The extremal generalized $\theta-$graphs with respect to Hosoya index

Guibin Ou[1], Zhongxun Zhu[2*]

[1] College of Science, Wuhan University of Science and Engineering ,Wuhan, 430073, P.R. China

[2] Faculty of Mathematics and Statistics, South Central University for Nationalities, Wuhan 430074, P.R. China

Abstract. For a graph G, the Hosoya index is defined as the total number of its matchings. A generalized $\theta-$graph $\theta(r_1, r_2, \cdots, r_k)$ consists of a pair of end vertices joined by k internally disjoint paths of lengths $r_1+1, r_2+1, \cdots, r_k+1$. Let Θ_n^k denote the set of generalized $\theta-$graphs with $k \geq 4$. In this paper, we obtain the smallest and the largest Hosoya index of the generalized $\theta-$graph in Θ_n^k, respectively. At the same time, we characterize the corresponding extremal graphs.

Keywords: Hosoya index ; generalized $\theta-$graph; extremal graph

AMS subject classification: 05C69, 05C05

1. Introduction

All graphs considered in this paper are finite, undirected and simple. Let $G=(V,E)$ be a graph on n vertices. Two edges of G are said to be independent if they are not adjacent in G. A $k-$matching of G is a set of k mutually independent edges. Denote by $Z(G,k)$ the number of $k-$matchings of G. For convenience, we regard the empty edge set as a matching. Then $Z(G,0)=1$ for any graph G. The *Hosoya index*, denoted by $z(G)$, is defined to be the total number of matchings, namely,

$$Z(G)=\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} Z(G,k).$$

The *Hosoya index* was introduced by Hosoya [1] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling

* Corresponding author. E-mail: zzxun73@mail.scuec.edu.cn (Z. Zhu)

The Project was Supported by the Special Fund for Basic Scientific Research of Central Colleges, South-Central University for Nationalities.

point, entropy or heat of vaporization are well studied. Especially, because of its important application to chemistry and physics, graphs with extremal Hosoya index are studied by numerous scholars. Now the research on Hosoya index mainly focuses on graphs with pendent vertices, e.g., trees, unicyclic graphs, bicyclic graphs and tricyclic graphs; see[2-11]. On the other hand, only a few papers reported the progrèss on Hosoya index of graphs without pendent vertices. In [12], Alameddine determined the sharp bounds for Hosoya index of a maximal outer planar graph. Gutman [13], Zhang and Tian [14] studied the Hosoya indices of hexagonal chains and catacondensed systems, respectively. Ren and Zhang [15] determined the minimal Hosoya index of double hexagonal chains. L. Tan and Z. Zhu [16] determined the sharp bounds for Hosoya index of $\theta-$graphs. Here we continue this line of research by investigating sharp upper and lower bounds of so called generalized $\theta-$graphs.

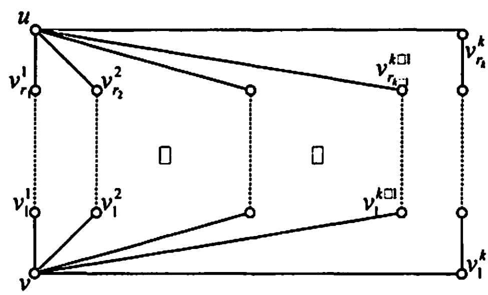

Figure 1: $\theta(r_1, r_2, \cdots, r_k)$

A generalized $\theta-$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). Since the case of $k=3$ has been discussed in [16], in this paper, we only consider the case of $k \geq 4$. We denote the set of $n-$vertex generalized $\theta-$graphs with $k \geq 4$ by Θ_n^k, that is, $\Theta_n^k = \{\theta(r_1, r_2, \cdots, r_k) : r_1 + r_2 + \cdots + r_k = n-2, r_1 \leq r_2 \leq \cdots \leq r_k, k \geq 4\}$.

In order to present our results, we introduce some notations and terminologies. For other undefined notations we refer to Bollobás [17]. If $W \subset V(G)$, we denote by $G-W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E \subset E(G)$, 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, C_n the path, the cycle on n vertices, respectively. Let $N(v) = \{u | uv \in E(G)\}$, $N[v] = N(v) \cup \{v\}$.

Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. Then $z(P_n) = F_n$. For convenience, we let $F_n = 0$ for $n < 0$. Note that $F_{n+m} = F_n F_m + F_{n-1} F_{m-1}$.

The following Lemma will be used in the proof of our main results repeatedly.

Lemma 1.1 ([13]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G - uv) + z(G - \{u, v\})$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G - v) + \sum_{u \in N(v)} z(G - \{u, v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

2. Graphs in Θ_n^k with minimal Hosoya index

We first consider the lower bound of generalized θ−graph in Θ_n^k with respect to the Hosoya index. Let

$$\begin{aligned} T_0 &= \theta(r_1, r_2, \cdots, r_k) - \{uv_{r_1}^1, \cdots, uv_{r_{k-1}}^{k-1}\}, \\ T_1 &= \theta(r_1, r_2, \cdots, r_k) - \{u, v_{r_1}^1\}, \\ T_i &= \theta(r_1, r_2, \cdots, r_k) - \{uv_{r_1}^1, \cdots, uv_{r_{i-1}}^{i-1}\} - \{u, v_{r_i}^i\}, i = 2, \cdots, k-1. \end{aligned}$$

Obviously, $T_i \cong \theta(r_1, r_2, \cdots, r_k) - \{u, v_{r_i}^i\}$ for $i = 1, \cdots, k-1$. By Lemma 1.1 (i, iii), we have

$$\begin{aligned} & z(\theta(r_1, r_2, \cdots, r_k)) \\ = \ & z(\theta(r_1, r_2, \cdots, r_k) - uv_{r_1}^1) + z(\theta(r_1, r_2, \cdots, r_k) - \{u, v_{r_1}^1\}) \\ = \ & z(\theta(r_1, r_2, \cdots, r_k) - \{uv_{r_1}^1, uv_{r_2}^2\}) + \\ & z(\theta(r_1, r_2, \cdots, r_k) - uv_{r_1}^1 - \{u, v_{r_2}^2\}) + z(\theta(r_1, r_2, \cdots, r_k) - \{u, v_{r_1}^1\}) \\ = \ & \cdots \\ = \ & z(\theta(r_1, r_2, \cdots, r_k) - \{uv_{r_1}^1, uv_{r_2}^2, \cdots, uv_{r_{k-1}}^{k-1}\}) + \\ & z(\theta(r_1, r_2, \cdots, r_k) - \{uv_{r_1}^1, \cdots, uv_{r_{k-2}}^{k-2}\} - \{u, v_{r_{k-1}}^{k-1}\}) + \cdots \\ & + z(\theta(r_1, r_2, \cdots, r_k) - uv_{r_1}^1 - \{u, v_{r_2}^2\}) + z(\theta(r_1, r_2, \cdots, r_k) - \{u, v_{r_1}^1\}) \\ = \ & \sum_{i=0}^{k-1} z(T_i), \end{aligned} \tag{2.1}$$

