*Journal of Mathematical Chemistry, Vol. 43, No. 2, February 2008 (© 2007)*
DOI: 10.1007/s10910-006-9224-4

# The first and second largest Merrifield–Simmons indices of trees with prescribed pendent vertices

Maolin Wang,* Hongbo Hua, and Dongdong Wang

*Department of Computing Science, Huaiyin Institute of Technology, Huaian, Jiangsu 223000, People's Republic of China*
E-mail: mlw.math@gmail.com

The Merrifield–Simmons index $\sigma(G)$ of a graph $G$ is defined as the number of subsets of the vertex set, in which any two vertices are non-adjacent, i.e., the number of independent-vertex sets of $G$. By $T(n, k)$ we denote the set of trees with $n$ vertices and with $k$ pendent vertices. In this paper, we investigate the Merrifield–Simmons index $\sigma(T)$ for a tree $T$ in $T(n, k)$. For all trees in $T(n, k)$, we determined unique trees with the first and second largest Merrifield–Simmons index, respectively.

**KEY WORDS:** Merrifield–Simmons index, trees with $k$ pendent vertices

## 1. Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of $v$ as $N_G(v)$. By $n(G)$, we denote the number of vertices of $G$. All graphs considered here are both finite and simple.We denote, respectively, by $S_n$ and $P_n$ the star and path with $n$ vertices.

For any given graph $G$, its Merrifield–Simmons index, simply denoted as $\sigma(G)$, is defined as the number of subsets of the vertex set, in which any two vertices are non-adjacent, i.e., in graph-theoretical terminology, the number of independent-vertex subsets of $G$, including the empty set. For example, for the cycle $C_4 = v_0v_1v_2v_3$, the independent-vertex subsets of $V(C_4)$ of all size are as follows: $\emptyset, \{v_0\}, \{v_1\}, \{v_2\}, \{v_3\}, \{v_0,\ v_2\}, \{v_1,\ v_3\}$, and then $\sigma(C_4) = 7$. As for the path $P_n$, $\sigma(G)$ is exactly equal to the Fibonacci number $F_{n+2}$. This is perhaps why some researchers call the Merrifield–Simmons index "Fibonacci number." The concept of a (molecular) graph is introduced in [13], and discussed later in [1]. The Merrifield–Simmons index for a molecular graph was extensively investigated in [10], where its chemical applications were demonstrated. In [6], Li et al. gave its other properties and applications. Wang and Hua [15] gave sharp lower and upper bounds for Merrifield–Simmons index among all unicycle graphs.

*Corresponding author.

More recently, Yu et al. [16] determined the unique trees with the first greatest value of Merrifield–Simmons index among all trees with $k$ pendent vertices. There have been many literature studying the Merrifield–Simmons index. For further details, see [3–9, 11, 12, 14, 17] and the cited references therein.

By $T - u$ and $T - uv$, we denote, respectively, the graphs that arises from $T$ by deleting the vertex $u \in V(T)$ and the edge $uv \in E(T)$. Likewise, $T + uv$ denotes the graph that arises from $T$ by adding an edge $uv \notin E(T)$. Let $T(n,k)$ denote the set of trees of $n$ vertices and with $k$ pendent vertices. Let $T_{n_1,n_2,\ldots,n_k}$ be a tree in $T(n,k)$ obtained from a star $S_{k+1}$ by attaching paths of orders $n_1,\ n_2,\ldots n_k$ to $k$ pendent vertices of $S_{k+1}$. A caterpillar is a tree if deleting all its pendent vertices will reduce it to a path. By $S_{m,n}$, we denote a double star which is obtained by identifying one pendent vertex of $S_{n+2}$ with the center of $S_{m+1}$.

Let $(G_1, v_1)$ and $(G_2, v_2)$ be two graphs rooted at $v_1$ and $v_2$, respectively, then $G = (G_1, v_1) \bowtie (G_1, v_2)$ denote the graph obtained by identifying $v_1$ with $v_2$ as one common vertex.

