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The Merrifield-Simmons Indices and Hosoya Indices of Trees with a Given Maximum Degree

Xuezheng LV[a*] **Aimei YU**[b†]

[a]Department of Mathematics, Renmin University of China, Beijing 100872, China.

[b] Department of Mathematics, Beijing Jiaotong University, Beijing 100044, China.

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Abstract

The Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph and the Hosoya index of a graph is defined as the total number of the matchings of the graph. Let $\mathcal{T}(n, \Delta)$ denote the set of trees with order n and maximum degree Δ. We present a conjecture on the structure of the tree in $\mathcal{T}(n, \Delta)$ with maximal Merrifield-Simmons index or minimal Hosoya index, and verify it for $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq n-2$.

1. Introduction

Let G be a graph on n vertices. Two vertices of G are said to be independent if they are not adjacent in G. A k-independent set of G is a set of k mutually independent vertices. Denote by $i(G, k)$ the number of the k-independent sets of G. For convenience, we regard the empty vertex set as 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 $i(G) = \sum_{k=0}^{n} i(G, k)$. So $i(G)$ is equal to the total number of the independent sets of G. Similarly, 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 the k-matchings of G. For

*email: xzlv@ruc.edu.cn

†email: yuaimeimath@yeah.net. Partially supported by the fund of Beijing Jiaotong University, No. 2005RC027

convenience, we regard the empty edge set as a matching. Then $z(G,0)=1$ for any graph G. The *Hosoya index* of G, denoted by $z(G)$, is defined as $z(G)=\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G,k)$. Obviously, $z(G)$ is equal to the total number of matchings of G.

The Merrifield-Simmons index was introduced in 1982 in a paper of Prodinger and Tichy [17], although it is called Fibonacci number of a graph there. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [15]. There Merrifield and Simmons showed the correlation between this index and boiling points. Now there have been many papers studying the Merrifield-Simmons index (see [1, 8, 13, 16, 17],[19]-[22],[24, 25]). The Hosoya index of a graph was introduced by Hosoya in 1971 [11] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures ([15, 18]). Since then, many authors have investigated the Hosoya index (e.g., see [3]-[10], [12],[18]-[22],[24, 25]).

For Merrifield-Simmons index and Hosoya index, a direction is to determine the graph with extremal index in a given class of graphs. Here we consider the trees with n vertices and given maximum degree. Let $\mathcal{T}(n,\Delta)$ be the set of all the trees with n vertices and maximum degree Δ. Denote by T^* the tree in $\mathcal{T}(n,\Delta)$ such that $i(T)\le i(T^*)$ or $z(T)\ge z(T^*)$ for any $T\in\mathcal{T}(n,\Delta)$. In other words, T^* has the maximal Merrifield-Simmons index or minimal Hosoya index among all the trees with n vertices and maximum degree Δ. In this paper, we present a conjecture on the structure of T^*, and verify it for $\lceil \frac{n+1}{3} \rceil \le \Delta \le n-2$.

In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to [2]. 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 $\bigcup_{i=1}^{t} G_i$. For a vertex v of G, we denote $N_G[v]=\{v\}\cup\{\ u\mid uv\in E(G)\}$.

2. Lemmas and results

According to the definitions of the Merrifield-Simmons index and Hosoya index, we immediately get the following results.

Lemma 2.1 *Let G be a graph and uv be an edge of G. Then*

(1) $i(G) = i(G - uv) - i(G - (N_G[u] \cup N_G[v]))$,

(2) **(see [9])** $z(G) = z(G - uv) + z(G - \{u, v\})$.

Lemma 2.2 (see [9]) *Let v be a vertex of G. Then*

(1) $i(G) = i(G - v) + i(G - N_G[v])$,

(2) $z(G) = z(G - v) + \sum_u z(G - \{u, v\})$, *where the summation extends over all vertices adjacent to v.*

In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $i(G) = i(G - v) + i(G - \{u, v\})$ and $z(G) = z(G - v) + z(G - \{u, v\})$.

