On the skew energy of oriented unicyclic digraphs *

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Abstract

The concept of the skew energy of a digraph was introduced by Adiga, Balakrishnan and So in 2010. Let $\overrightarrow{G}$ be an oriented graph of order n and $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote all the eigenvalues of the skew-adjacency matrix of $\overrightarrow{G}$. The skew energy $\varepsilon_s(\overrightarrow{G}) = \sum_{i=1}^{n} |\lambda_i|$. Hou, Shen and Zhang determined the minimal and the second minimal skew energy of the oriented unicyclic graphs. In this paper, the oriented unicyclic graphs with the third, fourth and fifth minimal skew energy are characterized, respectively.

Keywords: unicyclic graphs; oriented graph; skew-adjacency matrix; skew energy

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1 Introduction

An important quantum-chemical characteristic of a conjugated molecule is its total π-electron energy. The energy of a graph has closed links to chemistry. Since the concept of the energy of simple undirected graphs was introduced by Gutman in [5], there have been lots of research papers on this topic. For the extremal energy of unicyclic graph, Hou [7] showed that S_n^3 is the graph with minimal energy in all unicyclic graphs; In [6], Huo and Li showed that P_n^6 is the

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graph with maximal energy in all unicyclic graphs. For the energy of graphs, Li, Shi and Gutman published a paper on this subject; see [11].

The concept of the skew energy of a digraph was introduced by Adiga, Balakrishnan and So in [1]. Let $\overrightarrow{G}$ be a digraph of order n with vertex set $V(\overrightarrow{G}) = \{v_1, v_2, \cdots, v_n\}$, and arc set $\Gamma(\overrightarrow{G}) \subset V(\overrightarrow{G}) \times V(\overrightarrow{G})$. Throughout this paper, we assume that $\overrightarrow{G}$ does not have loop and multiple arcs, i.e., $(v_i, v_i) \notin \Gamma(\overrightarrow{G})$ of all i and $(v_i, v_j) \in \Gamma(\overrightarrow{G})$ implies that $(v_j, v_i) \notin \Gamma(\overrightarrow{G})$. Hence the underlying undirected graph G of $\overrightarrow{G}$ is a simple graph. The *skew-adjacency matrix* of $\overrightarrow{G}$ is the $n \times n$ matrix $S(\overrightarrow{G}) = [s_{ij}]$, where $s_{ij} = 1$ whenever $(v_i, v_j) \in \Gamma(\overrightarrow{G})$, $s_{ij} = -1$ whenever $(v_j, v_i) \in \Gamma(\overrightarrow{G})$, and $s_{ij} = 0$ otherwise. If we denote *the skew energy* of $\overrightarrow{G}$ by $\varepsilon_s(\overrightarrow{G})$, then $\varepsilon_s(\overrightarrow{G}) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the all eigenvalues of $S(\overrightarrow{G})$. For more detail on the skew energy of oriented graphs, we refer to the survey paper by Li and Lian [12].

Let $P(\overrightarrow{G_1}, x) = \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(\overrightarrow{G_1})x^{n-2i}$ and $P(\overrightarrow{G_2}, x) = \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(\overrightarrow{G_2})x^{n-2i}$ be the skew-characteristic polynomials of two oriented graphs $\overrightarrow{G_1}$ and $\overrightarrow{G_2}$ of order n, respectively. If $a_{2i}(\overrightarrow{G_1}) \leq a_{2i}(\overrightarrow{G_1})$, for all $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$, then denote $\overrightarrow{G_1} \preceq \overrightarrow{G_2}$ implies that $\varepsilon_s(\overrightarrow{G_1}) \leq \varepsilon_s(\overrightarrow{G_2})$; If $\overrightarrow{G_1} \preceq \overrightarrow{G_2}$ and there exists at least one such i that $a_{2i}(\overrightarrow{G_1}) < a_{2i}(\overrightarrow{G_1})$, then denote $\overrightarrow{G_1} \prec \overrightarrow{G_2}$, which implies that $\varepsilon_s(\overrightarrow{G_1}) < \varepsilon_s(\overrightarrow{G_2})$.

An *unicyclic graph* is the connected graph with the same number of vertices and edges. In [7], Hou, Shen and Zhang determined the orientations of unicyclic graphs with extremal skew energy. Let $G(n, \ell)$ be the set of all connected unicyclic graphs on n vertices with girth ℓ. Denote, as usual, the n-vertex path and cycle by P_n and C_n, respectively. Let P_n^ℓ be the unicyclic graph obtained by connecting a vertex of C_ℓ with a terminal vertex of $P_{n-\ell}$. Let S_n^ℓ be the graph obtained by connecting $n - \ell$ pendant vertices to a vertex u_1 of the cycle C_ℓ (see Figure 1). We call the vertex u_1 a *bonding vertex* of S_n^ℓ.