Other notations and terminology not defined here will conform to those in [2].

Let $F_n$ denote the $n-th$ Fibonacci number, we have $F_n + F_{n+1} = F_{n+2}$ with initial conditions $F_1 = F_2 = 1$.

In this paper, we also investigate the Merrifield–Simmons index for trees in $T(n,k)$. By presenting a new proof of Yu et al., results in [16], we determined the unique trees with the first greatest value of Merrifield–Simmons index among all trees in $T(n,k)$. Moreover, all trees in $T(n,k)$ with the second largest Merrifield–Simmons index are uniquely determined.

## 2. Some known results

We begin with several important lemmas from [6,13] will be helpful to the proofs of our main results.

**Lemma 1.** For any graph $G$ with any $v \in V(G)$, we have

$$\sigma(G) = \sigma(G - v) + \sigma(G - [v]),$$

where $[v] = N_G(v) \bigcup \{v\}$.

**Lemma 2.** Let $G$ be a graph with $m$ components $G_1,\ G_2,\ldots G_m$. Then $\sigma(G) = \prod_{i=1}^{m} \sigma(G_i)$.

**Lemma 3.** Let $T$ be a tree. Then $F_{n+2} \leqslant \sigma(T) \leqslant 2^{n-1} + 1$ and $\sigma(T) = F_{n+2}$ if and only if $T \cong P_n$ and $\sigma(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$.

**Lemma 4.** Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs. If $V(G_1) = V(G_2)$ and $E(G_1) \subset E(G_2)$, then $\sigma(G_1) > \sigma(G_2)$.

## 3. Trees in $T(n,k)$ with the first largest value of Merrifield–Simmons index

In this section, we investigate the first largest value of Merrifield–Simmons index for trees in $T(n,k)$. Before we introduce our main results, we need to state and prove the following lemma.

**Lemma 5.** Let $G_1$ be a connected graph and $T$ a tree of order $n$. Let $G = (G_1, r_i) \bowtie (T, r_i)$, then we have $\sigma(G) \leqslant \sigma((G_1, r_i) \bowtie (S_n, r_i))$ with equality holds if and only if $T \cong S_n$. Moreover, $r_i$ is the center of $S_n$.

*Proof.* It follows from lemma 1. that

$$\sigma(G) = \sigma(G - r_i) + \sigma(G - [r_i]). \tag{1}$$

Let $N_{G_1}(r_i) = \{x_1, \ldots x_p\}$ and $N_T(r_i) = \{y_1, \ldots y_q\}$, where $p, q \geqslant 1$.
Note first from lemma 2. that

$$\sigma(G - r_i) = \sigma[(G_1 - r_i) \bigcup (T - r_i)] = \sigma(G_1 - r_i)\sigma\left(\bigcup_{i=1}^{q} T_i\right). \tag{2}$$

where each $T_i$ denote the subtree of $T - r_i$ containing $y_i$ for $i = 1, \ldots q$.
Note also from lemma 2. that

$$\begin{aligned}\sigma(G - [r_i]) &= \sigma\left[(G_1 - [r_i]) \bigcup (T - [r_i])\right] \\ &= \sigma[(G_1 - [r_i])]\sigma[(T - [r_i])] \\ &= \sigma(G_1 - [r_i])\sigma\left(\bigcup_{i=1}^{s} T_j\right),\end{aligned} \tag{3}$$

where $T_j$ denote the subtree of $T - [r_i]$.
Moreover, from lemma 1. it follows that

$$\begin{aligned}\sigma(G_1 - [r_i]) &= \sigma[(G_1 - r_i - x_1 - \cdots x_p) \\ &= \sigma(G_1 - r_i - x_1 - \cdots x_{p-1}) - \sigma(G_1 - r_i - x_1 - \cdots x_{p-1} - [x_p]) \\ &= \cdots \\ &= \sigma(G_1 - r_i) - \sigma(G_1 - r_i - [x_1]) - \cdots - \sigma(G_1 - r_i - x_1 \\ &\quad - \cdots x_{p-1} - [x_p])\end{aligned} \tag{4}$$

