Sharp bounds on Merrifield-Simmons index of the generalized θ-graph

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Abstract. For a graph G, the Merrifield-Simmons index $i(G)$ is defined as the total number of its independent sets. In this paper, we determine sharp upper and lower bounds on Merrifield-Simmons index of generalized θ- graph, which is obtained by subdividing the edges of the multigraph consisting of k parallel edges, denoted by $\theta(r_1, r_2, ..., r_k)$. The corresponding extremal graphs are also characterized.

Keywords: Merrifield-Simmons index; Generalized θ-graph; Sharp bounds

AMS subject classification: 05C69, 05C05

1. Introduction

Graph theory has provided chemist with a variety of useful tools, such as topological indices. Molecules and molecular compounds are often modeled by molecular graph. Topological indices and graph invariants based on the stable sets are used for characterizing molecular graphs. Also, topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure-activity relationships (QSAR) [28]. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [19]. There Merrifield and Simmons showed the correlation between this index and boiling points.

Let G be a graph on n vertices. 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 $\emptyset$ 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 $i(G) = \Sigma_{k=0}^{n} i(G, k)$.

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Now the research on Merrifield-Simmons index mainly focuses on graphs with pendent vertices, e.g., trees, unicyclic graphs, bicyclic graphs and tricyclic graphs; see [4, 5, 11, 12, 13, 14, 15, 18, 20, 21, 24, 25]. On the other hand, only a few papers reported the progress on Merrifield-Simmons index of graphs without pendent vertices. In [1], Alameddine determined the sharp bounds for Merrifield-Simmons index of a maximal outer planar graph. Gutman [10], Zhang and Tian [22, 23] studied the Merrifield-Simmons indices of hexagonal chains and catacondensed systems, respectively. Ren and Zhang [26] determined the minimal Merrifield-Simmons index of double hexagonal chains. Here we continue this line of research by investigating sharp upper and lower bounds of so called generalized θ-graphs.

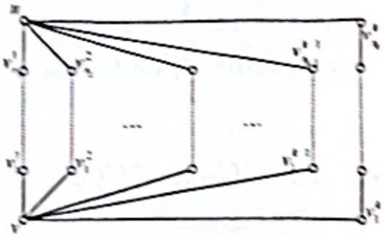

Figure 1: $\theta(r_1, r_2, \cdots, r_k)$

A generalized θ-graph $\theta(r_1, r_2, \cdots, r_k)$ consists of a pair of end vertices joined by k internally disjoint paths of lengths $r_1+1, r_2+1, \cdots, r_k+1$ (see Fig.1). We denote the set of n-vertex generalized θ-graphs by $\Theta_n^k = \theta(r_1, r_2, \ldots, r_k)$, $r_1+r_2+\cdots+r_k = n-2$, $r_1 \le r_2 \le \cdots \le r_k$, $k \ge 3$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobs [2]. We only consider finite, simple and undirected graphs. 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. We denote by P_n the path on n vertices. Let $N(v) = \{u|uv \subseteq E(G)\}$, $N[v] = N(v)\bigcup\{v\}$.

We list the following results which will be used in this paper.

Lemma 1.1. *([5])Let $G=(V,E)$ be a graph*

(i) *If $uv \in E(G)$, then $i(G) = i(G-uv) - i(G-(N[u]\bigcup N[v]))$;*

(ii) *If* $v \in V(G)$, *then* $i(G) = i(G - v) + i(G - N[v])$;

(iii) *If* $G_1, G_2, \ldots, G_t$ *are the components of the graph* G, *then* $i(G) = \prod_{j=1}^{t} i(G_j)$.

According to the definition of the Merrifield-Simmons index of a graph G, by Lemma 1.1, if v is a vertex of G, then $i(G) > i(G-v)$. In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $i(G) = i(G - v) + i(G - \{u, v\})$. So it is easy to see that $i(P_0) = 1, i(P_1) = 2$ and $i(P_n) = i(P_{n-1}) + i(P_{n-2})$ for $n \geq 2$. Let F_n be the nth Fibonacci number, defined by $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. Therefore,

$$i(P_n) = F_{n+1} = \frac{1}{\sqrt{5}}[(\frac{1+\sqrt{5}}{2})^{n+2} - (\frac{1-\sqrt{5}}{2})^{n+2}].$$

Note that $F_{n+m} = F_n F_m + F_{n-1} F_{m-1}$. For convenience, we let $F_n = 0$ for $n < 0$. Our main result in this paper is the following.

