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# The Merrifield–Simmons indices and Hosoya indices of trees with $k$ pendant vertices

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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. In this paper, we characterize the trees with maximal Merrifield–Simmons indices and minimal Hosoya indices, respectively, among the trees with $k$ pendant vertices.

**KEY WORDS:** Merrifield–Simmons index, Hosoya index, tree, pendant vertex

## 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 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 [15], although it is called Fibonacci number of a graph there.

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The Merrifield–Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [13]. There Merrifield and Simmons showed the correlation between this index and boiling points. Now there have been many papers studying the Merrifield–Simmons index. In [15], Prodinger and Tichy showed that, for $n$-vertex trees, the star has the maximal Merrifield–Simmons index and the path has the minimal Merrifield–Simmons index. In [1], Alameddine studied bounds for the Merrifield–Simmons index of a maximal outerplanar graph. Gutman [7], Zhang [17], Zhang [18], Zhang and Tian [19, 20] studied the Merrifield–Simmons indices of hexagonal chains and catacondensed systems, respectively. In [12], Li et al characterized the tree with the maximal Merrifield–Simmons index among the trees with given diameter. In [14], Pedersen and Vestergaard studied the Merrifield–Simmons indices of the unicyclic graphs. In [21], Yu and Tian studied the Merrifield–Simmons indices of the graphs with given edge-independence number and cyclomatic number.

The Hosoya index of a graph was introduced by Hosoya [10] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [13, 16]. Since then, many authors have investigated the Hosoya index (e.g., see [3–6, 8, 9, 16]). An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. In [7], Gutman showed that linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. In [17], Zhang showed that zig–zag hexagonal chain is the unique chain with maximal Hosoya index among all hexagonal chains. In [19], Zhang and Tian gave another proof on Gutman's and Zhang's results above mentioned. In [18], Zhang determined the graph with the second minimal Hosoya index among all hexagonal chains. In [20], Zhang and Tian determined the graphs with minimal and second minimal Hosoya indices among catacondensed systems. As for $n$-vertex trees, it has been shown that the path has the maximal Hosoya index and the star has the minimal Hosoya index (see [8]). Recently, Hou [11] characterized the trees with a given size of matching and having minimal and second minimal Hosoya index, respectively. In [21], Yu and Tian studied the graphs with given edge-independence number and cyclomatic number and having the minimal Merrifield–Simmons indices.

Let $\mathcal{T}_{n,k}$ be the set of all trees with $n$ vertices and $k$ pendant vertices. In this paper, we show that $P_{n,k}$ (as shown in figure 1) is the tree with maximal Merrifield–Simmons index and the minimal Hosoya index in $\mathcal{T}_{n,k}$.

In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to Bondy and Murty [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 $G_1,\ G_2, \ldots, G_t$, then $G$ is

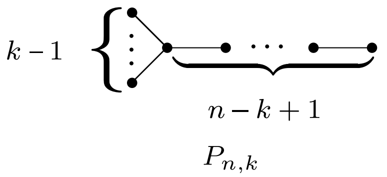


Figure 1

denoted by $\bigcup_{i=1}^{t} G_i$. For a vertex $v$ of $G$, we denote $N_G[v] = \{v\} \cup \{\, u \mid uv \in E(G)\}$. We denote by $P_n$ and $S_n$ the path and the star on $n$ vertices, respectively.

## 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 [8]) $z(G) = z(G - uv) + z(G - \{u, v\})$.

From lemma 2.1, we have $z(G) > z(G - uv)$, if $uv$ is an edge of $G$.

**Lemma 2.2** (see [8]). 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 $v$.

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 $z(G) > z(G - v)$.

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 $z(G) = z(G-v)+z(G-\{u, v\})$. 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 $n \geqslant 2$. Denote by $F_n$ the $n$th Fibonacci number. Recall that $F_n = F_{n-1}+F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. We have

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

Similarly, we have $z(P_0) = 1$, $z(P_1) = 1$ and $z(P_n) = z(P_{n-1}) + z(P_{n-2})$ for $n \geqslant 2$. Thus

$$z(P_n) = F_n = \left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1}\right] / \sqrt{5}.$$

