(2, 2, 2))) \\ & \geq m(2P_7 \cup (n-8)P_2 \cup P_1, k-1) - m(T_3(3, 3, 3) \cup (n-6)P_2 \cup P_1, k-1) \\ & = [m(P_7 \cup P_4 \cup P_3 \cup (n-8)P_2 \cup P_1, k-1) \\ & + m(P_7 \cup P_3 \cup (n-7)P_2 \cup P_1, k-2)] \\ & - [m(P_7 \cup P_3 \cup (n-6)P_2 \cup P_1, k-1) + m(2P_3 \cup (n-5)P_2 \cup P_1, k-2)] \geq 0 . \end{aligned}$$

The above inequality is strict for $k = 3$, the proof completed. □

Similarly, we can prove that

Lemma 15. $S(B_n^*(4, 3)) \succ S(\theta_n^*(1, 2, 2))$ for $n \geq 6$; $S(\theta_n^*(4, 3)) \succ S(\theta_n^*(1, 2, 2))$ for $n \geq 5$.

Theorem 4. *Let G be a bicyclic graph on n vertices. (a) if $6 \leq n \leq 30$, then $IE(G) \geq IE(\theta_n^*(2, 2, 2))$ with equality if and only if $G \cong \theta_n^*(2, 2, 2)$; (b) if $n \geq 31$, then $IE(G) \geq IE(\theta_n^*(1, 2, 2))$ with equality if and only if $G \cong \theta_n^*(1, 2, 2)$.*

Proof. By Lemmas 11, 12, 13, 14, and 15, we only need to compare the incidence energies of $\theta_n^*(1, 2, 2)$ and $\theta_n^*(2, 2, 2)$.

It is easy to obtain that the Q-polynomial of $\theta_n^*(1, 2, 2)$ and $\theta_n^*(2, 2, 2)$ are

$$Q_{\theta_n^*(1,2,2)}(x) = (x - 2)(x - 1)^{n-4}(x^3 - (n + 4)x^2 + 4nx - 8)$$

and

$$Q_{\theta_n^*(2,2,2)}(x) = x(x - 2)^2(x - 1)^{n-6}(x^3 - (n + 4)x^2 + (5n - 2)x - 3n) .$$

So, the polynomial of $S(\theta_n^*(1, 2, 2))$ and $S(\theta_n^*(2, 2, 2))$ are

$$P_{S(\theta_n^*(1,2,2))}(x) = x(x^2 - 2)(x^2 - 1)^{n-4}(x^6 - (n + 4)x^4 + 4nx^2 - 8)$$

and

$$P_{S(\theta_n^*(2,2,2))}(x) = x^3(x^2 - 2)^2(x^2 - 1)^{n-6}(x^6 - (n + 4)x^4 + (5n - 2)x^2 - 3n)$$

respectively. Let x_1, x_2, x_3 ($x_1 \geq x_2 \geq x_3$) are the three positive roots of $h(x) = x^6 - (n + 4)x^4 + 4nx^2 - 8$, and y_1, y_2, y_3 ($y_1 \geq y_2 \geq y_3$) are the three positive roots of $r(x) = x^6 - (n + 4)x^4 + (5n - 2)x^2 - 3n$. Then

$$IE(\theta_n^*(1, 2, 2)) = \frac{1}{2}E(S(\theta_n^*(1, 2, 2))) = n - 4 + \sqrt{2} + x_1 + x_2 + x_3$$

$$IE(\theta_n^*(2, 2, 2)) = \frac{1}{2}E(S(\theta_n^*(2, 2, 2))) = n - 6 + 2\sqrt{2} + y_1 + y_2 + y_3 .$$

Clearly, $y_1 = \sqrt{q_1(\theta_n^*(2, 2, 2))} \geq \sqrt{\Delta + 1} = \sqrt{n - 1}$. By direct calculation it is easy to prove the result for $6 \leq n \leq 45$. Suppose that $n \geq 46$, we have that $r(0.834) = -2.989795891 - 0.006018149n < 0$, $r(2.065) = -3.72388436 + 0.13751015n > 0$, $r(2.2) = 9.997504 - 2.2256n < 0$, $h(0) = -8 < 0$, $h(0.21) = -8.007693474 + 0.17445519n > 0$, $h(2) = -8 < 0$, and

$$\begin{aligned} h(\sqrt{n-1} + 0.1) &= -0.91n^2 + 0.2\sqrt{n-1}n^2 - 1.584\sqrt{n-1}n \\ &\quad - 12.611899 + 5.5614n + 2.16406\sqrt{n-1} \\ &> -0.91n^2 + 0.2\sqrt{n-1}n^2 - 1.584\sqrt{n-1}n \\ &> 0.4n^2 - 1.584\sqrt{n-1}n > 0 . \end{aligned}$$

Thus it follows that for $n \geq 46$, $y_1 \geq \sqrt{n-1}$, $y_2 \geq 2.065$, $y_3 \geq 0.834$ and $x_1 \leq \sqrt{n-1} + 0.1$, $x_2 \leq 2$, $x_3 \leq 0.21$. Thus we have

$$\begin{aligned} IE(\theta_n^*(2, 2, 2)) &= n - 6 + 2\sqrt{2} + y_1 + y_2 + y_3 > n - 6 + 2\sqrt{2} + 2.899 + \sqrt{n-1} \\ &> (n - 4) + \sqrt{2} + \sqrt{n-1} + 0.1 + 0.21 + 2 \\ &> IE(\theta_n^*(1, 2, 2)) \end{aligned}$$

which completes the proof. \square

Remark: It is easy to prove that $E(P_{2n}^6) < E(P_{2n+1}^{6,6})$ for $n \geq 8$, and $E(S(U_n^3)) < E(S(\theta^*(1, 2, 2)))$ for $n \geq 31$. By Theorem 1, 2, 3 and 4 it follows that for a connected graph with n vertices and m edges ($31 \leq n \leq m \leq n + 1$), then

$$IE(U_n^3) \leq IE(G) \leq IE(P_n^{3,3})$$

with left (right, respectively) equality if and only if $G \cong U_n^3$ ($G \cong P_n^{3,3}$, respectively).

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