Theorem 1.2. *For any generalized* θ*-graph* $\theta(r_1, r_2, \cdots, r_k) \in \Theta_n^k$.

(i) *([27])If* $k = 3$, $n \geq 7$, *then* $F_n + F_{n-3} \leq i(\theta(r_1, r_2, r_3)) \leq F_n - 1 + 3F_n - 3$. *The equality holds on the left if and only if* $\theta(r_1, r_2, r_3) \cong \theta(0, 1, n-3))$. *The equality holds on the right if and only if* $\theta(r_1, r_2, r_3) \cong \theta(1, 1, n-4))$.

(ii) *If* $k = 4$, *then* $10F_{n-5} + 7F_{n-6} \leq i(\theta(r_1, r_2, r_3, r_4)) \leq (2^3 + 1)F_{n-4} + F_{n-5}$. *The equality holds on the left if and only if* $\theta(r_1, r_2, r_3, r_4) \cong \theta(0, 2, 2, n-6)$, *or* $\theta(0, 1, 2, n-5)$. *The equality holds on the right if and only if* $\theta(r_1, r_2, r_3, r_4) \cong \theta(1, 1, 1, n-5)$.

(iii) *If* $k \geq 5$, *then* $2 \cdot 3^{k-2} F_{n-2k+3} + 2^{k-1} F_{n-2k+2} \leq i(\theta(r_1, r_2, \ldots, r_k)) \leq (2^{k-1} + 1)F_{n-k} + F_{n-k-1}$. *The equality holds on the left if and only if* $\theta(r_1, r_2, \ldots, r_k) \cong \theta(0, 2, 2, \ldots, 2, n-2k-4)$. *The equality holds on the right if and only if* $\theta(r_1, r_2, \ldots, r_k) \cong \theta(1, 1, 1, \ldots, 1, n-k-1)$.

2. Proof of Theorem 1.2

We first give some lemmas that will be used in the proof of our main results.

Lemma 2.1. *Let* $\theta(r_1, r_2, \ldots, r_k) \in \Theta_n^k$ *be from Figure 1. Then* $i(\theta(r_1, r_2, \ldots, r_k)) = F_{r_1+1} F_{r_2+1} \ldots F_{r_k+1} + 2F_{r_1} F_{r_2} \ldots F_{r_k} + F_{r_1-1} F_{r_2-1} \ldots F_{r_k-1}$. *Especially, when* $r_1 = \cdots = r_{k-1} = 1$, $i(\theta(1, 1, \ldots, 1, n-k-1)) = (2^{k-1} + 1)F_{n-k} + F_{n-k-1}$.

Proof. By Lemma 1.1, we have

$$\begin{aligned}
& i(\theta(r_1,r_2,\ldots,r_k)) \\
= & \ i(\theta(r_1,r_2,\ldots,r_k)-u)+i(\theta(r_1,r_2,\ldots,r_k)-N[u]) \\
= & \ i(\theta(r_1,r_2,\ldots,r_k)-u-v)+i(\theta(r_1,r_2,\ldots,r_k)-u-N[v])+ \\
& \ i(\theta(r_1,r_2,\ldots,r_k)-N[u]-v)+i(\theta(r_1,r_2,\ldots,r_k)-N[u]-N[v]) \\
= & \ i(P_{r_1}\cup P_{r_2}\cup\ldots\cup P_{r_k})+2i(P_{r_1-1}\cup P_{r_2-1}\cup\ldots\cup P_{r_k-1})+ \\
& \ i(P_{r_1-2}\cup P_{r_2-2}\cup\ldots\cup P_{r_k-2}) \\
= & \ F_{r_1+1}F_{r_2+1}\ldots F_{r_k+1}+2F_{r_1}F_{r_2}\ldots F_{r_k}+F_{r_1-1}F_{r_2-1}\ldots F_{r_k-1}.
\end{aligned}$$

