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Extremal trees with respect to Hosoya Index and Merrifield-Simmons Index.*

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Abstract

We characterize the trees T with n vertices whose Hosoya index (total number of matchings) is $Z(T) > 16f_{n-5}$ resp. the trees whose Merrifield-Simmons index (total number of independent subsets) is $\sigma(T) < 18f_{n-5} + 21f_{n-6}$, where f_k is the k-th Fibonacci number. It turns out that all the trees satisfying the inequality are tripodes (trees with exactly three leaves) and the path in both cases. Furthermore, we show that the remarkable correspondence $Z(T)+\sigma(T) = f_{n+3}$ holds for all these trees. These results are achieved by modifying and enhancing methods due to Li and Zhao, who found the trees of second- and third-smallest Merrifield-Simmons index.

1 Introduction

The Hosoya- or Z-index $Z(G)$ and the Merrifield-Simmons- or σ-index $\sigma(G)$ of a graph G are two prominent examples of topological indices which are of interest in combinatorial chemistry. They are defined as the number of matchings (independent edge subsets) resp. number of independent vertex subsets of a graph.

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The Z-index was introduced by Hosoya [5, 6] 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 point, entropy or heat of vaporization are well studied.

Similar connections are known for the σ-index, introduced by Merrifield and Simmons [11] in 1989. For detailed information on the chemical applications, we refer to [4, 11, 13] and the references therein.

Several papers deal with the characterization of the extremal graphs with respect to these two indices in several given graph classes – usually, trees and certain structures involving pentagonal and hexagonal cycles are of major interest [2, 7, 8, 9, 10, 15, 16]. It turns out that typically the graphs of minimal Hosoya index coincide with those of maximal Merrifield-Simmons index and vice versa. In view of the similar definitions, this might not be too surprising; however, the correlations between these two indices are not fully understood yet (cf. also [3, 14]).

Trees with maximal and minimal Merrifield-Simmons index were the topic of a paper of Lin and Lin [10]; some of their results were rediscovered and extended by Gutman, Li and Zhao [8, 9]. In particular, Li and Zhao characterize the trees of second- and third-smallest σ-index in their paper [8] (the path has been proved to be the tree of minimal σ-index before in [12]). In this paper, their approach is extended to a much larger range – it is shown that a tree T with σ-index $\sigma(T) < 18f_{n-5} + 21f_{n-6}$ has at most three leaves; on the other hand, $\sigma(T) < 18f_{n-5} + 21f_{n-6}$ holds for almost all tripodes (i.e. trees with three leaves). Most results together with their proofs hold in almost literally the same way for the Z-index. Finally, there is a remarkable correspondence between the Z-index and σ-index of tripodes.

2 Preliminaries

In the following, $G = (V(G), E(G))$ denotes a graph with vertex set $V(G)$ and edge set $E(G)$. All graphs considered here are finite and simple. For graph-theoretical terminology and notation, we refer to [1].

We will mainly be concerned with trees, though some theorems are stated for more general graphs. For a tree T and a vertex v of T, we call the components of $T \setminus \{v\}$ the *subtrees* of T at v.

We denote the sequence of Fibonacci numbers by f_n, i.e. $f_0 = 0$, $f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$. f_n is extended to negative values of n via Binet's formula $f_n = \frac{1}{\sqrt{5}}\left(\phi^n - (-\phi)^{-n}\right)$, where $\phi = \frac{1+\sqrt{5}}{2}$. Analogously, the Lucas numbers are denoted by l_n, i.e. $l_0 = 2$, $l_1 = 1$,

$l_{n+1} = l_n + l_{n-1}$ and $l_n = \phi^n + (-\phi)^{-n}$.

