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Extremal Unicyclic Graphs with Respect to Merrifield-Simmons Index *

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Abstract

We obtain smallest, second- and third- smallest value of Merrifield-Simmons index(total number of independent subsets) for unicyclic graphs with n vertices and girth $k(3 \leq k < n)$.

1 Introduction

All graphs considered here are finite, simple and undirected. Undefined notations and terminology will conform to those in [1].

The Merrifield-Simmons-, or σ-index $\sigma(G)$ of a (molecular) graph G is a prominent example of topological index which is of interest in combinatorial chemistry. It is defined as the number of independent vertex subsets of a graph. σ-index was introduced by Merrifield and Simmons [8] in 1989. For detailed information on the chemical application, we refer to [3,8] and the references therein.

For a graph G, we denote by $V(G)$ the vertex set of G and by $E(G)$ the edge set of G. For two graphs G and H, we denote by $G \cup H$ the disjoint union of G and H and mH the disjoint union of m copies of H. The girth of G is the length of a shortest cycle in G, or ∞ if it has no cycle. We denote by P_n, S_n and C_n the path, the star, the circle of n vertices, respectively. A graph is called unicyclic if it is connected and contains exactly one cycle. $C(n,k)$ denotes unicyclic graphs set of order n and girth $k(3 \leq k < n)$. $C_{k,n-k}$ denotes a graph obtained by identifying an endvertex of P_{n-k+1} with a vertex of C_k. For a vertex v of G, we denote $N_G[v] = \{v\} \cup \{u \mid uv \in E(G)\}$. If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E^{'} \subseteq E(G)$, we denote by $G - E^{'}$ the subgraph of G obtained by deleting the edges of $E^{'}$. If $W = \{v\}$ and $E^{'} = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. If a graph G has components $G_1, G_2, \cdots, G_t$, then G is denoted by $\bigcup_{i=1}^{t} G_i$. We denote the sequence

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of Fibonacci numbers by F_n, i.e., $F_0 = 0,\ F_1 = 1$ and $F_{n+1} = F_n + F_{n-1}$. Analogously, the Lucas numbers are denoted by L_n, i.e., $L_0 = 2, L_1 = 1, L_{n+1} = L_n + L_{n-1}$. Furthermore, $F_nF_m = \frac{1}{5}[L_{m+n} - (-1)^n L_{m-n}]$ and $F_{n+m} = F_{n-1}F_m + F_nF_{m+1}$.

Several papers deal with the characterization of the extremal graphs with respect to σ-index in several given classes-usually, trees and certain structures involving pentagonal and hexagonal cycles are of major interest [2,4,5,6,7,9,10].

Zhao and Li characterized the trees of second- and third-smallest σ-index in [5]. Wagner showed that a tree T with $\sigma(T) < 18F_{n-5} + 21F_{n-6}$ had at most three leaves in [4]. Pedersen and Vestergaard obtained the smallest value of σ-index among all unicyclic graphs of order n in [12]. In this paper, we obtain smallest, second- and third-smallest value of σ-index about unicyclic graphs with n vertices and girth $k(3 \le k < n)$.

Let T be a tree with $n(T)$ vertices, From [11],we can find

Lemma 1. Let T be a tree with $n(T) = n$, then $F_{n+2} \le \sigma(T) \le 2^{n-1} + 1$ and $\sigma(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$ and $\sigma(T) = F_{n+2}$ if and only if $T \cong P_n$.

The graphs shown in Figure 1 are frequently used throughout the paper.

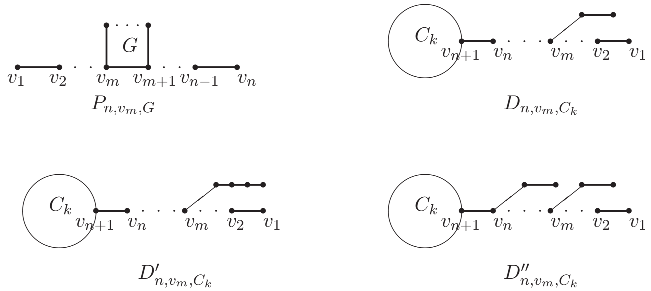


Figure 1. Graphs $P_{n,v_m,G}$, D_{n,v_m,C_k}, D'_{n,v_m,C_k} and D''_{n,v_m,C_k}

2 Preliminaries

Lemma 2.([3]) Let G be a graph with k components $G_1, G_2, \ldots, G_k$. Then $\sigma(G) = \prod_{i=1}^{k} \sigma(G_i)$.

Lemma 3.([3]) Let G be a graph and uv be an edge of G and v be a vertex of G. Then

(i) $\sigma(G) = \sigma(G - uv) - \sigma(G - (N_G[u] \cup N_G[v]))$;

(ii) $\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v])$.

When v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $\sigma(G) = \sigma(G - v) + \sigma(G - \{u, v\})$.

Lemma 4.([5]) Let $G \not\cong P_1$ be a connected graph and choose $v \in V(G)$. Denote by $P'_{n,v_k,G}$ the graph obtained by identifying v with the vertex v_k of a path $v_1, v_2, \cdots, v_n$. Now, let $n = 4m + i, i \in \{1, 2, 3, 4\}, m \geq 2$. Then

$$\sigma(P'_{n,v_2,G}) > \sigma(P'_{n,v_4,G}) > \cdots > \sigma(P'_{n,v_{2m+2\rho},G}) >$$
$$\sigma(P'_{n,v_{2m+1},G}) > \cdots \sigma(P'_{n,v_3,G}) > \sigma(P'_{n,v_1,G}),$$

where $\rho = 0$ if $i = 1$ or 2 and $\rho = 1$ if $i = 3$ or 4.