where

$$\begin{aligned}
& z(T_0) \\
= \ & z(T_0 - v) + \sum_{x \in N(v)} z(T_0 - \{v, x\}) \\
= \ & z(P_{r_1} \cup \cdots \cup P_{r_{k-1}} \cup P_{r_k+1}) + z(P_{r_1-1} \cup P_{r_2} \cup \cdots \cup P_{r_{k-1}} \cup P_{r_k+1}) \\
& + z(P_{r_1} \cup P_{r_2-1} \cup P_{r_3} \cup \cdots \cup P_{r_{k-1}} \cup P_{r_k+1}) + \cdots + \\
& z(P_{r_1} \cup P_{r_2} \cup \cdots \cup P_{r_{k-1}-1} \cup P_{r_k+1}) + z(P_{r_1} \cup \cdots \cup P_{r_{k-1}} \cup P_{r_k}) \\
= \ & F_{r_1} \cdots F_{r_{k-1}} F_{r_k+1} + F_{r_1-1} F_{r_2} \cdots F_{r_{k-1}} F_{r_k+1} + \\
& F_{r_1} F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}} F_{r_k+1} + \cdots + \\
& F_{r_1} F_{r_2} \cdots F_{r_{k-1}-1} F_{r_k+1} + F_{r_1} \cdots F_{r_{k-1}} F_{r_k}, \\
& z(T_1) \\
= \ & F_{r_1-1} F_{r_2} \cdots F_{r_k} + F_{r_1-2} F_{r_2} \cdots F_{r_k} + F_{r_1-1} F_{r_2-1} F_{r_3} \cdots F_{r_k} + \\
& F_{r_1-1} F_{r_2} F_{r_3-1} F_{r_4} \cdots F_{r_k} + \cdots + F_{r_1-1} F_{r_2} \cdots F_{r_{k-1}} F_{r_k-1}, \\
& z(T_2) \\
= \ & F_{r_1} F_{r_2-1} F_{r_3} \cdots F_{r_k} + F_{r_1-1} F_{r_2-1} F_{r_3} \cdots F_{r_k} + F_{r_1} F_{r_2-2} F_{r_3} \cdots F_{r_k} + \\
& F_{r_1} F_{r_2-1} F_{r_3-1} \cdots F_{r_k} + \cdots + F_{r_1} F_{r_2-1} F_{r_3} \cdots F_{r_k-1},
\end{aligned}$$

$\vdots$

$$\begin{aligned}
& z(T_{k-1}) \\
= \ & F_{r_1} F_{r_2} \cdots F_{r_{k-1}-1} F_{r_k} + F_{r_1-1} F_{r_2} \cdots F_{r_{k-1}-1} F_{r_k} \\
& + F_{r_1} F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}-1} F_{r_k} + \cdots + F_{r_1} F_{r_2} \cdots F_{r_{k-1}-2} F_{r_k} + \\
& F_{r_1} F_{r_2} \cdots F_{r_{k-1}-1} F_{r_k-1}. \qquad (2.2)
\end{aligned}$$

Lemma 2.1. *Let $\theta(r_1, r_2, \cdots, r_k) \in \Theta_n^k$ with $r_1 > 1$, then*

$$z(\theta(r_1, r_2, \cdots, r_k)) > z(\theta(1, r_2, \cdots, r_1 + r_k - 1)).$$

Proof. Let

$$\begin{aligned}
T_0' &= \theta(1, r_2, \cdots, r_1 + r_k - 1) - \{uv_{r_1}^1, \cdots, uv_{r_{k-1}}^{k-1}\}, \\
T_1' &= \theta(1, r_2, \cdots, r_1 + r_k - 1) - \{u, v_{r_1}^1\}, \\
T_i' &= \theta(1, r_2, \cdots, r_1 + r_k - 1) - \{uv_{r_1}^1, \cdots, uv_{r_{i-1}}^{i-1}\} - \{u, v_{r_i}^i\}, \\
& \quad i = 2, \cdots, k-1.
\end{aligned}$$

By Lemma 1.1, we have

$$z(\theta(1, r_2, \cdots, r_1 + r_k - 1)) = \sum_{i=0}^{k-1} z(T_i'), \qquad (2.3)$$

where

$$
\begin{aligned}
& z(T_0') \\
= \ & F_{r_2}\cdots F_{r_{k-1}}F_{r_1+r_k} + F_{r_2}\cdots F_{r_{k-1}}F_{r_1+r_k} + F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1+r_k} \\
& +\cdots + F_{r_2}\cdots F_{r_{k-1}-1}F_{r_1+r_k} + F_{r_2}\cdots F_{r_{k-1}}F_{r_1+r_k-1} \\
& z(T_1') \\
= \ & F_{r_2}\cdots F_{r_{k-1}}F_{r_1+r_k-1} + F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1+r_k-1} + \\
& F_{r_2}F_{r_3-1}F_{r_4}\cdots F_{r_{k-1}}F_{r_1+r_k-1} + \cdots + F_{r_2}\cdots F_{r_{k-1}}F_{r_1+r_k-2} \\
& z(T_2') \\
= \ & 2F_{r_2-1}F_{r_3}\cdots F_{r_1+r_k-1} + F_{r_2-2}F_{r_3}\cdots F_{r_1+r_k-1} + F_{r_2-1}F_{r_3-1}\cdots F_{r_1+r_k-1} \\
& +F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1}F_{r_1+r_k-1} + F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1+r_k-2} \\
\vdots \\
& z(T_{k-1}') \\
= \ & 2F_{r_2}\cdots F_{r_{k-2}}F_{r_{k-1}-1}F_{r_1+r_k-1} + F_{r_2-1}F_{r_3}\cdots F_{r_{k-2}}F_{r_{k-1}-1}F_{r_1+r_k-1} \\
& +\cdots + F_{r_2}\cdots F_{r_{k-2}-1}F_{r_{k-1}-1}F_{r_1+r_k-1} + F_{r_2}\cdots F_{r_{k-2}}F_{r_{k-1}-2}F_{r_1+r_k-1} \\
& +F_{r_2}\cdots F_{r_{k-2}}F_{r_{k-1}-1}F_{r_1+r_k-2}
\end{aligned} \tag{2.4}
$$