We will make use of the following two well-known lemmas on the Merrifield-Simmons index and Hosoya index:

Lemma 1 Let G be a graph and $v \in V(G)$, and let $v_1, \ldots, v_k$ be the neighbors of v. Then we have

$$Z(G) = Z(G \setminus v) + \sum_{i=1}^{k} Z(G \setminus \{v, v_i\})$$

and

$$\sigma(G) = \sigma(G \setminus v) + \sigma(G \setminus \{v, v_1, \ldots, v_k\}).$$

If G is a graph whose connected components are $G_1, \ldots, G_l$, we have

$$Z(G) = \prod_{i=1}^{l} Z(G_i) \text{ and } \sigma(G) = \prod_{i=1}^{l} \sigma(G_i).$$

Lemma 2 For a given number of vertices n, the tree of maximal Hosoya index and minimal Merrifield-Simmons index is the path P_n. We have $Z(P_n) = f_{n+1}$ and $\sigma(P_n) = f_{n+2}$.

Next, we define two special classes of trees that will be in the center of our interest.

Definition 1 We call a tree with only one vertex v of degree $d > 2$ a *d-pode*. In particular, we use the term *tripode* for 3-podes. v is called the *center*. To each partition $(c_1, \ldots, c_d)$ of $n-1$, there is exacty one corresponding d-pode (s. Figure 1), which we denote by $R(c_1, \ldots, c_d)$. Here, c_i is the length of the i-th "ray" going out from the center.

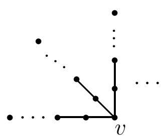

Figure 1: The d-pode $R(c_1, \ldots, c_d)$.

Definition 2 Let a, b_{ij} be positive integers with $a + b_{11} + b_{12} + b_{21} + b_{22} = n$. Then, the n-vertex tree that is shown in Figure 2 is denoted by $H(a, b_{11}, b_{12}, b_{21}, b_{22})$. Here, $a = 1$ means that v_1 and v_a coincide.

REMARK: It is easy to see that every tree with 3 leaves is a tripode, and that every tree with 4 leaves is of the form $H(a, b_{11}, b_{12}, b_{21}, b_{22})$.

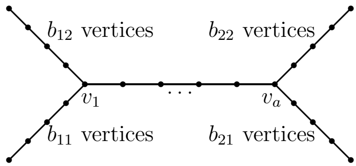

Figure 2: The tree $H(a, b_{11}, b_{12}, b_{21}, b_{22})$.

Lemmas 1 and 2 can be used to give explicit formulas for the Hosoya- and Merrifield-Simmons indices of these special trees:

Proposition 3 The following formulas hold for all $a, b_{ij}, c_i \geq 1$:

$$Z(R(c_1, \dots, c_d)) = \prod_{i=1}^{d} f_{c_i+1} + \sum_{i=1}^{d} f_{c_i} \prod_{\substack{j=1 \\ j \neq i}}^{d} f_{c_j+1},$$

$$\sigma(R(c_1, \dots, c_d)) = \prod_{i=1}^{d} f_{c_i+2} + \prod_{i=1}^{d} f_{c_i+1}.$$

and

$$Z(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = \prod_{1 \leq i,j \leq 2} f_{b_{ij}+1} \cdot \left(f_{a-1} \left(1 + \sum_{1 \leq i,j \leq 2} \frac{f_{b_{ij}}}{f_{b_{ij}+1}} + \sum_{1 \leq i,j \leq 2} \frac{f_{b_{1i}} f_{b_{2j}}}{f_{b_{1i}+1} f_{b_{2j}+1}} \right) + f_{a-2} \left(2 + \sum_{1 \leq i,j \leq 2} \frac{f_{b_{ij}}}{f_{b_{ij}+1}} \right) + f_{a-3} \right),$$

$$\sigma(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = f_a \prod_{1 \leq i,j \leq 2} f_{b_{ij}+2} + f_{a-1} \left(\prod_{1 \leq i,j \leq 2} f_{b_{ij}+i} + \prod_{1 \leq i,j \leq 2} f_{b_{ij}+3-i} \right) + f_{a-2} \prod_{1 \leq i,j \leq 2} f_{b_{ij}+1}.$$