Analogous to Lemma 4, we have the following Lemma 5:

Lemma 5. Let $G \not\cong P_1, P_2$ be a connected graph and choose $e \in E(G)$. $P_{n,v_m,G}$ then denotes the graph that results from identifying e with the edge $v_m v_{m+1}$ of a path $v_1, v_2, \cdots, v_n$. If $n = 4m + i, i \in \{2, 3, 4, 5\}, m \geq 0, G - N_G[v_m] \cong G - N_G[v_{m+1}]$. Then

$$\sigma(P_{n,v_2,G}) > \sigma(P_{n,v_4,G}) > \cdots > \sigma(P_{n,v_{2m+2l},G}) >$$
$$\sigma(P_{n,v_{2m+1},G}) > \cdots \sigma(P_{n,v_3,G}) > \sigma(P_{n,v_1,G}),$$

where $l = \lfloor \frac{i-2}{2} \rfloor$.

Proof. Set $A = \sigma(G - \{v_m, v_{m+1}\}), B = \sigma(G - N_G[v_m]), C = \sigma(G - N_G[v_{m+1}])$. Clearly, each independent subset of $(G - N_G[v_m])$, $(G - N_G[v_{m+1}])$ is also a independent subset $(G - \{v_m, v_{m+1}\})$, but not vice versa, so $A > B, A > C$. A independent subset of $P_{n,v_m,G}$ has to satisfy exactly one of the following conditions:

• it contains neither vertex v_m nor v_{m+1}. If these vertices are removed, three subgraphs remain: $G - \{v_m, v_{m+1}\}$ and two paths with $m - 1$ resp. $n - m - 1$ vertices. Therefore, there are $\sigma(G - \{v_m, v_{m+1}\})\sigma(P_{m-1})\sigma(P_{n-m-1}) = AF_{m+1}F_{n-m+1}$ such independent subsets.

• it contains vertex v_m. Then it contains no other vertex adjacent to v_m. Again, three subgraphs remain: $G - N_G[v_m]$ and two paths with $m-2$ resp. $n-m-1$ vertices. Therefore, there are $\sigma(G - N_G[v_m])\sigma(P_{m-2})\sigma(P_{n-m-1}) = BF_m F_{n-m+1}$ such independent subsets.

• it contains vertex v_{m+1}. Analogously, there are $CF_{m+1}F_{n-m}$ such independent subsets.

So, we have

$$\sigma(G) = AF_{m+1}F_{n-m+1} + BF_m F_{n-m+1} + CF_{m+1}F_{n-m}$$
$$= \frac{A}{5}[L_{n+2} - (-1)^{m+1}L_{n-2m}] + \frac{B}{5}[L_{n+1} - (-1)^m L_{n-2m+1}] + \frac{C}{5}[L_{n+1} - (-1)^{m+1}L_{n-2m-1}]$$
$$= \frac{1}{5}[(AL_{n+2} + BL_{n+1} + CL_{n+1}) - (-1)^{m+1}(AL_{n-2m} - BL_{n-2m+1} + CL_{n-2m-1})]$$
$$= \frac{1}{5}[(AL_{n+2} + BL_{n+1} + CL_{n+1}) - (-1)^{m+1}((A - B)L_{n-2m} + (C - B)L_{n-2m-1})]$$

The only term depending on m is $\frac{1}{5}[-(-1)^{m+1}((A - B)L_{n-2m} + (C - B)L_{n-2m-1})]$.

We have $B = C$ for $G - N_G[v_m] \cong G - N_G[v_{m+1}]$. We may assume $m \leq \frac{n}{2}$, since

$P_{n,v_m,G} \cong P_{n,v_{n-m},G}$. So $(A-B)L_{n-2m}$ is always positive and monotonically decreasing

in k. The result follows immediately.□

Especially, when $G \cong C_k$, we have

let $n = 4m + i, i \in \{2, 3, 4, 5\}, m \geq 0$. Then

$$\begin{aligned}\sigma(P_{n,v_2,C_k}) > \sigma(P_{n,v_4,C_k}) > \cdots > \sigma(P_{n,v_{2m+2l},C_k}) > \\ \sigma(P_{n,v_{2m+1},C_k}) > \cdots \sigma(P_{n,v_3,C_k}) > \sigma(P_{n,v_1,C_k}),\end{aligned}$$

where $l = \lfloor \frac{i-2}{2} \rfloor$.

The following Lemma 6 results from Lemma 2, 3.

Lemma 6.
(i) if $j = 2i + 1,\ i = 0, 1, 2, \cdots, \lfloor \frac{n-k-4}{4} \rfloor,\ k \geq 3$, then

$\sigma(D_{n-k-2,v_j,C_k}) < \sigma(D_{n-k-2,v_{n-k-1-j},C_k})$;

(ii) if $l = 2m + 1,\ m = 1, 2, \cdots, \lfloor \frac{n-k-4}{4} \rfloor,\ k \geq 3$, then

$\sigma(D_{n-k-2,v_{n+1-k-l},C_k}) < \sigma(D_{n-k-2,v_l,C_k})$;

Proof. (i) if $j = 2i + 1,\ i = 1, 2, \cdots, \lfloor \frac{n-k-4}{4} \rfloor,\ k \geq 3$, then

$$\begin{aligned}
& \sigma(D_{n-k-2,v_j,C_k}) - \sigma(D_{n-k-2,v_{n-k-1-j},C_k}) \\
= \ & \sigma(P_2 \cup C_{k,n-k-2}) - \sigma(P_{j-2} \cup C_{k,n-k-3-j}) \\
& -[\sigma(P_2 \cup C_{k,n-k-2}) - \sigma(P_{n-k-3-j} \cup C_{k,j-2})] \\
= \ & F_{n-k-1-j}(F_{k-1}F_{j-1} + F_{k+1}F_j) - F_j(F_{k-1}F_{n-k-2-j} + F_{k+1}F_{n-k-1-j}) \\
= \ & F_{k-1}F_{j-1}F_{n-k-1-j} - F_{k-1}F_jF_{n-k-2-j} \\
= \ & F_{k-1}(F_{j-1}F_{n-k-1-j} - F_jF_{n-k-2-j}) \\
= \ & F_{k-1}[\frac{1}{5}(L_{n-k-2} - (-1)^{j-1}L_{n-k-2j}) - \frac{1}{5}(L_{n-k-2} - (-1)^jL_{n-k-2-2j})] \\
= \ & \frac{(-1)^jF_{k-1}}{5}(L_{n-k-2j} + L_{n-k-2-2j}) \\
< \ & 0
\end{aligned}$$

$i = 0$ also satisfies the above equality by direct calculation.

