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The Maximal Merrifield-Simmons Indices and Minimal Hosoya Indices of Unicyclic Graphs

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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. In this paper, we characterize the unicyclic graphs with maximal Merrifield-Simmons indices and minimal Hosoya indices, respectively, among all unicyclic graphs with n vertices and k pendent vertices.

1. Introduction

Given a molecular graph G, the *Merrifield-Simmons index* $\sigma = \sigma(G)$ and the *Hosoya index* $z = z(G)$ are defined as the number of subsets of $V(G)$ in which no two vertices are adjacent and the number of subsets of $E(G)$ in which no edges are incident, respectively, i.e., in graph-theoretical terminology, the total number of the independent vertex sets of the graph and the total number of the independent edge sets of the graph G.

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The Hosoya index of a (molecular) graph was introduced by Hosoya in 1971 [9] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures ([13, 15]). Merrifield and Simmons [13] developed a topological approach to structural chemistry. The cardinality of the topological space in their theory turns out to be equal to $\sigma(G)$ of the respective molecular graph G. In [6], Gutman first uses "Merrifield-Simmons index" to name the quantity. Since then, many authors have investigated the Hosoya index and Merrifield-Simmons index (e.g., see [2]-[8], [11], [16]-[21]). An important direction is to determine the graphs with maximal or minimal Hosoya indices (or Merrifield-Simmons indices, resp.) in a given class of graphs. It had been shown in [7, 12] that the path P_n has the minimal Merrifield-Simmons index (or the maximal Hosoys index, resp.) and the star S_n has the maximal Merrifield-Simmons index (or the minimal Hosoys index, resp.) for all the trees with n vertices. Pedersen and Vestergaad [14] studied the Merrifield-Simmons indices of the unicyclic graphs.

Here, unicyclic graphs with n vertices and k pendent vertices are considered, and the maximal Merrifield-Simmons indices and minimal Hosoya indices are given, and the corresponding extremal graphs are characterized.

In order to discuss our results, we first introduce some terminologies and notations of graphs. Other undefined notations may refer to [1]. Let $G = (V, E)$ be a 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 *pendent vertex* is a vertex of degree 1. Let $V_0(G)$ be the set of all pendent vertices in G. Let C_q be a cycle of order q and P_s be a path of order s. We 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 *pendent chain* $P_s^0 = v_0v_1 \cdots v_s$ of the graph G is a sequence of vertices $v_0, v_1, \ldots, v_s$ such that v_0 is a pendent 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 pendent chain P_s^0, respectively. Denote $\mathscr{U}_{n,k} = \{G : G$ is a unicyclic graph with n vertices and k pendent vertices, $0 \leq k \leq n-3\}$.

2. Lemmas

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

Lemma 2.1 ([7]). *Let G be a graph and uv be an edge of G. Then*

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

(ii) $z(G) = z(G - uv) + z(G - \{u, v\}).$ ■

Lemma 2.2 ([7]). *Let v be a vertex of G. Then*

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

(ii) $z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\}).$ ■

From Lemma 2.2, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$. Moreover, if G is a graph with at least one edge incident with v, then $z(G) > z(G - v)$.

Lemma 2.3 ([7]). *If $G_1, G_2, \cdots, G_t$ are the components of a graph G, we have*

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

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

In order to formulate our results, we need to define two graphs U_n^k $(0 \le k \le n-3)$ and $S_{a,b}$ (shown in Figure 1) as follows: U_n^k $(0 \ge k \le n-3)$ is a graph created from C_{n-k} by attaching k pendent vertices to one vertex of the cycle C_{n-k}; $S_{a,b}$ $(a, b \ge 1)$ is a graph created from a path $P_a = v_0 v_1 \cdots v_{a-1}$ by attaching b pendent vertices to v_{a-1}, and the vertex v_0 is called the tail of the graph $S_{a,b}$. Note that $U_n^0 \cong C_n$, $S_{n-1,1} \cong P_n$, $S_{2,n-2} \cong K_{1,n-1}$, $S_{1,n-1} \cong K_{1,n-1}$ and the unique non-pendent vertex is the tail of $S_{1,n-1}$.