From Lemma 2.1, if uv is an edge of G, then $z(G) > z(G - uv)$. From Lemma 2.2, if v is a vertex of G, then $i(G) > i(G - v)$. Moreover, if G is a graph with at least one edge, then $z(G) > z(G - v)$.

Lemma 2.3 (see [9]) *If $G_1, G_2, \cdots, G_t$ are the components of a graph G, we have*

(1) $i(G) = \prod_{i=1}^{t} i(G_i)$,

(2) $z(G) = \prod_{i=1}^{t} z(G_i)$.

For a vertex v of a tree T, if $d_T(v) \geq 2$, we call v an internal vertex of T. Otherwise we call v a pendent vertex. Recall that T^* is the tree with maximal Merrifield-Simmons index or minimal Hosoya index in $\mathcal{T}(n, \Delta)$. Now we show T^* has the properties shown in the following two lemmas.

Lemma 2.4 *There are no two interval vertices u, v in T^* such that $d(u) < \Delta$ and $d(v) < \Delta$.*

Proof. We show the result by contradiction. Assume u and v are two internal vertices of T^* such that $d(u) = k+1 < \Delta$ and $d(v) = s+1 < \Delta$. Then T^* can be seen as the graph shown in Fig. 1, where X_i and Y_j are the subtrees of T^* with root x_i $(1 \leq i \leq k)$ and y_j $(1 \leq j \leq s)$, respectively, and T_1 is the component that join u and v together. Note that $ux_i \in E(T^*)$, $vy_j \in E(T^*)$ $(1 \leq i \leq k,\ 1 \leq j \leq s)$, $V(T_1)$ is an empty set if $uv \in E(T^*)$ and $u_1 = v_1$ if $d(u, v) = 2$. We denote $N_{X_i}[x_i] = U_i$ and $N_{Y_j}[y_j] = V_j$. T' and T'' are the trees obtained from T^*.

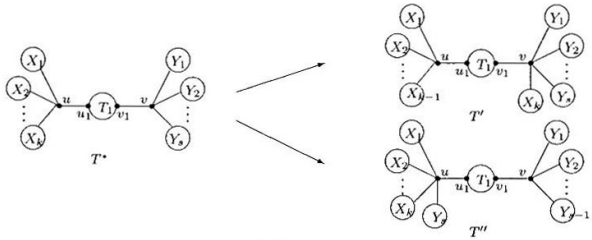

Fig. 1

To show the lemma, it is sufficient to show that

(1) $i(T') > i(T^*)$ or $i(T'') > i(T^*)$;

(2) $z(T') < z(T^*)$ or $z(T'') < z(T^*)$.

We first show $i(T') > i(T^*)$ or $i(T'') > i(T^*)$. Denote $L_j = \prod_{i=1}^{j} i(X_i)$, $L'_j = \prod_{i=1}^{j} i(X_i - x_i)$ $(1 \le j \le k)$ and $R_j = \prod_{i=1}^{j} i(Y_i)$, $R'_j = \prod_{i=1}^{j} i(Y_i - y_i)$ $(1 \le j \le s)$.

If $d(u, v) \ge 3$, then by Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
i(T^*) &= L_k R_s \cdot i(T_1) + L'_k R'_s \cdot i(T_1 - \{u_1, v_1\}) + L_k R'_s \cdot i(T_1 - v_1) + L'_k R_s \cdot i(T_1 - u_1), \\
i(T') &= L_k R_s \cdot i(T_1) + L'_k R'_s \cdot i(T_1 - \{u_1, v_1\}) \\
&\quad + L_{k-1} R'_s \cdot i(X_k - x_k) i(T_1 - v_1) + L'_{k-1} R_s \cdot i(X_k) i(T_1 - u_1), \\
i(T'') &= L_k R_s \cdot i(T_1) + L'_k R'_s \cdot i(T_1 - \{u_1, v_1\}) \\
&\quad + i(Y_s) \cdot L_k R'_{s-1} \cdot i(T_1 - v_1) + i(Y_s - y_s) \cdot L'_k R_{s-1} \cdot i(T_1 - u_1).
\end{aligned}$$

