A Unified Approach to the Extremal Trees without Perfect Matching for Different Indices

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Abstract

In this paper, we present a unified and simple approach to extremal acyclic graphs without perfect matching for the energy, the Merrifield-Simmons index and Hosoya index.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph. For a vertex u of G, we denote the neighborhood and the degree of u by $N_G(u)$ and $d_G(u)$, respectively. Denote $N_G[u] = N_G(u) \cup \{u\}$. A *pendant vertex* is a vertex of degree 1. The *maximum degree* of G is denoted by $\Delta = \Delta(G)$. We also use $G - u$ or $G - uv$ to denote the graph that arises from G by deleting the vertex $u \in V(G)$ or the edge $uv \in E(G)$. Similarly, $G + uv$ is a graph that arises from G by adding an edge $uv \notin E(G)$, where u, $v \in V(G)$. A *pendant*

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chain $P_s^0 = v_0 v_1 \cdots v_s$ of the graph G is a sequence of vertices $v_0, v_1, \cdots, v_s$ such that v_0 is a pendant vertex of G, $d_G(v_1) = \cdots = d_G(v_{s-1}) = 2$ (unless $s = 1$) and $d_G(v_s) \geq 3$. We also call that v_s and s the end-vertex and the length of the pendant chain P_s^0, respectively. If $s = 1$, then the pendant chain P_s^0 is a pendant edge. If a graph G has components $G_1, G_2, \ldots, G_t$, then G is denoted by $\bigcup_{i=1}^t G_i$. We denote by P_n the path of order n.

Let T be a tree. If there is a unique vertex $u \in V(T)$ such that $d_T(u) = k \geq 3$ and for any other vertex $v \in V(T)$, $d(v) \leq 2$, then we call that T is a *k-tree*. Let $T_{i,j,k}$ $(i, j, k \geq 1)$ (see Figure 1) be a 3-tree such that $T_{i,j,k} - u = P_i \cup P_j \cup P_k$, where u is the vertex of degree 3.

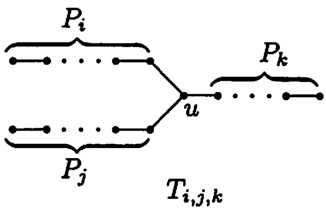


Figure 1

The Hosoya index $z(G)$ and the Merrifield-Simmons 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) and the number of independent vertex subsets of a graph, respectively.

The Hosoya index was introduced by Hosoya [10] 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 Merrifield-Simmons index, introduced by Merrifield and Simmons [18] in 1989. For detailed information on the chemical applications, we refer to [2, 4, 18, 20] and the references therein.

Let G be a graph of order n and $A(G)$ the adjacency matrix of G. Then the characteristic polynomial of $A(G)$, denoted by $\phi(G) = |xI - A(G)|$, is called the characteristic polynomial of G. The n roots of the equation $\phi(G) = 0$, denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$, are called the eigenvalues of G. Since $A(G)$ is real and symmetric, all eigenvalues of G are real. The *energy* of G, denoted by $e(G)$, is defined as

$$e(G) = \sum_{i=1}^{n} |\lambda_i|.$$

This concept was introduced by I. Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-electron energy of a molecule (see, e.g., [3], [4]). It is well-known (see [4]) that for a bipartite graph G of order n,

$$\phi(G) = |xI - A(G)| = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G,k) x^{n-2k},$$

where $b(G,k)$ is the number of k-matchings of G. Note that $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b(G,k)$. The energy of bipartite graph G can be expressed as the Coulson integral formula (see [12])

$$e(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \ln \left[1 + \sum_{k=1}^{\lfloor n/2 \rfloor} b(G,k) x^{2k} \right].$$

It is easy to see that $e(G)$ is a strictly monotonously increasing function of $b(G,k)$. This fact inspired Gutman to define a quasiordering $\succeq$ or $\preceq$ to compare the energies for trees and further for a set of graphs. Let G_1 and G_2 be two bipartite graphs of order n, whose characteristic polynomials are

$$\phi(G_1) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G_1,k) x^{n-2k} \quad \text{and} \quad \phi(G_2) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G_2,k) x^{n-2k}.$$