Theorem 1.1 *Among all orientations of unicyclic graphs on n vertices, $\overrightarrow{S_n^3}$ has the minimal skew energy and $\overrightarrow{S_n^4}^-$ has the second minimal skew energy for $n \geq 6$; Both $\overrightarrow{S_5^3}$ and $\overrightarrow{S_5^4}^-$ have the minimal skew energy, $\overrightarrow{S_5^4}^+$ has the second minimal skew energy for $n = 5$; $\overrightarrow{C^4}^-$ has the minimal skew energy, $\overrightarrow{S_4^3}^-$ has the second minimal skew energy for $n = 4$.*

Energy sequencing problem is important. For example, the authors [3] investigated the unicyclic graphs with maximal energy. Later, Gutman et al. [6] studied the unicyclic graphs with studied the unicyclic graphs with the second-maximal and third-maximal energy.

In this paper, we are interested in studying the orientations of unicyclic graphs with third, fourth and fifth minimal skew energy. Let $H_n^{\ell,1}$ be a graph obtained from the graph S_{n-1}^{ℓ} and a new vertex v_2 by adding an edge u_2v_2 such that u_1, u_2 has a common vertex on the cycle C_ℓ, where u_1 is the bonding vertex of S_{n-1}^{ℓ} (see Figure 1). Let $H_n^{\ell,2}$ be a graph obtained from the graph S_{n-2}^{ℓ} and two new vertices v_2, v_3 by adding two edges u_2v_2, u_2v_3 such that u_1, u_2 has a common vertex on the cycle C_ℓ, where u_1 is the bonding vertex of S_{n-2}^{ℓ} (see Figure 1).

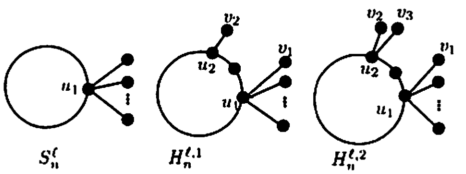

Figure 1. Graphs S_n^{ℓ}, $H_n^{\ell,1}$ and $H_n^{\ell,2}$.

Theorem 1.2 *Among all orientations of unicyclic graphs on n vertices, we have the following results.*

- *For $n \geq 10$, $\overrightarrow{S_n^3}$ has the minimal skew energy, $\overrightarrow{S_n^4}^-$ has the second minimal skew energy, $\overrightarrow{H_n^{3,1}}$ has the third minimal skew energy, $\overrightarrow{S_n^4}^+$ has the fourth minimal skew energy and $\overrightarrow{H_n^{3,2}}$ or $\overrightarrow{H_n^{4,1}}^-$ has the fifth minimal skew energy;*
- *For $7 \leq n \leq 9$, $\overrightarrow{S_n^3}$ has the minimal skew energy, $\overrightarrow{S_n^4}^-$ has the second minimal skew energy, $\overrightarrow{H_n^{3,1}}$ has the third minimal skew energy, and $\overrightarrow{H_n^{3,2}}$ or $\overrightarrow{H_n^{4,1}}^-$ has the fourth minimal skew energy;*
- *For $n = 6$, $\overrightarrow{S_6^3}$ has the minimal skew energy, $\overrightarrow{S_6^4}^-$ has the second minimal skew energy, and $\overrightarrow{H_6^{3,1}} = \overrightarrow{H_6^{3,2}}$ or $\overrightarrow{H_6^{4,1}}^-$ has the third minimal skew energy;*
- *For $n = 5$, both $\overrightarrow{S_5^3}$ and $\overrightarrow{S_5^4}^-$ have the minimal skew energy, $\overrightarrow{H_5^{3,1}}$ has the second minimal skew energy, $\overrightarrow{H_4}$ has the third minimal skew energy, and $\overrightarrow{S_5^4}^+$ has the fourth minimal skew energy;*
- *For $n = 4$, $\overrightarrow{C_4}^-$ has the minimal skew energy, and $\overrightarrow{S_4^3}^-$ has the second minimal skew energy.*

2 Preliminary

Let G be a graph. A *linear subgraph* L of G is a disjoint union of some edges and some cycles in G. A *k-matching* of G is a disjoint union of k-edges. If $2k$

is the order of G, then k-matching of G is called a *perfect matching* of G. The number of k-matching is denoted by $m(G, k)$.