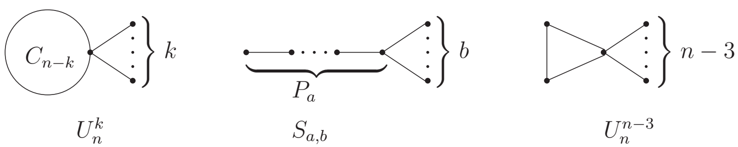

Figure 1

Let F_n be the nth Fibonacci number, i.e., $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$, $n \ge 2$. Then $\sigma(P_n) = F_{n+1}$ and $z(P_n) = F_n$. From Lemmas 2.1-2.3, we can easily get the following:

Lemma 2.4. *Let U_n^k be the graph shown in Figure 1, where $0 \le k \le n-3$. Then*

(i) $\sigma(U_n^k) = 2^k F_{n-k} + F_{n-k-2}$;

(ii) $z(U_n^k) = 2F_{n-k} + (k-1)F_{n-k-1}$.

In the following, we introduce three kinds of graph transformations.

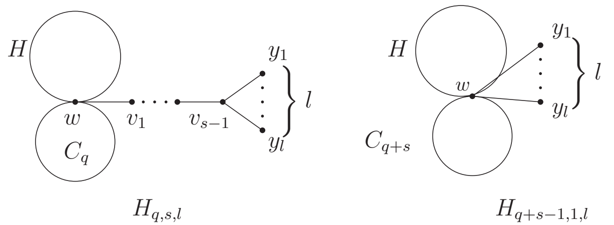

Figure 2

Lemma 2.5. *Let $H_{q,s,l}$ $(s \ge 2)$ (see Figure 2) be a graph obtained from a graph H $(H \ncong P_1)$ by attaching a cycle C_q and a graph $S_{s,l}$ at a vertex w of H, where the tail of $S_{s,l}$ identifies with w. Then*

(i) $\sigma(H_{q,s,l}) < \sigma(H_{q+s-1,1,l})$;

(ii) $z(H_{q,s,l}) > z(H_{q+s-1,1,l})$.

Proof. Let $H_{q,s,l} = G$ and $H_{q+s-1,1,l} = G_1$. Let $N_G(w) = \{w_1, w_2, x_1, \cdots, x_t, v_1\}$, where $w_1, w_2 \in V(C_q)$, $x_1, \ldots, x_t \in V(H)$. Set $F_{-1} = 0$.

(i) By Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
\sigma(G) &= \sigma(G-w) + \sigma(G - N_G[w]) \\
&= F_q(2^l F_{s-1} + F_{s-2})\sigma(H-w) + F_{q-2}(2^l F_{s-2} + F_{s-3})\sigma(H - N_H[w]), \\
\sigma(G_1) &= \sigma(G_1 - w) + \sigma(G_1 - N_{G_1}[w]) \\
&= F_{q+s-1}2^l\sigma(H-w) + F_{q+s-3}\sigma(H - N_H[w]).
\end{aligned}$$

Thus

$$\begin{aligned}
& \sigma(G) - \sigma(G_1) \\
= \ & \sigma(H-w)(2^l F_q F_{s-1} + F_q F_{s-2} - 2^l F_{q+s-1}) \\
& + \sigma(H - N_H[w])(2^l F_{q-2}F_{s-2} + F_{q-2}F_{s-3} - F_{q+s-3}) \\
= \ & \sigma(H-w)F_{s-2}(F_q - 2^l F_{q-1}) + \sigma(H - N_H[w])F_{s-2}(2^l F_{q-2} - F_{q-1})
\end{aligned}$$