The second part of this lemma is obvious by direct computing. □

Lemma 2.2. *Let* $\theta(0,r_2,\ldots,r_1+r_k)\in\Theta_n^k$. *Then* $i(\theta(0,r_2,\ldots,r_1+r_k)) = F_{r_2+1}F_{r_3+1}\ldots F_{r_1+r_k+1}+2F_{r_2}F_{r_3}\ldots F_{r_1+r_k}+F_{r_2-1}F_{r_3-1}\ldots F_{r_1+r_k-1}$.

Proof. By Lemma 1.1, we have

$$\begin{aligned}
& i(\theta(0,r_2,\ldots,r_{k-1},r_1+r_k)) \\
= & \ i(\theta(0,r_2,\ldots,r_1+r_k)-u)+i(\theta(0,r_2,\ldots,r_1+r_k)-N[u]) \\
= & \ F_{r_2+1}F_{r_3+1}\ldots F_{r_1+r_k+1}+2F_{r_2}F_{r_3}\ldots F_{r_1+r_k}+ \\
& \ F_{r_2-1}F_{r_3-1}\ldots F_{r_1+r_k-1}.
\end{aligned}$$

□

Lemma 2.3. *Let* $r_1,r_2,\ldots,r_{k-1}$ *be positive integers with* $2\le r_1\le r_2\le\cdots\le r_{k-1}$. *Then* $F_{r_2+1}\cdots F_{r_{k-1}+1}+F_{r_2-1}\cdots F_{r_{k-1}-1}-2F_{r_2}\cdots F_{r_{k-1}}>0$.

Proof. In fact,

$$\begin{aligned}
& F_{r_2+1}\cdots F_{r_{k-1}+1}+F_{r_2-1}\cdots F_{r_{k-1}-1}-2F_{r_2}\cdots F_{r_{k-1}} \\
= & \ (F_{r_2}+F_{r_2-1})\cdots(F_{r_{k-1}}+F_{r_{k-1}-1})+F_{r_2-1}\cdots F_{r_{k-1}-1}-F_{r_2}\cdots F_{r_{k-1}} \\
& -(F_{r_2-1}+F_{r_2-2})\cdots(F_{r_{k-1}-1}+F_{r_{k-1}-2}).
\end{aligned}$$

Let

$$\begin{aligned}
g_1 &= (F_{r_2}+F_{r_2-1})\cdots(F_{r_{k-1}}+F_{r_{k-1}-1})+F_{r_2-1}\cdots F_{r_{k-1}-1}- \\
& \quad F_{r_2}\cdots F_{r_{k-1}} && (2.1)\\
g_2 &= (F_{r_2-1}+F_{r_2-2})\cdots(F_{r_{k-1}-1}+F_{r_{k-1}-2}) && (2.2)
\end{aligned}$$

Note that the last term in (2.1) will be canceled when we simplify the expression of g_1. On the other hand, the total number of terms of (2.1) is 2^{k-2}, which is equal to that of (2.2). The largest term in g_2 is $F_{r_2-1}\cdots F_{r_{k-1}-1}$, for each other term, say $F_{r_2-i_1}F_{r_3-i_2}\cdots F_{r_{k-1}-i_{k-2}}$, in (2.2), there is a term $F_{r_2-i_1+1}F_{r_3-i_2+1}\cdots F_{r_{k-1}-i_{k-2}+1}$, in (2.1) such that

$$F_{r_2-i_1}F_{r_3-i_2}\cdots F_{r_{k-1}-i_{k-2}} < F_{r_2-i_1+1}F_{r_3-i_2+1}\cdots F_{r_{k-1}-i_{k-2}+1},$$

where $i_j = 1$ or 2, $j = 1, 2, \ldots, k-2$. Notice that the term $F_{r_2-1}\cdots F_{r_{k-1}-1}$is also contained in (2.1). Therefore, we obtain that $g_1 > g_2$, as desired. □