(ii) if $l = 2m + 1,\ m = 1, 2, \cdots, \lfloor \frac{n-k-4}{4} \rfloor,\ k \geq 3$, then

$$\begin{aligned}
& \sigma(D_{n-k-2,v_l,C_k}) - \sigma(D_{n-k-2,v_{n+1-k-l},C_k}) \\
= \ & \sigma(P_{n-k-1-l} \cup C_{k,l-4}) - \sigma(P_{l-2} \cup C_{k,n-k-3-l}) \\
= \ & F_{n-k+1-l}(F_{k-1}F_{l-3} + F_{k+1}F_{l-2}) - F_l(F_{k-1}F_{n-k-2-l} + F_{k+1}F_{n-k-1-l}) \\
= \ & F_{n-k+1-l}(F_{k-1}F_l + F_{k-2}F_{l-2}) - F_l(F_{k-1}F_{n-k+1-l} + F_{k-2}F_{n-k-1-l}) \\
= \ & F_{k-2}(F_{l-2}F_{n-k+1-l} - F_lF_{n-k-1-l})
\end{aligned}$$

$$
\begin{aligned}
&= \frac{F_{k-2}}{5}[-(-1)^{l-2}L_{n-k+3-2l} + (-1)^l L_{n-k-1-2l}] \\
&= \frac{-(-1)^l F_{k-2}}{5}(L_{n-k+3-2l} - L_{n-k-1-2l}) \\
&= \frac{-(-1)^l F_{k-2}}{5}(L_{n-k+2-2l} + L_{n-k-2l}) \\
&> 0
\end{aligned}
$$

which completes the proof of Lemma 6. □

Lemma 7 If $t = 2r+1$, $r = 0,1,2,\cdots,\lfloor\frac{n-k-4}{4}\rfloor, k \geq 3, 1 \leq s \leq n-k-1$, $s \neq t, s \neq n-k-1-t$, and $s \neq \lfloor\frac{n-k}{2}\rfloor$, then

$$
\begin{aligned}
&\sigma(D_{n-k-2,v_1,C_k}) < \sigma(D_{n-k-2,v_{n-k-2},C_k}) < \sigma(D_{n-k-2,v_3,C_k}) < \sigma(D_{n-k-2,v_{n-k-4},C_k}) \\
&\quad < \cdots < \sigma(D_{n-k-2,v_t,C_k}) < \sigma(D_{n-k-2,v_{n-k-1-t},C_k}) < \sigma(D_{n-k-2,v_s,C_k}).
\end{aligned}
$$

and $\sigma(D_{n-k-2,v_3,C_k}) \leq \sigma(D_{n-k-2,v_{\lfloor\frac{n-k}{2}\rfloor},C_k})$ with equality if and only if $\lfloor\frac{n-k}{2}\rfloor = 3$. Especially, $\sigma(D_{n-5,v_i,C_3}) \leq \sigma(P_{n-1,v_3,C_3})$ with equality if and only if $n = 2i+3$.

Proof. By Lemma 2, 3, 6, we shall distinguish the following cases:

Case 1 if $1 \leq i \leq \lfloor\frac{n-k-2}{2}\rfloor, k \geq 3$, then

$$
\begin{aligned}
& \sigma(D_{n-k-2,v_i,C_k}) \\
=\ & \sigma(P_2 \cup C_{k,n-k-2}) - \sigma(P_{i-2} \cup C_{k,n-k-3-i}) \\
=\ & 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - F_i(F_{k-1}F_{n-k-2-i} + F_{k+1}F_{n-k-1-i}) \\
=\ & 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{F_{k-1}}{5}[L_{n-k-2} - (-1)^i L_{n-k-2-2i}] \\
& -\frac{F_{k+1}}{5}[L_{n-k-1} - (-1)^i L_{n-k-1-2i}] \\
=\ & 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{1}{5}(F_{k-1}L_{n-k-2} + F_{k+1}L_{n-k-1}) \\
& +\frac{(-1)^i}{5}(F_{k-1}L_{n-k-2-2i} + F_{k+1}L_{n-k-1-2i})
\end{aligned}
$$

The only term depending on i is $\frac{(-1)^i}{5}(F_{k-1}L_{n-k-2-2i} + F_{k+1}L_{n-k-1-2i})$. For $1 \leq i \leq \lfloor\frac{n-k-2}{2}\rfloor$($i = 1, 2$ also satisfies the above equality by direct calculation), $F_{k-1}L_{n-k-2-2i} + F_{k+1}L_{n-k-1-2i}$ is always positive and monotonically decreasing in i.

Case 2 if $\lceil\frac{n-k+1}{2}\rceil \leq i \leq n-k-1, k \geq 3$, then

$$
\begin{aligned}
& \sigma(D_{n-k-2,v_i,C_k}) \\
=\ & 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{F_{k-1}}{5}[L_{n-k-2} - (-1)^{n-k-2-i}L_{2i+k+2-n}] \\
& -\frac{F_{k+1}}{5}[L_{n-k-1} - (-1)^{n-k-1-i}L_{2i+k+1-n}]
\end{aligned}
$$

$$
\begin{aligned}
&= 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{1}{5}(F_{k-1}L_{n-k-2} + F_{k+1}L_{n-k-1}) \\
&\quad + \frac{(-1)^{n-k-2-i}}{5}(F_{k-1}L_{2i+k+2-n} - F_{k+1}L_{2i+k+1-n}) \\
&= 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{1}{5}(F_{k-1}L_{n-k-2} + F_{k+1}L_{n-k-1}) \\
&\quad + \frac{(-1)^{n-k-2-i}}{5}(-F_kL_{2i+k+1-n} + F_{k-1}L_{2i+k-n}) \\
&= 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{1}{5}(F_{k-1}L_{n-k-2} + F_{k+1}L_{n-k-1}) \\
&\quad + \frac{(-1)^{n-k-2-i}}{5}(-F_{k-2}L_{2i+k+1-n} - F_{k-1}L_{2i+k-1-n}) \\
&= 3(F_{k-1}F_{n-k-1} + F_{k+1}F_{n-k}) - \frac{1}{5}(F_{k-1}L_{n-k-2} + F_{k+1}L_{n-k-1}) \\
&\quad - \frac{(-1)^{n-k-2-i}}{5}(F_{k-2}L_{2i+k+1-n} + F_{k-1}L_{2i+k-1-n})
\end{aligned}
$$