Remark: From the explicit formulas, the recursions

$$Z(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = Z(H(a-1, b_{11}, b_{12}, b_{21}, b_{22})) + Z(H(a-2, b_{11}, b_{12}, b_{21}, b_{22})),$$
$$Z(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = Z(H(a, b_{11}-1, b_{12}, b_{21}, b_{22})) + Z(H(a, b_{11}-2, b_{12}, b_{21}, b_{22})),$$
$$\sigma(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = \sigma(H(a-1, b_{11}, b_{12}, b_{21}, b_{22})) + \sigma(H(a-2, b_{11}, b_{12}, b_{21}, b_{22})),$$
$$\sigma(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = \sigma(H(a, b_{11}-1, b_{12}, b_{21}, b_{22})) + \sigma(H(a, b_{11}-2, b_{12}, b_{21}, b_{22}))$$

follow easily.

Corollary 4 The formulas

$$Z(R(c_1,c_2,c_3)) = \frac{1}{5}\Big(f_{n+2} + 3f_{n+1} + (-1)^{c_1} f_{n-2c_1-1} + (-1)^{c_2} f_{n-2c_2-1} + (-1)^{c_3} f_{n-2c_3-1}\Big)$$

and

$$\sigma(R(c_1,c_2,c_3)) = \frac{1}{5}\Big(4f_{n+2} + 2f_{n+1} - (-1)^{c_1} f_{n-2c_1-1} - (-1)^{c_2} f_{n-2c_2-1} - (-1)^{c_3} f_{n-2c_3-1}\Big)$$

hold for all $c_1, c_2, c_3 \geq 1$ with $c_1 + c_2 + c_3 + 1 = n$. It follows that

$$Z(R(c_1,c_2,c_3)) + \sigma(R(c_1,c_2,c_3)) = f_{n+3}.$$

Proof: From Binet's formula, we easily obtain

$$f_u f_v f_w = \frac{1}{5}\Big(f_{u+v+w} - (-1)^u f_{-u+v+w} - (-1)^v f_{u-v+w} - (-1)^w f_{u+v-w}\Big),$$

and the corollary follows upon some elementary simplifications. □

3 Auxiliary results

First, we need a lemma on graphs which are constructed by attaching an arbitrary graph G to a path P_n. For the Merrifield-Simmons index, this lemma was given in [8], therefore, we only state a proof for the Hosoya index:

Lemma 5 Let $G \not\cong P_1$ be a connected graph and choose $v \in V(G)$. $P(n,k,G,v)$ then denotes the graph that results from identifying v with the vertex v_k of a simple path $v_1, \ldots, v_n$ (Figure 3).

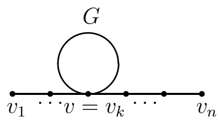

Figure 3: The graph $P(n,k,G,v)$.

Now, let $n = 4m + i$, $i \in 1,2,3,4$, $m \geq 0$. Then

$$Z(P(n,2,G,v)) < Z(P(n,4,G,v)) < \ldots < Z(P(n,2m+2l,G,v)) <$$
$$Z(P(n,2m+1,G,v)) < \ldots < Z(P(n,3,G,v)) < Z(P(n,1,G,v))$$

and

$$\sigma(P(n,2,G,v)) > \sigma(P(n,4,G,v)) > \ldots > \sigma(P(n,2m+2l,G,v)) >$$
$$\sigma(P(n,2m+1,G,v)) > \ldots > \sigma(P(n,3,G,v)) > \sigma(P(n,1,G,v)),$$

where $l = \lfloor \frac{i-1}{2} \rfloor$.

