Extremal Multi-bridge Graphs With Respect To Merrifield-Simmons Index

Shubo Chen[a], Weijun Liu[b*]
[a] Department of Mathematics and Computer Science, Hunan City University, Yiyang, Hunan 413000, P. R. China
[b] School of Sciences, Nantong University, Nantong, Jiangsu, 226007, P. R. China

Abstract

The Merrifield-Simmons index of a graph G, denoted by $i(G)$, is defined to be the total number of its independent sets, including the empty set. Let $\theta(a_1, a_2, \cdots, a_k)$ denote the graph obtained by connecting two distinct vertices with k independent paths of lengths a_1, $a_2, \cdots, a_k$ respectively, we named it as multi-bridge graphs for convenience. Tight upper and lower bounds for the Merrifield-Simmons index of $\theta(a_1, a_2, \cdots, a_k)$ are established in this paper.

1 Introduction

The Merrifield-Simmons index was introduced in 1982 in a paper written by Prodinger and Tichy [1], although it was called Fibonacci number of a graph there. It is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [2-5]. Let $G = (V, E)$ be a graph whose sets of vertices and edges are $V(G)$ and $E(G)$, respectively. Two vertices of G are said to be independent if they are not adjacent in G. An independent k set is a set of k vertices, no two of which are adjacent. Denote by $i(G, k)$ the number of the k-independent sets of G. It follows directly from the definition that is an independent set. Then $i(G, 0) = 1$ for any graph G. The Merrifield-Simmons index of G, denoted by $i(G)$, is defined as

$$i(G) = \sum_{k=0}^{n} i(G, k)$$

The Merrifield-Simmons index is one of the topological indices whose mathematical properties were studied in some detail, whereas its applicability for QSPR and QSAR was examined to a much lesser extent. In [1], Prodinger and Tichy shown that, for n-vertex trees, the star(S_n) has the maximal Merrifield-Simmons index and the path(P_n) has the minimal Merrifield-Simmons index. In [6], Alameddine determined the sharp bounds for the Merrifield-Simmons index of a maximal outer planar graph. Gutman [7], Zhang and Tian [8,9] studied the Merrifield-Simmons indices

*Corresponding author: wjliu6210@126.com, shubochen@gmail.com

of hexagonal chains and catacondensed systems, respectively. Ren and Zhang [10] determined the minimal Merrifield-Simmons index of double hexagonal chains. In [11], Li et al. characterized the tree with the maximal Merrifield-Simmons index among the trees with given diameter. In [12], Yu and Tian studied the Merrifield-Simmons index of the graphs with given edge-independence number and cyclomatic number. Yu and Lv [13, 14] studied the Merrifield-Simmons indices of trees with maximal degree and given pendent vertices, respectively. Ye et al., ordered the unicyclic graphs with given girth according to the Merrifield-Simmons index in [15]. Pedersen and Vestergaard [16] determined upper and lower bounds for the number of independent sets in a unicyclic graph in terms of its order. Li and Zhu [17] determined the sharp upper bound for the number of independent sets in a unicyclic graph of a given diameter. In [18], Deng et al., determined the upper bounds for number of independent sets among bicyclic graphs. In [19], Li et al., determined tricyclic graphs with maximum Merrifield-Simmons index. In [20], Deng characterized (n,n+1)-graphs with the smallest Merrifield-Simmons index. For a more detailed study of the properties of the Merrifield-Simmons index we refer to[21-26].

All graphs considered here are both connected and simple if not stated in particular. For any $v \in V(G)$, we use $N_G(v)$ to denote the set of the neighbors of v, and let $N_G[v] = v \cup N_G(v)$, let $d(v)$ be the number of edges incident with v. For each integer $k \geq 2$, let θ_k be the multigraph with 2 vertices and k edges. For any $a_1, a_2, \cdots, a_k \in \mathbb{N}$, we denote $\theta(a_1, a_2, \cdots, a_k)$ the graph obtained by replacing the edges of θ_k with paths of length $a_1, a_2, \cdots, a_k$ respectively. The graph $\theta(a_1, a_2, \cdots, a_k)$ is called a multi-bridge(or more precisely, a k-bridge graph). $\theta(1, a_2, a_3)$ is called a θ graph and $\theta(a_1, a_2, a_3)$ is called a generalized θ graph. Note that if $a_1 = 0$, then $\theta(a_1, a_2, \cdots, a_k)$ is a graph obtained by gluing C_{a_2+2}, C_{a_3+2}, C_{a_k+2} at a common edge, which is a polygon tree.