Let $A = \sigma\left(\bigcup_{i=1}^{q} T_i\right)$ and $B = \sigma\left(\bigcup_{j=1}^{s} T_j\right)$. Combining (1)–(4) we obtain that

$$\begin{aligned}\sigma(G) &= A\sigma(G_1-r_i)+B[\sigma(G_1-r_i)-\sigma(G_1-r_i-[x_1])-\cdots-\sigma(G_1-r_i-x_1-\cdots x_{p-1}-[x_p])]\\ &= (A+B)\sigma(G_1-r_i)-B[\sigma(G_1-r_i-[x_1])+\cdots+\sigma(G_1-r_i-x_1-\cdots x_{p-1}-[x_p])].\end{aligned}$$

It is easy to see that $\sigma(G_1-r_i) > 0$ and $\sigma(G_1-r_i-[x_1])+\cdots+\sigma(G_1-r_i-x_1-\cdots x_{p-1}-[x_p]) > 0$. In order for $\sigma(T)$ to be large enough, we must have that $A+B$ is large enough while $B$ is small enough. It follows that $A = (A+B)+(-B)$ is large enough.

It follows from lemmas 2. and 3. that

$$A = \sigma\left(\bigcup_{i=1}^{q} T_i\right) = \prod_{i=1}^{q} \sigma(T_i) \leqslant 2^{\sum_{i=1}^{q} n(T_i)} = 2^{n-1}, \tag{5}$$

where $n(T_i)$ denotes the order of $T_i$.

It's not difficult to see that the equality in (5) holds if and only if $\bigcup_{i=1}^{q} T_i = (n-1)P_1$. It implies that $T \cong S_n$ and $r_i$ is the center of $S_n$. This completes the proof. □

When $k = n-1$ or $k = 2$, $T$ is a star or a path. We can easily determine its Merrifield–Simmons index, so we will assume that $3 \leqslant k \leqslant n-2$ in the following.

**Colollary 6.** For $3 \leqslant k \leqslant n-2$, let $T$ be a tree in $T(n,k)$ such that $\sigma(T)$ is large enough, then $T$ is a caterpillar with at least two branched vertices or $T \cong T_{1,1,\ldots,1,s,t}$, where $\min\{s,t\} \geqslant 1$ and $\max\{s,t\} \geqslant 2$.

*Proof.* Let $T$ be a tree in $T(n,k)$ such that $\sigma(T)$ is large enough, where $3 \leqslant k \leqslant n-2$.

Since $k \leqslant n-2$, then $T \ncong S_n$. So there exists a diametrical path $P_{d+1} = v_0v_1\ldots v_d$ in $T$ with $d \geqslant 3$. Since $k \geqslant 3$, there exist at least one vertex $v_i$ in $P_{d+1}$ such that $d(v_i) \geqslant 3$ where $1 \leqslant i \leqslant d-1$.

Note that, for any tree $T$, we have

$$T = (T_1, r) \bowtie (T_2, r), \tag{6}$$

where $T_1$ and $T_2$ denote trees of order $n_1$ and $n_2$, respectively, and $n_1+n_2 = n+1$.

Suppose there exists exactly one vertex, say $v_j$ in $P_{d+1}$ such that $d(v_i) \geqslant 3$ where $1 \leqslant j \leqslant d-1$. Then by (6) and lemma 5., we have $T(v_j) \cong S_{n(T(v_j))}$, where $T(v_j)$ denotes the subtree containing $v_j$ of $T - \{v_{j-1}v_j,\ v_jv_{j+1}\}$. Thus, $T \cong T_{1,1,\ldots,1,s,t}$.