Let $\overrightarrow{G}$ be an oriented unicyclic graph and C be an undirected even cycle of a graph G. Then C is said to be *evenly oriented* relative to $\overrightarrow{G}$ if it has an even number of edges oriented in clockwise direction (and now it also has an even number of edges oriented in anticlockwise direction, since C is an even cycle); otherwise C is *oddly oriented*. Denote by $\overrightarrow{G}^-$ ($\overrightarrow{G}^+$, resp.) the orientation of G in first (second, resp) case above.

We call a linear subgraph L of G *evenly linear* if L contains no odd cycle and denote by $L \in \varepsilon L_i(G)$ (or $L \in \varepsilon L_i$ for short) the set of all evenly linear subgraph of G with i vertices. For a linear subgraph $L \in \varepsilon L_i$ denote by $p_e^{(L)}$(resp., $p_o(L)$) the number of evenly (resp., oddly) oriented cycles in L relative to $\overrightarrow{G}$. Denote the characteristic polynomial of $S(\overrightarrow{G})$ by

$$P_s(\overrightarrow{G}, x) = det(xI - S(\overrightarrow{G})) = \sum_{i=1}^{n} a_i x^{n-i}$$

Then $(i) b_0 = 1$, $(ii) b_2$ is the number of edges of G, (iii) all $b_i \geq 0$ and $(iv) b_i = 0$ for all odd i since the determinant of every real skew symmetric matrix is non-negative and is 0 if its order is odd.

Lemma 2.1 [13] *Let G be a graph of order n and uv be an edge of G. Then*

$$m(G, k) = m(G - uv, k) + m(G - v - u, k - 1) \left(1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor\right)$$

Lemma 2.2 [14] *Let $a + b = c + d$ with $0 \leq a \leq b$, $0 \leq c \leq d$ and $a < c$.*

(1) If a is even, then $m(P_a \cup P_b, i) \geq m(P_c \cup P_d, i)$. Furthermore, there exists at least one index i such that the above inequality is strict.

(2) If a is odd, then $m(P_a \cup P_b, i) \leq m(P_c \cup P_d, i)$. Furthermore, there exists at least one index i such that the above inequality is strict.

Lemma 2.3 [9] *If H is a subgraph of G. Then $m(H, k) \leq m(G, k), k \geq 1$. Moreover, if H is a proper subgraph of G, then the inequality is strict.*

Lemma 2.4 [8] *Let $\overrightarrow{G}$ be an orientation of a graph G. Then*

$$a_i(\overrightarrow{G}) = \sum_{L \in \varepsilon L_i} (-2)^{p_e(L)} 2^{p_o(L)}$$

Where $p_e(L)$ is the number of evenly oriented cycles of L and $p_o(L)$ is the number of oddly oriented cycles of L relative to $\overrightarrow{G}$.

Lemma 2.5 [8] *Let $G \in G(n,l)$ and $\overrightarrow{G}$ be an orientation of G. Then we have:*

(1) If l is odd, the $a_{2i}(\overrightarrow{G}) = m(G,i)$

(2) If l is even and C_ℓ is oddly oriented, then $a_{2i}(\overrightarrow{G}) = m(G,i) + 2m(G - C_\ell, i - \frac{l}{2})$

(3) If l is even and C_ℓ is evenly oriented, then $a_{2i}(\overrightarrow{G}) = m(G,i) - 2m(G - C_\ell, i - \frac{l}{2})$

Let $P_n(a,b,c)$ be a tree of order n obtained by attaching three pendent paths of length a, b and c to an isolated vertex u where $a + b + c = n - 1$ (see Figure 2).

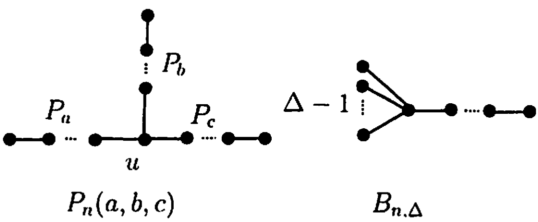

Figure 2. Graphs $P_n(a,b,c)$ and $B_{n,\Delta}$.

Lemma 2.6 [16] *Let $P_n(a,b,c)$ be a tree with diameter $n-2$. Then*

$$m(P_n(1,1,n-3),k) \leq m(P_n(i,1,n-i-2),k)$$

The *broom* $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n - \Delta - 1$ attached to an arbitrary pendent vertex of the star (see Figure 2).