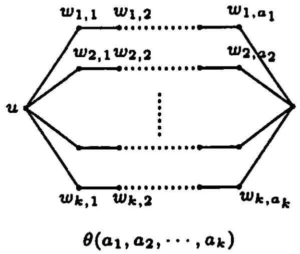

Figure 1. The graph $\theta(a_1, a_2, \cdots, a_k)$

Let $\Theta_n^k = \{\theta(a_1, a_2, \cdots, a_k) : a_1 + a_2 + \cdots + a_k = n - 2\}$, without loss of generality, we assume that $a_1 \leq a_2 \leq \cdots \leq a_k, k \geq 4$. In this paper, we shall determine upper and lower bounds for the Merrifield-Simmons index of graphs in Θ_n^k, and characterize the graph in Θ_n^k with the largest and smallest Merrifield-Simmons index.

2 Preliminaries

Let $E' \subseteq E(G)$, we denote by $G-E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G-W$ denote the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If a graph G has components $G_1, G_2, \cdots, G_t$, then G is denoted by $\bigcup_{i=0}^{t} G_i$.

Let $F(n)$ denote the n-th Fibonacci number. Recall that $F(n) = F(n-1) + F(n-2)$ with initial conditions $F(0) = 0, F(1) = 1$.

The following basic results will be used and can be found in the references cited.

Lemma 1. Let x and y be two vertices in G. Then

(i) $i(G) = i(G - \{x\}) + i(G - N_G[x])$;

(ii) If x and y are not adjacent in G, then

$$i(G) = i(G - \{x, y\}) + i(G - \{x\} \cup N_G[y]) + i(G - \{y\} \cup N_G[x]) + i(G - N_G[x] \cup N_G[y])$$

(iii) If x and y are adjacent in G, then

$$i(G) = i(G - \{x, y\}) + i(G - N_G[y]) + i(G - N_G[x]);$$

(iv) If G is a graph with components G_1, G_2, G_3, $\cdots$, G_k. Then

$$i(G) = \prod_{i=1}^{k} i(G_i).$$

(v) $i(P_n) = F(n+2)$, $i(S_n) = 1 + 2^{n-1}$.

(vi) Given for all k, l, $F(k+l) = F(k-1)F(l) + F(k)F(l+1)$.

3 Graphs in Θ_n^k with maximal Merrifield-Simmons index

We consider the upper bounds of Θ_n^k with respect to the Merrifield-Simmons index in this section.

Let $T_1 = \theta(a_1, a_2, \cdots, a_k) - u$;

$T_2 = \theta(a_1, a_2, \cdots, a_k) - \{u, w_{1,1}, w_{2,1}, \cdots, w_{k,1}\}$.

Theorem 1. Let $\theta(a_1, a_2, \cdots, a_k)$ be the multi-bridge graph depicted in Figure 1, then

$$i(\theta(a_1, a_2, \cdots, a_k)) = \prod_{i=1}^{k} F(a_i + 2) + 2\prod_{i=1}^{k} F(a_i + 1) + \prod_{i=1}^{k} F(a_i)$$

Proof. Let $G = \theta(a_1, a_2, \cdots, a_k)$, by definition of Merrifield-Simmons index and Lemma 1, we have

$$\begin{aligned} i(G) &= i(G-u) + i(G - \{u, w_{1,1}, w_{2,1}, \cdots, w_{k,1}\}) \\ &= i(T_1) + i(T_2) \\ &= i(T_1 - v) + i(T_1 - \{v, w_{1,a_2}, w_{2,a_2}, \cdots, w_{k,a_k}\}) + i(T_2 - v) \\ &\quad + i(T_2 - \{v, w_{1,a_1}, w_{2,a_2}, \cdots, w_{k,a_k}\}) \\ &= F(a_1+2)F(a_2+2)\cdots F(a_k+2) + 2F(a_1+1)F(a_2+1)\cdots \\ &\quad F(a_k+1) + F(a_1)F(a_2)\cdots F(a_k) \\ &= \prod_{i=1}^{k} F(a_i+2) + 2\prod_{i=1}^{k} F(a_i+1) + \prod_{i=1}^{k} F(a_i) \end{aligned}$$

This completes the proof.