Note that $i(X_k) = i(X_k - x_k) + i(X_k - U_k)$ and $i(Y_s) = i(Y_s - y_s) + i(Y_s - V_s)$, we have

$$\begin{aligned}
i(T') - i(T^*) &= i(X_k - U_k)(L'_{k-1} R_s \cdot i(T_1 - u_1) - L_{k-1} R'_s \cdot i(T_1 - v_1)), \\
i(T'') - i(T^*) &= i(Y_s - V_s)(L_k R'_{s-1} \cdot i(T_1 - v_1) - L'_k R_{s-1} \cdot i(T_1 - u_1)).
\end{aligned}$$

If $i(T') - i(T^*) \le 0$, since $i(X_k - U_k) > 0$, we have

$$L'_{k-1} R_s \cdot i(T_1 - u_1) - L_{k-1} R'_s \cdot i(T_1 - v_1) \le 0.$$

Since $R_s > 0$ and $i(X_k - x_k) > 0$, we have

$$L'_k \cdot i(T_1 - u_1) \le \frac{L_{k-1} R'_s \cdot i(T_1 - v_1) i(X_k - x_k)}{R_s}.$$

So

$$L_k R'_{s-1} \cdot i(T_1 - v_1) - L'_k R_{s-1} \cdot i(T_1 - u_1)$$

$$\begin{aligned}
&\geq L_k R'_{s-1} \cdot i(T_1 - v_1) - R_{s-1} \cdot \frac{L_{k-1} R'_s \cdot i(T_1 - v_1) i(X_k - x_k)}{R_s} \\
&= L_{k-1} R'_{s-1} \cdot i(T_1 - v_1) \cdot (i(X_k) - \frac{i(Y_s - y_s)}{i(Y_s)} i(X_k - x_k)) \\
&> 0.
\end{aligned}$$

Note that $i(Y_s - V_s) > 0$, we have $i(T'') > i(T^*)$.

If $d(u, v) \leq 2$, it is easy to see that

$$\begin{aligned}
i(T') - i(T^*) &= i(X_k - U_k)(L'_{k-1} R_s - L_{k-1} R'_s), \\
i(T'') - i(T^*) &= i(Y_s - V_s)(L_k R'_{s-1} - L'_k R_{s-1}).
\end{aligned}$$

Similarly, we can show $i(T') > i(T^*)$ or $i(T'') > i(T^*)$.

Now we show that $z(T') < z(T^*)$ or $z(T'') < z(T^*)$. Denote $P_j = \prod_{i=1}^{j} z(X_i)$, $P'_j = \sum_{i=1}^{j} \frac{z(X_i - x_i)}{z(X_i)}$ $(1 \leq j \leq k)$ and $Q_j = \prod_{i=1}^{j} z(Y_i)$, $Q'_j = \sum_{i=1}^{j} \frac{z(Y_i - y_i)}{z(Y_i)}$ $(1 \leq j \leq s)$. By Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
z(T^*) &= P_k Q_s [(1 + P'_k)(z(T_1) + z(T_1 - v_1) + z(T_1) Q'_s) \\
&\quad + z(T_1 - u_1) + z(T_1 - \{u_1, v_1\}) + z(T_1 - u_1) Q'_s], \\
z(T') &= P_k Q_s [(1 + P'_{k-1})(z(T_1) + z(T_1 - v_1) + z(T_1) Q'_s + z(T_1) \frac{z(X_k - x_k)}{z(X_k)}) \\
&\quad + z(T_1 - u_1) + z(T_1 - \{u_1, v_1\}) + z(T_1 - u_1) Q'_s + z(T_1 - u_1) \frac{z(X_k - x_k)}{z(X_k)}], \\
z(T'') &= P_k Q_s [(1 + P'_k + \frac{z(Y_s - y_s)}{z(Y_s)})(z(T_1) + z(T_1 - v_1) + z(T_1) Q'_{s-1}) \\
&\quad + z(T_1 - u_1) + z(T_1 - \{u_1, v_1\}) + z(T_1 - u_1) Q'_{s-1}].
\end{aligned}$$