Lemma 2.7 [16] *Let d be a positive integer more than one, and let T be a tree with n vertices having diameter at least d. Then $m(B_{n,n-d+1},k) \leq m(T,k)$.*

Lemma 2.8 [9] *Let $\overrightarrow{G}$ be an orientation of a unicyclic graph $G \in G(n,\ell), G \neq S_n^\ell$. If unique cycle C_ℓ in $\overrightarrow{G}$ and S_n^ℓ is the same orientation, then $\overrightarrow{G} \succ S_n^\ell$.*

Lemma 2.9 [9] *Let $n \geq \ell \geq 6$ or $n > \ell = 5$, then $\overrightarrow{S_n^4}^- \prec \overrightarrow{S_n^4}^+ \prec \overrightarrow{S_n^\ell}^- \prec \overrightarrow{S_n^\ell}^+$*

Lemma 2.10 [9] *Let $e = uv$ be an edge of G that is on no even cycle of G. Then*

$$b_{2k}(\overrightarrow{G}) = b_{2k}(\overrightarrow{G} - e) + b_{2k-2}(\overrightarrow{G} - u - v).$$

Furthermore, if $e = uv$ is a pendant edge with the pendant vertex v. Then

$$b_{2k}(\overrightarrow{G}) = b_{2k}(\overrightarrow{G} - v) + b_{2k-2}(\overrightarrow{G} - u - v).$$

Lemma 2.11 [2] *The skew-adjacency matrices of a graph G are all cospectral if and only if G has no even cycles.*

3 Proof of Theorem 1.2

We are now in a position to prove Theorem 1.2.

Lemma 3.1 *Let $\overrightarrow{G}$ be an orientation of an unicyclic graph $G \in G(n, \ell)$, and let $G \neq S_n^\ell$ and $G \neq H_n^{\ell,1}$. If the unique cycle C_ℓ is in $\overrightarrow{G}$, and S_n^ℓ and $H_n^{\ell,1}$ is the same orientation, then $\overrightarrow{G} \succ H_n^{\ell,1}$.*

Proof. We prove this statement by induction on n. Since $G \neq S_n^\ell$, it follows that $n \geq \ell + 2$. Suppose $n = \ell + 2$. One can see that $G = P_{\ell+2}$ or $G = H_1$ (see Figure 3). By Lemma 2.1, we have

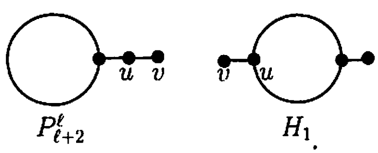

Figure 3. Graphs for Lemma 3.1

$$\begin{aligned} b_{2k}(\overrightarrow{P_{\ell+2}^\ell}) &= b_{2k}(\overrightarrow{P_{\ell+1}^\ell}) + b_{2k-2}(\overrightarrow{C_\ell}) \\ b_{2k}(\overrightarrow{H_1}) &= b_{2k}(\overrightarrow{P_{\ell+1}^\ell}) + b_{2k-2}(\overrightarrow{P_\ell(i, 1, \ell - i - 2)}) \end{aligned}$$

Observe that

$$b_{2k}(\overrightarrow{H_{\ell+2}^{\ell,1}}) = b_{2k}(\overrightarrow{P_{\ell+1}^\ell}) + b_{2k-2}(\overrightarrow{P_\ell(1, 1, \ell - 3)}).$$

If $k \leq \frac{\ell}{2}$, then it follows from Lemma 2.1 that

$$\begin{aligned} b_{2k-2}(\overrightarrow{C_\ell}) &= m(C_\ell, k - 1) \\ &= m(P_\ell, k - 1) + m(P_{\ell-2}, k - 2) \\ b_{2k-2}(\overrightarrow{P_\ell(1, 1, \ell - 3)}) &= m(P_\ell(1, 1, \ell - 3), k - 1) \\ &= m(P_{\ell-1}, k - 1) + m(P_{\ell-3}, k - 2) \end{aligned}$$

For $k \geq \frac{\ell}{2}$, one can see that $b_{2k-2}(\overrightarrow{P_\ell(1, 1, \ell - 3)}) = 0$.

By Lemmas 2.1 and 2.6, we have

$$m(P_\ell(1,1,\ell-3),k-1) \leq m(T,k-1)$$
$$m(P_\ell(1,1,\ell-3),k-1) \leq m(C_\ell,k-1)$$

The result holds immediately for $n=\ell+2$.