Theorem 2. Let $\theta(a_1, a_2, \cdots, a_k) \in \Theta_n^k$ with $a_1 > 1$, then

$$i(\theta(a_1, a_2, \cdots, a_k)) < i(\theta(1, a_2, \cdots, a_1 + a_k - 1)).$$

Proof. By Theorem 1, we have

$$\begin{aligned} & i(\theta(1, a_2, \cdots, a_1 + a_k - 1)) \\ = & \prod_{i=2}^{k-1} F(a_i+2)F(3)F(a_1+a_k+1) + 2\prod_{i=2}^{k-1} F(a_i+1)F(2) \\ & F(a_1+a_k) + \prod_{i=2}^{k-1} F(a_i)F(1)F(a_1+a_k-1) \\ = & 2F(a_1+a_k+1)\prod_{i=2}^{k-1} F(a_i+2) + 2F(a_1+a_k)\prod_{i=2}^{k-1} F(a_i+1) \\ & + F(a_1+a_k-1)\prod_{i=2}^{k-1} F(a_i) \end{aligned}$$

Thus,

$$\begin{aligned} \Delta &= i(\theta(a_1, a_2, \cdots, +a_k)) - i(\theta(1, a_2, \cdots, a_1 + a_k - 1)) \\ &= \prod_{i=2}^{k-1} F(a_i+2)[F(a_1+2)F(a_k+2) - 2F(a_1+a_k+1)] + \\ &\quad 2\prod_{i=2}^{k-1} F(a_i+1)[F(a_1+1)F(a_k+1) - F(a_1+a_k)] + \\ &\quad \prod_{i=2}^{k-1} F(a_i)[F(a_1)F(a_k) - F(a_1+a_k-1)] \end{aligned}$$

By Lemma 1(vi), we have

$$\begin{aligned} & F(a_1+2)F(a_k+2) - 2F(a_1+a_k+1) \\ = & F(a_1+2)F(a_k+2) - 2[F(a_1)F(a_k) + F(a_1+1)F(a_k+1)] \\ = & \cdots \\ = & -F(a_1-1)F(a_k-1) \end{aligned}$$

Similarly, $F(a_1+1)F(a_k+1) - F(a_1+a_k) = F(a_1-1)F(a_k-1)$; $F(a_1)F(a_k) - F(a_1+a_k-1) = -F(a_1-1)F(a_k-1)$.

By combing above, we arrive at

$$\Delta = F(a_1-1)F(a_k-1)[2\prod_{i=2}^{k-1}F(a_i+1)-\prod_{i=2}^{k-1}F(a_i+2)-\prod_{i=2}^{k-1}F(a_i)]$$

Let $I_1 = 2\prod_{i=2}^{k-1}F(a_i+1)-\prod_{i=2}^{k-1}F(a_i+2)-\prod_{i=2}^{k-1}F(a_i)$. We have

CLAIM 1: $I_1 < 0$.

We prove it by induction on $i (2 \le i \le k-1)$.

(i) When $i = 2$. In this case,

$I_1 = 2F(a_2+1) - F(a_2+2) - F(a_2) = -F(a_2-2) < 0$

(ii) Assume that the claim 1 holds for $i = j$ such that $2 < j < k-1$. Then we have

$$2F(a_2+1)F(a_3+1)\cdots F(a_j+1) < F(a_2+2)F(a_3+2)\cdots F(a_j+2) + F(a_2)F(a_3)\cdots F(a_j)$$