Then we have

$$\begin{aligned}
z(T') - z(T^*) &= P_k Q_s \frac{z(X_k - x_k)}{z(X_k)} \left(z(T_1) P'_{k-1} - z(T_1) Q'_s - z(T_1 - v_1) + z(T_1 - u_1) \right), \\
z(T'') - z(T^*) &= P_k Q_s \frac{z(Y_s - y_s)}{z(Y_s)} \left(z(T_1) Q'_{s-1} - z(T_1) P'_k + z(T_1 - v_1) - z(T_1 - u_1) \right).
\end{aligned}$$

If $z(T') \geq z(T^*)$ and $z(T'') \geq z(T^*)$, we have

$$\begin{aligned}
A &= z(T_1) P'_{k-1} - z(T_1) Q'_s - z(T_1 - v_1) + z(T_1 - u_1) \geq 0, \\
B &= z(T_1) Q'_{s-1} - z(T_1) P'_k + z(T_1 - v_1) - z(T_1 - u_1) \geq 0.
\end{aligned}$$

But we have

$$A + B = -z(T_1) \left(\frac{z(X_k - x_k)}{z(X_k)} + \frac{z(Y_s - y_s)}{z(Y_s)} \right) < 0,$$

a contradiction. Hence $z(T') < z(T^*)$ or $z(T'') < z(T^*)$.

If $d(u,v) \leq 2$, similarly we can show $z(T') < z(T^*)$ or $z(T'') < z(T^*)$. This completes the proof of Lemma 2.4. ∎

Lemma 2.5 *If $u_1u_2\ldots u_{k-1}u_k$ is a longest path in T^*, $k \geq 5$ and $\Delta \geq 3$, then $d(u_2) = d(u_{k-1}) = \Delta$.*

Proof. We show the result by contradiction. Without loss of generality, we assume $d(u_2) = x+1 < \Delta$. Then by Lemma 2.4, we know all the other internal vertices of T^* have degree Δ. Since $u_1u_2\ldots u_k$ is a longest path in T^*, T^* can be seen as the graph shown in Fig. 2, where $y_1 + y_2 = \Delta - 2$ and $|V(T_1)| > 1$.

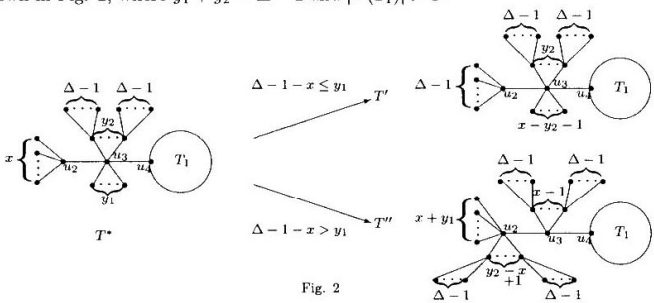

Fig. 2

If $\Delta - 1 - x \leq y_1$, we have $y_1 \geq 1$ since $x + 1 < \Delta$. Then as shown in Fig. 2, we can get T'. It is easy to see that $T' \in \mathcal{T}(n,\Delta)$. By Lemmas 2.1, 2.2 and 2.3, we have