Suppose that for $G \in G(n',\ell)$, $\overrightarrow{G} \succ \overrightarrow{H_{n'}^{\ell,1}}$ for all $n' < n$. Since $\overrightarrow{G}$ is a unicyclic digraph, there is at least a pendant edge uv with pendant vertex v in $\overrightarrow{G}$. First, we consider the case $G-v \neq S_{n-1}^{\ell}$. Let u_1 be the vertex of $\overrightarrow{H_n^{\ell,1}}$ with degree $n-\ell+1$, and let v_1 be a pendent vertex adjacent to u_1. By Lemma 2.10, we have

$$\begin{aligned} b_{2k}(\overrightarrow{G}) &= b_{2k}(\overrightarrow{G}-v)+b_{2k-2}(\overrightarrow{G}-v-u) \\ b_{2k}(\overrightarrow{H_n^{\ell,1}}) &= b_{2k}(\overrightarrow{H_{n-1}^{\ell,1}}-v_1)+b_{2k-2}(\overrightarrow{P_l(1,1,\ell-3)}) \end{aligned}$$

By induction assumption, it suffices to prove that

$$b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{P_l(1,1,\ell-3)}), \quad (1 \leq k \leq \lfloor n/2 \rfloor)$$

Observe that $b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{P_\ell(1,1,\ell-3)}) = 0$ for $k > \lfloor \frac{\ell}{2} \rfloor$. So we assume that $0 \leq k \leq \lfloor \frac{\ell}{2} \rfloor$. Note that $G-v \neq S_{n-1}^{\ell}$. Then the order of the graph $G-v-u$ is n_1 $(n_1 \geq \ell)$, and the size of the graph $G-v-u$ is at least ℓ, and $G-v-u$ contains a path of length $\ell-2$. By Lemmas 2.3 and 2.6, we have

$$b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{P_\ell(1,1,\ell-3)}).$$

Next, we consider the case $G-v = S_{n-1}^{\ell}$. Then $G=H_2$ or $G=H_3$ (see Figure 4).

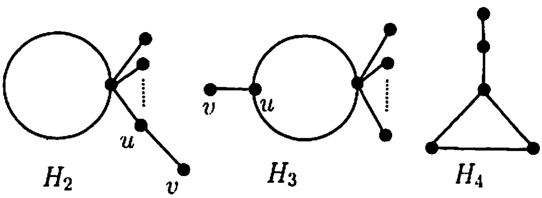

Figure 4. Graphs for Lemma 3.1.

If $G=H_2$, then $H_2-v-u=S_{n-2}^{\ell}$, as desired. Furthermore, by Lemma 2.6, we have

$$\begin{aligned} b_{2k}(\overrightarrow{H_2}) &= b_{2k}(\overrightarrow{S_{n-1}^{\ell}})+b_{2k}(\overrightarrow{S_{n-2}^{\ell}}) \\ b_{2k}(\overrightarrow{H_n^{\ell,1}}) &= b_{2k}(\overrightarrow{S_{n-1}^{\ell}})+b_{2k}(\overrightarrow{B_{n-2,n-\ell+1}}) \end{aligned}$$

Because $B_{n-2,n-\ell}$ is a subgraph of S^{ℓ}_{n-2}, $P_{\ell-3}$ is a subgraph of $B_{n-4,n-\ell}$. By Lemma 2.3, we have

$$\begin{aligned} m(B_{n-2,n-\ell},k) &= m(B_{n-3,n-\ell},k) + m(B_{n-4,n-\ell},k-1) \\ m(B_{n-2,n-\ell+1},k) &= m(B_{n-3,n-\ell},k) + m(P_{\ell-3},k-1) \end{aligned}$$

Then $\overrightarrow{H_2} \succ \overrightarrow{H^{\ell,1}_n}$.

If $G = H_3$, then the order of the graph $G - v - u$ is n_1 $(n_1 \geq \ell)$, and the size of the graph $G - v - u$ is at least ℓ, and $G - v - u$ contains a path of length $\ell - 2$.

By Lemmas 2.3 and 2.6, we have

$$b_{2k-2}(\overrightarrow{G} - v - u) \geq b_{2k-2}(\overrightarrow{P_\ell(1,1,\ell-3)}).$$

∎

Lemma 3.2 *Let n be an integer with $n \geq 6$. Then* $\overrightarrow{S^3_n} \prec \overrightarrow{S^4_n}^- \prec \overrightarrow{H^{3,1}_n} \prec \overrightarrow{S^4_n}^+ \prec \overrightarrow{S^5_n}$.