When $i = j+1$,

$$\begin{aligned}
&2\prod_{i=2}^{j+1}F(a_i+1)-\prod_{i=2}^{j+1}F(a_i+2)-\prod_{i=2}^{j+1}F(a_i)\\
&< [\prod_{i=2}^{j}F(a_i+2)+\prod_{i=2}^{j}F(a_i)]F(a_{j+1}+1)-\prod_{i=2}^{j+1}F(a_i+2)-\prod_{i=2}^{j+1}F(a_i)\\
&= \prod_{i=2}^{j}F(a_i+2)[F(a_{j+1}+1)-F(a_{j+1}+2)]+\prod_{i=2}^{j}F(a_i)[F(a_{j+1}+1)\\
&\quad -F(a_{j+1})]\\
&= -F(a_{j+1})\prod_{i=2}^{j}F(a_i+2)+F(a_{j+1}-1)\prod_{i=2}^{j}F(a_i)\\
&< 0
\end{aligned}$$

Therefore, for any $2 \le i \le k-1$, the claim 1 follows.

Hence, $\Delta < 0$, i.e., $i(\theta(a_1, a_2, \cdots, a_k)) < i(\theta(1, a_2, \cdots, a_1 + a_k - 1))$.

The proof is completed.

Repeating using Theorem 2, we arrive at

Corollary 3. Let $\theta(a_1, a_2, \cdots, a_k) \in \Theta_n^k$ with $a_1 \ge 1$, then

$$i(\theta(a_1, a_2, \cdots, a_{k-1}, a_k)) \le i(\theta(\underbrace{1, 1, \cdots, 1}_{k-1}, n-k-1)).$$

Note that, $i(\theta(\underbrace{1, 1, \cdots, 1}_{k-1}, n-k-1)) = 2^{k-1}F(n+1-k) + F(n+2-k)$.

Lemma 4. Let $\theta(a_1, a_2, \cdots, a_k) \in \Theta_n^k$ with $a_1 \ge 1$, then

$$i(\theta(0, a_2, \cdots, a_1 + a_k)) < i(\theta(a_1, a_2, \cdots, a_k)).$$

Proof. By Theorem 1, we have

$$\begin{aligned} & i(\theta(0,a_2,\cdots,a_1+a_k)) \\ = \; & F(a_1+a_k+2)\prod_{i=2}^{k-1}F(a_i+2)+2F(a_1+a_k+1)\prod_{i=2}^{k-1}F(a_i+1) \end{aligned}$$

Thus,

$$\begin{aligned} & \Delta' \\ & = i(\theta(a_1,a_2,\cdots,a_k)) - i(\theta(0,a_2,\cdots,a_1+a_k)) \\ & = \prod_{i=2}^{k-1}F(a_i+2)[F(a_1+2)F(a_k+2)-F(a_1+a_k+2)] \\ & \quad +2\prod_{i=2}^{k-1}F(a_i+1)[F(a_1+1)F(a_k+1)-F(a_1+a_k+1)]+\prod_{i=2}^{k-1}F(a_i) \\ & = F(a_1)F(a_k)[\prod_{i=2}^{k-1}F(a_i+2)-2\prod_{i=2}^{k-1}F(a_i+1)+\prod_{i=2}^{k-1}F(a_i)] \\ & > 0 \end{aligned}$$

By Corollary 3 and Lemma 4, we obtain

Theorem 5. Let $\theta(a_1,a_2,\cdots,a_k)\in\Theta_n^k$, then

$$i(\theta(a_1,a_2,\cdots,a_k)) \le 2^{k-1}F(n+1-k)+F(n+2-k)$$

the equality holds if and only if $\theta(a_1,a_2,\cdots,a_k)\cong\theta(\underbrace{1,1,\cdots,1}_{k-1},n-k-1)$.

4 Graphs in Θ_n^k with minimal Merrifield-Simmons index

We consider the lower bounds of Θ_n^k with respect to the Merrifield-Simmons index in this section.

By Theorem 1, we have

$$\begin{aligned} & i(\theta(0,2,a_3,\cdots,a_{k-1},a_1+a_2+a_k-2)) \\ & = 3F(a_1+a_2+a_k)\prod_{i=3}^{k-1}F(a_i+2)+4F(a_1+a_2+a_k-1)\prod_{i=3}^{k-1}F(a_i+1) \end{aligned}$$