So, we may assume that there exist at least two vertices, say $v_i$ and $v_j$ in $T$ such that $d(v_i) \geqslant 3$ and $d(v_j) \geqslant 3$. Let $T = (T_1, r) \bowtie (T_2, r)$. Assume that $T_1$ denote the subtree containing $v_j$ of $T - \{v_{j-1}v_j,\ v_jv_{j+1}\}$. By lemma 5. , $T_1 \cong S_{n(T(v_j))}$. Also, we have $T_2 \ncong S_{n+1-n(T(v_j))}$ for otherwise $T \cong S_n$, contradicting $k \leqslant n-2$. Similarly, we have $T(v_i) \cong S_{n(T(v_i))}$. Consequently, $T$ is a caterpillar with at least two branched vertices.

Therefore, the proof is complete. □

If $T$ is a tree in $T(n,k)$ such that $\sigma(T)$ is large enough, then we call it a *maximal tree*.

**Lemma 7.** Let $T$ be a tree in $T(n,k)$ with $3 \leqslant k \leqslant n-2$ such that $\sigma(T)$ is large enough, then $T \cong T_{1,1,\ldots,1,s,t}$, where $\min\{s,t\} \geqslant 1$ and $\max\{s,t\} \geqslant 2$.

*Proof.* Let $T$ be a maximal tree in $T(n,k)$ with $3 \leqslant k \leqslant n-2$. From corollary 6., we have $T \cong T_{1,1,\ldots,1,s,t}$ or $T$ is a caterpillar having at least two branched vertices.

In the following, we will show that $T$ can not be a caterpillar with at least two branched vertices.

Suppose, to the contrary, that $T$ is a caterpillar with at least two branched vertices. Let $P_{d+1} = v_0v_1\ldots v_d$ be a diametrical path in $T$. For $1 \leqslant i \leqslant d-1$, let $n_i$ denote the number of neighbors of $v_i$ lying outside the path $P_{d+1}$. We will complete the proof by distinguishing the following two cases.

*Case 1.* There exists some $v_j$ $(1 \leqslant i \leqslant d-1)$ such that $n_j \geqslant 2$.

Since $T$ has at least two branched vertices, let $v_i$ be another branched vertex. Let $N(v_i) - \{v_{i-1}, v_{i+1}\} = \{x_1, \ldots, x_{n_i}\}$ and $N(v_j) - \{v_{j-1}, v_{j+1}\} = \{y_1, \ldots, y_{n_j}\}$.

Let $T^{'}$ be obtained as follows.

$$T^{'} = T - v_ix_1 - \cdots - v_ix_{n_i} + v_jx_1 + \cdots + v_jx_{n_i}.$$

We will show that $\sigma(T^{'}) > \sigma(T)$ by induction on the order of $T$. Assume that the result holds for any maximal tree $T$ in $T(n,k)$ of order less than $n$.

Now, let $T$ be a maximal tree of order $n$ in $T(n,k)$.

From lemma 1., we have

$$\sigma(T^{'}) = \sigma(T^{'} - y_1) + \sigma(T^{'} - [y_1]) \tag{7}$$

and

$$\sigma(T) = \sigma(T - y_1) + \sigma(T - [y_1]). \tag{8}$$

From induction hypothesis it follows that

$$\sigma(T^{'} - y_1) > \sigma(T - y_1). \tag{9}$$

Let $T_1$ and $T_2$ denote the subtrees of $T^{'} - [y_1]$ containing $v_{j-1}$ and $v_{j+1}$, respectively. Without loss of generality we may suppose that $v_i \in T_1$.

From lemma 2, we obtain

$$\sigma(T^{'} - [y_1]) = \sigma\left[T_1 \bigcup T_2 \bigcup (n_i + n_j - 1)P_1\right]$$
$$= 2^{n_j - 1}\sigma\left(T_1 \bigcup n_i P_1\right)\sigma(T_2) \tag{10}$$

and

$$\sigma(T - [y_1]) = 2^{n_j - 1}\sigma(T_3)\sigma(T_2), \tag{11}$$

where $T_3$ denotes the subtree of $T - [y_1]$ containing $v_{j-1}$. Then $v_i \in T_3$.