By (2.2) and (2.4), we have

$$
\begin{aligned}
& z(T_0) - z(T_0') \\
= \ & F_{r_2}\cdots F_{r_{k-1}}(F_{r_1}F_{r_k+1} - F_{r_1+r_k}) + F_{r_2}\cdots F_{r_{k-1}}(F_{r_1}F_{r_k+1} - F_{r_1+r_k}) + \\
& \{F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}(F_{r_1}F_{r_k+1} - F_{r_1+r_k}) + \cdots + \\
& F_{r_2}\cdots F_{r_{k-1}-1}(F_{r_1}F_{r_k+1} - F_{r_1+r_k})\} + F_{r_2}\cdots F_{r_{k-1}}(F_{r_1}F_{r_k+1} - F_{r_1+r_k-1}) \\
= \ & F_{r_2}\cdots F_{r_{k-1}}(F_{r_1-2}F_{r_k-1} - F_{r_1-2}F_{r_k} + F_{r_1-2}F_{r_k-2}) + \\
& \{F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-2}F_{r_k-1} + \cdots + F_{r_2}\cdots F_{r_{k-1}-1}F_{r_1-2}F_{r_k-1}\} \\
= \ & F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-2}F_{r_k-1} + \cdots + F_{r_2}\cdots F_{r_{k-1}-1}F_{r_1-2}F_{r_k-1} \\
& z(T_1) - z(T_1') \\
= \ & -(F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-2}F_{r_k-1} + \cdots + F_{r_2}\cdots F_{r_{k-1}-1}F_{r_1-2}F_{r_k-1}) \\
& z(T_2) - z(T_2') \\
= \ & F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}(F_{r_1}F_{r_k} - F_{r_1+r_k-1} + F_{r_1-1}F_{r_k} - F_{r_1+r_k-1} + F_{r_1}F_{r_k-1} \\
& -F_{r_1+r_k-2}) + (F_{r_2-2}F_{r_3}\cdots F_{r_{k-1}} + F_{r_2-1}F_{r_3-1}\cdots F_{r_{k-1}} + \cdots + \\
& F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1})F_{r_1-2}F_{r_k-2} \\
= \ & (F_{r_2-2}F_{r_3}\cdots F_{r_{k-1}} + F_{r_2-1}F_{r_3-1}\cdots F_{r_{k-1}} + \cdots + F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1}) \\
& F_{r_1-2}F_{r_k-2}
\end{aligned}
$$

$\vdots$

$$\begin{aligned} & z(T_{k-1}) - z(T'_{k-1}) \\ = & (F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1} + F_{r_2}F_{r_3-1}\cdots F_{r_{k-1}-1} + \cdots + F_{r_2}F_{r_3}\cdots F_{r_{k-1}-2}) \\ & F_{r_1-2}F_{r_k-2}. \end{aligned} \tag{2.5}$$

By (2.1),(2.3) and (2.5), we have

$$\begin{aligned} & z(\theta(r_1, r_2, \cdots, r_k)) - z(\theta(1, r_2, \cdots, r_1 + r_k - 1)) \\ = & \sum_{i=0}^{k-1} z(T_i) - \sum_{i=0}^{k-1} z(T'_i) \geq z(T_2) - z(T'_2) > F_{r_2-2}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-2}F_{r_k-2} \\ > & 0. \end{aligned}$$

Hence, we obtain the desirable result. □

Lemma 2.2. *If* $r_1, r_2, \cdots, r_i > 1$ *and* $i \geq 2$, *then* $z(\theta(\underbrace{1, \cdots, 1}_{i-1}, r_i, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_{i-1} - i + 1)) > z(\theta(\underbrace{1, \cdots, 1}_{i}, r_{i+1}, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_i - i))$.

Proof. Let

$$\begin{aligned} T_0^i &= \theta(\underbrace{1, \cdots, 1}_{i}, r_{i+1}, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_i - i) - \{uv_{r_1}^1, \cdots, uv_{r_{k-1}}^{k-1}\}, \\ T_1^i &= \theta(\underbrace{1, \cdots, 1}_{i}, r_{i+1}, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_i - i) - \{u, v_{r_1}^1\}, \\ T_j^i &= \theta(\underbrace{1, \cdots, 1}_{i}, r_{i+1}, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_i - i) - \{uv_{r_1}^1, \cdots, uv_{r_{j-1}}^{j-1}\} \\ & \quad -\{u, v_{r_j}^j\}, j = 2, \cdots, k-1. \end{aligned}$$

By Lemma 1.1, we have

$$z(\theta(\underbrace{1, \cdots, 1}_{i}, r_{i+1}, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_i - i)) = \sum_{j=0}^{k-1} z(T_j^i) \tag{2.6}$$

where

$$\begin{aligned} z(T_0^i) = & (i+1)F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i+1} + \\ & F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i+1} + \cdots + \\ & F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i+1} + F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} \end{aligned}$$

$$
\begin{aligned}
z(T_1^i) &= iF_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \cdots + \\
&\quad +F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i-1} \\
z(T_j^i) &= z(T_1^i), j = 2, \cdots, i, \\
z(T_{i+1}^i) &= (i+1)F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-2}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \cdots + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i-1}, \\
z(T_{i+2}^i) &= (i+1)F_{r_{i+1}}F_{r_{i+2}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}}F_{r_{i+2}-2}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i} + \cdots + \\
&\quad F_{r_{i+1}}F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i} \\
&\quad +F_{r_{i+1}}F_{r_{i+2}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_i-i-1}, \\
&\quad \vdots \\
z(T_{k-1}^i) &= (i+1)F_{r_{i+1}}F_{r_{i+2}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}}F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i} + \cdots + \\
&\quad F_{r_{i+1}}F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-2}F_{r_k+r_1+\cdots+r_i-i} + \\
&\quad F_{r_{i+1}}F_{r_{i+2}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_i-i-1}
\end{aligned}
$$