**Lemma 2.3** (see [8]). If $G_1, G_2, \ldots, G_t$ are the components of a graph $G$, we have

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

Let $P = v_0v_1\ldots v_k$ $(k \geqslant 1)$ be a path of a tree $T$. If $d_T(v_0) \geqslant 3$, $d_T(v_k) \geqslant 3$ and $d_T(v_i) = 2$ $(0 < i < k)$, we call $P$ an internal path of $T$. If $d_T(v_0) \geqslant 3$, $d_T(v_k) = 1$ and $d_T(v_i) = 2$ $(0 < i < k)$, we call $P$ a pendant path of $T$ with root $v_0$ and particularly when $k = 1$, we call $P$ a pendant edge. Let $s(T)$ be the number of vertices in $T$ with degree more than 2 and $p(T)$ the number of pendent paths in $T$ with length more than 1. For example, we consider the tree $T$ as shown in figure 2. $v_3v_4v_5v_6$ is an internal path of $T$, while $v_6v_7v_8v_9v_{10}$, $v_6v_{11}$, $v_3v_1$, and $v_3v_2$ are all pendant paths of $T$; $s(T) = 2$ and $p(T) = 1$.

In the following, we shall define two kinds of operations of $T \in \mathcal{T}_{n,k}$ and show that these two kinds of operations make the Merrifield–Simmons indices of the trees increase strictly and the Hosoya indices of the trees decrease strictly.

If $T \in \mathcal{T}_{n,k}$ $(3 \leqslant k \leqslant n-2)$, $T \not\cong P_{n,k}$ and $p(T) \neq 0$, then $T$ can be seen as the tree as shown in figure 3, where $P_s$ $(s \geqslant 3)$ is the pendant path of $T$ with $s$ vertices and root $u$, $T_1$ and $T_2$ are two subtrees of $T$ with vertices $v$ and $u$ as

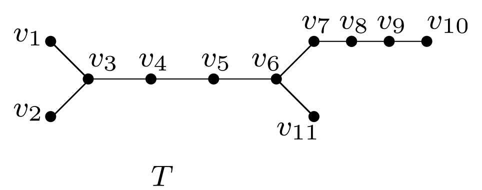


Figure 2

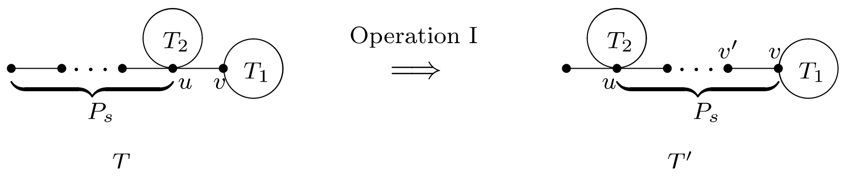


Figure 3

roots, respectively, and $T_1, T_2 \ncong P_1$. If $T'$ is obtained from $T$ by replacing $P_s$ with a pendant edge and replacing the edge $uv$ with a path $P_s$, we say that $T'$ is obtained from $T$ by operation I (as shown in figure 3). It is easy to see that $T' \in \mathcal{T}_{n,k}$.

Now we show that operation I makes the Merrifield–Simmons indices of the trees increase strictly and the Hosoya indices of the trees decrease strictly. In the following proofs, we shall use the same notations as above.

**Lemma 2.4.** If $T'$ is obtained from $T$ by operation I, then

$$(1)\ i(T') > i(T),$$
$$(2)\ z(T') < z(T).$$

*Proof.* (1) Let $N_{T_1}[v] = V_1$ and $N_{T_2}[u] = V_2$. If $s \geqslant 4$, by lemmas 2.2 and 2.3, we have

$$\begin{aligned} i(T) &= i(T-v) + i(T - N_T[v]) \\ &= i(T_1 - v)(i(T_2 - u)\cdot i(P_{s-1}) + i(T_2 - V_2)\cdot i(P_{s-2})) \\ &\quad + i(T_1 - V_1)\cdot i(T_2 - u)\cdot i(P_{s-1}), \\ i(T') &= i(T'-v) + i(T' - N_{T'}[v]) \\ &= i(T_1 - v)(2\cdot i(T_2 - u)\cdot i(P_{s-2}) + i(T_2 - V_2)\cdot i(P_{s-3})) \\ &\quad + i(T_1 - V_1)(2\cdot i(T_2 - u)\cdot i(P_{s-3}) + i(T_2 - V_2)\cdot i(P_{s-4})). \end{aligned}$$

Since $i(P_0) = 1$, $i(P_1) = 2$ and $i(P_n) = i(P_{n-1}) + i(P_{n-2})$ for $n \geqslant 2$, we have

$$i(T') - i(T) = i(P_{s-4})(i(T_1 - v) - i(T_1 - V_1))(i(T_2 - u) - i(T_2 - V_2)).$$

Since $s \geqslant 4$, $i(P_{s-4}) > 0$. Noting that $T_1, T_2 \ncong P_1$, by lemma 2.2, we have $i(T_1 - v) - i(T_1 - V_1) > 0$ and $i(T_2 - u) - i(T_2 - V_2) > 0$. Therefore, $i(T') - i(T) > 0$.