Note that $V(T_1 \bigcup n_i P_1) = V(T_3)$ and $E(T_1 \bigcup n_i P_1) = E(T_3) - \{v_i x_1, \ldots v_i x_{n_i}\} \subset E(T_3)$. So $\sigma(T_1 \bigcup n_i P_1) > \sigma(T_3)$ by lemma 4.

Combining (7)–(9) with (10)–(11), we get $\sigma(T^{'}) > \sigma(T)$. So in this case, we have shown that $\sigma(T^{'}) > \sigma(T)$ for any maximal tree $T$ in $T(n,k)$ by the principle of mathematical induction. But then it contradicts the maximality of $\sigma(T)$.

*Case 2*. For each $1 \leqslant i \leqslant d-1$, $n_i = 1$.

Let $v_j$ be a vertex with $n_j = 1$. we obtain $T^{'}$ by deleting all the pendent edges of $T$ incident with each $v_i$ ($1 \leqslant i \leqslant d-1$ and $i \neq j$) and attaching all the deleted edges to the vertex $v_j$.

Let $S = \{v_i | n_i = 1, 1 \leqslant i \leqslant d-1\}$. If $|S| = 2$, we can easily check that $\sigma(T^{'}) > \sigma(T)$, a contradiction to the choice of $T$.

Suppose $|S| \geqslant 3$. We will show that $\sigma(T^{'}) > \sigma(T)$ by induction on the order of $T$ in the following. Assume that the result holds for maximal trees $T$ in $T(n,k)$ of order less than $n$.

Now, let $T$ be a maximal tree of order $n$ in $T(n,k)$. Let $N(v_j) - \{v_{j-1}, v_{j+1}\} = \{y_1\}$, we have

$$\sigma(T^{'}) = \sigma(T^{'} - y_1) + \sigma(T^{'} - [y_1]) \tag{12}$$

and

$$\sigma(T) = \sigma(T - y_1) + \sigma(T - [y_1]). \tag{13}$$

By induction assumption, we get

$$\sigma(T^{'} - y_1) > \sigma(T - y_1). \tag{14}$$

Also,

$$\sigma(T^{'} - [y_1]) = \sigma\left[P_j \bigcup P_{d-j} \bigcup (|S| - 1)P_1\right]. \tag{15}$$

One can easily see that $V(P_j \bigcup P_{d-j} \bigcup (|S| - 1)P_1]) = V(T - [y_1])$ and $E(P_j \bigcup P_{d-j} \bigcup (|S| - 1)P_1]) \subset E(T - [y_1])$. So

$$\sigma(T^{'} - [y_1]) = \sigma\left(P_j \bigcup P_{d-j} \bigcup (|S| - 1)P_1\right) > \sigma(T - [y_1]) \tag{16}$$

by lemma 4.

Combining (12) and (13) with (14) and (15), we get $\sigma(T^{'}) > \sigma(T)$. Thus, by the principle of mathematical induction, we know that $\sigma(T^{'}) > \sigma(T)$ for any maximal tree $T$ in $T(n,k)$ in this case. It is a contradiction to the choice of $T$.

Therefore, the desired result follows from the proofs of cases 1 and 2. □

In the following, we will determine the unique trees in $T(n,k)$ having the first largest Merrifield–Simmons index.

**Theorem 8.** Let $T$ be a tree in $T(n,k)$ with $3 \leqslant k \leqslant n-2$, then $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,(n-k)})$ with equality holds if and only if $T \cong T_{1,1,\ldots 1,(n-k)}$.