$$
z(\theta(\underbrace{1,\cdots,1}_{i-1}, r_i, \cdots, r_{k-1}, r_k + r_1 + \cdots + r_{i-1} - i + 1)) = \sum_{j=0}^{k-1} z(T_j^{i-1}), \tag{2.7}
$$

where

$$
\begin{aligned}
z(T_0^{i-1}) &= iF_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+2} + \\
&\quad F_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+2} + \cdots + \\
&\quad F_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+2} + \\
&\quad F_{r_i}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1}
\end{aligned}
$$

$$
\begin{aligned}
z(T_1^{i-1}) &= (i-1)F_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad \cdots + F_{r_i}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i} \\
z(T_j^{i-1}) &= z(T_1^{i-1}), j = 2, \cdots, i-1, \\
z(T_i^{i-1}) &= iF_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-2}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}-1}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \cdots + \\
&\quad F_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i}, \\
z(T_{i+1}^{i-1}) &= iF_{r_i}F_{r_{i+1}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i}F_{r_{i+1}-2}F_{r_{i+2}}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \cdots + \\
&\quad F_{r_i}F_{r_{i+1}-1}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i}F_{r_{i+1}-1}\cdots F_{r_{k-1}}F_{r_k+r_1+\cdots+r_{i-1}-i}, \\
&\quad \vdots \\
z(T_{k-1}^{i-1}) &= iF_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i-1}F_{r_{i+1}}F_{r_{i+2}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \cdots + \\
&\quad F_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}-2}F_{r_k+r_1+\cdots+r_{i-1}-i+1} + \\
&\quad F_{r_i}F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_k+r_1+\cdots+r_{i-1}-i}
\end{aligned}
$$

Then

$$
\begin{aligned}
&z(T_0^{i-1}) - z(T_0^i) \\
= \;& (i-1)F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i} + \\
& F_{r_{i+1}-1}\cdots F_{r_{k-1}}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i} \\
& + \cdots + F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i}; \\
&z(T_i^{i-1}) - z(T_i^i) \\
= \;& (1-i)F_{r_{i+1}}\cdots F_{r_{k-1}}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i} - \\
& F_{r_{i+1}-1}\cdots F_{r_{k-1}}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i} \\
& - \cdots - F_{r_{i+1}}\cdots F_{r_{k-1}-1}F_{r_i-2}F_{r_k+r_1+\cdots+r_{i-1}-i}.
\end{aligned}
$$

And for $j = 1, \cdots, i-1$, we have

$$\begin{aligned}
& z(T_j^{i-1}) - z(T_j^i) \\
= \;& (i-2)F_{r_{i+1}} \cdots F_{r_{k-1}} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} + \\
& F_{r_{i+1}-1} \cdots F_{r_{k-1}} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} \\
& + \cdots + F_{r_{i+1}} \cdots F_{r_{k-1}-1} F_{r_{i-2}} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1},
\end{aligned}$$

for $j = i+1, \cdots, k-1$, we have

$$\begin{aligned}
& z(T_{i+1}^{i-1}) - z(T_{i+1}^i) \\
= \;& (i-1)F_{r_{i+1}-1} \cdots F_{r_{k-1}} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} + \\
& F_{r_{i+1}-1} \cdots F_{r_{k-1}} F_{r_i - 1} F_{r_k + r_1 + \cdots + r_{i-1} - i + 1} + \\
& F_{r_{i+1}-2} F_{r_{i+2}} \cdots F_{r_{k-1}} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} + \cdots + \\
& F_{r_{i+1}-1} \cdots F_{r_{k-1}-1} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1}, \\
& \vdots \\
& z(T_{k-1}^{i-1}) - z(T_{k-1}^i) \\
= \;& (i-1)F_{r_{i+1}} \cdots F_{r_{k-1}-1} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} + \\
& F_{r_{i+1}} \cdots F_{r_{k-1}-1} F_{r_i - 1} F_{r_k + r_1 + \cdots + r_{i-1} - i + 1} + \\
& F_{r_{i+1}-1} F_{r_{i+2}} \cdots F_{r_{k-1}-1} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} + \cdots + \\
& F_{r_{i+1}} \cdots F_{r_{k-1}-2} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1}.
\end{aligned}$$

Hence

$$\begin{aligned}
\sum_{j=0}^{k-1} z(T_j^{i-1}) - \sum_{j=0}^{k-1} z(T_j^i) \;&\geq\; z(T_1^{i-1}) - z(T_1^i) \\
&\geq\; F_{r_{i+1}-1} \cdots F_{r_{k-1}} F_{r_i - 2} F_{r_k + r_1 + \cdots + r_{i-1} - i - 1} > 0,
\end{aligned}$$

as desired. □

Repeated using Lemma 2.1 and 2.2, we have

Corollary 2.3. *Let $\theta(r_1, r_2, \cdots, r_k) \in \Theta_n^k$ with $r_1 \geq 1$, then*

$$z(\theta(r_1, r_2, \cdots, r_k)) \geq z(\theta(1, 1, \cdots, 1, n-k-1)),$$

the equality holds if and only if $\theta(r_1, r_2, \cdots, r_k) \cong \theta(1, 1, \cdots, 1, n-k-1)$.

Lemma 2.4. *If $r_1 \geq 1$, then $z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k)) > z(\theta(r_1, r_2, \cdots, r_k))$.*

Proof. Let

$$\begin{aligned}
A_0 &= \theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{uv, uv_{r_2}^2, \cdots, uv_{r_{k-1}}^{k-1}\}, \\
A_1 &= \theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{u, v\}, \\
A_i &= \theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{uv, uv_{r_2}^2, \cdots, uv_{r_{i-1}}^{i-1}\} - \{u, v_{r_i}^i\},
\end{aligned}$$

$i = 2, \cdots, k-1$.