Proof. By Lemma 2.4, the characteristic polynomials of $\overrightarrow{S^3_n}, \overrightarrow{S^4_n}^-, \overrightarrow{H^{3,1}_n}, \overrightarrow{S^4_n}^+, \overrightarrow{S^5_n}$ are shown as follows.

$$\begin{aligned} P(\overrightarrow{S^3_n},x) &= x^{n-4}(x^4 + nx^2 + n - 3) \\ P(\overrightarrow{S^4_n}^-,x) &= x^{n-4}(x^4 + nx^2 + 2n - 8) \\ P(\overrightarrow{H^{3,1}_n},x) &= x^{n-4}(x^4 + nx^2 + 2n - 7) \\ P(\overrightarrow{S^4_n}^+,x) &= x^{n-4}(x^4 + nx^2 + 2n - 4) \\ P(\overrightarrow{S^5_n},x) &= x^{n-6}(x^6 + nx^4 + (3n-10)x^2 + n - 5) \end{aligned}$$

One can easily see that $\overrightarrow{S^3_n} \prec \overrightarrow{S^4_n}^- \prec \overrightarrow{H^{3,1}_n} \prec \overrightarrow{S^4_n}^+ \prec \overrightarrow{S^5_n}$. ∎

Lemma 3.3 *Let n be an integer with $6 \leq n \leq 9$. Then* $\overrightarrow{H^{3,1}_n} \preceq \overrightarrow{H^{4,1}_n}^- \preceq \overrightarrow{S^4_n}^+ \prec \overrightarrow{S^5_n}$.

Proof. By Lemma 2.4, the characteristic polynomials of $\overrightarrow{H^{3,1}_n}, \overrightarrow{N^{4,1}_n}^-, \overrightarrow{S^4_n}^+, \overrightarrow{S^5_n}$ are shown as follows.

$$\begin{aligned} P(\overrightarrow{H^{3,1}_n},x) &= x^{n-4}(x^4 + nx^2 + 2n - 7) \\ P(\overrightarrow{H^{4,1}_n}^-,x) &= x^{n-4}(x^4 + nx^2 + 3n - 13) \\ P(\overrightarrow{S^4_n}^+,x) &= x^{n-4}(x^4 + nx^2 + 2n - 4) \\ P(\overrightarrow{S^5_n},x) &= x^{n-6}(x^6 + nx^4 + (3n-10)x^2 + n - 5) \end{aligned}$$

One can see that $\overrightarrow{H_n^{3,1}} \prec \overrightarrow{H_n^{4,1}}^- \prec \overrightarrow{S_n^4}^+$, as desired. ∎

Corollary 3.4 *Let n be an integer with $n \geq 10$. Then $\overrightarrow{H_n^{3,1}} \prec \overrightarrow{S_n^4}^+ \prec \overrightarrow{H_n^{4,1}}^- \prec \overrightarrow{S_n^5}$.*

In [9], Hou, Shen and Zhang studied the oriented unicyclic graphs with extremal skew energy, and claimed to show both $\overrightarrow{S_5^3}$ and $\overrightarrow{S_5^4}^-$ have the minimal skew energy, and $\overrightarrow{S_5^4}^+$ has the second minimal skew energy for $n = 5$. But, we prove that $\overrightarrow{H_5^{3,1}}$ has the second minimal skew energy.

Lemma 3.5 *Let n be an integer with $n = 5$. Then $\overrightarrow{S_5^3} = \overrightarrow{S_5^4}^- \prec \overrightarrow{H_5^{3,1}} \prec \overrightarrow{H_4} \prec \overrightarrow{S_5^4}^+$.*

Proof. By Lemma 2.4, the characteristic polynomials of $\overrightarrow{S_5^3}, \overrightarrow{S_5^4}^-, \overrightarrow{H_5^{3,1}}, \overrightarrow{H_4}, \overrightarrow{S_5^4}^+$ are shown as follows.

$$
\begin{aligned}
P(\overrightarrow{S_5^3}, x) &= x^{n-4}(x^4 + 5x^2 + 2) \\
P(\overrightarrow{S_5^4}^-, x) &= x^{n-4}(x^4 + 5x^2 + 2) \\
P(\overrightarrow{H_5^{3,1}}, x) &= x^{n-4}(x^4 + 5x^2 + 3) \\
P(\overrightarrow{H_4}, x) &= x^{n-4}(x^4 + 5x^2 + 4) \\
P(\overrightarrow{S_5^4}^+, x) &= x^{n-4}(x^4 + 5x^2 + 6)
\end{aligned}
$$