If $s = 3$, similarly, we have

$$i(T') - i(T) = (i(T_1 - v) - i(T_1 - V_1))(i(T_2 - u) - i(T_2 - V_2)) > 0.$$

Therefore $i(T') > i(T)$, if $T'$ is obtained from $T$ by operation I.

(2) Let $A_l$ and $B_l$ be the trees as shown in figure 4.

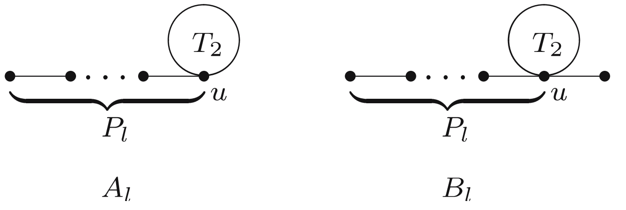


Figure 4

By lemmas 2.1 – 2.3, we have

$$
\begin{aligned}
z(T) &= z(T - uv) + z(T - \{u, v\}) \\
&= z(T_1) \cdot z(A_s) + z(T_1 - v) \cdot z(T_2 - u) \cdot z(P_{s-1}) \\
&= z(T_1) \cdot z(A_{s-1}) + z(T_1) \cdot z(A_{s-2}) + z(T_1 - v) \cdot z(T_2 - u) \cdot z(P_{s-1}), \\
z(T') &= z(T' - v'v) + z(T' - \{v', v\}) \\
&= z(T_1) \cdot z(B_{s-1}) + z(T_1 - v) \cdot z(B_{s-2}) \\
&= z(T_1) \cdot z(A_{s-1}) + z(T_1) \cdot z(T_2 - u) \cdot z(P_{s-2}) + z(T_1 - v) \cdot z(A_{s-2}) \\
&\quad + z(T_1 - v) \cdot z(T_2 - u) \cdot z(P_{s-3}).
\end{aligned}
$$

Since $z(P_0) = 1$, $z(P_1) = 1$ and $z(P_n) = z(P_{n-1}) + z(P_{n-2})$ for $n \geqslant 2$, we have

$$z(T) - z(T') = (z(T_1) - z(T_1 - v))(z(A_{s-2}) - z(T_2 - u) \cdot z(P_{s-2})).$$

Noting that $T_1, T_2 \ncong P_1$, by lemmas 2.1 and 2.2, we have $z(A_{s-2}) - z(T_2 - u) \cdot z(P_{s-2}) > 0$ and $z(T_1) - z(T_1 - v) > 0$. So $z(T) - z(T') > 0$. Therefore if $T'$ is obtained from $T$ by operation I, $z(T') < z(T)$. □

From lemma 2.4, we immediately get the following result.

**Lemma 2.5.** Let $T \in \mathcal{T}_{n,k}$ $(3 \leqslant k \leqslant n - 2)$, $T \ncong P_{n,k}$ and $p(T) \neq 0$.

(1) If $s(T) = 1$, we can finally get a tree $T'$ by operation I with $i(T') > i(T)$, $z(T') < z(T)$, and $p(T') = 1$; it is easy to see that $T' \cong P_{n,k}$;

(2) if $s(T) \geqslant 2$, we can finally get a tree $T'$ by operation I with $i(T') > i(T)$, $z(T') < z(T)$, and $p(T') = 0$.

If $T \in \mathcal{T}_{n,k}$ $(3 \leqslant k \leqslant n-2)$, $T \ncong P_{n,k}$ and $p(T) = 0$, then we always can find two pendant vertices $u_1$ and $v_1$ of $T$ such that $d(u_1, v_1) = \max\{d(u, v) : u, v \in V(T)\}$. Let $u_1u, v_1v \in E(T)$, then $N_T(u) = \{u_1, u_2, \ldots, u_s, w\}$ $(s \geqslant 2)$, $N_T(v) = \{v_1, v_2, \ldots, v_t, w'\}(t \geqslant 2)$, where $u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t$ are pendant vertices of $T$, $d_T(w) \geqslant 2$ and $d_T(w') \geqslant 2$. Note that $w = w'$, when $d(u_1, v_1) = 3$. If $T' = T - \{vv_2, \ldots, vv_t\} + \{uv_2, \ldots, uv_t\}$ and $T'' = T - \{uu_2, \ldots, uu_s\} + \{vu_2, \ldots, vu_s\}$, we say that $T'$ and $T''$ are obtained from $T$ by operation II, respectively. It is easy to see that $T', T'' \in \mathcal{T}_{n,k}$, $p(T') = p(T'') = 1$ and $s(T') = s(T'') = s(T) - 1$.