The only term depending on i is $-\frac{(-1)^{n-k-2-i}}{5}(F_{k-2}L_{2i+k+1-n} + F_{k-1}L_{2i+k-1-n})$. For $\lceil \frac{n-k+1}{2} \rceil \le i \le n-k-1$ ($i = n-k-2, n-k-1$ also satisfies the above equality by direct calculation), $F_{k-2}L_{2i+k+1-n} + F_{k-1}L_{2i+k-1-n}$ is always positive and monotonically increasing in i.

Case 3 $i = \lfloor \frac{n-k}{2} \rfloor, k \ge 3$. By direct calculation we have $\sigma(D_{n-k-2,v_3,C_k}) \le \sigma(D_{n-k-2,v_{\lfloor \frac{n-k}{2} \rfloor},C_k})$ with equality if and only if $\lfloor \frac{n-k}{2} \rfloor = 3$

Especially, if $k = 3$ we analogously have $\sigma(D_{n-5,v_i,C_3}) \le \sigma(P_{n-1,v_3,C_3})$ with equality if and only if $n = 2i+3$, which completes the proof of Lemma 7. □

Lemma 8
(i) if $n \ge k+8,\ k \ge 3$, then $\sigma(D'_{n-k-4,v_{n-k-4},C_k}) \le \sigma(D_{n-k-2,v_3,C_k})$ with equality if and only if $n = k+8$ and $k = 4$.

(ii) if $2 \le m \le n-k-4,\ k \ge 3$, then $\sigma(D'_{n-k-4,v_{n-k-4},C_k}) < \sigma(D''_{n-k-4,v_m,C_k})$.

Proof. (i) if $n \ge k+8,\ k \ge 3$, then

$$
\begin{aligned}
&\quad\ \sigma(D'_{n-k-4,v_{n-k-4},C_k}) - \sigma(D_{n-k-2,v_3,C_k}) \\
&= 8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2} - [F_{k-1}(3F_{n-k-1} - 2F_{n-k-5}) \\
&\quad + F_{k+1}(3F_{n-k} - 2F_{n-k-4})] \\
&= F_{k-1}(8F_{n-k-3} - 3F_{n-k-1} + 2F_{n-k-5}) + F_{k+1}(F_{n-k+2} - 3F_{n-k} + 2F_{n-k-4}) \\
&= F_{k-1}(2F_{n-k-5} + F_{n-k-7}) - F_{k+1}F_{n-k-5} \\
&= F_{k-1}F_{n-k-7} - F_{k-2}F_{n-k-5} \\
&\le F_{k-1}F_{n-k-7} - 2F_{k-2}F_{n-k-7} \\
&= -F_{k-4}F_{n-k-7} \\
&\le 0
\end{aligned}
$$

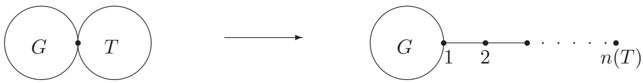
(ii) if $2 \le m \le n-k-4,\ k \ge 3$, then

$$
\sigma(D'_{n-k-4,v_{n-k-4},C_k}) - \sigma(D''_{n-k-4,v_m,C_k})
$$

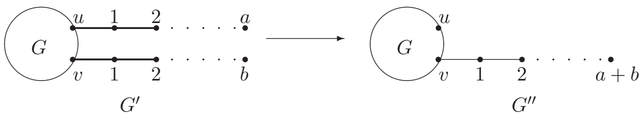
$$
\begin{aligned}
&= 8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2} \\
&\quad -[3\sigma(D_{n-k-4,v_{n-k-4},C_k}) - \sigma(P_{m-2} \cup D_{n-k-m-5,v_{n-k-m-5},C_k})] \\
&= 8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2} \\
&\quad -[3(F_{k+1}F_{n-k} + 3F_{k-1}F_{n-k-3}) - F_m(F_{k+1}F_{n-k-m-1} + 3F_{k-1}F_{n-k-m-4})] \\
&= F_{k+1}F_mF_{n-k-m-1} + 3F_{k-1}F_mF_{n-k-m-4} - F_{k+1}F_{n-k-2} - F_{k-1}F_{n-k-3} \\
&= F_{k+1}(F_mF_{n-k-m-1} - F_{n-k-2}) + F_{k-1}(3F_mF_{n-k-m-4} - F_{n-k-3}) \\
&= -F_{k+1}F_{m-1}F_{n-k-m-2} + F_{k-1}(2F_mF_{n-k-m-4} - F_{m+1}F_{n-k-m-3}) \\
&= -F_{k+1}F_{m-1}F_{n-k-m-2} + F_{k-1}(F_mF_{n-k-m-4} - F_mF_{n-k-m-5} - F_{m-1}F_{n-k-m-3}) \\
&= -F_{k+1}F_{m-1}F_{n-k-m-2} + F_{k-1}(F_mF_{n-k-m-6} - F_{m-1}F_{n-k-m-3}) \\
&< -F_{k+1}F_{m-1}F_{n-k-m-2} + F_{k-1}(F_mF_{n-k-m-6} - 2F_{m-1}F_{n-k-m-6}) \\
&= -F_{k+1}F_{m-1}F_{n-k-m-2} - F_{k-1}F_{m-3}F_{n-k-m-6} \\
&< 0
\end{aligned}
$$

which completes the proof of Lemma 8. □

lemma 9. σ-index decreases in the transformation I and II.(See Figure 2)