By Lemma 1.1, we have

$$\begin{aligned}
& z\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k)) \\
= \; & z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - uv) + z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{u, v\}) \\
= \; & z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{uv, uv_{r_2}^2\}) + z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) \\
& -uv - \{u, v_{r_2}^2\}) + z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{u, v\}) \\
= \; & \cdots \\
= \; & z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{uv, uv_{r_2}^2, \cdots, uv_{r_{k-1}}^{k-1}\}) \\
& + z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - \{uv, uv_{r_2}^2, \cdots, uv_{r_{k-2}}^{k-2}\} - \{u, v_{r_{k-1}}^{k-1}\}) + \cdots \\
& z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k) - uv - \{u, v_{r_2}^2\}) + z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k \\
& -\{u, v\}) \\
= \; & \sum_{i=0}^{k-1} z(A_i),
\end{aligned}$$

where

$$\begin{aligned}
z(A_0) &= F_{r_2} \cdots F_{r_{k-1}} F_{r_1+r_k+1} + F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}} F_{r_1+r_k+1} + \cdots + \\
& \quad F_{r_2} \cdots F_{r_{k-1}-1} F_{r_1+r_k+1} + F_{r_2} \cdots F_{r_{k-1}} F_{r_1+r_k}, \\
z(A_1) &= F_{r_2} \cdots F_{r_{k-1}} F_{r_1+r_k}, \\
z(A_2) &= F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}} F_{r_1+r_k} + F_{r_2-2} F_{r_3} \cdots F_{r_{k-1}} F_{r_1+r_k} + \\
& \quad F_{r_2-1} F_{r_3-1} \cdots F_{r_{k-1}} F_{r_1+r_k} \\
& \quad + \cdots + F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}-1} F_{r_1+r_k} + F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}} F_{r_1+r_k-1}, \\
& \vdots \\
z(A_{k-1}) &= F_{r_2} F_{r_3} \cdots F_{r_{k-1}-1} F_{r_1+r_k} + F_{r_2-1} F_{r_3} \cdots F_{r_{k-1}-1} F_{r_1+r_k} + \\
& \quad F_{r_2} F_{r_3-1} \cdots F_{r_{k-1}-1} F_{r_1+r_k} \\
& \quad + \cdots + F_{r_2} F_{r_3} \cdots F_{r_{k-1}-2} F_{r_1+r_k} + F_{r_2} F_{r_3} \cdots F_{r_{k-1}-1} F_{r_1+r_k-1}.
\end{aligned}$$

Then

$$\begin{aligned}
& z(A_0) - z(T_0) \\
= \ & F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k} + F_{r_2}F_{r_3-1}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k} + \cdots + \\
& F_{r_2}F_{r_3}\cdots F_{r_{k-1}-1}F_{r_1-1}F_{r_k} \\
& z(A_1) - z(T_1) \\
= \ & -(F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k} + F_{r_2}F_{r_3-1}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k} \\
& + \cdots + F_{r_2}F_{r_3}\cdots F_{r_{k-1}-1}F_{r_1-1}F_{r_k})
\end{aligned}$$

$$\begin{aligned}
& z(A_2) - z(T_2) \\
= \ & F_{r_2-2}F_{r_3}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k-1} + F_{r_2-1}F_{r_3-1}F_{r_4}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k-1} \\
& + \cdots + F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1}F_{r_1-1}F_{r_k-1}
\end{aligned}$$

$\vdots$

$$\begin{aligned}
& z(A_{k-1}) - z(T_{k-1}) \\
= \ & F_{r_2-1}F_{r_3}\cdots F_{r_{k-1}-1}F_{r_1-1}F_{r_k-1} + F_{r_2}F_{r_3-1}F_{r_4}\cdots F_{r_{k-1}-1}F_{r_1-1}F_{r_k-1} \\
& + \cdots + F_{r_2}F_{r_3}\cdots F_{r_{k-1}-2}F_{r_1-1}F_{r_k-1}.
\end{aligned}$$

$$\begin{aligned}
& z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k)) - z(\theta(r_1, r_2, \cdots, r_k)) \\
= \ & \sum_{i=0}^{k-1} A_i - \sum_{i=0}^{k-1} T_i \geq z(A_2) - z(T_2) \geq F_{r_2-1}F_{r_3-1}F_{r_4}\cdots F_{r_{k-1}}F_{r_1-1}F_{r_k-1} \\
> \ & 0.
\end{aligned}$$

Then $z(\theta(0, r_2, \cdots, r_{k-1}, r_1 + r_k)) > z(\theta(r_1, r_2, \cdots, r_k))$. As desired. □

By direct calculation,

$$\begin{aligned}
& z(\theta(1, 1, \cdots, 1, n-k-1)) \\
= \ & kF_{n-k} + F_{n-k-1} + (k-1)[(k-1)F_{n-k-1} + F_{n-k-2}]. \quad (2.8)
\end{aligned}$$

By (2.8), Corollary 2.3 and Lemma 2.4, we have

Theorem 2.5. *Let $\theta(r_1, r_2, \cdots, r_k) \in \Theta_n^k$, then*

$$z(\theta(r_1, r_2, \cdots, r_k)) \geq kF_{n-k} + F_{n-k-1} + (k-1)[(k-1)F_{n-k-1} + F_{n-k-2}],$$

the equality holds if and only if $\theta(r_1, r_2, \cdots, r_k) \cong \theta(1, 1, \cdots, 1, n-k-1)$.

3. Graphs in Θ_n^k with maximal Hosoya index

Now, we consider the upper bound of generalized θ–graphs with respect to the Hosoya index.

Lemma 3.1. *If* $r_2 \geq 3$, *then* $z(\theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2)) > z(\theta(0,r_2,\cdots,r_1+r_k))$.

Proof. Let

$$\begin{aligned}
B_0 &= \theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2)-\{uv,uv_{r_2}^2,\cdots,uv_{r_{k-1}}^{k-1}\},\\
B_1 &= \theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2)-\{u,v\},\\
B_i &= \theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2)-\{uv,uv_{r_2}^2,\cdots,uv_{r_{i-1}}^{i-1}\}-\\
&\quad \{u,v_{r_i}^i\}, i=2,\cdots,k-1.
\end{aligned}$$

By Lemma 1.1, we have

$$z(\theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2))=\sum_{i=0}^{k-1}z(B_i)$$