$$\begin{aligned}
i(T^*) &= i(T^* - u_3) + i(T^* - N_{T^*}[u_3]) \\
&= i(T_1) \times 2^{y_1}(1+2^x)(1+2^{\Delta-1})^{y_2} + i(T_1 - u_4) \times 2^{x+(\Delta-1)y_2}, \\
i(T') &= i(T' - u_3) + i(T' - N_{T'}[u_3]) \\
&= i(T_1) \times 2^{x-y_2-1}(1+2^{\Delta-1})^{y_2+1} + i(T_1 - u_4) \times 2^{(\Delta-1)(y_2+1)}, \\
z(T^*) &= z(T^* - u_3) + \sum_{u_3w \in E(T^*)} z(T^* - \{u_3, w\}) \\
&= (1+x)\Delta^{y_2} z(T_1) + [\Delta^{y_2} + y_1\Delta^{y_2}(1+x) + y_2\Delta^{y_2-1}(1+x)]z(T_1) \\
&\quad +(1+x)\Delta^{y_2} z(T_1 - u_4), \\
z(T') &= z(T' - u_3) + \sum_{u_3w \in E(T')} z(T' - \{u_3, w\}) \\
&= \Delta^{y_2+1} z(T_1) + [(y_2+1)\Delta^{y_2} + (x - y_2 - 1)\Delta^{y_2+1}]z(T_1) + \Delta^{y_2+1} z(T_1 - u_4).
\end{aligned}$$

Note that the above four equations also hold when $y_2 = 0$. It is easy to see that

$$i(T') - i(T^*) = (2^{\Delta-x-1} - 1)2^{x-y_2-1}[2 \cdot i(T_1 - u_4)2^{\Delta y_2} - i(T_1)(1 + 2^{\Delta-1})^{y_2}];$$

Since $2^\Delta > 1+2^{\Delta-1}$ and $2i(T_1-u_4) > i(T_1)$, we can get $i(T')-i(T^*) > 0$ which contradicts with the choice of T^*.

And if $y_2 > 0$, we have

$$z(T^*) - z(T') = \Delta^{y_2-1}(\Delta - x - 1)[y_2(\Delta - 1)z(T_1) + \Delta(z(T_1) - z(T_1 - u_4))].$$

If $y_2 = 0$, then $y_1 = \Delta - 2$, we have

$$z(T^*) - z(T') = (\Delta - x - 1)(z(T_1) - z(T_1 - u_4)).$$

Since $x < \Delta - 1$ and $z(T_1) > z(T_1 - u_4)$, we get $z(T') < z(T^*)$ in either case which contradicts with the choice of T^*. This completes the proof when $\Delta - 1 - x \leq y_1$.

If $\Delta - 1 - x > y_1$, we have $y_2 \geq x$, then as shown in Fig. 2, we can get T''. Obviously, $T'' \in \mathcal{T}(n, \Delta)$. Similarly we have

$$\begin{aligned}
i(T'') &= i(T'' \curlywedge u_3) + i(T'' - N_{T''}[u_3]) \\
&= i(T_1) \times 2^{x+y_1}(1 + 2^{\Delta-1})^{y_2} + i(T_1) \times 2^{(\Delta-1)(y_2-x+1)}(1 + 2^{\Delta-1})^{x-1} \\
&\quad + i(T_1 - u_4) \times 2^{\Delta x - y_2 - 1}(1 + 2^{\Delta-1})^{y_2-x+1}, \\
z(T'') &= z(T'' - u_3) + \sum_{u_3 w \in E(T'')} z(T'' - \{u_3, w\}) \\
&= z(T_1)\Delta^{y_2-2}[(2 + x + y_1)\Delta^2 + y_2\Delta + (x-1)(x+y_1)\Delta + (x-1)(y_2 - x + 1)] \\
&\quad + z(T_1 - u_4)\Delta^{y_2-1}[(x + y_1 + 1)\Delta + (y_2 - x + 1)].
\end{aligned}$$