Theorem 6. If $a_2\ge 3$, then

$$\begin{cases} i(\theta(0,2,a_3,\cdots,a_{k-1},a_1+a_2+a_k-2)) > i(\theta(0,a_2,\cdots,a_1+a_k)), \\ \qquad\qquad \text{if } k=4; \\ i(\theta(0,2,a_3,\cdots,a_{k-1},a_1+a_2+a_k-2)) < i(\theta(0,a_2,\cdots,a_1+a_k)), \\ \qquad\qquad \text{if } k>4. \end{cases}$$

Proof. By Theorem 1, we have

$$
\begin{aligned}
&\Delta'' \\
&= i(\theta(0, a_2, \cdots, a_1 + a_k)) - i(\theta(0, 2, a_3, \cdots, a_{k-1}, a_1 + a_2 + a_k - 2)) \\
&= \prod_{i=3}^{k-1} F(a_i + 2)[F(a_2 + 2)F(a_1 + a_k + 2) - 3F(a_1 + a_2 + a_k)] + \\
&\quad 2\prod_{i=3}^{k-1} F(a_i + 1)[F(a_2 + 1)F(a_1 + a_k + 1) - 2F(a_1 + a_2 + a_k - 1)] \\
&= F(a_2 - 2)F(a_1 + a_k - 2)[\prod_{i=3}^{k-1} F(a_i + 2) - 2\prod_{i=3}^{k-1} F(a_i + 1)]
\end{aligned}
$$

Let $I_2 = \prod_{i=3}^{k-1} F(a_i + 2) - 2\prod_{i=3}^{k-1} F(a_i + 1)$. We have

CLAIM 2: $\begin{cases} I_2 < 0, & \text{if } k = 4; \\ I_2 > 0, & \text{if } k > 4. \end{cases}$

We prove it by induction on k, note that $k \geq 4$.

Case 1. When $k = 4$. $I_2 = F(a_3 + 2) - 2F(a_3 + 1) = -F(a_3 - 1) < 0$.

Case 2. When $k > 4$.

(i) Let $k = 5$, it is suffice to see that

$$
\begin{aligned}
I_2 &= F(a_3 + 2)F(a_4 + 2) - 2F(a_3 + 1)F(a_4 + 1) \\
&= [F(a_3 + 1) + F(a_3)][F(a_4 + 1) + F(a_4)] - 2F(a_3 + 1)F(a_4 + 1) \\
&= 2F(a_3)F(a_4) - F(a_3 - 1)F(a_4 - 1) > 0
\end{aligned}
$$

(ii) Assume that the claim holds for $k = j > 4$, then we have

$$\prod_{i=3}^{j} F(a_i + 2) > 2\prod_{i=3}^{j} F(a_i + 1)$$

and

$$
\begin{aligned}
&\prod_{i=3}^{j+1} F(a_i + 2) - 2\prod_{i=3}^{j+1} F(a_i + 1) \\
&> 2\prod_{i=3}^{j} F(a_i + 1)F(a_{j+1} + 2) - 2\prod_{i=3}^{j} F(a_i + 1)F(a_{j+1} + 1) \\
&= 2\prod_{i=3}^{j} F(a_i + 1)[F(a_{j+1} + 2) - F(a_{j+1} + 1)] \\
&= 2\prod_{i=3}^{j} F(a_i + 1)F(a_{j+1}) \\
&> 0
\end{aligned}
$$

Therefore, the claim follows.

Hence, $\Delta'' < 0$ when $k = 4$, and $\Delta'' > 0$ when $k > 4$.

The proof is completed.

Similar to Theorem 6, we have

Corollary 7. If $a_1, a_2, \cdots, a_{i+1} \geq 3, i \geq 1$, then

$$i(\theta(0,\underbrace{2,2,\cdots,2}_{i},a_{i+2},\cdots,a_{k-1},a_1+a_2+\cdots+a_{i+1}+a_k-2i))$$
$$< i(\theta(0,\underbrace{2,2,\cdots,2}_{i-1},a_{i+1},\cdots,a_{k-1},a_1+a_2+\cdots+a_i+a_k-2i+2))$$

By Corollary 7, we have

Remark I:

$$i(\theta(0,2,a_3,\cdots,a_{k-1},a_1+a_2+a_k-2))$$
$$> i(\theta(0,2,2,a_4,\cdots,a_{k-1},a_1+a_2+a_3+a_k-2))$$
$$> \cdots$$
$$> i(\theta(0,\underbrace{2,2,\cdots,2}_{k-2},n-2k+2))$$