Now we show that operation II makes the Merrifield–Simmons indices of the trees increase strictly and the Hosoya indices of the trees decrease strictly. In the following proofs, we shall use the same notations as above.

**Lemma 2.6.** If $T'$ and $T''$ are obtained from $T$ by Operation II, then

(1) either $i(T') > i(T)$ or $i(T'') > i(T)$,

(2) either $z(T') < z(T)$ or $z(T'') < z(T)$.

*Proof.* (1) Let $u_1$, $v_1$ be the pendant vertices such that $d(u_1, v_1) = \max\{d(u, v) : u, v \in V(T)\}$. If $d(u_1, v_1) \geqslant 4$, without loss of generality, we suppose $u_1u$, $v_1v$, $uw \in E(T)$ and $d_T(w) \geqslant 2$. Then $w \neq v$. In this case, $T, T', T''$ can be seen as the trees as shown in figure 5.

Denote $N_{T_1}[v] = V_1$ and $N_{T_1-w}[v] = V_2$. Note that if $d(u_1, v_1) = 4$, then $V_1 = \{v, w\}$ and $V_2 = \{v\}$; if $d(u_1, v_1) > 4$, then $V_1 = \{v, w'\}$ and $V_2 = \{v, w'\}$. By lemmas 2.2 and 2.3, we have

$$\begin{aligned} i(T) &= i(T-u) + i(T - N_T[u]) \\ &= 2^s(2^t \cdot i(T_1 - v) + i(T_1 - V_1)) + 2^t \cdot i(T_1 - \{w, v\}) + i(T_1 - (\{w\} \cup V_2)), \\ i(T') &= i(T'-u) + i(T' - N_{T'}[u]) \\ &= 2^{s+t-1}(2 \cdot i(T_1 - v) + i(T_1 - V_1)) + 2 \cdot i(T_1 - \{w, v\}) + i(T_1 - (\{w\} \cup V_2)), \\ i(T'') &= i(T''-u) + i(T'' - \{u, w, u_1\}) \\ &= 2(2^{s+t-1} \cdot i(T_1 - v) + i(T_1 - V_1)) + 2^{s+t-1} \cdot i(T_1 - \{w, v\}) + i(T_1 - (\{w\} \cup V_2)). \end{aligned}$$

It is easy to see that

$$\begin{aligned} i(T') - i(T) &= 2(2^{t-1} - 1)(2^{s-1} \cdot i(T_1 - V_1) - i(T_1 - \{w, v\})), \\ i(T'') - i(T) &= 2(2^{s-1} - 1)(2^{t-1} \cdot i(T_1 - \{w, v\}) - i(T_1 - V_1)). \end{aligned}$$

Note that $s, t \geqslant 2$. If $i(T') - i(T) \leqslant 0$, we have $2^{s-1} \cdot i(T_1 - V_1) \leqslant i(T_1 - \{w, v\})$. Then we have

$$i(T'') - i(T) \geqslant 2(2^{s-1} - 1)(2^{t-1} \cdot 2^{s-1} - 1) \cdot i(T_1 - V_1) > 0.$$

If $d(u_1, v_1) = 3$, we have $T' \cong T''$ and

$$\begin{aligned} i(T') - i(T) &= (2^{s+t} + 2^{s+t-1} + 2) - (2^{s+t} + 2^s + 2^t) \\ &= 2(2^{t-1} - 1)(2^{s-1} - 1) > 0. \end{aligned}$$