Note that the above two equations also hold when $y_1 = 0$. Then

$$\begin{aligned}
i(T'') - i(T^*) &= 2^{\Delta-2-y_2}((1 + 2^{\Delta-1})^{y_2-x+1} - 2^{\Delta y_2 - \Delta x + x + 1}) \\
&\quad \times (2i(T_1 - u_4)2^{\Delta(x-1)} - i(T_1)(1 + 2^{\Delta-1})^{x-1}), \\
z(T^*) - z(T'') &= (y_1\Delta^{y_2} + y_2\Delta^{y_2-1} - (x-1)\Delta^{y_2-1})(z(T_1) - z(T_1 - u_4)) \\
&\quad + (x-1)z(T_1)\Delta^{y_2-2}[(y_1\Delta - y_1 + y_2 - x)\Delta + \Delta - y_2 + x - 1].
\end{aligned}$$

Since $(\Delta-1)(y_2-x+1) \geq \Delta y_2 - \Delta x + x + 1$, $2i(T_1-u_4) > i(T_1)$ and $2^\Delta > 1+2^{\Delta-1}$, we have $i(T'') > i(T^*)$ which contradicts with the choice of T^*. And since $\Delta - 2 \geq y_2 > x - 1 \geq 0$ and $z(T_1) > z(T_1 - u_4)$, we have $z(T^*) > z(T'')$ which contradicts with the choice of T^*. ■

Definition 2.1 (see [6]) *Let $\Delta \geq 3$ and $R \in \{\Delta - 1, \Delta\}$. For every n the family $\mathcal{G}(R, \Delta)$ of trees has a unique member T of order n up to isomorphism which we now define together with a natural plane embedding.*

Let $M_0(R, \Delta) = 1$ and $M_k(R, \Delta) = 1 + R + R(\Delta - 1) + \cdots + R(\Delta - 1)^{k-1}$ for $k \geq 1$. Let

$$M_k(R, \Delta) \leq n < M_{k+1}(R, \Delta)$$

for some $k \geq 0$. Let $n - M_k(R, \Delta) = m(\Delta - 1) + r$ for some $0 \leq r < \Delta - 1$. Let T be the tree of order n embedded in the plane such that

(i) all vertices of T lie on some line $R \times \{i\}$ for $0 \leq i \leq k + 1$,

(ii) there is a unique vertex on line $R \times \{0\}$ which has exactly $min\{n - 1, R\}$ neighbors that lie on line $R \times \{1\}$,

(iii) for $1 \leq j \leq k - 1$ every vertex on line $R \times \{j\}$ has a unique neighbor on line $R \times \{j - 1\}$ and $\Delta - 1$ neighbors on line $R \times \{j + 1\}$,

(iv) if $v_1, v_2, \ldots, v_{m+1}$ are the $m + 1$ leftmost vertices on line $R \times \{k\}$ such that v_i lies left of v_j for $i < j$, then each of $v_1, v_2, \ldots, v_m$ has $\Delta - 1$ neighbors on line $R \times \{k + 1\}$ and v_{m+1} has r neighbors on line $R \times \{k + 1\}$.

For a tree in $\mathcal{G}(R, \Delta)$, we give each vertex a label for convenience. Label the vertex in $R \times \{0\}$ by 0 and $R \times \{1\}$ by $1, 2, 3 \ldots, R$ respectively. For $j \geq 2$ and $v \in R \times \{j\}$, we label v with $i_1 i_2 i_3 \ldots i_{j-1} i_j$ if $N_{R \times \{j-1\}}(v) = i_1 i_2 i_3 \ldots i_{j-1}$. It is easy to see that there are $\Delta - 1$ vertices in $R \times \{j\}$ whose labels are same except for the last number, we will denote them by $i_1 i_2 \ldots i_{j-1} 1$, $i_1 i_2 \ldots i_{j-1} 2$, ..., $i_1 i_2 \ldots i_{j-1}(\Delta - 1)$ respectively. Without loss of generality, we may assume the vertices in $R \times \{j\}$ can be arranged from left to right according to the order from $11 \cdots 1$ to $R(\Delta - 1)(\Delta - 1) \cdots (\Delta - 1)$. Fig. 3 gives us an example of a tree in $\mathcal{G}(R, \Delta)$ and its labelling where $R = \Delta = 3$ and $n = M_2(R, \Delta) + 5(\Delta - 1) + 1$.