Lemma 8. If $a_{j+2}\geq 3, j\geq 1$, then

$$i(\theta(0,\underbrace{1,\cdots,1}_{j},2,a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+2}a_i+a_k-j-2))$$
$$< i(\theta(0,\underbrace{1,\cdots,1}_{j},a_{j+2},a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+1}a_i+a_k-j-2))$$

Proof. Theorem 1, we have

$$\begin{aligned} & i(\theta(0,\underbrace{1,\cdots,1}_{j},2,a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+2}a_i+a_k-j-2)) \\ = \; & 3\cdot 2^j\cdot F(a_1+\cdots+a_{j+2}+a_k-j)\prod_{i=j+3}^{k-1}F(a_i+2) \\ & +4F(a_1+\cdots+a_{j+2}+a_k-j-1)\prod_{i=j+3}^{k-1}F(a_i+1) \end{aligned}$$

and

$$\begin{aligned} & i(\theta(0,\underbrace{1,\cdots,1}_{j},a_{j+2},a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+1}a_i+a_k-j)) \\ = \; & 2^j\cdot F(a_1+\cdots+a_{j+2}+a_k-j+2)\prod_{i=j+2}^{k-1}F(a_i+2) \\ & +2F(a_1+\cdots+a_{j+1}+a_k-j+1)\prod_{i=j+2}^{k-1}F(a_i+1) \end{aligned}$$

Thus

$$\Delta = i(\theta(0,\underbrace{1,\cdots,1}_{j},2,a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+2}a_i+a_k-j-2))$$
$$-i(\theta(0,\underbrace{1,\cdots,1}_{j},a_{j+2},a_{j+3},\cdots,a_{k-1},\sum_{i=1}^{j+1}a_i+a_k-j))$$
$$=F(a_{j+2}-2)F(a_1+\cdots+a_{j+1}+a_k-j-2)$$
$$[-2^j\prod_{i=j+3}^{k-1}F(a_i+2)+2\prod_{i=j+3}^{k-1}F(a_i+1)]$$
$$<0$$

Since,

$$3F(a_1+\cdots+a_{j+1}+a_{j+2}+a_k-j)$$
$$-F(a_{j+2}+2)F(a_1+\cdots+a_{j+1}+a_k-j+2)$$
$$=3[F(a_1+\cdots+a_{j+1}+a_k-j-1)F(a_{j+2})+F(a_1+\cdots+a_{j+1}$$
$$+a_k-j)F(a_{j+2}+1)]-[F(a_{j+2}+1)+F(a_{j+2})][F(a_1+\cdots+$$
$$a_{j+1}+a_k-j+1)+F(a_1+\cdots+a_{j+1}+a_k-j)]$$
$$=-F(a_{j+2}-2)F(a_1+\cdots+a_{j+1}+a_k-j-2)$$

and

$$2F(a_1+\cdots+a_{j+1}+a_{j+2}+a_k-j-1)-F(a_{j+2}+1)$$
$$F(a_1+\cdots+a_{j+1}+a_k-j-2)$$
$$=2[F(a_1+\cdots+a_{j+1}+a_k-j-1)F(a_j-1)$$
$$+F(a_1+\cdots+a_{j+1}+a_k-j)F(a_{j+2})]$$
$$-[F(a_{j+2})+F(a_{j+2}-1)][F(a_1+\cdots+a_{j+1}+a_k-j)$$
$$+F(a_1+\cdots+a_{j+1}+a_k-j-1)]$$
$$=F(a_{j+2}-2)F(a_1+\cdots+a_{j+1}+a_k-j-2)$$

The proof is completed.