Lemma 2.4. *Let $\theta(r_1, \ldots, r_k) \in \Theta_n^k$ with $r_1 > 1$. Then $i(\theta(r_1, \ldots, r_k)) < i(\theta(1, r_2, \ldots, r_k + r_1 - 1)$.*

Proof. By Lemma 2.2, we have

$$\begin{aligned} i(\theta(1, r_2, \ldots, r_k + r_1 - 1)) &= F_{r_2}F_{r_2+1}\cdots F_{r_k+r_1} + 2F_1F_{r_2}\cdots F_{r_k+r_1-1} + \\ &\quad F_0F_{r_2-1}\cdots F_{r_k+r_1-2}. \end{aligned}$$

Let $\Delta i = i(\theta(1, r_2, \ldots, r_k + r_1 - 1)) - i(\theta(r_1, r_2, \ldots, r_k))$. Hence,

$$\begin{aligned} \Delta i &= F_{r_1-2}F_{r_k-2}(F_{r_2+1}\cdots F_{r_{k-1}+1} + F_{r_2-1}\cdots F_{r_{k-1}-1} - 2F_{r_2}\cdots F_{r_k-1}) \\ &< 0. \end{aligned}$$

□

Lemma 2.5. *If $r_1, \ldots, r_i > 1$, then $i(\theta(\underbrace{1, \ldots, 1}_{i}, r_{i+1}, \ldots, r_{k-1}, r_k + r_1 + \cdots + r_i - i)) > i(\theta(\underbrace{1, \ldots, 1}_{i-1}, r_i, \ldots, r_{k-1}, r_k + r_1 + \cdots + r_{i-1} - i + 1))$.*

Proof. Let

$$\begin{aligned} A &= i(\theta(\underbrace{1, \ldots, 1}_{i}, r_{i+1}, \ldots, r_{k-1}, r_k + r_1 + \cdots + r_i - i)), \\ B &= i(\theta(\underbrace{1, \ldots, 1}_{i-1}, r_i, \ldots, r_{k-1}, r_k + r_1 + \cdots + r_{i-1} - i + 1)). \end{aligned}$$

By Lemma 2.1, we have

$$\begin{aligned} A &= 2^iF_{r_{i+1}+1}\ldots F_{r_{k-1}+1}F_{r_k+r_1+\cdots+r_i-i+1} + \\ &\quad 2F_{r_{i+1}}\ldots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} \\ &\quad +F_{r_{i+1}-1}\ldots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i+1}, \\ B &= 2^{i-1}F_{r_i+1}\ldots F_{r_{k-1}+1}F_{r_k+r_1+\cdots+r_{i-1}-i+2} + \\ &\quad 2F_{r_i}\ldots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} \\ &\quad +F_{r_i-1}\ldots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i}. \end{aligned}$$

This yields,

$$\begin{aligned}
A-B &= (2^{i-1}F_{r_{i+1}+1}\dots F_{r_{k-1}+1}-2F_{r_{i+1}}\cdots F_{r_{k-1}} \\
&\quad +F_{r_{i+1}-1}\dots F_{r_{k-1}-1})F_{r_i-2}F_{r_k+r_1+\dots+r_{i-1}-i-1} \\
&= [(2^{i-1}-1)F_{r_{i+1}+1}\dots F_{r_{k-1}+1}+(F_{r_{i+1}+1}\dots F_{r_{k-1}+1}- \\
&\quad 2F_{r_{i+1}}\dots F_{r_{k-1}}+F_{r_{i+1}-1}\dots F_{r_{k-1}-1})]F_{r_i-2}F_{r_k+r_1+\dots+r_{i-1}-i-1} \\
&\geq (F_{r_{i+1}+1}\dots F_{r_{k-1}+1}-2F_{r_{i+1}}\dots F_{r_{k-1}}+ \\
&\quad F_{r_{i+1}-1}\dots F_{r_{k-1}-1})F_{r_i-2}F_{r_k+r_1+\dots+r_{i-1}-i-1}>0,
\end{aligned}$$

where the last inequality follows from Lemma 2.3 and the assumption that $r_1,\dots,r_i>1$. This completes the proof. □