Proof: Set $A = Z(G)$ and $B = Z(G \setminus \{v\})$. Clearly, each matching of $G \setminus \{v\}$ is also a matching of G, but not vice versa, so $A > B$. A matching of $P(n, k, G, v)$ has to satisfy exactly one of the following conditions:

- it contains neither (v_{k-1}, v_k) nor (v_k, v_{k+1}). If these edges are removed, three subgraphs remain: G and two paths with $k-1$ resp. $n-k$ vertices. Therefore, there are $Z(G)Z(P_{k-1})Z(P_{n-k}) = Af_kf_{n-k+1}$ such matchings.
- it contains (v_{k-1}, v_k). Then it contains no other edge going out from v_{k-1} or v_k. Again, three subgraphs remain: $G\setminus\{v\}$ and two paths with $k-2$ resp. $n-k$ vertices. Therefore, there are $Z(G \setminus \{v\})Z(P_{k-2})Z(P_{n-k}) = Bf_{k-1}f_{n-k+1}$ such matchings.
- it contains (v_k, v_{k+1}). Analogously, there are Bf_kf_{n-k} such matchings.

So we have

$$\begin{aligned} Z(G) &= Af_kf_{n-k+1} + Bf_{k-1}f_{n-k+1} + Bf_kf_{n-k} \\ &= B(f_kf_{n-k+1} + f_{k-1}f_{n-k+1} + f_kf_{n-k}) + (A-B)f_kf_{n-k+1} \\ &= B(f_{k+1}f_{n-k+1} + f_kf_{n-k}) + (A-B)\cdot(l_{n+1} - (-1)^k l_{n-2k+1})/5 \\ &= Bf_{n+1} + (A-B)l_{n+1}/5 - (A-B)(-1)^k l_{n-2k+1}/5. \end{aligned}$$

The only term depending on k is $-(A-B)(-1)^k l_{n-2k+1}/5$. We may assume $k \leq (n+1)/2$, since $P(n,k,G,v) \simeq P(n, n+1-k, G, v)$. So l_{n-2k+1} is always positive and monotonically decreasing in k. The result follows immediately. □

Remark: The fact $Z(P(n,k,G,v)) < Z(P(n,1,G,v))$ $(1 < k < n)$ implies the following: if two subtrees of a tree T at some vertex v are paths, the Hosoya index increases if these subtrees are replaced by a single path starting in v and preserving the number of vertices (s. Figure 4). Analogously, the Merrifield-Simmons index decreases by this transformation.

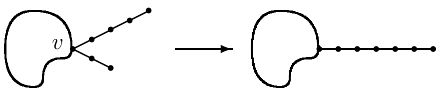

Figure 4: Transformation of subtrees I.

Lemma 6 Let T be a tree, v any vertex of T. Furthermore, let S be one of the subtrees at v that contains more than one leaf. S can be replaced in such a way that the resulting tree T' has exactly one leaf less than T and larger Z-index resp. smaller σ-index.

Proof: Let w be a vertex of degree ≥ 3 in S that has largest distance from v (such a vertex exists, as S has more than one leaf). Then, by maximality, all subtrees of T at w except the subtree containing v must be paths. If we replace two of them by a single path preserving the number of vertices, the number of leaves decreases by 1, and the Z-index increases by the previous remark, while the σ-index decreases. □

Corollary 7 If a subtree of a tree T at some vertex v is replaced by a path starting in v (s. Figure 5), the Z-index increases, whereas the σ-index decreases.

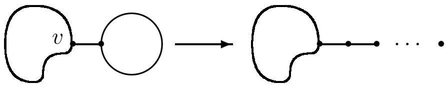

Figure 5: Transformation of subtrees II.

Proof: If a subtree is not a path, we may apply the previous lemma iteratively until the subtree contains only one leaf. The Z-index increases with every step, and at the end, the subtree must be a path. □

4 Main results

Theorem 8 *For a given number n of vertices and given maximal degree d, the tree T with maximal Z-index and minimal σ-index is*

$$\begin{cases} R(\underbrace{2,\ldots,2}_{n-1-d},\underbrace{1,\ldots,1}_{2d-n+1}) & \text{if } d \geq \frac{n-1}{2}, \\ R(\underbrace{2,\ldots,2}_{d-1}, n-2d+1) & \text{if } d \leq \frac{n-1}{2}. \end{cases}$$

The Z-index of these trees is $2^{n-d-2}(3d-n+3)$ and $2^{d-2}((d+1)f_{n-2d+2}+2f_{n-2d+1})$ respectively, and the σ-index of these trees is $\left(\frac{3}{2}\right)^{n-1}\left(\frac{4}{3}\right)^{d}+2^{n-d-1}$ and $3^{d-1}f_{n-2d+3}+2^{d-1}f_{n-2d+2}$ respectively.