By Lemma 2.4, we have

$$\begin{aligned}
& z(B_0)-z(A_0)\\
=\ & F_{r_3}\cdots F_{r_{k-1}}(F_2F_{r_1+r_2+r_k-1}-F_{r_2}F_{r_1+r_k+1})+\\
& F_{r_3}\cdots F_{r_{k-1}}(F_1F_{r_1+r_2+r_k-1}-F_{r_2-1}F_{r_1+r_k+1})\\
& F_{r_3-1}\cdots F_{r_{k-1}}(F_2F_{r_1+r_2+r_k-1}-F_{r_2}F_{r_1+r_k+1})+\cdots\\
& +F_{r_3}\cdots F_{r_{k-1}-1}(F_2F_{r_1+r_2+r_k-1}-F_{r_2}F_{r_1+r_k+1})+\\
& F_{r_3}\cdots F_{r_{k-1}}(F_2F_{r_1+r_2+r_k-2}-F_{r_2}F_{r_1+r_k})\\
=\ & (F_{r_3-1}\cdots F_{r_{k-1}}+\cdots+F_{r_3}\cdots F_{r_{k-1}-1})F_{r_2-3}F_{r_1+r_k-2}\\
& z(B_2)-z(A_2)\\
=\ & -(F_{r_3-1}\cdots F_{r_{k-1}}+\cdots+F_{r_3}\cdots F_{r_{k-1}-1})F_{r_2-3}F_{r_1+r_k-2}\\
& z(B_1)-z(A_1)\\
=\ & F_{r_3}\cdots F_{r_{k-1}}F_{r_2-3}F_{r_1+r_k-3}\\
& \vdots\\
& z(B_{k-1})-z(A_{k-1})\\
=\ & (F_{r_3-1}F_{r_4}\cdots F_{r_{k-1}-1}+F_{r_3}F_{r_4-1}\cdots F_{r_{k-1}-1}+\cdots+F_{r_3}\cdots F_{r_{k-1}-2})\\
& F_{r_2-3}F_{r_1+r_k-3}
\end{aligned}$$

Hence,

$$\begin{aligned} & z(\theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_k-2)) - z(\theta(0,r_2,\cdots,r_1+r_k)) \\ = & \sum_{i=0}^{k-1}(z(B_i)-z(A_i)) \geq z(B_1)-z(A_1) > F_{r_3}\cdots F_{r_{k-1}}F_{r_2-3}F_{r_1+r_k-3} \\ > & \ 0, \end{aligned}$$

as desired. □

Similar to Lemma 3.1, we have

Lemma 3.2. *If* $r_1,\cdots,r_{i+1}\geq 3, i\geq 1$, *then*

$$\begin{aligned} & z(\theta(0,\underbrace{2,\cdots,2}_{i},r_{i+2},\cdots,r_{k-1},r_1+r_2+\cdots+r_{i+1}+r_k-2i)) \\ & > z(\theta(0,\underbrace{2,\cdots,2}_{i-1},r_{i+1},\cdots,r_{k-1},r_1+r_2+\cdots+r_i+r_k-2i+2)). \end{aligned}$$

By Lemma 3.2, we have

$$\begin{aligned} & z(\theta(0,2,r_3,\cdots,r_{k-1},r_1+r_2+r_3+r_k-2)) \\ < & \ z(\theta(0,2,2,r_4,\cdots,r_{k-1},r_1+r_2+r_3+r_k-4)) \\ < & \ \cdots < z(\theta(0,2,\cdots,2,n-2k+2)) \end{aligned} \tag{3.9}$$

Lemma 3.3. *If* $r_{i+2}\geq 3, i\geq 1$, *then*

$$\begin{aligned} & z(\theta(0,\underbrace{1,\cdots,1}_{i},2,r_{i+3},\cdots,r_{k-1},r_1+r_2+\cdots+r_{i+2}+r_k-i-2)) \\ & > z(\theta(0,\underbrace{1,\cdots,1}_{i},r_{i+2},r_{i+3},\cdots,r_{k-1},r_1+r_2+\cdots+r_i+r_{i+1}+r_k-i)). \end{aligned}$$

Proof. Let

$$\begin{aligned} D &= \theta(0,\underbrace{1,\cdots,1}_{i},2,r_{i+3},\cdots,r_{k-1},r_1+r_2+\cdots+r_{i+2}+r_k-i-2) \\ D_0 &= D-\{uv,uv_{r_2}^2,\cdots,uv_{r_{k-1}}^{k-1}\}, \\ D_1 &= D-\{u,v\}, \\ D_i &= D-\{uv,uv_{r_2}^2,\cdots,uv_{r_{i-1}}^{i-1}\}-\{u,v_{r_i}^i\}, i=2,\cdots,k-1. \end{aligned}$$

By Lemma 1.1, we have

$$z(\theta(0,\underbrace{1,\cdots,1}_{i},2,r_{i+3},\cdots,r_{k-1},r_1+r_2+\cdots+r_{i+2}+r_k-i-2)) = \sum_{i=0}^{k-1} z(D_i),$$

where

$$
\begin{aligned}
& z(D_0) \\
= \; & (i+1)F_2F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-1} + \\
& F_1F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-1} + \\
& F_2F_{r_{i+3}-1}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-1} + \cdots + \\
& F_2F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-1} \\
& +F_2F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} \\
& z(D_1) \\
= \; & F_2F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} \\
& z(D_2) \\
= \; & iF_2F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \\
& F_1F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \\
& F_2F_{r_{i+3}-1}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \cdots + \\
& F_2F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} \\
& +F_2F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-3} \\
& \vdots \\
& z(D_{k-1}) \\
= \; & (i+1)F_2F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \\
& F_1F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} \\
& +F_2F_{r_{i+3}-1}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \cdots + \\
& F_2F_{r_{i+3}}\cdots F_{r_{k-1}-2}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-2} + \\
& F_2F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+2}+r_k-i-3}
\end{aligned}
$$

Similarly, let

$$
\begin{aligned}
E &= \theta(0, \underbrace{1, \cdots, 1}_{i}, r_{i+2}, r_{i+3}, \cdots, r_{k-1}, r_1 + r_2 + \cdots + r_{i+1} + r_k - i) \\
E_0 &= E - \{uv, uv_{r_2}^2, \cdots, uv_{r_{k-1}}^{k-1}\}, \\
E_1 &= E - \{u, v\}, \\
E_i &= E - \{uv, uv_{r_2}^2, \cdots, uv_{r_{i-1}}^{i-1}\} - \{u, v_{r_i}^i\}, i = 2, \cdots, k-1.
\end{aligned}
$$