Transformation I



Transformation II and Graphs G', G''

Figure 2: Transformation I and II

Proof. Let $G \in C(n,k)$, $u, v \in V(C_k)$ and T be a tree with $n(T)$ vertices. According to Lemma 4, σ-index decreases in the transformation I. Now we prove σ-index decreases in the transformation II. We shall distinguish the following cases:

Case 1. u and v are adjacent. Without loss of generality, assuming $\sigma(G-[v]) \geq \sigma(G-[u])$. By lemma 2, 3, we have

$$
\begin{aligned}
\sigma(G') &= F_{a+2}F_{b+2}\sigma(G-\{u,v\}) + F_{a+2}F_{b+1}\sigma(G-[v]) \\
&\quad + F_{a+1}F_{b+2}\sigma(G-[u]) \\
\sigma(G'') &= F_{a+b+2}\sigma(G-\{u,v\}) + F_{a+b+2}\sigma(G-[u]) + F_{a+b+1}\sigma(G-[v]) \\
\sigma(G') - \sigma(G'') &= (F_{a+2}F_{b+2} - F_{a+b+2})\sigma(G-\{u,v\}) \\
&\quad + (F_{a+2}F_{b+1} - F_{a+b+1})\sigma(G-[v]) \\
&\quad + (F_{a+1}F_{b+2} - F_{a+b+2})\sigma(G-[u]) \\
&= F_aF_b\sigma(G-\{u,v\}) + F_aF_{b-1}\sigma(G-[v]) - F_aF_{b+1}\sigma(G-[u])
\end{aligned}
$$

$$
\begin{aligned}
&> F_aF_b\sigma(G-[v]) + F_aF_{b-1}\sigma(G-[v]) - F_aF_{b+1}\sigma(G-[u]) \\
&\geq F_aF_b\sigma(G-[u]) + F_aF_{b-1}\sigma(G-[u]) - F_aF_{b+1}\sigma(G-[u]) \\
&= 0
\end{aligned}
$$

Case 2. u and v aren't adjacent. Without loss of generality, assuming

$\sigma(G-\{u,[v]\}) \geq \sigma(G-\{[u],v\})$. Let $\{u,[v]\} = \{u\} \cup \{v\} \cup \{y \mid vy \in E(G)\}$ and $\{[u],[v]\} = \{u\} \cup \{x \mid ux \in E(G)\} \cup \{v\} \cup \{y \mid vy \in E(G)\}$. By lemma 2, 3, we have

$$
\begin{aligned}
\sigma(G') &= F_{a+2}F_{b+2}\sigma(G-\{u,v\}) + F_{a+2}F_{b+1}\sigma(G-\{u,[v]\}) \\
&\quad +F_{a+1}F_{b+2}\sigma(G-\{[u],v\}) + F_{a+1}F_{b+1}\sigma(G-\{[u],[v]\}) \\
\sigma(G'') &= F_{a+b+2}\sigma(G-\{u,v\}) + F_{a+b+2}\sigma(G-\{[u],v\}) \\
&\quad +F_{a+b+1}\sigma(G-\{u,[v]\}) + F_{a+b+1}\sigma(G-\{[u],[v]\}) \\
\sigma(G')-\sigma(G'') &= F_aF_b\sigma(G-\{u,v\}) + F_aF_{b-1}\sigma(G-\{u,[v]\}) \\
&\quad -F_aF_{b+1}\sigma(G-\{[u],v\}) - F_aF_b\sigma(G-\{[u],[v]\}) \\
&> F_aF_b\sigma(G-[v]) + F_aF_{b-1}\sigma(G-\{u,[v]\}) \\
&\quad -F_aF_{b+1}\sigma(G-\{[u],v\}) - F_aF_b\sigma(G-\{[u],[v]\}) \\
&= F_aF_b(\sigma(G-\{u,[v]\}) + \sigma(G-\{[u],[v]\})) + F_aF_{b-1}\sigma(G-\{u,[v]\}) \\
&\quad -F_aF_{b+1}\sigma(G-\{[u],v\}) - F_aF_b\sigma(G-\{[u],[v]\}) \\
&\geq F_aF_b\sigma(G-\{[u],v\}) + F_aF_{b-1}\sigma(G-\{[u],v\}) \\
&\quad -F_aF_{b+1}\sigma(G-\{[u],v\}) \\
&= 0
\end{aligned}
$$

Which completes the proof of Lemma 9. □

From Lemma 9, we have the following Corollary 1 from which the smallest value of $\sigma(G)$ for $G \in C(n,k)$ is obtained.

Corollary 1. Let $G \in C(n,k)$. Then $\sigma(G) \geq F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k+2}$ with equality if and only if $G \cong C_{k,n-k}$. □

3 The second- and third- smallest value of σ-index about unicyclic graphs of girth 3 and order n

Theorem 1. Let $n \geq 11$ and $|V(G)| = n$. If $G \in C(n,3) - C_{3,n-3}$, then $\sigma(G) \geq 3F_{n-1} + 3F_{n-4}$ with equality if and only if $G \cong D_{n-5,v_{n-5},C_3}$. If $G \in C(n,3) - C_{3,n-3} - D_{n-5,v_{n-5},C_3}$, then $\sigma(G) \geq F_{n+1} + F_{n-1} + F_{n-6} + F_{n-10}$ with equality if and only if $G \cong D'_{n-7,v_{n-7},C_3}$.

Proof. We shall distinguish the following cases:

Case 1. Three vertices of C_3 are attached trees.

From Lemma 9, the trees must be paths and only two vertices are attached paths. We shall consider it in case 2.

Case 2. Two vertices of C_3 are attached trees.

We only need to consider P_{n-1,v_m,C_3} according to Lemma 9.

Case 3. One vertices of C_3 is attached tree.

We only need to consider D_{n-5,v_m,C_3} according to Corollary 1 and Lemma 4.