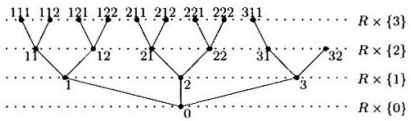

Fig. 3

If T is a tree in $\mathcal{G}(R, \Delta)$ with order $n = M_k(R, \Delta)$, then we denote T by $T_{k,R}$. If T is a tree in $\mathcal{G}(R, \Delta)$ with order $M_k(R, \Delta) \leq n < M_{k+1}(R, \Delta)$, for a vertex $v \in R \times \{i\}$ $(1 \leq i \leq k)$, let T_v denote the maximal subtree of T that contains v and has only vertices on lines $R \times \{j\}$ for $j \geq i$. Let $u_1, u_2, \ldots, u_m$ be m vertices of the graph G,

and $G(u_1, u_2, \ldots, u_m)(a_1, a_2, \ldots, a_m)$ denote the graph obtained from G by attaching a_i pendent vertices to the vertex u_i $(1 \leq i \leq m)$.

Definition 2.2 *Suppose $T_\Delta^* \in \mathcal{T}(n, \Delta)$ with order $M_k(\Delta, \Delta) \leq n < M_{k+1}(\Delta, \Delta)$. Suppose $n - M_k(\Delta, \Delta) = m(\Delta - 1) + r$ where $0 \leq r < \Delta - 1$. We call T_Δ^* a Δ star-tree, if*

(i) $m = r = 0$, $T_\Delta^* = T_{k,\Delta}$;

(ii) $m \neq 0, r = 0$, $T_\Delta^* = T_{k,\Delta}(v_1, v_2, \cdots, v_m)(\Delta-1, \Delta-1, \cdots, \Delta-1)$ where $v_1, v_2, \cdots, v_m$ are the leftmost m vertices on line $R \times \{k\}$ of $T_{k,\Delta}$;

(iii) $m \neq 0$ and $r \neq 0$, suppose $v_1, v_2, \cdots, v_m, v_{m+1}$ are the leftmost $m+1$ vertices on line $R \times \{k\}$ of $T_{k,\Delta}$ and the label of v_{m+1} is $i_1 i_2 \ldots i_{k-1} i_k$, T_Δ^* is obtained from $T_{k,\Delta}(v_1, v_2, \cdots, v_m, v_{m+1})(\Delta - 1, \Delta - 1, \cdots, \Delta - 1, r)$ by switching the subtrees

$$T_{i_1 i_2 \ldots i_{k-1}(i_k+1)}, T_{i_1 i_2 \ldots i_{k-1}(i_k+2)}, \ldots, T_{i_1 i_2 \ldots i_{k-1}(i_k+(\Delta-1-r))}$$

from vertex $i_1 i_2 \ldots i_{k-1}$ to vertex $i_1 i_2 \ldots i_{k-1} i_k$, where the addition is module $\Delta - 1$ addition.

In order to explain how to switch the subtrees when $m \neq 0$ and $r \neq 0$, we give an example in Fig. 4 where $\Delta = 4$ and $m = r = 1$.