Proof: We only state the proof for the Z-index; the proof for the σ-index is completely analogous. Let v be a vertex of maximal degree. If we replace all subtrees at v by paths, the Z-index increases by Corollary 7. Therefore, the tree of maximal Z-index for given maximal degree d is of the form $R(c_1,\ldots,c_d)$.

It is easy to see that $R(c_1,\ldots,c_d) \simeq P(c_i+c_j+1, c_i+1, G, v)$ for all $1 \leq i < j \leq d$, where

$$G \simeq R(c_1,\ldots,c_{i-1},c_{i+1},\ldots,c_{j-1},c_{j+1},\ldots,c_n).$$

If $(c_1, \ldots, c_d)$ contains two elements $c_i, c_j \geq 3$, the Z-index increases by Lemma 5 if they are replaced by $2, c_i + c_j - 2$. On the other hand, if it contains an element $c_i \geq 3$ and an element 1, the Z-index increases by Lemma 5 if they are replaced by $2, c_i - 1$.

Therefore, $Z(R(c_1, \ldots, c_d))$ is maximal if $(c_1, \ldots, c_d)$ either contains only 2's and 1's or only one element $\neq 2$, which yields the stated result. The formulas follow easily from Proposition 3. □

Now, we are going to characterize all trees T with n vertices whose Hosoya index is $Z(T) > 16f_{n-5}$ resp. all trees whose Merrifield-Simmons index is $\sigma(T) < 18f_{n-5} + 21f_{n-6}$. Parts of the following results have already been given in the paper of Li and Zhao ([8]) for the σ-index. Therefore, all proofs are stated mainly for the Z-index; however, it is not difficult to see that the proofs for the σ-index are completely analogous.

Lemma 9 If T is a tree with $n \geq 9$ vertices and exactly four leaves, $Z(T) \leq 16f_{n-5}$. Equality occurs if either $T \simeq H(2, n-8, 2, 2, 2)$ or $T \simeq H(n-8, 2, 2, 2, 2)$. Furthermore, $\sigma(T) \leq 18f_{n-5} + 21f_{n-6}$, with equality if $T \simeq H(2, n-8, 2, 2, 2)$.

Proof: Again, we only give the proof for the Z-index. We proceed by induction on n. For $n = 9$ and $n = 10$, the proof is easily done by direct computation. For $n \geq 11$, we consider two cases:

- $\max(b_{11}, b_{12}, b_{21}, b_{22}) \geq 3$. Without loss of generality, let $b_{11} \geq 3$. From the remark after Proposition 3, we know that

  $$Z(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = Z(H(a, b_{11}-1, b_{12}, b_{21}, b_{22})) + Z(H(a, b_{11}-2, b_{12}, b_{21}, b_{22})).$$

  By the induction hypothesis, $Z(H(a, b_{11}, b_{12}, b_{21}, b_{22}))$ is maximal if

  $$H(a, b_{11} - 1, b_{12}, b_{21}, b_{22}) \simeq H(2, n-9, 2, 2, 2) \text{ or } H(n-9, 2, 2, 2, 2)$$

  and

  $$H(a, b_{11} - 2, b_{12}, b_{21}, b_{22}) \simeq H(2, n-10, 2, 2, 2) \text{ or } H(n-10, 2, 2, 2, 2),$$

  which happens if and only if $a = 2$, $b_{11} = n - 8$, $b_{12} = b_{21} = b_{22} = 2$.