We can compare $\sigma(P_{n-1,v_3,C_3})$ with $\sigma(D_{n-5,v_{n-5},C_3})$ to obtain second-smallest value of σ-index according to Lemma 5 and Lemma 7.

Analogously, we can compare $\sigma(D'_{n-7,v_{n-7},C_3})$ with $\sigma(D''_{n-7,v_m,C_3})$ to obtain third-smallest value of σ-index according to Lemma 7 and Lemma 8, Which completes the proof of Theorem 1. □

4 The second- and third- smallest value of σ-index about unicyclic graphs of girth $k(k \geq 4)$ and order n

After the results presented in the previous section, it might be natural to conjecture analogous results hold for unicyclic graphs of girth $k(k \geq 4)$. However, the latter hasn't the same results to the former by the following Theorem 2 and 3.

Theorem 2. Let $k \geq 4$ and $G \in C(n,k) - C_{k,n-k}$. If $n \geq 2k+2$ and k is even or $k+5 \leq n \leq 2k$ and $n-k$ is even, then $\sigma(G) \geq 3F_{n-1} + 2F_{k-1}F_{n-k}$ with equality if and only if $G \cong P_{n-k+2,v_3,C_k}$; if $n \geq 2k+2$ and k is odd or $k+5 \leq n \leq 2k$ and $n-k$ is odd, then $\sigma(G) \geq F_{k+1}F_{n-k+2} + 3F_{k-1}F_{n-k-1}$ with equality if and only if $G \cong D_{n-k-2,v_{n-k-2},C_k}$; if $n = 2k+1$ then $\sigma(G) \geq 3F_{2k} + 2F_{k-1}F_{k+1}$ with equality if and only if $G \cong P_{n-k+2,v_3,C_k}$ or $G \cong D_{n-k-2,v_{n-k-2},C_k}$;

Proof. Before the proof of Theorem 2, we claim a fact.

Claim 1. σ-index decreases in the transformation III. (See Figure 3)

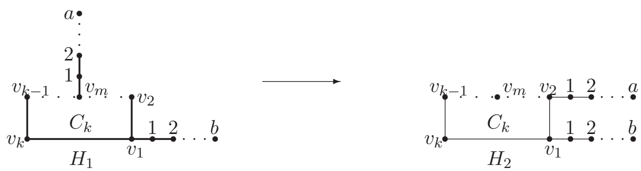


Figure 3: Transformation III and Graphs H_1, H_2

Proof of Claim 1. When $m \neq 1,2,k,\ \ a \geq 1,\ b \geq 2$, from Lemma 2, 3, we have

$$\sigma(H_1) = \sigma(C_{k,a} \cup P_{b-1}) + \sigma(H' \cup P_{b-2})$$

$$\sigma(H_2) = \sigma(C_{k,a} \cup P_{b-1}) + \sigma(P_{k+a-1} \cup P_{b-2})$$

where H' is a graph obtained by identifying an endvertex of P_{a+1} with vertex v_m of a path $v_2v_3 \cdots v_k$, from Lemma 4 we have $\sigma(P_{k+a-1}) < \sigma(H')$ and claim 1 holds.

Proof of Theorem 2. Analogous to the proof of Theorem 1, the proof of Theorem 2 only need to compare $\sigma(P_{n-k+2,v_3,C_k})$ with $\sigma(D_{n-k-2,v_{n-k-2},C_k})$. Then

$$\begin{aligned}
& \sigma(P_{n-k+2,v_3,C_k}) - \sigma(D_{n-k-2,v_{n-k-2},C_k}) \\
= \; & 3F_{n-1} + 2F_{k-1}F_{n-k} - (F_{k+1}F_{n-k+2} + 3F_{k-1}F_{n-k-1}) \\
= \; & 3F_{n-1} - F_{k+1}F_{n-k+2} + F_{k-1}(2F_{n-k} - 3F_{n-k-1}) \\
= \; & F_{n+1} + F_{n-3} - F_{k+1}F_{n-k+2} + F_{k-1}F_{n-k-4} \\
= \; & F_kF_{n-k} + F_{k+1}F_{n-k+1} - F_{k+1}F_{n-k+2} + F_{n-3} + F_{k-1}F_{n-k-4} \\
= \; & -F_{k-1}F_{n-k} + F_{n-3} + F_{k-1}F_{n-k-4} \\
= \; & F_{n-3} - F_{k-1}(F_{n-k-1} + F_{n-k-3}) \\
= \; & F_{k-1}F_{n-k-1} + F_{k-2}F_{n-k-2} - F_{k-1}(F_{n-k-1} + F_{n-k-3}) \\
= \; & F_{k-2}F_{n-k-2} - F_{k-1}F_{n-k-3}
\end{aligned}$$

If $n \geq 2k+2$, then

$$\begin{aligned}
& F_{k-2}F_{n-k-2} - F_{k-1}F_{n-k-3} \\
= \; & \frac{1}{5}[L_{n-4} - (-1)^{k-2}L_{n-2k}] - \frac{1}{5}[L_{n-4} - (-1)^{k-1}L_{n-2k-2}] \\
= \; & \frac{-(-1)^{k-2}}{5}(L_{n-2k} + L_{n-2k-2})
\end{aligned}$$

when k is even, $\frac{-(-1)^{k-2}}{5} < 0$; otherwise, $\frac{-(-1)^{k-2}}{5} > 0$.