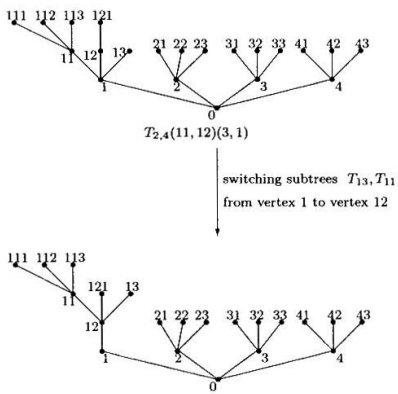

Fig. 4

Conjecture. *Suppose $T \in \mathcal{T}(n, \Delta)$ with order $M_k(\Delta, \Delta) \leq n < M_{k+1}(\Delta, \Delta)$ where $k \geq 1$, then*

(i) $i(T) \leq i(T^*_\Delta)$ *and the equality holds if and only if* $T = T^*_\Delta$;

(ii) $z(T) \geq z(T^*_\Delta)$ *and the equality holds if and only if* $T = T^*_\Delta$.

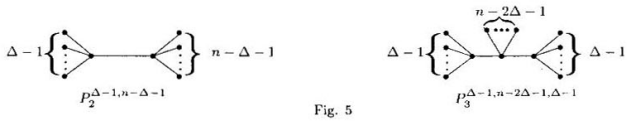

Fig. 5

Now we verify our conjecture for $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq n-2$.

Theorem 2.1 *Let* T *be a tree in* $\mathcal{T}(n,\Delta)$, $P_2^{\Delta-1,n-\Delta-1}$ *and* $P_3^{\Delta-1,\Delta-1,n-2\Delta-1}$ *are the trees as shown in Fig. 5. If* $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq n-2$, *then* $i(T) \leq i(T^*)$ *and* $z(T) \geq z(T^*)$ *with the equality hold if and only if* $T \cong T^*$, *where* $T^* \cong P_2^{\Delta-1,n-\Delta-1}$ *if* $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, *and* $T^* \cong P_3^{\Delta-1,\Delta-1,n-2\Delta-1}$ *if* $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq \lceil \frac{n}{2} \rceil - 1$.

Proof. Suppose T^* is a tree in $\mathcal{T}(n,\Delta)$ with maximal Merrifield-Simmons index. Let $P = u_1u_2\cdots u_k$ be a longest path in T^*, then we know u_1, u_k are the pendent vertices of T^*. By lemma 2.4, we know at most one of $u_2, u_3, \cdots, u_{k-1}$ has degree less than Δ, then we have $n \geq \Delta + (k-4)(\Delta-1) + 2$.

If $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, then we must have $k = 4$. Without loss of generality, we may assume $d(u_2) = \Delta$. Then it is easy to see that $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$ and $T^* \cong P_2^{\Delta-1,n-\Delta-1}$.

If $\lceil \frac{n+1}{3} \rceil \leq \Delta < \lceil \frac{n}{2} \rceil$, we must have $k = 5$. Then we may assume u_2, u_3, u_4 are the only three interval vertices of T^*, otherwise we also can get a contradiction with $\Delta \geq \lceil \frac{n+1}{3} \rceil$ by lemma 2.4. By Lemma 2.5, we know $d(u_2) = d(u_4) = \Delta$, and thus $T^* \cong P_3^{\Delta-1,\Delta-1,n-2\Delta-1}$. So we have proved that $i(T) \leq i(T^*)$ with the equality holds if and only if $T \cong T^*$.

Similarly we can prove $z(T) \geq z(T^*)$ with the equality holds if and only if $T \cong T^*$. ∎

Remark

From Theorem 3.2 [14], we can also get one result of Theorem 2.1:

Let T *be a tree in* $\mathcal{T}(n,\Delta)$ *and* $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq n-2$, *then* $z(T) \geq z(T^*)$ *with the equality holds if and only if* $T \cong T^*$, *where* $T^* \cong P_2^{\Delta-1,n-\Delta-1}$ *if* $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, *and* $T^* \cong P_3^{\Delta-1,\Delta-1,n-2\Delta-1}$ *if* $\lceil \frac{n+1}{3} \rceil \leq \Delta \leq \lceil \frac{n}{2} \rceil - 1$.

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