If $b(G_1,k) \geq b(G_2,k)$ holds for all $k \geq 0$, we call $G_1 \succeq G_2$ or $G_2 \preceq G_1$. If $G_1 \succeq G_2$ and there is a k such that $b(G_1,k) > b(G_2,k)$, we call $G_1 \succ G_2$. By the strict monotonicity of $e(G)$ and the definition of $z(G)$, we have

$$\text{if } G_1 \succeq G_2, \text{ then } e(G_1) \geq e(G_2) \text{ and } z(G_1) \geq z(G_2);$$
$$\text{if } G_1 \succ G_2, \text{ then } e(G_1) > e(G_2) \text{ and } z(G_1) > z(G_2).$$

Recently, there are a lot of results on $e(G)$, $\sigma(G)$ and $z(G)$ (see [6]-[9], [11]-[13], [15]-[17], [19], [21]-[31]). In [14], Li and Zheng put forward a problem, which *asked for a more unified approach that can cover extremal result for as many as chemical indices as possible.* Here, we present a unified and simple approach to extremal tree without perfect matching for the energy, the Merrifield-Simmons index and Hosoya index.

Let $\mathscr{T}_n = \{T : T \text{ is a tree of order } n\}$. It had been shown that P_n is the unique extremal graph that has maximal energy, maximal Hosoya index and minimal Merrifield-Simmons index in the set $\mathscr{T}_n$. Note that the path P_n contains no perfect matching if n is odd, and hence while studying the extremal trees without perfect matching for these indices one need only consider the case that the trees have even order. Let $\mathscr{T}_n^* = \{T \in \mathscr{T}_n : T$ contains no perfect matching and n is even$\}$. In this paper, the maximal energy, maximal Hosoya index and minimal Merrifield-Simmons index of trees in the set $\mathscr{T}_n^*$ are characterized. Moreover, the second maximal energy, the second maximal Hosoya index and the second minimal Merrifield-Simmons indexof trees in the set $\mathscr{T}_n$ are also characterized.

2. Preliminaries

According to the definition of Merrifield-Simmons index, we immediately obtain the following results.

Lemma 2.1 (see [4]). *Let G be a graph and uv be an edge of G. Then*

$$\sigma(G) = \sigma(G - uv) - \sigma\left(G - (N_G[u] \cup N_G[v])\right).$$

Lemma 2.2 (see [4]). *Let v be a vertex of G. Then*

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

From Lemma 2.2, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$.

Lemma 2.3 (see [4]). *If $G_1, G_2, \ldots, G_t$ are the components of a graph G, then $\sigma(G) = \prod_{i=1}^{t} \sigma(G_i)$.*

Let F_n be the nth Fibonacci number. Note that $\sigma(P_n) = F_{n+1}$ and $z(P_n) = F_n$. Since $F_0 = F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ $(n \geq 2)$, we have

$$F_{2i}F_{n-2i} - F_{2i-2}F_{n-2i+2} = -F_{n-4i+1}, \quad (1)$$

$$F_{2i+1}F_{n-2i-1} - F_{2i-1}F_{n-2i+1} = F_{n-4i-1}. \quad (2)$$

From Lemmas 2.2, 2.3 and the fact $\sigma(P_i) = F_{i+1}$, we can obtain the following result by calculations.

Lemma 2.4. *Let $T_{i,j,k}$ be a graph shown in Figure 1. Then*

$$\sigma(T_{i,j,k}) = F_{i+1}F_{j+1}F_{k+1} + F_iF_jF_k.$$

Let H_1, H_2 be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let $G = H_1vH_2$ be a graph defined by $V(G) = V(H_1) \cup V(H_2)$ and $E(G) = E(H_1) \cup E(H_2)$.

Lemma 2.5 [5]. *Let G be a graph, and let $P_n = v_1v_2 \cdots v_n$ be a path of order n. Then, for $n = 4k + i$, $i \in \{-1, 0, 1, 2\}$, $k \geq 1$,*

$$P_nv_1G \succ P_nv_3G \succ \cdots \succ P_nv_{2k+1}G \succ P_nv_{2k}G \succ P_nv_{2k-2}G \succ \cdots \succ P_nv_2G.$$

3. Operations

Now we first define three kinds of operations on graphs as follows.

Let G be a graph with two pendant chains $P_s^0 = u_0u_1\cdots u_s$ ($u_s = w$), $P_l^0 = v_0v_1\cdots v_l$ ($v_l = w$), where $w \in V(G)$ and $s, l \geq 1$ (see Figure 2).