One can see that $\overrightarrow{S_5^3} = \overrightarrow{S_5^4}^- \prec \overrightarrow{H_5^{3,1}} \prec \overrightarrow{H_4} \prec \overrightarrow{S_5^4}^+$, as desired. ∎

Lemma 3.6 *Let $\overrightarrow{G}$ be an orientation of a unicyclic graph $G \in G(n,3)$, where $n \geq 6, G \neq S_n^3, G \neq H_n^{3,1}, G \neq H_n^{3,2}, S_n^3 \neq H_n^{3,2}$. Then $\overrightarrow{G} \succ \overrightarrow{H_n^{3,2}} \succeq \overrightarrow{N_n^{3,1}}$.*

Proof. We prove the statement by induction on n. Since $G \neq S_n^3, S_n^3 \neq H_n^{3,2}$, it follows that $n \geq 6$. For $n = 6$, by Lemma 2.8, the result holds immediately for $n = 6$. Suppose that $\overrightarrow{G} \succ \overrightarrow{H_{n'}^{\ell,1}}$ for all $n' < n$. Since $\overrightarrow{G}$ is a unicyclic digraph, there is at least a pendant edge uv with pendant vertex v in $\overrightarrow{G}$.

First, we consider the case $G - v \neq S_{n-1}^3, G - v \neq H_n^{3,1}$. Let u_1 be the vertex of $\overrightarrow{H_n^{\ell,2}}$ with degree $n - \ell$, and v_1 is a pendent vertex adjacent to u_1. From Lemma 2.10, we get

$$
\begin{aligned}
b_{2k}(\overrightarrow{G}) &= b_{2k}(\overrightarrow{G} - v) + b_{2k-2}(\overrightarrow{G} - v - u) \\
b_{2k}(\overrightarrow{H_n^{\ell,2}}) &= b_{2k}(\overrightarrow{H_{n-1}^{\ell,2}} - v_1) + b_{2k-2}(\overrightarrow{S_4})
\end{aligned}
$$

By induction assumption, it suffices to prove that

$$b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{S_4}), \quad (1 \leq k \leq \lfloor n/2 \rfloor).$$

For $k > 1$, one can see that $b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{S_4}) = 0$. So we now suppose $0 \leq k \leq 1$. Note that $G - v \neq S_{n-1}^3, G - v \neq H_n^{3,1}$.

Then the order of the graph $G - v - u$ is n_1 $(n_1 \geq 4)$, and the size of the graph $G - v - u$ is at least 3. By Lemmas 2.6, Lemma 2.3, we have

$$b_{2k-2}(\overrightarrow{G}-v-u) \geq b_{2k-2}(\overrightarrow{S_4}).$$

Since $G - v = S_{n-1}^3$ or $G - v = H_n^{3,1}$, it follows that $G \in \{H_5, H_6, H_7, H_8\}$ (see Figure 5).

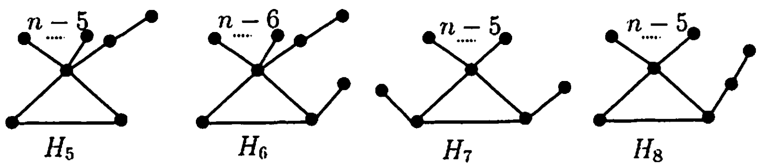

Figure 5. Graphs for Lemma 3.6.

By Lemma 2.4, the characteristic polynomials of $\overrightarrow{H_5}, \overrightarrow{H_6}, \overrightarrow{H_7}$ and $\overrightarrow{H_8}$ are shown as follows.

$$\begin{aligned}
P(\overrightarrow{H_n^{3,1}}, x) &= x^{n-4}(x^4 + nx^2 + 2n - 7) \\
P(\overrightarrow{H_n^{3,2}}, x) &= x^{n-4}(x^4 + nx^2 + 3n - 13) \\
P(\overrightarrow{H_5}, x) &= x^{n-6}(x^6 + nx^4 + (2n-6)x^2 + n - 5) \\
P(\overrightarrow{H_6}, x) &= x^{n-6}(x^6 + nx^4 + (3n-11)x^2 + 2n - 11) \\
P(\overrightarrow{H_7}, x) &= x^{n-6}(x^6 + nx^4 + (3n-12)x^2 + n - 5) \\
P(\overrightarrow{H_8}, x) &= x^{n-6}(x^6 + nx^4 + (3n-11)x^2 + n - 5)
\end{aligned}$$