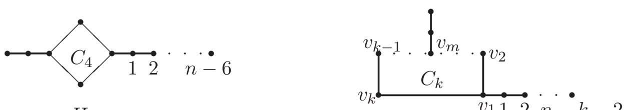
If $k+5 \leq n \leq 2k$, then

$$\begin{aligned}
& F_{k-2}F_{n-k-2} - F_{k-1}F_{n-k-3} \\
= \; & \frac{1}{5}[L_{n-4} - (-1)^{n-k-2}L_{2k-n}] - \frac{1}{5}[L_{n-4} - (-1)^{n-k-3}L_{2k+2-n}] \\
= \; & \frac{-(-1)^{n-k+2}}{5}(L_{2k-n} + L_{2k+2-n})
\end{aligned}$$

when $n-k$ is even, $\frac{-(-1)^{n-k+2}}{5} < 0$; otherwise, $\frac{-(-1)^{n-k+2}}{5} > 0$.

if $n = 2k+1$, then $F_{k-2}F_{n-k-2} - F_{k-1}F_{n-k-3} = 0$, which completes the proof of Theorem 2. □

From Theorem 2, we obtain second-smallest value of $\sigma(G)$ for $G \in C(n,k)$. Furthermore, we shall obtain third-smallest value of $\sigma(G)$. At first we pick up some graphs whose σ-index is greater than $\sigma(P_{n-k+2,v_3,C_k})$ when $n \geq k+7$. (See Figure 4)



H_3 H_4

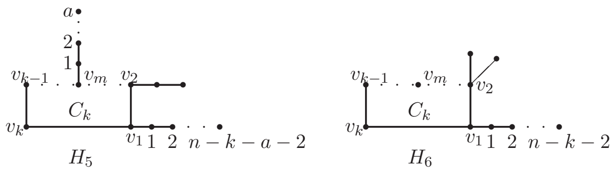


Figure 4. Graphs H_3, H_4, H_5 and H_6

Claim 2. If $n \geq k+7$, then $\sigma(H_i) > \sigma(P_{n-k+2,v_5,C_k})$ where $i = 3,4,5,6$.

Proof of Claim 2. (i) By direct calculation, we have $\sigma(H_3) > \sigma(P_{n-2,v_5,C_4})$.

(ii) When $k \geq 5, m \neq 1,2,k$, analogous to the proof of transformation III, we have $\sigma(H_4) > \sigma(P_{n-k+2,v_5,C_k})$.

(iii) When $k \geq 4, m \neq 1,2$, by transformation II and Lemma 5, we have $\sigma(H_5) > \sigma(P_{n-k+2,v_5,C_k})$.

(iv)

$$\begin{aligned}
& \sigma(H_6) - \sigma(P_{n-k+2,v_5,C_k}) \\
= \; & F_{n-k-1}(4F_k + 5F_{k-1}) + F_{n-k-2}(F_{k+2} + 2F_k) - (8F_{n-3} + 5F_{k-1}F_{n-k-2}) \\
= \; & 4F_kF_{n-k-1} + F_{n-k-2}(F_{k+2} + 2F_k) - 8F_{n-3} + 5F_{k-1}F_{n-k-3} \\
= \; & 4F_kF_{n-k-1} + F_{n-k-2}F_{k+2} - 2F_{k-1}F_{n-k-3} - 6F_{n-3} + 5F_{k-1}F_{n-k-3} \\
= \; & 4F_kF_{n-k-1} + F_{n-k-2}F_{k+2} - 3F_{n-3} - 3F_kF_{n-k-2} \\
= \; & 4F_kF_{n-k-1} - 3F_{n-3} - F_{k-2}F_{n-k-2} \\
= \; & F_kF_{n-k-1} - F_{k-2}F_{n-k-2} + 3(F_kF_{n-k-1} - F_{n-3}) \\
= \; & F_{k-1}F_{n-k-1} + F_{k-2}F_{n-k-3} + 3(F_{k-2}F_{n-k-1} - F_{k-2}F_{n-k-2}) \\
= \; & F_{k-1}F_{n-k-1} + 4F_{k-2}F_{n-k-3} \\
> \; & 0
\end{aligned}$$

which completes the proof of claim 2.

From Lemma 8, Theorem 2 and claim 2, it is necessary to prove the following Lemma 10 before obtaining third-smallest value of $\sigma(G)$ for $G \in C(n,k)$.

Lemma 10. (i) If $n = k+7, k = 4$, then $\sigma(P_{n-k+2,v_5,C_k}) = \sigma(D_{n-k-2,v_{n-k-2},C_k})$;

If $n \geq k+8, k = 4$, then $\sigma(P_{n-k+2,v_5,C_k}) < \sigma(D_{n-k-2,v_{n-k-2},C_k})$;

If $n \geq k+7, k \geq 5$, then $\sigma(P_{n-k+2,v_5,C_k}) > \sigma(D_{n-k-2,v_{n-k-2},C_k})$;

(ii) If $n \geq k+8$, then $\sigma(P_{n-k+2,v_3,C_k}) < \sigma(D'_{n-k-4,v_{n-k-4},C_k})$;

(iii) If $n = 2k+1, n \geq k+8$, when k is even, then $\sigma(P_{n-k+2,v_5,C_k}) > \sigma(D'_{n-k-4,v_{n-k-4},C_k})$; when k is odd, then $\sigma(P_{n-k+2,v_5,C_k}) < \sigma(D'_{n-k-4,v_{n-k-4},C_k})$;

Proof. (i) If $n \geq k+7, k \geq 5$, then

$$\sigma(P_{n-k+2,v_5,C_k}) - \sigma(D_{n-k-2,v_{n-k-2},C_k})$$

$$\begin{aligned}
&= 8F_{n-3} + 5F_{k-1}F_{n-k-2} - (F_{k+1}F_{n-k+2} + 3F_{k-1}F_{n-k-1}) \\
&= F_{n+1} + F_{n-3} + F_{n-7} - F_{k+1}F_{n-k+2} + F_{k-1}(5F_{n-k-2} - 3F_{n-k-1}) \\
&= F_{k-1}F_{n-k+1} + F_{n-3} + F_{n-7} - F_{k-1}F_{n-k+2} + F_{k-1}F_{n-k-6} \\
&= -F_{k-1}F_{n-k} + F_{n-3} + F_{n-7} + F_{k-1}F_{n-k-6} \\
&= F_{k-2}F_{n-k-2} - F_{k-1}F_{n-k-2} + F_{n-7} + F_{k-1}F_{n-k-6} \\
&= -F_{k-3}F_{n-k-2} + F_{n-7} + F_{k-1}F_{n-k-6} \\
&= F_{k-4}F_{n-k-4} - F_{k-3}F_{n-k-4} + F_{k-1}F_{n-k-6} \\
&= -F_{k-5}F_{n-k-4} + F_{k-1}F_{n-k-6} \\
&> -F_{k-5}F_{n-k-4} + 3F_{k-5}F_{n-k-6} \\
&= F_{k-5}F_{n-k-8} \\
&\geq 0
\end{aligned}$$

especially, if $n \geq k+7, k = 4$, then

$$\begin{aligned}
&\sigma(P_{n-k+2,v_5,C_k}) - \sigma(D_{n-k-2,v_{n-k-2},C_k}) \\
&= -F_{n-k-4} + 2F_{n-k-6} \\
&= -F_{n-k-7} \\
&\leq 0
\end{aligned}$$