$$
\begin{aligned}
&= F_{s-2}[(2^l F_{q-2} - F_{q-1})(\sigma(H - N_H[w]) - \sigma(H - w))] \\
&\quad + F_{s-2}[\sigma(H - w)(F_{q-2} - 2^l F_{q-3})] \\
&\leq F_{s-2}[(2F_{q-2} - F_{q-1})(\sigma(H - N_H[w]) - \sigma(H - w))] \\
&\quad + F_{s-2}[\sigma(H - w)(F_{q-2} - 2F_{q-3})] \\
&= F_{s-2}[F_{q-4}\sigma(H - N_H(w)) - F_{q-3}\sigma(H - w)] \\
&\leq F_{s-2}F_{q-3}(\sigma(H - N_H[w]) - \sigma(H - w)) < 0.
\end{aligned}
$$

(ii) By Lemmas 2.2 and 2.3, we have

$$
\begin{aligned}
z(G) &= z(G - w) + 2z(G - w - w_1) + z(G - w - v) + \sum_{i=1}^{t} z(G - w - x_i) \\
&= F_{q-1}(F_{s-1} + lF_{s-2})z(H - w) + 2F_{q-2}(F_{s-1} + lF_{s-2})z(H - w) \\
&\quad + F_{q-1}(F_{s-2} + lF^0_{s-3})z(H - w) + F_{q-1}(F_{s-1} + lF_{s-2})\sum_{i=1}^{t} z(H - w - x_i) \\
&= z(H - w)(F_{q+s-1} + F_{q-2}F_{s-1} + lF_{q+s-2} + lF_{q-2}F_{s-2}) \\
&\quad + F_{q-1}(F_{s-1} + lF_{s-2})\sum_{i=1}^{t} z(H - w - x_i), \\
z(G_1) &= z(G_1 - w) + 2z(G_1 - w - w_1) + lz(G_1 - w - y_1) + \sum_{i=1}^{t} z(G_1 - w - x_i) \\
&= F_{q+s-2}z(H - w) + 2F_{q+s-3}z(H - w) \\
&\quad + lF_{q+s-2}z(H - w) + F_{q+s-2}\sum_{i=1}^{t} z(H - w - x_i) \\
&= z(H - w)(F_{q+s-1} + F_{q+s-3} + lF_{q+s-2}) + F_{q+s-2}\sum_{i=1}^{t} z(H - w - x_i).
\end{aligned}
$$

So

$$
\begin{aligned}
&z(G) - z(G_1) \\
&= z(H - w)(lF_{q-2}F_{s-2} - F_{q-3}F_{s-2}) \\
&\quad + \sum_{i=1}^{t} z(H - w - x_i)(lF_{q-1}F_{s-2} - F_{q-2}F_{s-2}) \\
&= F_{s-2}[z(H - w)(lF_{q-2} - F_{q-3}) + \sum_{i=1}^{t} z(H - w - x_i)(lF_{q-1} - F_{q-2})]
\end{aligned}
$$

$$\geq F_{s-2}[z(H-w)(F_{q-2}-F_{q-3})+\sum_{i=1}^{t} z(H-w-x_i)(F_{q-1}-F_{q-2})]$$

$$\geq F_{s-2}F_{q-3}\sum_{i=1}^{t} z(H-w-x_i) > 0.$$

■

Lemma 2.6. *Let G be a connected graph and $u, v \in V(G)$. Suppose vv_i, uu_j are cut-edges of G, $1 \leq i \leq s$, $1 \leq j \leq t$ (shown in Figure. 3). Let G_1^* be the graph obtained from G by deleting the edges (u, u_j) and adding the edges (v, u_j) and G_2^* be the graph obtained from G by deleting the edges (v, v_j) and adding the edges (u, v_j). Then*

(i) $\sigma(G_1^*) > \sigma(G)$ *or* $\sigma(G_2^*) > \sigma(G)$;

(ii) $z(G_1^*) < \sigma(G)$ *or* $z(G_2^*) < \sigma(G)$.