- $\max(b_{11}, b_{12}, b_{21}, b_{22}) \leq 2$. Then $b_{11}+b_{12}+b_{21}+b_{22} \leq 8$, and as $a+b_{11}+b_{12}+b_{21}+b_{22} = n \geq 11$, we must have $a \geq 3$. By the remark after Proposition 3, the recursion

  $$Z(H(a, b_{11}, b_{12}, b_{21}, b_{22})) = Z(H(a-1, b_{11}, b_{12}, b_{21}, b_{22})) + Z(H(a-2, b_{11}, b_{12}, b_{21}, b_{22}))$$

  holds. Again, $Z(H(a, b_{11}, b_{12}, b_{21}, b_{22}))$ is maximal if

  $$H(a-1, b_{11}, b_{12}, b_{21}, b_{22}) \simeq H(2, n-9, 2, 2, 2) \text{ or } H(n-9, 2, 2, 2, 2)$$

and

$$H(a-2, b_{11}, b_{12}, b_{21}, b_{22}) \simeq H(2, n-10, 2, 2, 2) \text{ or } H(n-10, 2, 2, 2, 2),$$

which happens if and only if $a = n-8$, $b_{11} = b_{12} = b_{21} = b_{22} = 2$.

Finally, Proposition 3 shows that

$$Z(H(n-8, 2, 2, 2, 2)) = Z(H(2, n-8, 2, 2, 2)) = 16f_{n-5}$$

and

$$\sigma(H(2, n-8, 2, 2, 2)) = 18f_{n-5} + 21f_{n-6}.$$

This completes the proof. □

REMARK: By Lemma 6, $Z(T) \leq 16f_{n-5}$ even holds if T has *at least* four leaves, and equality occurs if either $T \simeq H(2, n-8, 2, 2, 2)$ or $T \simeq H(n-8, 2, 2, 2, 2)$. The analogous statement holds for the σ-index.

Theorem 10 *We define a relation on the set of positive integers by*

$$2 \rhd 4 \rhd 6 \rhd \ldots \rhd 5 \rhd 3 \rhd 1.$$

This induces a lexicographic order on the set of triples (c_1, c_2, c_3) *with* $c_1 \leq c_2 \leq c_3$ *and* $c_1 + c_2 + c_3 = n-1$ *in the following way:*

$$\begin{aligned}
&(2,2,n-5) \rhd (2,4,n-7) \rhd \ldots \rhd (2,3,n-6) \\
&\rhd (4,4,n-9) \rhd (4,6,n-11) \rhd \ldots \rhd (4,5,n-10) \\
&\ldots \\
&\rhd (3,4,n-8) \rhd \ldots \rhd (3,5,n-9) \rhd (3,3,n-7) \\
&\rhd (1,2,n-4) \rhd \ldots \rhd (1,3,n-5) \rhd (1,1,n-3).
\end{aligned}$$

Using this order, we have, for $n \geq 13$,

$$\begin{aligned}
&Z(R(1,1,n-3)) < Z(R(1,3,n-5)) < Z(H(2,n-8,2,2,2)) = Z(H(n-8,2,2,2,2)) \\
&= 16f_{n-5} < Z(R(1,5,n-7)) < \ldots < Z(R(2,2,n-5)) < Z(P_n)
\end{aligned}$$

and

$$\begin{aligned}
&\sigma(R(1,1,n-3)) > \sigma(R(1,3,n-5)) > \sigma(H(2,n-8,2,2,2)) = 18f_{n-5} + 21f_{n-6} \\
&> \sigma(R(1,5,n-7)) > \ldots > \sigma(R(2,2,n-5)) > \sigma(P_n).
\end{aligned}$$

There are no further trees T *with* n *vertices and* $16f_{n-5} \leq Z(T) \leq f_{n+1}$ *or* $18f_{n-5} + 21f_{n-6} \geq \sigma(T) \geq f_{n+2}$.