*Proof.* Suppose $T$ is a tree in $T(n,k)$ with $\sigma(T)$ taking the largest value. It follows from lemma 7 that $T \cong T_{1,1,\ldots,1,s,t}$, where $\min\{s,t\} \geqslant 1$ and $\max\{s,t\} \geqslant 2$. without loss of generality, we may assume that $t \geqslant s$ hereinafter.

In the following, we will prove that $T \cong T_{1,1,\ldots 1,(n-k)}$.

Suppose that $t = 2$. If $s = 1$, then $T \cong T_{1,1,\ldots 1,2}$ and the result holds. So, we may assume that $s = 2$.

Let $u$ be the unique branched vertex in $T$. Let $uv_1^s v_2^s$ and $uv_1^t v_2^t$ denote the path with respect to $s$ and $t$, respectively.

Let $T^{'}$ be obtained as follows

$$T^{'} = T - v_1^s v_2^s + v_2^s v_2^t.$$

Let $t$ be the number of pendent vertices in $N(u)$. Since $T \cong T_{1,1,\cdots 1,s,t}$ and $T \ncong S_n$, then $t \leqslant k-1$.

One can easily get that

$$\sigma(T^{'}) = \sigma(T^{'}-u) + \sigma(T^{'}-[u]) = 5.2^{t+1}3^{k-t-1} + 3.2^{k-t-2}$$

and

$$\sigma(T) = \sigma(T-u) + \sigma(T-[u]) = 2^t 3^{k-t} + 2^{k-t}.$$

Then $\sigma(T^{'}) – \sigma(T) = 7.2^t 3^{k-t-1} – 2^{k-t-2} > 0$, a contradiction to the choice of $T$.

So we may assume that $t \geqslant 3$. By $uv_1 \ldots v_t$, we denote the path with respect to $t$. We will show that $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,(k-1)})$ by induction on the order of $T$.

Assume that the result holds for all trees $T$ in $T(n,k)$ with small values of $n$.

Since $t \geqslant 3$, then $T - v_t \in T(n-1,k)$ and $T - [v_t] \in T(n-2,k)$. Hence by inductive hypothesis, we have

$$\sigma(T - v_t) \leqslant \sigma(T_{1,1,\ldots 1,(n-k-1)})$$

with equality holds if and only if $T \cong T_{1,1,\ldots 1,(n-k-1)}$ and

$$\sigma(T - [v_t]) \leqslant \sigma(T_{1,1,\ldots 1,(n-k-2)})$$

with equality holds if and only if $T \cong T_{1,1,\ldots 1,(n-k-2)}$.

Therefore

$$\begin{aligned}\sigma(T) &= \sigma(T - v_t) + \sigma(T - [v_t]) \\ &\leqslant \sigma(T_{1,1,\ldots,1,(n-k-1)}) + \sigma(T_{1,1,\ldots,1,(n-k-2)}) \\ &= \sigma(T_{1,1,\ldots,1,(n-k)}).\end{aligned}$$

It is not difficult to see that the above equality holds if and only if $T - v_t \cong T_{1,1,\ldots,1,(n-k-1)}$ and $T - [v_t] \cong T_{1,1,\ldots,1,(n-k-2)}$, which implies that $T \cong T_{1,1,\ldots,1,(n-k)}$. This completes the proof. □

## 3. Trees in $T(n,k)$ with the second largest value of Merrifield–Simmons index

We begin with an important lemma which is crucial to the proofs of our main results in this section.

**Lemma 9.** For $2 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$, $i \neq 3$ and $n \geqslant 6$, we have $F_3 F_{n+1} > F_5 F_{n-1} > F_{i+2} F_{n+2-i}$.