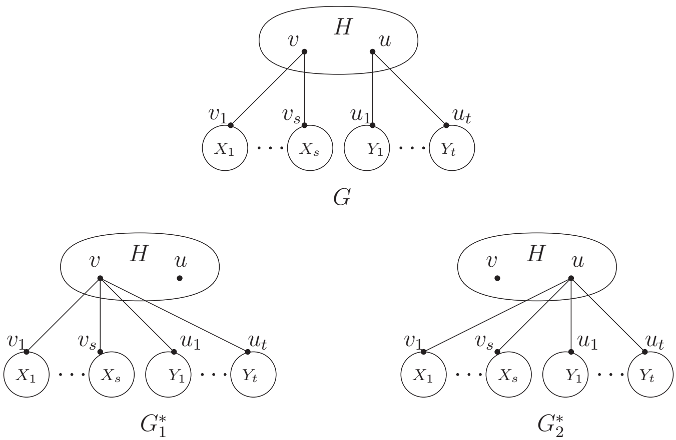

Figure 3

Proof. Let $G' = G - \{vv_1, \cdots, vv_s, uu_1, \cdots, uu_t\} = H \cup X_1 \cup \cdots \cup X_s \cup Y_1 \cup \cdots \cup Y_t$ (shown in Figure. 3), where H is a component containing u, v, and X_k is a component containing v_k, $1 \leq k \leq s$, and Y_j is a component containing u_j, $1 \leq j \leq t$, respectively.

(i) Denote $a = \prod_{k=1}^{s} \sigma(X_k)$, $a' = \prod_{k=1}^{s} \sigma(X_k - v_k)$ and $b = \prod_{k=1}^{t} \sigma(Y_k)$, $b' = \prod_{k=1}^{t} \sigma(Y_k - u_k)$. Then $a > a' > 0$ and $b > b' > 0$. Let $i_{u,v}$ be the number of independent vertex subsets in H containing both u and v. By Lemma 2.2 and Lemma 2.3, we have

$$\begin{aligned}\sigma(G) &= \sigma(G-v)+\sigma(G-N_G[v]) \\ &= ab\sigma(H-v-u)+ab'\sigma(H-v-N_H[u])+a'b\sigma(H-u-N_H[v])+a'b'i_{u,v}.\end{aligned}$$

Similarly, we have

$$\begin{aligned}\sigma(G_1^*) &= ab[\sigma(H-v-u)+\sigma(H-v-N_H[u])]+a'b'[\sigma(H-u-N_H[v])+i_{u,v}], \\ \sigma(G_2^*) &= ab[\sigma(H-v-u)+\sigma(H-u-N_H[v])]+a'b'[\sigma(H-v-N_H[u])+i_{u,v}].\end{aligned}$$

Therefore

$$\begin{aligned}\sigma(G)-\sigma(G_1^*) &= a'(b-b')\sigma(H-u-N_H[v])-a(b-b')\sigma(H-v-N_H[u]), \\ \sigma(G)-\sigma(G_2^*) &= b'(a-a')\sigma(H-v-N_H[u])-b(a-a')\sigma(H-u-N_H[v]).\end{aligned}$$

If $\sigma(G)-\sigma(G_1^*)\geq 0$, then $(b-b')[a'\sigma(H-u-N_H[v])-a\sigma(H-v-N_H[u])]\geq 0$. Since $a>a'$ and $b>b'$, we have

$$\sigma(H-u-N_H[v])>\sigma(H-v-N_H[u]).$$

So

$$\begin{aligned}\sigma(G)-\sigma(G_2^*) &= (a-a')[b'\sigma(H-v-N_H[u])-b\sigma(H-u-N_H[v])] \\ &< (a-a')[b'\sigma(H-v-N_H[u])-b\sigma(H-v-N_H[u])] \\ &= (a-a')(b'-b)\sigma(H-v-N_H[u])<0.\end{aligned}$$