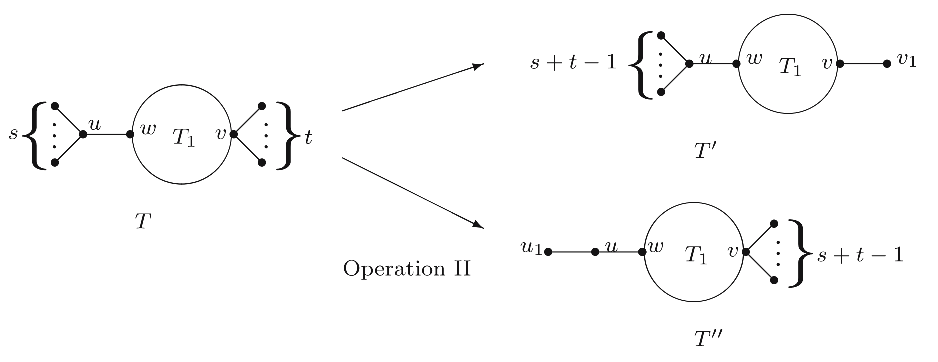


Figure 5

Therefore, if $T'$ and $T''$ are obtained from $T$ by operation II, then either $i(T') > i(T)$ or $i(T'') > i(T)$.

(2) Let $u_1$, $v_1$ be the pendant vertices such that $d(u_1, v_1) = \max\{d(u, v) : u, v \in V(T)\}$. If $d(u_1, v_1) \geqslant 4$, without loss of generality, we suppose $u_1u$, $v_1v$, $uw \in E(T)$ and $d_T(w) \geqslant 2$. Then $w \neq v$. In this case, $T, T', T''$ can be seen as the trees as shown in figure 5.

Denote $A = \sum_{v'v \in E(T_1)} z(T_1 - \{v', v\})$ and $B = \sum_{v'v \in E(T_1 - w)} z(T_1 - \{v', v, w\})$. By Lemmas 2.1 – 2.3, we have

$$\begin{aligned} z(T) &= z(T - uw) + z(T - \{u, w\}) \\ &= (s+1)((t+1) \cdot z(T_1 - v) + A) + (t+1) \cdot z(T_1 - \{w, v\}) + B, \\ z(T') &= z(T' - uw) + z(T' - \{u, w\}) \\ &= (s+t)(2 \cdot z(T_1 - v) + A) + 2 \cdot z(T_1 - \{w, v\}) + B, \\ z(T'') &= z(T'' - uw) + z(T'' - \{u, w\}) \\ &= 2((s+t) \cdot z(T_1 - v) + A) + (s+t) \cdot z(T_1 - \{w, v\}) + B. \end{aligned}$$

It is easy to see that

$$\begin{aligned} z(T) - z(T') &= (t-1)((s-1) \cdot z(T_1 - v) - A + z(T_1 - \{w, v\})), \\ z(T) - z(T'') &= (s-1)((t-1) \cdot z(T_1 - v) + A - z(T_1 - \{w, v\})). \end{aligned}$$

Note that $s, t \geqslant 2$. If $z(T) - z(T') \leqslant 0$, we have

$$(s-1) \cdot z(T_1 - v) + z(T_1 - \{w, v\}) \leqslant A.$$

Then we have

$$z(T) - z(T'') \geqslant (s-1)(t+s-2) \cdot z(T_1 - v) > 0.$$

If $d(u_1, v_1) = 3$, we have $T' \cong T''$ and

$$\begin{aligned} z(T) - z(T') &= (s+1)(t+1) + 1 - (2(s+t) + 1) \\ &= (t-1)(s-1) > 0. \end{aligned}$$

Therefore, if $T'$ and $T''$ are obtained from $T$ by operation II, then either $z(T') < z(T)$ or $z(T'') < z(T)$. □

**Theorem 2.1.** Let $T \in \mathcal{T}_{n,k}$. Then

(1) $i(T) \leqslant 2^{k-1} \cdot F_{n-k+1} + F_{n-k}$, the equality holds if and only if $T \cong P_{n,k}$;

(2) $z(T) \geqslant k \cdot F_{n-k} + F_{n-k-1}$, the equality holds if and only if $T \cong P_{n,k}$.

*Proof.* (1) By lemma 2.2 (1), it is easy to see that

$$i(P_{n,k}) = 2^{k-1} i(P_{n-k}) + i(P_{n-k-1}) = 2^{k-1} \cdot F_{n-k+1} + F_{n-k}.$$

Since $\mathcal{T}_{n,2} = \{P_n\}$ and $P_n \cong P_{n,2}$, $\mathcal{T}_{n,n-1} = \{S_n\}$ and $S_n \cong P_{n,n-1}$, we may assume $3 \leqslant k \leqslant n-2$ and it is sufficient to show that $i(T) < i(P_{n,k})$ for any $T \in \mathcal{T}_{n,k}$ and $T \ncong P_{n,k}$.