*Proof.* It is easy to prove that $F_3 F_{n+1} > F_5 F_{n-1}$ and $F_5 F_{n-1} > F_4 F_n$. So we need only to prove that $F_5 F_{n-1} > F_{i+2} F_{n-i+2}$ for $4 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$. Note that

$$\begin{aligned}F_{i+2}F_{n-i+2} - F_{i+1}F_{n-i+3} &= (F_{i+1} + F_i)F_{n-i+2} - F_{i+1}(F_{n-i+2} + F_{n-i+1}) \\ &= -(F_{i+1}F_{n-i+1} - F_i F_{n-i+2}) \\ &= (F_i + F_{i-1})F_{n-i+2} - F_i(F_{n-i+1} + F_{n-i}) \\ &= F_i F_{n-i} - F_{i-1}F_{n-i+1} \\ &= \cdots \\ &= (-1)^i (F_2 F_{n-2i+2} - F_1 F_{n-2i+3}) \\ &= (-1)^{i+1} F_{n-2i+1}.\end{aligned}$$

So, for $4 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$, we have $F_{i+2}F_{n-i+2} - F_5 F_{n-1} = (F_{n-9} - F_{n-7}) + (F_{n-13} - F_{n-11}) + \cdots < 0$, that is $F_5 F_{n-1} > F_{i+2}F_{n-i+2}$. This completes the proof. □

The proof of the following lemma is trivial, so we omit here.

**Lemma 10.** Let $T$ be a tree in $T(n,k)$ with $3 \leqslant k \leqslant n-2$. If $T \ncong T_{1,1,\ldots,1,(n-k)}$, then $\sigma(T) \leqslant \sigma(T_{1,1,\ldots,1,s,t})$ with equality holds if and only if $T \cong T_{1,1,\ldots,1,s,t}$, where $t \geqslant s \geqslant 2$ and $s + t = n - k + 1$.

**Theorem 11.** Let $T$ be a tree in $T(n,k)$ with $3 \leqslant k \leqslant n-5$. If $T \ncong T_{1,1,\ldots,1,(n-k)}$, then $\sigma(T) \leqslant \sigma(T_{1,1,\ldots,1,3,(n-k-2)})$ with equality holds if and only if $T \cong T_{1,1,\ldots,1,3,(n-k-2)}$.

*Proof.* Let $T$ be a tree in $T(n,k)$ with $3 \leqslant k \leqslant n-5$ such that $T \ncong T_{1,1,\ldots 1,(n-k)}$. By lemma 10, $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,s,\ t})$ where $t \geqslant s \geqslant 2$ and $s+t = n-k+1$. Moreover, the above equality holds if and only if $T \cong T_{1,1,\ldots 1,\ s,\ t}$. So it is sufficient to prove that $\sigma(T_{1,1,\ldots 1,s,\ t}) \leqslant \sigma(T_{1,1,\ldots 1,3,(n-k-2)})$ with equality holds if and only if $T_{1,1,\ldots 1,s,\ t} \cong T_{1,1,\ldots 1,3,(n-k-2)}$.

Let $T \cong T_{1,1,\ldots s,\ t}$ and $u$ be the unique branched vertex in $T$. Since $k \geqslant 3$, there must exist one pendent vertex, say $w$ in $T$, which is adjacent to $u$. Applying induction on $n$ and $k$.

It follows from lemma 1. that

$$\begin{aligned}\sigma(T) &= \sigma(T-w) + \sigma(T-[w]) \\ &= \sigma(T') + 2^{k-3}\sigma(P_s)\sigma(P_t) \\ &= \sigma(T') + 2^{k-3}F_{s+2}F_{t+2},\end{aligned}$$

where $T' = T - w \in T(n-1, k-1)$.