(ii) Denote $p=\prod_{k=1}^{s} z(X_k)$, $p'=\sum_{k=1}^{s}\frac{z(X_k-v_k)}{z(X_k)}$, $q=\prod_{k=1}^{t} z(Y_k)$, $q'=\sum_{k=1}^{t}\frac{z(Y_k-u_k)}{z(Y_k)}$, $r_u=\sum\limits_{u'\in N_{G-v}(u)\backslash\{u_1,\dots,u_t\}} z(H-v-u-u')$, $r_v=\sum\limits_{v'\in N_G(v)\backslash\{u,v_1,\dots,v_s\}} z(H-v-u-v')$, $r_0=\sum\limits_{v'\in N_G(v)\backslash\{v_1,\dots,v_s,u\}}\ \sum\limits_{u'\in N_{G-v-v'}(u)\backslash\{u_1,\dots,u_t\}} z(G-v-u-v'-u')$. Let $e_0=1$ if $uv\in E(G)$; and $e_0=2$ if $uv\notin E(G)$.

By Lemmas 2.2 and 2.3, we have

$$z(G) = z(G-v)+\sum_{v'\in N_G(v)} z(G-v-v')$$

$$
\begin{aligned}
&= z(G-v-u) + \sum_{u' \in N_{G-v}(u)} z(G-v-u-u') \\
&\quad + \sum_{v' \in N_G(v)} z(G-v-v'-u) + \sum_{v' \in N_G(v)} \sum_{u' \in N_{G-v-v'}(u)} z(G-v-v'-u-u') \\
&= e_0 z(G-v-u) + \sum_{j=1}^{t} z(G-v-u-u_j) + \sum_{u' \in N_{G-v}(u)\setminus\{u_1,\ldots,u_t\}} z(G-v-u-u') \\
&\quad + \sum_{j=1}^{s}\sum_{k=1}^{t} z(G-v-u-v_j-u_k) + \sum_{v' \in N_G(v)\setminus\{v_1,\ldots,v_s,u\}} z(G-v-u-v') \\
&\quad + \sum_{j=1}^{s} z(G-v-u-v_j) + \sum_{j=1}^{s} \sum_{u' \in N_{G-v-v_j}(u)\setminus\{u_1,\ldots,u_t\}} z(G-v-u-v_j-u') \\
&\quad + \sum_{v' \in N_G(v)\setminus\{v_1,\ldots,v_s,u\}} \sum_{k=1}^{t} z(G-v-u-v'-u_k) \\
&\quad + \sum_{v' \in N_G(v)\setminus\{v_1,\ldots,v_s,u\}} \sum_{u' \in N_{G-v-v'}(u)\setminus\{u_1,\ldots,u_t\}} z(G-v-u-v'-u') \\
&= pq \cdot [e_0 z(H-v-u) + q' z(H-v-u) + r_u + p'q' z(H-v-u) + r_v \\
&\quad + p' z(H-v-u) + r_u p' + r_v q' + r_0] \\
&= pq[e_0 z(H-v-u)(1+q'+p'+p'q') + r_v(1+q') + r_u(1+p') + r_0].
\end{aligned}
$$

Similarly, we get

$$
\begin{aligned}
z(G_1^*) &= pq[z(H-v-u)(e_0+q'+p') + r_u(1+p'+q') + r_v + r_0], \\
z(G_2^*) &= pq[z(H-v-u)(e_0+q'+p') + r_v(1+p'+q') + r_u + r_0].
\end{aligned}
$$

Thus

$$
\begin{aligned}
z(G) - z(G_1^*) &= pqq'[z(H-v-u)p' + r_v - r_u], \\
z(G) - z(G_2^*) &= pqp'[z(H-v-u)q' + r_u - r_v].
\end{aligned}
$$