Similar to Lemma 8, we have

Lemma 9. If $a_{i+j+2}\geq 3, i,j\geq 1$, then

$$i(\theta(0,\underbrace{1,\cdots,1}_{i},\underbrace{2,\cdots,2}_{j+1},a_{i+j+3},\cdots,a_{k-1},a_1+a_2+\cdots+a_{i+j+2}$$
$$+a_k-i-2j-2))$$
$$<i(\theta(0,\underbrace{1,\cdots,1}_{i},\underbrace{1,\cdots,1}_{j},a_{i+j+2},a_{j+3},\cdots,a_{k-1},a_1+a_2+\cdots$$
$$+a_{i+j+1}+a_k-i-2j))$$

Remark II: In order to find the lower bound on the Merrifield-Simmons index of graphs in Θ_n^k, by **Remark I**, Theorem 6, Lemma 8 and Lemma 9, it suffices to determine

$$\min\{i(\theta(0,\underbrace{2,2,\cdots,2}_{k-2},n-2k+2)),i(\theta(0,1,\underbrace{2,2,\cdots,2}_{k-3},n-2k+3)),$$
$$i(\theta(0,1,1,\underbrace{2,2,\cdots,2}_{k-4},n-2k+4)),\cdots,i(\theta(0,\underbrace{1,1,\cdots,1}_{k-2},n-k))\}$$

Lemma 10.

$$i(\theta(0,\underbrace{1,1,\cdots,1}_{i},\underbrace{2,2,\cdots,2}_{k-i-2},n-2k+i+2))$$
$$\leq i(\theta(0,\underbrace{1,1,\cdots,1}_{i+1},\underbrace{2,2,\cdots,2}_{k-i-3},n-2k+i+3))$$

the equality holds if and only $i=1$ and $k=4$.

Proof. By a simple calculation, we have

$$i(\theta(0,\underbrace{1,1,\cdots,1}_{i},\underbrace{2,2,\cdots,2}_{k-i-2},n-2k+i+2))$$
$$=(\tfrac{2}{3})^i 3^{k-2}F(n+4-2k+i)+2^{k-i-1}F(n+3-2k+i)$$
$$i(\theta(0,\underbrace{1,1,\cdots,1}_{i+1},\underbrace{2,2,\cdots,2}_{k-i-3},n-2k+i+3))$$
$$=(\tfrac{2}{3})^i\cdot 2\cdot 3^{k-3}F(n+5-2k+i)+2^{k-i-2}F(n+4-2k+i)$$

So,

$$\begin{aligned}\Delta &= i(\theta(0,\underbrace{1,1,\cdots,1}_{i},\underbrace{2,2,\cdots,2}_{k-i-2},n-2k+i+2))-\\ &\quad i(\theta(0,\underbrace{1,1,\cdots,1}_{i+1},\underbrace{2,2,\cdots,2}_{k-i-3},n-2k+i+3))\\ &= (\tfrac{2}{3})^i 3^{k-3}[3F(n+4-2k+i)-2F(n+5-2k+i)]+2^{k-i-2}\\ &\quad [2F(n+3-2k+i)-F(n+4-2k+i)]\\ &= F(n+1-2k+i)(2^{k-i-2}-\tfrac{2^i}{3}\cdot 3^{k-i-2})\\ &\leq 0(\text{ with equality if and only if } i=1, \text{ and } k=4)\end{aligned}$$

Using Lemma 10 repeatedly, we arrive at

$$\min\{i(\theta(0,\underbrace{2,2,\cdots,2}_{k-2},n-2k+2)),i(\theta(0,1,\underbrace{2,2,\cdots,2}_{k-3},n-2k+3)),$$
$$i(\theta(0,1,1,\underbrace{2,2,\cdots,2}_{k-4},n-2k+4)),\cdots,i(\theta(0,\underbrace{1,1,\cdots,1}_{k-2},n-k))\}$$
$$=i(\theta(0,\underbrace{2,2,\cdots,2}_{k-2},n-2k+2))$$
$$=3^{k-2}F(n-2k+4)+2^{k-1}F(n-2k+3)$$

Summing up, we have

Theorem 11. Let $\theta(a_1,a_2,\cdots,a_k)\in\Theta_n^k$, then $i(\theta(a_1,a_2,\cdots,a_k))\geq 3^{k-2}F(n-2k+4)+2^{k-1}F(n-2k+3)$ the equality holds if and only if

$$\theta(a_1,a_2,\cdots,a_k)\cong\theta(0,\underbrace{2,2,\cdots,2}_{k-2},n-2k+2).$$

Acknowledgements: The authors sincerely thank the anonymous referees for their valuable comments, which have considerably improved the presentation of this paper. Projects Supported by the NNSFC(10871205) and Research Foundation of Education Bureau of Hunan Province, China(Grant

References

[1] H. Prodinger, R. F. Tichy, Fibonacci numbers of graphs, Fibonacci Quart. 20 (1982) 16-21.