By Lemma 1.1, we have

$$z(\theta(0,\underbrace{1,\cdots,1}_{i},r_{i+2},r_{i+3},\cdots,r_{k-1},r_1+r_2+\cdots+r_{i+1}+r_k-i))=\sum_{i=0}^{k-1}z(E_i),$$

where

$$\begin{aligned}
& z(E_0) \\
= \; & (i+1)F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i+1}+ \\
& F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i+1}+ \\
& F_{r_{i+2}}F_{r_{i+3}-1}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i+1}+\cdots+ \\
& F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i+1}+ \\
& F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i} \\
& z(E_1) \\
= \; & F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i} \\
& z(E_2) \\
= \; & iF_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+ \\
& F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+ \\
& F_{r_{i+2}}F_{r_{i+3}-1}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+\cdots+ \\
& F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+ \\
& F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-1} \\
& \vdots \\
& z(E_{k-1}) \\
= \; & (i+1)F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+ \\
& F_{r_{i+2}-1}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i} \\
& +F_{r_{i+2}}F_{r_{i+3}-1}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i}+\cdots+ \\
& F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-2}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i} \\
& +F_{r_{i+2}}F_{r_{i+3}}\cdots F_{r_{k-1}-1}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-1}
\end{aligned}$$

So

$$\begin{aligned}
z(D_0)-z(E_0) &= (F_{r_{i+3}-1}\cdots F_{r_{k-1}}+\cdots+F_{r_3}\cdots F_{r_{k-1}-1}) \\
& \quad F_{r_{i+2}-3}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-2} \\
z(D_2)-z(E_2) &= -(F_{r_{i+3}-1}\cdots F_{r_{k-1}}+\cdots+F_{r_3}\cdots F_{r_{k-1}-1}) \\
& \quad F_{r_{i+2}-3}F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-2}
\end{aligned}$$

$$
\begin{aligned}
z(D_1) - z(E_1) &= F_{r_{i+3}-1}\cdots F_{r_{k-1}} F_{r_{i+2}-3} F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-3} \\
&\vdots \\
z(D_{k-1}) - z(E_{k-1}) & \\
&= iF_{r_{i+3}-1} F_{r_{i+4}}\cdots F_{r_{k-1}} F_{r_{i+2}-3} F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-3} \\
&\quad +(F_{r_{i+3}-1} F_{r_{i+4}}\cdots F_{r_{k-1}} + \cdots + F_{r_3}\cdots F_{r_{k-1}-2}) \\
&\quad F_{r_{i+2}-3} F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-3}
\end{aligned}
$$

Hence

$$
\begin{aligned}
& \sum_{i=0}^{k-1} (z(D_i) - z(E_i)) \geq z(D_1) - z(E_1) \\
> \;& F_{r_{i+3}-1}\cdots F_{r_{k-1}} F_{r_{i+2}-3} F_{r_1+r_2+\cdots+r_{i+1}+r_k-i-3} > 0,
\end{aligned}
$$

as desired. □

Similar to Lemma 3.3, we have

Lemma 3.4. *If* $r_{i+j+2} \geq 3, i, j \geq 1$, *then*

$$
\begin{aligned}
& z(\theta(0, \underbrace{1, \cdots, 1}_{i}, \underbrace{2, \cdots, 2}_{j+1}, r_{i+j+3}, \cdots, r_{k-1}, \\
& r_1 + r_2 + \cdots + r_{i+j+2} + r_k - i - 2j - 2)) \\
> \;& z(\theta(0, \underbrace{1, \cdots, 1}_{i}, \underbrace{2, \cdots, 2}_{j}, r_{i+j+2}, \cdots, r_{k-1}, \\
& r_1 + r_2 + \cdots + r_{i+j+1} + r_k - i - 2j)).
\end{aligned}
$$

Remark: In order to find the upper bound on Hosoya index of graph in Θ_n^k, by (3.9), Lemma 3.1, 3.3 and 3.4, it suffices to determine

$$
\max\{z(\theta(0,2,\cdots,2,n-2k+2)), z(\theta(0,1,2,\cdots,2,n-2k+3)),
$$

$$
z(\theta(0,1,1,2,\cdots,2,n-2k+4)), \cdots, z(\theta(0,1,\cdots,1,n-k))\}.
$$

Lemma 3.5.

$$
\begin{aligned}
& z(\theta(0, \underbrace{1, \cdots, 1}_{i}, \underbrace{2, \cdots, 2}_{k-i-2}, n-2k+i+2)) \\
> \;& z(\theta(0, \underbrace{1, \cdots, 1}_{i+1}, \underbrace{2, \cdots, 2}_{k-i-3}, n-2k+i+3)).
\end{aligned}
$$

Proof. Let

$$
\begin{aligned}
W &= \theta(0,\underbrace{1,\cdots,1}_{i},\underbrace{2,\cdots,2}_{k-i-2},n-2k+i+2) \\
W_0 &= F-\{uv,uv_{r_2}^2,\cdots,uv_{r_{k-1}}^{k-1}\}, \\
W_1 &= F-\{u,v\}, \\
W_i &= F-\{uv,uv_{r_2}^2,\cdots,uv_{r_{i-1}}^{i-1}\}-\{u,v_{r_i}^i\}, i=2,\cdots,k-1.
\end{aligned}
$$

By Lemma 1.1, we have

$$
z(\theta(0,\underbrace{1,\cdots,1}_{i},\underbrace{2,\cdots,2}_{k-i-2},n-2k+i+2))=\sum_{i=0}^{k-1}z(F_i),
$$

where

$$
\begin{aligned}
z(W_0) &= (i+1)2^{k-i-2}F_{n-2k+i+3}+(k-i-2)2^{k-i-3}F_{n-2k+i+5}+ \\
&\quad 2^{k-i-2}F_{n-2k+i+2}, \\
z(W_1) &= 2^{k-i-2}F_{n-2k+i+2} \\
z(W_2) &= i2^{k-i-2}F_{n-2k+i+2}+(k-i-2)2^{k-i-3}F_{n-2k+i+4}+ \\
&\quad 2^{k-i-2}F_{n-2k+i+1}, \\
z(W_j) &= z(F_2), j=3,\cdots,i+1, \\
z(W_{i+2}) &= (i+2)2^{k-i-3}F_{n-2k+i+2}+(k-i-3)2^{k-i-4}F_{n-2k+i+2}+ \\
&\quad 2^{k-i-3}F_{n-2k+i+1}, \\
z(W_j) &= z(F_2), j=i+2,\cdots,k-1.
\end{aligned}
$$