If $z(G) - z(G_1^*) \leq 0$, then $pqq'[z(H-v-u)p' + r_v - r_u] \leq 0$, that is,

$$
r_u - r_v \geq z(H-v-u)p'.
$$

So

$$
\begin{aligned}
z(H-v-u)q' + r_u - r_v &\geq z(H-v-u)q' + z(H-v-u)p' \\
&= z(H-v-u)(q'+p') > 0.
\end{aligned}
$$

Note that $pqp' > 0$, and hence $z(G_2^*) < z(G)$. ∎

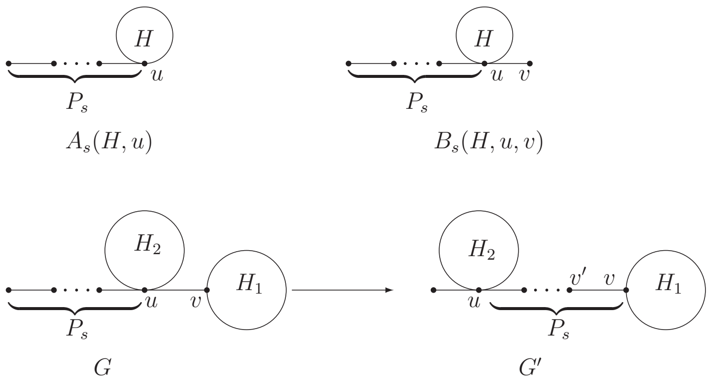

Figure 4

Let $A_s(H,u)$ $(s \geq 3)$ be a graph obtaining from a graph H by attaching a path P_s at one vertex u of H, and let $B_s(H,u,v)$ be a graph obtained from $A_s(H,u)$ by attaching a pendent vertex v to u (see Figure 4).

Lemma 2.7. *Let G be a graph obtained from $B_s(H_2,u,v)(s \geq 3)$ by attaching a graph H_1 to the vertex v, where $H_1, H_2 \ncong P_1$. If G' is obtained from G by replacing P_s with a pendent edge and replacing the edge uv with a path P_s (see Figure 4), then*

(i) $\sigma(G') > \sigma(G)$;

(ii) $z(G') < z(G)$.

Proof. (i) Let $N_{H_1}[v] = V_1$ and $N_{H_2}[u] = V_2$. By Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
\sigma(G) &= \sigma(G-v) + \sigma(G - N_G[v]) \\
&= \sigma(G-v-u) + \sigma(G-v-N_{G-v}[u]) + \sigma(G-N_G[v]) \\
&= F_s\sigma(H_1-v)\sigma(H_2-u) + F_{s-1}\sigma(H_1-v)\sigma(H_2-V_2) + F_s\sigma(H_1-V_1)\sigma(H_2-u), \\
\sigma(G') &= \sigma(G'-v) + \sigma(G'-N_{G'}[v]) \\
&= \sigma(G'-v-u) + \sigma(G'-v-N_{G'-v}[u]) + \sigma(G'-N_{G'}[v]-u) \\
&\quad + \sigma(G'-N_{G'}[v]-N_{G'-N_{G'}[v]}[u]) \\
&= 2F_{s-1}\sigma(H_1-v)\sigma(H_2-u) + F_{s-2}\sigma(H_1-v)\sigma(H_2-V_2) \\
&\quad + 2F_{s-2}\sigma(H_1-V_1)\sigma(H_2-u) + F_{s-3}\sigma(H_1-V_1)\sigma(H_2-V_2).
\end{aligned}$$

Since $F_0 = 1$, $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$, we have

$$\sigma(G') - \sigma(G) = F_{s-3}(\sigma(H_1 - v) - \sigma(H_1 - V_1))(\sigma(H_2 - u) - \sigma(H_2 - V_2)) > 0.$$