Lemma 2.6. *Let $\theta(r_1,\cdots,r_k)\in\Theta_n^k$ with $r_1>1$. Then $i(\theta(r_1,\dots,r_k))>i(\theta(0,r_2,\dots,r_1+r_k))$.*

Proof. Let $\Delta i'=i(\theta(r_1,r_2,\dots,r_k))-i(\theta(0,r_2,\dots,r_1+r_k))$. By lemmas 2.1 and 2.2, we have

$$\begin{aligned}
\Delta i' &= [(F_{r_2}\cdots F_{r_{k-3}}F_{r_{k-2}-1}F_{r_{k-1}}-F_{r_2}\cdots F_{r_{k-2}-1}F_{r_{k-1}-2})+ \\
&\quad (F_{r_2}\cdots F_{r_{k-3}}F_{r_{k-2}-1}F_{r_{k-1}-1}-F_{r_2}\cdots F_{r_{k-3}}F_{r_{k-2}-2}F_{r_{k-1}-2})+ \\
&\quad F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}}F_{r_{k-1}}+ \\
&\quad F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}-1}F_{r_{k-1}} \\
&\quad +F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}-1}F_{r_{k-1}-1}+ \\
&\quad F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}}F_{r_{k-1}-1}+\cdots)]F_{r_1-1}F_{r_k-1} \\
&\quad -(F_{r_1-1}F_{r_2-1}\cdots F_{r_{k-1}-1}F_{r_k-2}+F_{r_1-2}F_{r_2-1}\cdots F_{r_{k-1}-1}F_{r_k-1}) \\
&> (F_{r_1-1}F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}}F_{r_{k-1}}F_{r_k-1} \\
&\quad +F_{r_1-1}F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}-1}F_{r_{k-1}}F_{r_k-1} \\
&\quad +F_{r_1-1}F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}-1}F_{r_{k-1}-1}F_{r_k-1}) \\
&\quad -(F_{r_1-1}F_{r_2-1}\cdots F_{r_{k-1}-1}F_{r_k-2}+F_{r_1-2}F_{r_2-1}\cdots F_{r_{k-1}-1}F_{r_k-1}) \\
&> F_{r_1-1}F_{r_2}\cdots F_{r_{k-4}}F_{r_{k-3}-1}F_{r_{k-2}}F_{r_{k-1}}F_{r_k-1}>0.
\end{aligned}$$

Hence $i(\theta(r_1,r_2,\dots,r_k))>i(\theta(0,r_2,\dots,r_1+r_k))$. □

Lemma 2.7. *Let $\theta(0,r_2,r_3,\dots,r_{k-1},r_1+r_k)$,$\theta(0,2,r_3,\dots,r_{k-1},r_1+r_2+r_k-2)\in\Theta_n^k$. Then*

$$i(\theta(0,r_2,r_3,\dots,r_{k-1},r_1+r_k))>i(\theta(0,2,r_3,\dots,r_{k-1},r_1+r_2+r_k-2)),$$

for $r_1,r_2>2$.

Proof. By Lemma 2.3, we have $i(\theta(0, 2, r_3, \ldots, r_1 + r_2 + r_k - 2)) =$

$$F_3 F_{r_3+1} \cdots F_{r_1+r_2+r_k-1} + 2F_2 F_{r_3} \cdots F_{r_1+r_2+r_k-2} + F_{r_3-1} \cdots F_{r_1+r_2+r_k-3} \quad (2.3)$$

Let $\Delta = i(\theta(0, r_2, r_3, \ldots, r_1 + r_k)) - i(\theta(0, 2, r_3, \ldots, r_1 + r_2 + r_k - 2))$. By (2.3) and Lemma 2.4,

$$\begin{aligned} \Delta &= (F_{r_3+1} \cdots F_{r_{k-1}+1} - 2F_{r_3} \cdots F_{r_{k-1}} + \\ &\quad F_{r_3-1} \cdots F_{r_{k-1}-1}) F_{r_2-3} F_{r_1+r_k-3} > 0, \end{aligned}$$

where the last inequality follows from Lemma 2.3 and the assumption $r_1, r_2 > 2$. This completes the proof. □