Similarly, let

$$
\begin{aligned}
H &= \theta(0,\underbrace{1,\cdots,1}_{i+1},\underbrace{2,\cdots,2}_{k-i-3},n-2k+i+3) \\
H_0 &= H-\{uv,uv_{r_2}^2,\cdots,uv_{r_{k-1}}^{k-1}\}, \\
H_1 &= H-\{u,v\}, \\
H_i &= H-\{uv,uv_{r_2}^2,\cdots,uv_{r_{i-1}}^{i-1}\}-\{u,v_{r_i}^i\}, i=2,\cdots,k-1.
\end{aligned}
$$

By Lemma 1.1, we have

$$
z(\theta(0,\underbrace{1,\cdots,1}_{i+1},\underbrace{2,\cdots,2}_{k-i-3},n-2k+i+3))=\sum_{i=0}^{k-1}z(H_i),
$$

where

$$
\begin{aligned}
z(H_0) &= (i+2)2^{k-i-3}F_{n-2k+i+4} + (k-i-3)2^{k-i-4}F_{n-2k+i+4} + \\
&\quad 2^{k-i-3}F_{n-2k+i+3}, \\
z(H_1) &= 2^{k-i-3}F_{n-2k+i+3} \\
z(H_2) &= (i+1)2^{k-i-3}F_{n-2k+i+3} + (k-i-3)2^{k-i-4}F_{n-2k+i+3} + \\
&\quad 2^{k-i-3}F_{n-2k+i+2}, \\
z(H_j) &= z(H_2), j = 3, \cdots, i+2, \\
z(H_{i+3}) &= (i+3)2^{k-i-4}F_{n-2k+i+3} + (k-i-4)2^{k-i-5}F_{n-2k+i+3} + \\
&\quad 2^{k-i-4}F_{n-2k+i+2}, \\
z(H_j) &= z(H_2), j = i+2, \cdots, k-1.
\end{aligned}
$$

So

$$
\begin{aligned}
z(W_0) - z(H_0) &= i2^{k-i-3}F_{n-2k+i+3} + (k-i-3)2^{k-i-4}F_{n-2k+i} \\
z(W_1) - z(H_1) &= 2^{k-i-3}F_{n-2k+i}
\end{aligned}
$$

For $j = 2, \cdots, i+1$,

$$
\begin{aligned}
z(W_j) - z(H_j) &= (i+1)2^{k-i-3}F_{n-2k+i+1} + \\
&\quad (k-i-3)2^{k-i-4}F_{n-2k+i} + 2^{k-i-3}F_{n-2k+i-1}, \\
z(W_{i+2}) - z(H_{i+2}) &= -(i2^{k-i-3}F_{n-2k+i+3} + (k-i-3)2^{k-i-4}F_{n-2k+i})
\end{aligned}
$$

For $j = i+3, \cdots, k-1$,

$$
z(W_j) - z(H_j) = (i+1)2^{k-i-4}F_{n-2k+i+2} + (k-i-4)2^{k-i-5}F_{n-2k+i}.
$$

Hence

$$
\sum_{i=0}^{k-1}(z(W_i) - z(H_i)) \geq z(W_1) - z(H_1) = 2^{k-i-3}F_{n-2k+i} > 0,
$$

as desired. □

Using Lemma 3.5 repeatedly, we have

$$
\begin{aligned}
& \max\{z(\theta(0,2,\cdots,2,n-2k+2)), z(\theta(0,1,2,\cdots,2,n-2k+3)), \\
& z(\theta(0,1,1,2,\cdots,2,n-2k+4)), \cdots, z(\theta(0,1,\cdots,1,n-k))\} \\
= \; & z(\theta(0,2,\cdots,2,n-2k+2)). \qquad (3.10)
\end{aligned}
$$

By direct calculation,

$$\begin{aligned}
& z(\theta(0,2,\cdots,2,n-2k+2)) \\
= \; & k\cdot 2^{k-3}F_{n-2k+3}+(k^2-k+6)\cdot 2^{k-4}F_{n-2k+2}+ \\
& (k-2)\cdot 2^{k-3}F_{n-2k+1}.
\end{aligned} \tag{3.11}$$

Hence, by (3.10), (3.11) and **Remark**, we have

Theorem 3.6. *Let $\theta(r_1,r_2,\cdots,r_k)\in\Theta_n^k$, then $z(\theta(r_1,r_2,\cdots,r_k))\leq k\cdot 2^{k-3}F_{n-2k+3}+(k^2-k+6)\cdot 2^{k-4}F_{n-2k+2}+(k-2)\cdot 2^{k-3}F_{n-2k+1}$, the equality holds if and only if $\theta(r_1,r_2,\cdots,r_k)\cong\theta(0,2,\cdots,2,n-2k+2)$.*

References

[1] H. Hosoya, Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Jpn. 44(1971)2332-2339.

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

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

[4] H. Q. Liu, X. Yan and Z. Yan, On the Merrifield-Simmons indices and Hosoya indices of trees with a prescribed diameter, MATCH Commun. Math. Comput. Chem., 57(2007)371-384.

[5] X. Li, Z. Li, L. Wang, The inverse problems for some topological indices in combinatorial chemistry, J. Comput. Biol. 10 (2003) 47-55.

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

[7] H. Q. Liu and M. Lu, A unified approach to extremal cacti for different indices, MATCH Commun. Math. Comput. Chem., 58(2007)193-204.

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

[9] S. Wagner, Extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index. MATCH Commun. Math. Comput. Chem. 57 (2007)221–233.

[10] H. Hua, Minimizing a class of unicyclic graphs by means of Hosoya index, Mathematical and Computer Modelling, 48 (2008) 940-948.

[11] S. Li, X. Li, Z. Zhu, Hosoya indices of bicyclic graphs, Croat. Chem. Acta., 82(3) 2009 641-647.

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

[13] I. Gutman, Extremal hexagonal chains, J. Math. Chem. 12 (1993) 197-210.
[14] L. Zhang, F. Tian, Extremal catacondensed benzenoids. J. Math. Chem. 34(1-2) (2003) 111-122.
[15] H. Ren, F. Zhang, Double hexagonal chains with maximal Hosoya index and minimal Merrifield-Simmons index, J. Math. Chem. 42(2) (2007) 679-690.
[16] L. Tan, Z. Zhu, The extremal $\theta-$graphs with respect to Hosoya index and Merrifield-Simmons index, MATCH Commun. Math. Comput. Chem. 63 (2010) 789-798.
[17] B. Bollobás, Modern Graph Theory (Springer-Verlag, 1998).