Thus

$$\begin{aligned}
&\overrightarrow{H_6} \succ \overrightarrow{H_7^{3,2}} \succ \overrightarrow{H_7^{3,1}} \\
&\overrightarrow{H_7} \succ \overrightarrow{H_7^{3,2}} \succ \overrightarrow{H_7^{3,1}} \\
&\overrightarrow{H_8} \succ \overrightarrow{H_7^{3,2}} \succ \overrightarrow{H_7^{3,1}}.
\end{aligned}$$

For $G = H_5$, we have

$$\begin{aligned}
P(\overrightarrow{H_n^{3,2}}, x) &= x^{n-4}(x^4 + nx^2 + 3n - 13) \quad (1) \\
P(\overrightarrow{H_5}, x) &= x^{n-6}(x^6 + nx^4 + (2n-6)x^2 + n - 5) \quad (2)
\end{aligned}$$

For (1), we let $x^2 = y$; for (2), we let $x^2 = z$. Then $f(y) = y^2 + ny + 3n - 13$ and $g(z) = z^3 + nz^2 + (2n-6)z + n - 5 = (z+1)(z^2 + (n-1)z + n - 5)$. Observe that

$$\begin{aligned} y_1 + y_2 &= -n; \\ y_1 y_2 &= 3n - 13; \\ z_1 + z_2 + z_3 &= -n; \\ z_1 z_2 + z_2 z_3 + z_1 z_3 &= 2n - 6; \\ z_1 z_2 z_3 &= -n + 5. \end{aligned}$$

Without loss of generality, let $z_1 < z_2 < z_3$. Clearly, $n \geq 6$. Set $h(z) = (z^2 + (n-1)z + n - 5)$. One can see that $h(-1) < 0, h(0) > 0, h(-n+1) < 0$ and $h(-n+2) > 0$

By Hilbert's Nullstellensatz, we have $-n+1 < z_1 < -n+2$, $z_2 = -1$ and $-1 < z_3 < 0$. Therefore, $\sqrt{-z_1} + \sqrt{-z_2} + \sqrt{-z_3} > \sqrt{-z_1} > \sqrt{n-2} > \sqrt{n-5}$.

$$\begin{aligned} &(\sqrt{z_1 z_2} + \sqrt{z_1 z_3} + \sqrt{z_2 z_3})^2 \\ = \; &(z_1 z_2 + z_1 z_3 + z_2 z_3) + 2z_1\sqrt{z_2 z_3} + z_2\sqrt{z_1 z_3} + z_3\sqrt{z_1 z_2} \\ = \; &2n - 6 + 2\sqrt{-z_1 z_2 z_3}(\sqrt{-z_1} + \sqrt{-z_2} + \sqrt{-z_3}) \\ > \; &2n - 6 + 2\sqrt{n-5}\sqrt{n-5} = 4n - 16 > (\sqrt{y_1 y_2})^2 \end{aligned}$$

From the above, we have $\sqrt{z_1 z_2} + \sqrt{z_1 z_3} + \sqrt{z_2 z_3} > \sqrt{y_1 y_2}$.
Therefore,

$$\begin{aligned} ((\sqrt{z_1} + \sqrt{z_2} + \sqrt{z_3})/i)^2 &= (-z_1 - z_2 - z_3) + 2(\sqrt{z_1 z_2} + \sqrt{z_1 z_3} + \sqrt{z_2 z_3}) \\ &= n + 2(\sqrt{z_1 z_2} + \sqrt{z_1 z_3} + \sqrt{z_2 z_3}) \\ &> n + 2\sqrt{y_1 y_2} = ((\sqrt{y_1} + \sqrt{y_2})/i)^2 \end{aligned}$$

Therefore, $(\sqrt{z_1} + \sqrt{z_2} + \sqrt{z_3})/i > (\sqrt{y_1} + \sqrt{y_2})/i$ and hence $\varepsilon_s(H_5) = (\sqrt{z_1} + \sqrt{z_2} + \sqrt{z_3})/i > (\sqrt{y_1} + \sqrt{y_2})/i = \varepsilon_s(H_n^{3,2})$. ∎

By Lemmas 3.1 and 3.6, one can see that Theorem 1.2 holds.

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