Lemma 2.8. *Let* $\theta(0, \underbrace{2, \ldots, 2}_{i-1}, r_{i+1}, \ldots, r_{k-1}, r_1 + \cdots + r_i + r_k - 2i - 2)$, $\theta(0, \underbrace{2, \ldots, 2}_{i}, r_{i+2}, \ldots, r_{k-1}, r_1 + \cdots + r_{i+1} + r_k - 2i)) \in \Theta_n^k$ *with* $r_1, \ldots, r_{i+1} > 2, i \geq 1$. *Then* $i(\theta(0, \underbrace{2, \ldots, 2}_{i-1}, r_{i+1}, \ldots, r_{k-1}, r_1 + \cdots + r_i + r_k - 2i - 2)) > i(\theta(0, \underbrace{2, \ldots, 2}_{i}, r_{i+2}, \ldots, r_{k-1}, r_1 + \cdots + r_{i+1} + r_k - 2i))$.

Proof. Let

$$\begin{aligned} X &= i(\theta(0, \underbrace{2, \ldots, 2}_{i-1}, r_{i+1}, \ldots, r_{k-1}, r_1 + \cdots + r_i + r_k - 2i - 2)), \\ Y &= i(\theta(0, \underbrace{2, \ldots, 2}_{i}, r_{i+2}, \ldots, r_{k-1}, r_1 + \cdots + r_{i+1} + r_k - 2i)). \end{aligned}$$

By Lemma 2.2, we have

$$\begin{aligned} X &= 3^{i-1} F_{r_{i+1}+1} \cdots F_{r_{k-1}+1} F_{r_k+r_1+\cdots+r_i-2i+3} + \\ &\quad 2^i F_{r_{i+1}} \cdots F_{r_{k-1}+1} F_{r_k+r_1+\cdots+r_i-2i+2} + \\ &\quad F_{r_{i+1}-1} \cdots F_{r_{k-1}-1} F_{r_k+r_1+\cdots+r_i-2i+1}, \\ Y &= 3^i F_{r_{i+2}+1} \cdots F_{r_{k-1}+1} F_{r_k+r_1+\cdots+r_{i+1}-2i+1} + \\ &\quad 2^{i+1} F_{r_{i+2}} \cdots F_{r_{k-1}+1} F_{r_k+r_1+\cdots+r_{i+1}-2i} + \\ &\quad F_{r_{i+2}-1} \cdots F_{r_{k-1}-1} F_{r_k+r_1+\cdots+r_{i+1}-2i-1}. \end{aligned}$$

This yields

$$\begin{aligned} X - Y &= [(3^{i-1} - 1) F_{r_{i+2}+1} \cdots F_{r_{k-1}+1} - (2^i - 2) F_{r_{i+2}} \cdots F_{r_{k-1}} + \\ &\quad (F_{r_{i+2}+1} \cdots F_{r_{k-1}+1} - 2F_{r_{i+2}} \cdots F_{r_{k-1}} + \\ &\quad F_{r_{i+2}-1} \cdots F_{r_{k-1}-1})] F_{r_{i+1}-3} \cdots F_{r_k+r_1+\cdots+r_i-2i-1} \end{aligned}$$

$$> \quad (F_{r_{i+2}+1}\cdots F_{r_{k-1}+1} - 2F_{r_{i+2}}\cdots F_{r_{k-1}} + F_{r_{i+2}-1}\cdots F_{r_{k-1}-1})F_{r_{i+1}-3}\cdots F_{r_k+r_1+\cdots+r_i-2i-1} \geq 0$$

The last inequality follows form Lemma 2.3. This completes the proof. □

By Lemma 2.8, we have

$$i(\theta(0,2,r_3,\ldots,r_1+r_2+r_k-2)) > i(\theta(0,2,2,r_4,\ldots,r_1+r_2+r_k-2)) > \ldots > i(\theta(0,2,\ldots,2,n-2k+2)) \tag{2.4}$$