[2] R. E. Merrifield, H. E. Simmons, Topological Methods in Chemistry, John Wiley Son, New York, 1989.

[3] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[4] R. E. Merrifield, H. E. Simmons, Enumeration of structure-sensitive graphical subsets: theory, Proc. Natl. Acad. Sci. USA. 78 (1981) 692-695.

[5] R. E. Merrifield, H. E. Simmons, Enumeration of structure-sensitive graphical subsets: theory, Proc. Natl. Acad. Sci. USA 78 (1981) 1329-1332.

[6] A. F. Alameddine, Bounds on the Fibonacci number of a maximal outerplanar graph, Fibonacci Quart. 36 (1998) 206-210.

[7] I. Gutman, Extremal hexagonal chains, J. Math. Chem. 12 (1993) 197-210.

[8] L. Zhang, F. Tian, Extremal catacondensed benzenoids, J. Math. Chem. 34 (2003) 111-122.

[9] L. Zhang, F. Tian, Extremal hexagonal chains concerning largest eigenvalue, Sci. China Ser. A 44 (2001) 1089-1097.

[10] H. Ren and F. Zhang, Double hexagonal chains with maximal Hosoya index and minimal Merrifield-Simmons index. J. Math. Chem. 42(4)(2007)679-690.

[11] X. Li, H. Zhao, On the Fibonacci numbers of trees, Fibonacci Quarter. 44 (2006) 32-38.

[12] A. Yu, F. Tian, A kind of graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, MATCH Commun. Math. Comput. Chem. 55 (2006) 103-118.

[13] X. Lv, A. Yu, The Merrifield-Simmons indices and Hosoya indices of trees with a given maximum degree, MATCH Commun. Math. Comput. Chem. 56 (2006) 605-616.

[14] A. Yu, X. Lv, The Merrifield-Simmons indices and Hosoya indices of

[15] Y. Ye, X. F. Pan, and H. Liu, Ordering unicyclic graphs with respect to Hosoya indices and Merrifield-Simmons indices. MATCH Commun. Math. Comput. Chem. 59 (2008) 191-202.

[16] A. S. Pedersen, P. D. Vestergaard, The number of independent sets in unicyclic graphs, Discrete Appl. Math. 152 (2005) 246-256.

[17] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, Discrete Appl. Math. 157 (2009) 1387-1395.

[18] H. Deng, S. Chen, and J. Zhang, The Merrifield-Simmons index in (n, n+1)-graphs. J. Math. Chem. 43 (2008) 75-91.

[19] Z. Zhu, S. Li, L. Tan, Tricyclic graphs with maximum Merrifield-Simmons index, Discrete Appl. Math. 158 (2010) 204-212.

[20] H. Deng, The smallest Merrifield-Simmons index of (n, n+1)-graphs, Math. Comput. Modelling, 49(1-2) (2009) 320-26.

[21] H. Zhao and R. Liu, On the Merrifield-Simmons index of graphs, MATCH Commun. Math. Comput. Chem. 56 (2006) 617-624.

[22] L. Z. Zhang and F. J. Zhang, Extremal hexagonal chains concerning k-matchings and k-independent sets, J. Math. Chem. 27 (2000) 319-329.

[23] L. Z. Zhang, On the ordering of a class of hexagonal chains with respect to Merrifield-Simmons index, Systems Sci. Math. Sci. 13 (2000) 219-224.

[24] L. Z. Zhang. The proof of Gutman's conjectures concerning extremal hexagonal chains. J. Systems Sci. Math. Sci. 18 (1998) 460-465.

[25] Y. Zeng, The bounds of Hosoya index and Merrifield-Simmons index for polyomino chains, J. Math. Study. 41 (2008) 256-263.

[26] H. Deng and S. Chen, The extremal unicyclic graphs with respect to Hosoya index andMerrifield-Simmons index, MATCH Commun. Math. Comput. Chem. 59 (2008) 171-190.