Proof: By the remark after Lemma 9, all trees with at least four leaves have Z-index $\leq 16f_{n-5} = Z(H(2, n-8, 2, 2, 2)) = Z(H(n-8, 2, 2, 2, 2))$. Thus, all n-vertex trees T with $16f_{n-5} < Z(T) < f_{n+1}$ are tripodes. An analogous statement holds for the σ-index, so we only have to care about the order of tripodes with respect to the Z- and σ-index.

From Lemma 5, we already know that $Z(R(a, 1, n-a-2)) < Z(R(a, 3, n-a-4)) < \ldots < Z(R(a, 4, n-a-5)) < Z(R(a, 2, n-a-3))$ for all a. Therefore, it is sufficient to prove the following:

- $Z(R(2k-2, 2k-1, n-4k+2)) > Z(R(2k, 2k, n-4k-1))$ for all $2 \leq k \leq (n-1)/6$. By Corollary 4, this is equivalent to

$$\begin{aligned}&\frac{1}{5}\Big(f_{n+2} + 3f_{n+1} + f_{n-4k+3} - f_{n-4k+1} + (-1)^n f_{-n+8k-5}\Big)\\ &> \frac{1}{5}\Big(f_{n+2} + 3f_{n+1} + f_{n-4k-1} + f_{n-4k-1} - (-1)^n f_{-n+8k+1}\Big),\end{aligned}$$

  or

$$\begin{aligned}f_{n-4k} + f_{n-4k-2} &= f_{n-4k+3} - f_{n-4k+1} - 2f_{n-4k-1}\\ &> (-1)^{n-1}(f_{-n+8k-5} + f_{-n+8k+1}) = -f_{n-8k+5} - f_{n-8k-1}.\end{aligned}$$

  We have $n-4k > n-8k-1 > 4k-n$, as $2 \leq k \leq (n-1)/6$. Therefore,

$$f_{n-4k} > f_{|n-8k-1|} = |f_{n-8k-1}|.$$

  Similarly, $n-4k-2 > n-8k+5 > -n+4k+2$. Thus,

$$f_{n-4k-2} > f_{|n-8k+5|} = |f_{n-8k+5}|,$$

  which proves the claim.

- $Z(R(2k-1, 2k, n-4k)) < Z(R(2k+1, 2k+1, n-4k-3))$ for all $1 \leq k \leq (n-4)/6$. By Corollary 4, this is equivalent to

$$\begin{aligned}&\frac{1}{5}\Big(f_{n+2} + 3f_{n+1} - f_{n-4k+1} + f_{n-4k-1} + (-1)^n f_{-n+8k-1}\Big)\\ &< \frac{1}{5}\Big(f_{n+2} + 3f_{n+1} - f_{n-4k-3} - f_{n-4k-3} - (-1)^n f_{-n+8k+5}\Big),\end{aligned}$$

  or

$$\begin{aligned}f_{n-4k-2} + f_{n-4k-4} &= f_{n-4k+1} - f_{n-4k-1} - 2f_{n-4k-3}\\ &> (-1)^n(f_{-n+8k-1} + f_{-n+8k+5}) = f_{n-8k+1} + f_{n-8k-5}.\end{aligned}$$

  We have $n-4k-2 > n-8k+1 > -n+4k+2$, as $1 \leq k \leq (n-4)/6$. Therefore,

$$f_{n-4k-2} > f_{|n-8k+1|} = |f_{n-8k+1}|.$$

Similarly, $n-4k-4 > n-8k-5 > -n+4k+4$ if $1 \leq k \leq (n-5)/6$. In that case,

$$f_{n-4k-4} > f_{|n-8k-5|} = |f_{n-8k-5}|$$

and we are done. The only other case we have to consider is $k = (n-4)/6$. In this case, we are left with the inequality

$$f_{2k+2} + f_{2k} > f_{-2k+5} + f_{-2k-1} = f_{2k-5} + f_{2k+1}$$

(note that $2k+1$ has to be odd, so $f_{-2k-1} = f_{2k+1}$ and $f_{-2k+5} = f_{2k-5}$). By the recursion for f_n, this is equivalent to $5f_{2k-2} > 0$, which is obviously true for $k = (n-4)/6 > 1$. □