Lemma 2.9. *Let $r_k^* = r_k + r_{i+2} - 2$, $r_{i+2} > 2$, for $i \geq 1$,*

$$i(\theta(0,\underbrace{1,\ldots,1}_{i},r_{i+2},\ldots,r_{k-1},r_k) > i(\theta(0,\underbrace{1,\ldots,1}_{i},2,r_{i+3},\ldots,r_{k-1},r_k^*)).$$

Proof. Let

$$\begin{aligned} U &= i(\theta(0,\underbrace{1,\ldots,1}_{i},r_{i+2},\ldots,r_{k-1},r_k)), \\ V &= i(\theta(0,\underbrace{1,\ldots,1}_{i},2,r_{i+3},\ldots,r_{k-1},r_k^*)). \end{aligned}$$

By Lemma 1.1, we have

$$\begin{aligned} U &= 2^i F_{r_{i+2}+1}F_{r_{i+3}+1}\cdots F_{r_{k-1}+1}F_{r_k+1} + 2F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_k}, \\ V &= 2^i F_3 F_{r_{i+3}+1}\cdots F_{r_{k-1}+1}F_{r_{i+2}+r_k-1} + 2F_2 F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_{i+2}+r_k-2}. \end{aligned}$$

This yields, $U-V = F_{r_{i+2}-3}F_{r_k-3}[2^i F_{r_{i+3}+1}\cdots F_{r_{k-1}+1} + 2F_{r_{i+3}}\cdots F_{r_{k-1}}] > 0$. □

With the similar discussion in the proof of Lemma 2.9, we have

Lemma 2.10. *Let $r_k' = r_k + r_{i+j+2} - 2, r_{i+j+2} > 2$, for $i,j \geq 1$,*

$$\begin{aligned} & i(\theta(0,\underbrace{1,\ldots,1}_{i},\underbrace{2,\ldots,2}_{j},r_{i+j+2},\ldots,r_{k-1},r_k)) \\ > \quad & i(\theta(0,\underbrace{1,\ldots,1}_{i},\underbrace{2,\ldots,2}_{j+1},r_{i+j+3},\ldots,r_{k-1},r_k')). \end{aligned}$$

Remark: In order to find the lower bound on Merrifield-Simmons index of graphs in Θ_n^k, by (2.4), lemmas 2.9 and 2.10, it suffices to determine $\min\{i(\theta(0,2,\ldots,2,n-2k+2)), i(\theta(0,1,2,\ldots,2,n-2k+3)), \cdots i(\theta(0,1,1,\ldots,1,n-k-1)), i(\theta(0,1,1,\ldots,1,1,n-k))\}$.

Lemma 2.11. *For* $k \geq 5$, $i(\theta(0,\underbrace{1,\ldots,1}_{i+1},\underbrace{2,\ldots,2}_{k-i-3},n-2k+i+3)) > i(\theta(0,\underbrace{1,\ldots,1}_{i},\underbrace{2,\ldots,2}_{k-i-2},n-2k+i+2))$, *for* $i = 0,1,2\ldots,k-3$.

Proof. By Lemma 1.1, we have

$$\begin{aligned} & i(\theta(0,\underbrace{1,\ldots,1}_{i},\underbrace{2,\ldots,2}_{k-i-2},n-2k+i+2)) \\ = \quad & 2^i 3^{k-i-2} F_{n-2k+i+3} + 2^{k-i-1} F_{n-2k+i+2}. \end{aligned} \tag{2.5}$$

In view of (2.5), we have

$$\begin{aligned} & i(\theta(0,\underbrace{1,\ldots,1}_{i+1},\underbrace{2,\ldots,2}_{k-i-3},n-2k+i+3)) - \\ & i(\theta(0,\underbrace{1,\ldots,1}_{i},\underbrace{2,\ldots,2}_{k-i-2},n-2k+i+2)) = (2^i 3^{k-i-2} - 2^{k-i-2}) F_{n-2k+i}. \end{aligned}$$

Note that $n \geq 2k-i$, hence $F_{n-2k+i} > 0$. In order to complete the proof of Lemma 2.11, it suffices to show that $2^i 3^{k-i-2} - 2^{k-i-2} > 0$, which is equivalent to

$$k > \frac{i(\ln 3 - 2\ln 2) + 3\ln 3 - 2\ln 2}{ln3 - ln2},$$

for $i \geq 0$, i.e, $k > \frac{3\ln 3 - 2\ln 2}{ln3 - ln2} = 4.7095$. Namely, $k \geq 5$. □

Proof of Theorem 1.2. Here we only prove (ii) and (iii) of Theorem 1.2.