For $T \in \mathcal{T}_{n,k}$ $(3 \leqslant k \leqslant n-2)$ and $T \ncong P_{n,k}$, we know $1 \leqslant s(T) \leqslant n-k$, we shall show $i(T) < i(P_{n,k})$ by induction on $s(T)$. When $s(T) = 1$, since $T \ncong P_{n,k}$, we have $p(T) \geqslant 2$. By lemma 2.5 (1), we have $i(T) < i(P_{n,k})$. Suppose the result holds for any tree $T'$ with $s(T') = s-1$. Let $s(T) = s \geqslant 2$. If $p(T) \neq 0$, we can get a tree $T_1 \in \mathcal{T}_{n,k}$ such that $p(T_1) = 0$, $s(T_1) = s$ and $i(T_1) > i(T)$, by lemma 2.5 (2). By lemma 2.6 (1), we can get a tree $T_2 \in \mathcal{T}_{n,k}$ from $T_1$ such that $p(T_2) = 1$, $s(T_2) = s-1$ and $i(T_2) > i(T_1)$. Hence $i(T) < i(T_1) < i(T_2)$. By the induction hypothesis, we have

$$i(T) < i(T_1) < i(T_2) < i(P_{n,k}).$$

Therefore, if $T \in \mathcal{T}_{n,k}$, $i(T) \leqslant 2^{k-1} \cdot F_{n-k+1} + F_{n-k}$, the equality holds if and only if $T \cong P_{n,k}$.

(2) By lemma 2.2 (2), we have

$$z(P_{n,k}) = k \cdot z(P_{n-k}) + z(P_{n-k-1}) = k \cdot F_{n-k} + F_{n-k-1}.$$

Similarly, by lemmas 2.5 and 2.6 (2), we can show that, $z(T) \geqslant k \cdot F_{n-k} + F_{n-k-1}$, the equality holds if and only if $T \cong P_{n,k}$. □

**Lemma 2.7.** For $3 \leqslant k \leqslant n-1$, we have

(1) $i(P_{n,k}) > i(P_{n,k-1})$,

(2) $z(P_{n,k}) < z(P_{n,k-1})$.

*Proof.* (1) By lemma 2.2 (1), we have

$$i(P_{n,k}) = 2^{k-1} i(P_{n-k}) + i(P_{n-k-1}),$$
$$i(P_{n,k-1}) = 2^{k-2} i(P_{n-k+1}) + i(P_{n-k}).$$

Noting that, for $3 \leqslant k \leqslant n-1$, $i(P_{n-k+1}) = i(P_{n-k}) + i(P_{n-k-1})$ , we have

$$i(P_{n,k}) - i(P_{n,k-1}) = (2^{k-2} - 1)(i(P_{n-k}) - i(P_{n-k-1})) > 0.$$

Hence $i(P_{n,k}) > i(P_{n,k-1})$ for $3 \leqslant k \leqslant n-1$.

(2) By lemma 2.2 (2), we have

$$z(P_{n,k}) = k \cdot z(P_{n-k}) + z(P_{n-k-1}),$$
$$z(P_{n,k-1}) = (k-1) \cdot z(P_{n-k+1}) + z(P_{n-k}).$$

Noting that, for $3 \leqslant k \leqslant n-1$, $z(P_{n-k+1}) = z(P_{n-k}) + z(P_{n-k-1})$ , we have

$$z(P_{n,k}) - z(P_{n,k-1}) = -(k-2)z(P_{n-k-1}) < 0.$$

Hence $z(P_{n,k}) < z(P_{n,k-1})$ for $3 \leqslant k \leqslant n-1$. □

From theorem 2.1 and lemma 2.7, we immediately get the following results.

**Corollary 2.1.** Let $T$ be a tree with $n$ vertices. Then

(1) $i(T) \leqslant 2^{n-1} + 1$, the equality holds if and only if $T \cong S_n$;

(2) if $T \ncong S_n$, $i(T) \leqslant 3 \cdot 2^{n-3} + 2$, the equality holds if and only if $T \cong P_{n,n-2}$;

(3) $z(T) \geqslant n$, the equality holds if and only if $T \cong S_n$;

(4) if $T \ncong S_n$, $z(T) \geqslant 2n-3$, the equality holds if and only if $T \cong P_{n,n-2}$.

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