By induction assumption, we have $\sigma(T-w) = \sigma(T') \leqslant \sigma(T_{1,1,\ldots 1,3,(n-k-2)} - w')$, where $w'$ is one pendent vertex adjacent to the unique branched vertex $u'$ in $T_{1,1,\ldots 1,3,(n-k-2)}$. Also, it follows from lemma 9. that $F_{s+2}F_{t+2} \leqslant F_5F_{s+t-1}$ for all $2 \leqslant s \leqslant \lfloor \frac{s+t+4}{2} \rfloor$ with equality holds if and only if $s = 3$. since $T \ncong T_{1,1,\ldots 1,(n-k)}$, then $4 \leqslant s+2 \leqslant t+2$ and $\sigma(T-[w]) = 2^{k-3}F_{s+2}F_{t+2} \leqslant 2^{k-3}F_5F_{s+t-1} = \sigma(T_{1,1,\ldots 1,3,(n-k-2)} - [w'])$, where $w'$ is given as above. So

$$\begin{aligned}\sigma(T) &= \sigma(T-w) + \sigma(T-[w]) \\ &\leqslant \sigma(T_{1,1,\ldots 1,3,(n-k-2)} - w') + \sigma(T_{1,1,\ldots 1,3,(n-k-2)} - [w']) \\ &= \sigma(T_{1,1,\ldots 1,3,(n-k-2)}).\end{aligned}$$

Moreover, the above equality holds if and only if $T - w \cong T_{1,1,\ldots 1,3,(n-k-2)} - w'$ and $T - [w] \cong T_{1,1,\ldots 1,3,(n-k-2)} - [w']$, which leads to that $T \cong T_{1,1,\ldots 1,3,(n-k-2)}$. This completes the proof. □

When $n = k-4$, the next theorem determined the unique tree in $T(n, n-4)$ which attains the second largest value of Merrifield-Simmons index.

**Theorem 12.** Let $T$ be a tree in $T(n, n-4)$ and $T \ncong T_{1,1,\ldots 1,4}$, then $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,2,3})$ with equality if and only if $T \cong T_{1,1,\ldots 1,2,3}$.

*Proof.* For any tree $T$ in $T(n, n-4)$. If $T \ncong T_{1,1,\ldots 1,1,4}$, then by lemma 10., we have $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,s,t})$ where $t \geqslant s \geqslant 2$. Since the tree $T \cong T_{1,1,\ldots 1,2,3}$ is the unique tree of the form $T_{1,1,\ldots 1,s,t}$ with $t \geqslant s \geqslant 2$, then the desired result follows.

When $n = k-3$, one can easily get the following. □

**Theorem 13.** Let $T$ be a tree in $T(n, n-3)$ and $T \ncong T_{1,1,\ldots 1,1,3}$, then $\sigma(T) \leqslant \sigma(T_{1,1,\ldots 1,2,2})$ with equality holds if and only if $T \cong T_{1,1,\ldots 1,2,2}$.

The proof of this theorem is similar to that of theorem 12., so we omit here.

In the following, we determine the unique tree with the second largest Merrifiled-Simmons index among all trees in $T(n, n-2)$.

**Theorem 14.** Let $T$ be a tree in $T(n, n-2)$. If $T \ncong T_{1,1,\ldots 1,2}$, then $\sigma(T) \leqslant \sigma(S_{2,n-4})$ with equality holds if and only if $T \cong S_{2,n-4}$.

*Proof.* For any tree in $T(n, n-2)$, we must have $T \cong S_{a,b}(a \geqslant 1$ and $b \geqslant 1)$.

Since $T \ncong T_{1,1,\ldots 1,2}$ and $T_{1,1,\ldots 1,2} \cong S_{1,n-3}$, then we may assume that $T \cong S_{a,b}$ with $b \geqslant a \geqslant 2$. Noting that $\sigma(S_{a,b}) = 2^a(2^b+1)+2^b$. So $\sigma(S_{a-1,b+1}) - \sigma(S_{a,b}) = (2^{a-1} + 2^{b+1}) - (2^a + 2^b) = 2^b - 2^{a-1} > 0$. Then we have $\sigma(S_{a,b}) \leqslant \sigma(S_{2,n-4})$ for all trees $T$ in $T(n, n-2)$ and $T \ncong T_{1,1,\ldots 1,2}$ with equality holds if and only if $T \cong S_{2,n-4}$. □

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