(ii) When $k = 4$, for any $\theta(r_1,r_2,r_3,r_4) \in \Theta_n^4$, in view of lemmas 2.6, 2.7 and 2.8, we have $i(\theta(r_1,r_2,r_3,r_4)) \geq i(\theta(0,r_2,r_3,r_4+r_1)) \geq i(\theta(0,2,r_3,r_4+r_1+r_2-4)) \geq i(\theta(0,2,2,n-6))$. On the other hand, by direct computing, we have

$$i(\theta(0,2,2,n-6)) = i(\theta(0,1,2,n-5)) < i(\theta(0,1,1,n-4)).$$

By Lemmas 2.4 and 2.5, we have

$$i(\theta(r_1,r_2,r_3,r_4)) \leq i(\theta(1,r_2,r_3,r_4+r_1-3)) \leq i(\theta(1,1,1,n-5)),$$

the first equality holds if and only if $r_1 = 1$ and the second equality holds if and only if $r_2 = r_3 = 1$.

Therefore, by direct computing, for any $\theta(r_1,r_2,r_3,r_4) \in \Theta_n^4$, we have

$$10F_{n-5} + 7F_{n-6} \leq i(\theta(r_1,r_2,r_3,r_4)) \leq (2^3+1)F_{n-4} + F_{n-5}.$$

The equality holds on the left if and only if $\theta(r_1, r_2, r_3, r_4) \cong \theta(0, 2, 2, n-6)$, or $\theta(0, 1, 2, n-5)$. The equality holds on the right if and only if $\theta(r_1, r_2, r_3, r_4) \cong \theta(1, 1, 1, n-5)$.

(iii) When $k \geq 5$, for any $\theta(r_1, r_2, \ldots, r_k) \in \Theta_n^k$, in view of lemmas 2.6, 2.7 and 2.8, we have

$$\begin{aligned} i(\theta(r_1, r_2, \ldots, r_k)) &\geq i(\theta(0, r_2, \ldots, r_k + r_1)) \\ &\geq i(\theta(0, 2, r_3, \ldots, r_k + r_1 + r_2 - 4)) \\ &\geq i(\theta(0, 2, \ldots, 2, n - 2k - 4)). \end{aligned} \quad (2.6)$$

The first equality in (2.6) holds if $r_1 = 0$, and the i-th equality in (2.6) holds if only if $r_i = 2, i = 2, 3, \ldots, k-1$. By lemmas 2.4 and 2.5, we have $i(\theta(r_1, r_2, r_3, \ldots, r_k)) \leq i(\theta(1, r_2, r_3, \ldots, r_{k-1}, r_k + r_1 - 1)) \leq i(\theta(1, \ldots, 1, n-5))$, the first equality holds if and only if $r_1 = 1$ and the second equality holds if and only if $r_2 = r_3 = \cdots = r_{k-1} = 1$.

Therefore, by direct computing, for any $\theta(r_1, r_2, \ldots, r_k) \in \Theta_n^k$, we have $2 \cdot 3^{k-2} F_{n-2k+3} + 2^{k-1} F_{n-2k+2} \leq i(\theta(r_1, r_2, \ldots, r_k)) \leq (2^{k-1} + 1) F_{n-k} + F_{n-k-1}$. The equality holds on the left if and only if $\theta(r_1, r_2, \ldots, r_k) \cong \theta(0, 2, 2, \ldots, 2, n - 2k - 4)$. The equality holds on the right if and only if $\theta(r_1, r_2, \ldots, r_k) \cong \theta(1, 1, 1, \ldots, 1, n - k - 1)$. This completes the proof.

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