- Finally, we have to show that

$$Z(R(c_1, c_2, c_3)) > \frac{1}{5}\Big(f_{n+2} + 3f_{n+1}\Big) > Z(R(d_1, d_2, d_3))$$

if $c_1 \leq c_2 \leq c_3$, $d_1 \leq d_2 \leq d_3$, $c_1 + c_2 + c_3 = d_1 + d_2 + d_3 = n-1$, c_1 even and d_1 odd. By Corollary 4, the first inequality is equivalent to

$$(-1)^{c_1} f_{n-2c_1-1} + (-1)^{c_2} f_{n-2c_2-1} + (-1)^{c_3} f_{n-2c_3-1} > 0.$$

c_1 is even, so $(-1)^{c_1} = 1$. $c_1 \leq (n-1)/3$, so $f_{n-2c_1-1} > 0$. If $(-1)^{c_2} f_{n-2c_2-1} < 0$, we must have $c_2 > c_1$. From $c_1 + 1 \leq c_2 \leq n - c_1 - 2$, we get $n - 2c_1 - 3 \geq n - 2c_2 - 1 \geq 3 + 2c_1 - n$. Thus

$$f_{n-2c_1-3} \geq f_{|n-2c_2-1|} = |f_{n-2c_2-1}|$$

and analogously $f_{n-2c_1-3} \geq |f_{n-2c_3-1}|$ if $(-1)^{c_3} f_{n-2c_3-1} < 0$. This yields

$$(-1)^{c_1} f_{n-2c_1-1} + (-1)^{c_2} f_{n-2c_2-1} + (-1)^{c_3} f_{n-2c_3-1} \geq f_{n-2c_1-1} - 2f_{n-2c_1-3} = f_{n-2c_1-4} > 0,$$

as claimed. The second inequality is proved in an analogous manner. Finally, note that

$$Z(H(2, n-8, 2, 2, 2)) + \sigma(H(2, n-8, 2, 2, 2)) = 16f_{n-5} + 18f_{n-5} + 21f_{n-6} = f_{n+3}.$$

Furthermore, $Z(R(1, 3, n-5)) = 16f_{n-5} - f_{n-11} < 16f_{n-5}$ and $Z(R(1, 5, n-7)) = 16f_{n-5} + f_{n-12} > 16f_{n-5}$. Together with Corollary 4, this shows us that the order with resprect to the σ-index has to be the same as the order with respect to the Z-index. □

REMARK: Theorem 10 also provides information on the trees of maximal Hosoya index resp. minimal Merrifield-Simmons index for fixed diameter $d \geq \frac{2n}{3}$ – they are given by the tripodes $R(n-d-1, n-d-1, 2d-n+1)$ if $n-d-1$ is even and $R(n-d-1, n-d, 2d-n)$

otherwise.

REMARK: Theorem 10 suggests that the orders induced by the Z- resp. σ-index on the set of n-vertex trees are "almost the same". Indeed, this is true for small values of n. The first examples of two n-vertex trees T_1, T_2 with $Z(T_1) > Z(T_2)$ and $\sigma(T_1) > \sigma(T_2)$ occur for $n = 9$ – Figure 6 shows two trees T_1, T_2 with $Z(T_1) = 31 > 30 = Z(T_2)$ and $\sigma(T_1) = 126 > 124 = \sigma(T_2)$.

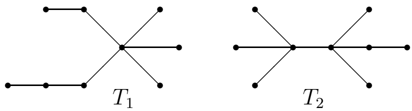

Figure 6: Two trees T_1, T_2 with $Z(T_1) > Z(T_2)$ and $\sigma(T_1) > \sigma(T_2)$.

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