(i) Set

$$G_1 = G - wu_{s-1} + v_0u_{s-1},$$

then we say that G_1 is obtained from G by Operation I.

(ii) If $s \geq 3$, $l \geq 1$ but $l \neq 2$ and

$$G_2 = G - u_{s-2}u_{s-3} + v_0u_{s-3},$$

then we say G_2 is obtained from G by Operation II.

(iii) If $s - l \geq 3$ and

$$G_3 = G - u_1u_2 + v_0u_1,$$

then we say G_3 is obtained from G by Operation III.

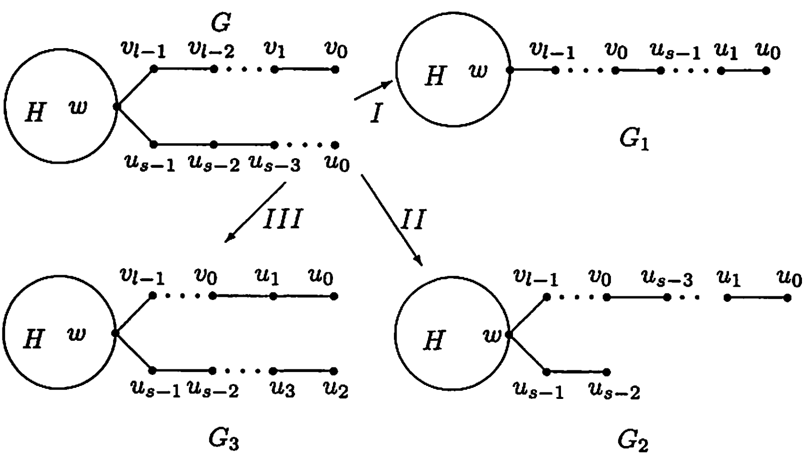


Figure 2

Lemma 3.1. *If G_1 is obtained from G by Operation I, then*

(i) $G_1 \succ G$;

(ii) $\sigma(G_1) < \sigma(G)$.

Proof. (i) The proof follows by Lemma 2.5.

(ii) By Lemma 2.2, we have

$$\begin{aligned}
& \sigma(G) - \sigma(G_1) \\
= & \ \sigma(G - w) + \sigma(G - N_G[w]) - \sigma(G_1 - w) - \sigma(G_1 - N_{G_1}[w]) \\
= & \ F_{s+1}F_{l+1}\sigma(H - w) + F_sF_l\sigma(H - N_H[w]) \\
& -F_{s+l+1}\sigma(H - w) - F_{s+l}\sigma(H - N_H[w]) \\
= & \ (F_{s+1}F_{l+1} - F_{s+l+1})\sigma(H - w) + (F_sF_l - F_{s+l})\sigma(H - N_H[w]) \\
= & \ F_{s-1}F_{l-1}(\sigma(H - w) - \sigma(H - N_H[w])) > 0.
\end{aligned}$$

■

Lemma 3.2. *If G_2 is obtained from G by Operation II, then*

(i) $G_2 \succ G$;

(ii) $\sigma(G_2) < \sigma(G)$.

Proof. (i) The proof follows by Lemma 2.5.

(ii) If $l, s \geq 3$, then

$$\begin{aligned}
\sigma(G) &= \sigma(G - w) + \sigma(G - N_G[w]), \\
&= F_{s+1}F_{l+1}\sigma(H - w) + F_sF_l\sigma(H - N_H[w]) \\
\sigma(G_2) &= \sigma(G_2 - w) - \sigma(G_2 - N_{G_2}[w]) \\
&= F_3F_{s+l-1}\sigma(H - w) + F_2F_{s+l-2}\sigma(H - N_H[w]).
\end{aligned}$$

Hence

$$\begin{aligned}
\sigma(G) - \sigma(G_2) &= (F_{s+1}F_{l+1} - F_3F_{s+l-1})\sigma(H - w) \\
&\quad +(F_sF_l - F_2F_{s+l-2})\sigma(H - N_H[w]) \\
&= F_{s-3}F_{l-3}[\sigma(H - w) - \sigma(H - N_H[w])] > 0.
\end{aligned}$$