(ii) if $n \geq k+8$, then

$$\begin{aligned}
&\sigma(P_{n-k+2,v_3,C_k}) - \sigma(D'_{n-k-4,v_{n-k-4},C_k}) \\
&= 3F_{n-1} + 2F_{k-1}F_{n-k} - (8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2}) \\
&= F_{n+1} + F_{n-3} - F_{k+1}F_{n-k+2} + F_{k-1}(2F_{n-k} - 8F_{n-k-3}) \\
&= F_kF_{n-k} + F_{n-3} - F_{k+1}F_{n-k} + F_{k-1}F_{n-k-6} \\
&= -F_{k-1}F_{n-k} + F_{n-3} + F_{k-1}F_{n-k-6} \\
&= -F_{k-1}F_{n-k} + F_{n-2} - F_{n-4} + F_{k-1}F_{n-k-6} \\
&= F_{k-2}F_{n-k-1} - F_{n-4} + F_{k-1}F_{n-k-6} \\
&= -F_{k-3}F_{n-k-2} + F_{k-1}F_{n-k-6} \\
&< -3F_{k-3}F_{n-k-6} + F_{k-1}F_{n-k-6} \\
&= -F_{k-5}F_{n-k-6} \\
&\leq 0
\end{aligned}$$

(iii) If $n = 2k+1, n \geq k+8$, then

$$\begin{aligned}
&\sigma(P_{n-k+2,v_5,C_k}) - \sigma(D'_{n-k-4,v_{n-k-4},C_k}) \\
&= 8F_{n-3} + 5F_{k-1}F_{n-k-2} - (8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2}) \\
&= 8F_kF_{n-k-2} + 5F_{k-1}F_{n-k-2} - F_{k+1}F_{n-k+2} \\
&= F_{k+5}F_{n-k-2} - F_{k+1}F_{n-k+2} \\
&= F_{k+5}F_{k-1} - F_{k+1}F_{k+3} \\
&= \frac{1}{5}[L_{2k+4} - (-1)^{k-1}L_6] - \frac{1}{5}[L_{2k+4} - (-1)^{k+1}L_2]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{5}[-18(-1)^{k-1} + 3(-1)^{k+1}] \\
&= 3(-1)^k
\end{aligned}
$$

which completes the proof of Lemma 10.

From Lemma 7, 8, 10, Theorem 2 and claim 2, we have the following Theorem 3 from which we obtain third-smallest value of $\sigma(G)$ for $G \in C(n,k)$.

Theorem 3. Let $G \in C(n,k)$ and $k \geq 4$.

(i) Let $G \in C(n,k) - C_{k,n-k} - P_{n-k+2,v_3,C_k}$, $n \geq 2k+2$ and k is even or $k+7 \leq n \leq 2k$ and $n-k$ is even.

If $n = k+7$ and $k = 4$, then $\sigma(G) \geq 218$ with equality if and only if $G \cong P_{9,v_5,C_4}$ or $G \cong D_{5,v_5,C_4}$;

If $n \geq k+8$ and $k = 4$, then $\sigma(G) \geq 8F_{n-3} + 10F_{n-6}$ with equality if and only if $G \cong P_{n-2,v_5,C_4}$;

if $n \geq k+7$ and $k \geq 5$, then $\sigma(G) \geq F_{k+1}F_{n-k+2} + 3F_{k-1}F_{n-k-1}$ with equality if and only if $G \cong D_{n-k-2,v_{n-k-2},C_k}$;

(ii) Let $G \in C(n,k) - C_{k,n-k} - D_{n-k-2,v_{n-k-2},C_k}$, $n \geq 2k+2$ and k is odd or $k+8 \leq n \leq 2k$ and $n-k$ is odd.

Then $\sigma(G) \geq 3F_{n-1} + 2F_{k-1}F_{n-k}$ with equality if and only if $G \cong P_{n-k+2,v_3,C_k}$;

(iii) Let $G \in C(n,k) - C_{k,n-k} - P_{n-k+2,v_3,C_k} - D_{n-k-2,v_{n-k-2},C_k}$, $n = 2k+1$ and $n \geq k+8$.

If k is even, then $\sigma(G) \geq 8F_{k-1}F_{n-k-3} + F_{k+1}F_{n-k+2}$ with equality if and only if $G \cong D'_{n-k-4,v_{n-k-4},C_k}$;

If k is odd, then $\sigma(G) \geq 8F_{n-3} + 5F_{k-1}F_{n-k-2}$ with equality if and only if $G \cong P_{n-k+2,v_5,C_k}$;

Proof of Theorem 3. According to Corollary 1 and Theorem 2, we only need to consider the graphs whose σ-index is greater than $\sigma(P_{n-k+2,v_3,C_k})$ or $\sigma(D_{n-k-2,v_{n-k-2},C_k})$ for obtaining third-smallest value of σ-index. From Lemma 5 and claim 2, we should consider P_{n-k+2,v_5,C_k}. On the other hand, we should consider D'_{n-k-4,v_{n-k-4},C_k} and D''_{n-k-4,v_m,C_k} from Lemma 4. By Lemma 8 and Lemma 10, Theorem 3 holds.

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