If $l = 1, s \geq 3$, then

$$\sigma(G) = \sigma(G - w) + \sigma(G - N_G[w])$$

$$
\begin{aligned}
&= F_{s+1}F_2\sigma(H-w)+F_s\sigma(H-N_H[w]) \\
\sigma(G_2) &= \sigma(G_2-w)+\sigma(G_2-N_{G_2}[w]) \\
&= F_3F_s\sigma(H-w)+F_2F_{s-1}\sigma(H-N_H[w]).
\end{aligned}
$$

Thus

$$
\begin{aligned}
&\sigma(G)-\sigma(G_2) \\
= &\ (F_{s+1}F_2-F_3F_s)\sigma(H-w)+(F_s-F_2F_{s-1})\sigma(H-N_H[w]) \\
= &\ F_{s-3}[\sigma(H-w)-\sigma(H-N_H[w])]>0.
\end{aligned}
$$

■

Lemma 3.3. *If G_3 is obtained from G by Operation III and l is odd, then*

(i) $G_3 \succ G$;

(ii) $\sigma(G_3)<\sigma(G)$.

Proof. (i) The proof follows by Lemma 2.5 and $l \neq 2$.

(ii) Since l is odd, $l+2$ is odd and $l+1$, $l+3$ are even. Thus by (1) and (2),

$$
\begin{aligned}
F_{l+3}F_{s-1}-F_{l+1}F_{s+1} &= -F_{s-l-3}, \\
F_{l+2}F_{s-2}-F_lF_s &= F_{s-l-3}.
\end{aligned}
$$

By Lemma 2.2, we have

$$
\begin{aligned}
&\sigma(G)-\sigma(G_3) \\
= &\ \sigma(G-w)+\sigma(G-N_G[w])-\sigma(G_3-w)-\sigma(G_3-N_{G_3}[w]) \\
= &\ \sigma(H-w)(F_{l+1}F_{s+1}-F_{l+3}F_{s-1}) \\
&+\sigma(H-N_H[w])(F_lF_s-F_{l+2}F_{s-2}) \\
= &\ [\sigma(H-w)-\sigma(H-N_H[w])]\,F_{s-l-3}>0.
\end{aligned}
$$

■

4. Main Results

By Lemmas 3.1 and 3.2, we first obtained the following result.

Theorem 4.1. *Let* $T \in \mathscr{T}_n \setminus \{P_n, T_{2,2,n-5}\}$, $n \geq 6$. *Then*

(i) $T_{2,2,n-5} \succ T$;

(ii) $\sigma(T) > \sigma(T_{2,2,n-5})$.

Proof. We only give the proof of (ii) here. The proof of (i) is similar.

We choose $T \in \mathscr{T}_n \setminus \{P_n, T_{2,2,n-5}\}$ such that $\sigma(T)$ is as small as possible. First we show the following result.

Claim A. *T is a k-tree,* $3 \leq k \leq \Delta$.

Proof of Claim A. Since $T \ncong P_n$, T has maximum degree $\Delta = \Delta(T) \geq 3$. Thus there is a vertex $u \in V(T)$ with $d_T(u) = k$ and $3 \leq k \leq \Delta$.

Let $V'(T) = \{v \;:\; v \in V(T) - \{u\},\ 2 < d_T(v) \leq \Delta\}$.

If $V'(T) \neq \emptyset$, then let $w \in V'(T)$ with $d_T(w) = s \geq 3$. By Lemma 3.1, we can obtain a tree T^* from T by Operation I such that $\sigma(T^*) < \sigma(T)$, a contradiction with our choice. Therefore $V'(T) = \emptyset$, i.e., T is a k-tree. ∎

Note that a $(k-1)$-tree can be obtained from a k-tree by Operation I, and hence, by Lemma 3.1 and Claim A, T is a 3-tree.

Since $T \ncong T_{2,2,n-5}$ and $T_{2,2,n-5}$ can be obtained from a 3-tree by Operation II at most twice, we have $\sigma(T_{2,2,n-5}) < \sigma(T)$ by Lemma 3.2. ∎

Lemma 4.2. *Let $T_{i,j,k}$ be a graph shown in Figure 1. If $k - j > 2$ and j is odd, then*

(i) $T_{i,j+2,k-2} \succ T_{i,j,k}$;

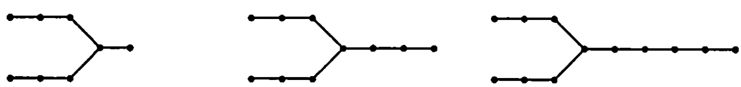
(ii) $\sigma(T_{i,j+2,k-2}) < \sigma(T_{i,j,k})$.

Proof. The lemma follows by Lemma 3.3. ∎

Lemma 4.3. *Let T be a tree of order $2k$ with $\Delta \geq 3$ and $V'(T) = \{v \in V(T) \;:\; 2 < d_T(v) \leq \Delta\} \neq \emptyset$. If there is only one odd component of $T - v$ for any $v \in V'(T)$, then T has a perfect matching.*

Proof. We proceed by induction on $k \geq 3$. If $k = 3$, then $T \in \{T_{1,2,2}, K_{1,5}, S_4\}$, where S_4 is a tree of order 6 obtained from $K_{1,4}$ by attaching a vertex to one pendant vertex of $K_{1,4}$. It is easily checked that $T \cong T_{1,2,2}$ and thus T has a perfect matching. We now suppose that $k \geq 4$ and the result holds for smaller than k. Since there is only one odd component of $T - v$ for any $v \in V'(T)$, every vertex of V is adjacent to at most one pendant vertex. Let $P = u_0u_1 \ldots u_s$ be a longest path in T. Then $d_T(u_0) = 1$, $d_T(u_1) = 2$, $d_T(u_s) = 1$ and $d_T(u_{s-1}) = 2$. Let $T^* = T - \{u_0, u_1\}$ and $T^{**} = T - \{u_s, u_{s-1}\}$. Then $|V(T^*)| = 2(k-1)$, $|V(T^{**})| = 2(k-1)$ and $V'(T^*) \neq \emptyset$ or $V'(T^{**}) \neq \emptyset$ as $k \geq 4$. Assume, without loss of generality, that $V'(T^*) \neq \emptyset$. By the induction hypothesis, T^* has a perfect matching M'. Let $M = M' \cup \{u_0u_1\}$. Then it is easy to see that M is a perfect matching in T. Therefore the proof of the lemma is complete. ∎

Note that if ijk and $i+j+k+1$ are even, then the 3-tree $T_{i,j,k}$ contains perfect matching. Thus we may assume that ijk is odd. Let T_n^* be a 3-tree $T_{i,j,k}$ with $|i-j| \leq 2$, $|j-k| \leq 2$ and $|k-i| \leq 2$. In Figure 3, we have drawn T_8^*, T_{10}^* and T_{12}^*.



T_8^* T_{10}^* T_{12}^*

Figure 3

Theorem 4.4. *Let $T \in \mathscr{T}_n^* \setminus \{T_n^*\}$, $n \geq 4$. Then*

(i) $T_n^* \succ T$;

(ii) $\sigma(T_n^*) < \sigma(T)$.

Proof. We only give the proof of (i) here. The proof of (ii) is similar.

Since $T \in \mathscr{T}_n^*$, $T \ncong P_n$. Thus $\Delta(T) \geq 3$. Let $V'(T) = \{v \in V(T) : 2 < d_T(v) \leq \Delta\}$. Then $V'(T) \neq \emptyset$. If there is only one odd component of $T - v$ for any $v \in V'(T)$, then, by Lemma 4.3, T has a perfect matching. This contradicts to $T \in \mathscr{T}_n^*$. Thus we can assume that there are at least three odd components of $T - v$ for some vertex $v \in V'(T)$. By an argument similar to the proof of Theorem 4.1, there is a 3-tree $T_{i,j,k}$, ijk is odd, such that $T_{i,j,k} \succeq T$. Note that $T_{i,j,k} \in \mathscr{T}_n^*$ when ijk is odd. Since $T_{i,j,k} \ncong T_n^*$, we may assume that $k > j + 2 \geq 3$ and $n \geq 6$. Since ijk is odd, we have $i(j+2)(k-2)$ is odd. Thus $T_{i,j+2,k-2} \in \mathscr{T}_n^*$. So, by Lemma 4.2, $T_{i,j+2,k-2} \succ T_{i,j,k}$. If $T_{i,j+2,k-2} \ncong T_n^*$, then, repeating the above step, we obtain

$$T_n^* \succeq \cdots \succ T_{i,j+2,k-2} \succ T_{i,j,k} \succeq T.$$

Therefore the proof of the theorem is complete. ■

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