(ii) Let $A_s = A_s(H_2, u)$ and $B_s = B_s(H_2, u, v)$. Then $z(A_l) = z(A_{l-1}) + z(A_{l-2})$ and $z(B_l) = z(A_l) + F_{l-1}z(H_2 - u)$. By Lemmas 2.1 – 2.3, we have

$$\begin{aligned} z(G) &= z(G - uv) + z(G - \{u,\ v\}) \\ &= z(H_1)z(A_s) + F_{s-1}z(H_1 - v)z(H_2 - u) \\ &= z(H_1)z(A_{s-1}) + z(H_1)z(A_{s-2}) + F_{s-1}z(H_1 - v)z(H_2 - u), \\ z(G') &= z(G' - v'v) + z(G' - \{v',\ v\}) \\ &= z(H_1)z(B_{s-1}) + z(H_1 - v)z(B_{s-2}). \\ &= z(H_1)z(A_{s-1}) + F_{s-2}z(H_1)z(H_2 - u) + z(H_1 - v)z(A_{s-2}) \\ &\quad + F_{s-3}z(H_1 - v)z(H_2 - u). \end{aligned}$$

Since $F_0 = F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$, we have

$$\begin{aligned} z(G) - z(G') &= (z(H_1) - z(H_1 - v))(z(A_{s-2}) - F_{s-2}z(H_2 - u)) \\ &= F_{s-3}(z(H_1) - z(H_1 - v)) \sum_{x \in N_{H_2}(u)} z(H_2 - u - x) > 0. \end{aligned}$$

3. Results

From Lemmas 2.4 – 2.7, we immediately get the following results.

Theorem 3.1. *Let $G \in \mathscr{U}_{n,k}$ $(0 \leq k \leq n-3)$. Then*

$$\sigma(G) \leq 2^k F_{n-k} + F_{n-k-2} \tag{1}$$

and

$$z(G) \geq 2F_{n-k} + (k-1)F_{n-k-1}. \tag{2}$$

Moreover, the equalities in (1) and (2) hold if and only if $G \cong U_n^k$.

Proof. First we note that if $G \cong U_n^k$, then (1) and (2) hold by Lemma 2.4.

Now we prove that if $G \in \mathscr{U}_{n,k}$, then (1) (or (2), resp.) holds and the equality in (1) (or (2), resp.) holds only if $G \cong U_n^k$.

Let $G \in \mathscr{U}_{n,k}$. If $k = 0$, then $G \cong C_n$ and hence the result holds obviously. So in the following proof, we assume that $k \geq 1$. We choose G such that $\sigma(G)$ is as large as possible. Let C be the unique cycle of order q in G. We will show some facts.

Fact 1. *There is only one vertex $w \in V(C)$ such that $d_G(w) \geq 3$.*

Proof of Fact 1. Assume that $d_G(w_i) \geq 3$, where $w_i \in V(C)$, $i = 1, 2$. Denote $N_G(w_1) = \{x_1, \ldots, x_s, u_1, u_2\}$ and $N_G(w_2) = \{y_1, \ldots, y_t, v_1, v_2\}$, where $u_1, u_2, v_1, v_2 \in V(C)$ and $s, t \geq 1$. Set $G_1 = G - \{w_2y_1, \ldots, w_2y_t\} + \{w_1y_1, \ldots, w_1y_t\}$ and $G_2 = G - \{w_1x_1, \ldots, w_1x_s\} + \{w_2x_1, \ldots, w_2x_s\}$. Then $G_1,\ G_2 \in \mathscr{U}_{n,k}$. By Lemma 2.6, we have $\sigma(G_1) > \sigma(G)$ or $\sigma(G_2) > \sigma(G)$, a contradiction with our choice. ■

By Fact 1, we let w be the unique vertex of C with $d_G(w) \geq 3$. Let $T_1, \cdots, T_m$ ($m \geq 1$) be the subtrees rooted at w with $|V(T_j)| = s_j + l_j$ and $|V(T_j) \cap (V_0(T_j) \setminus \{w\})| = l_j$, $1 \leq j \leq m$, respectively.

Fact 2. *Let $v \in V(T_j)$ with $N_T(v) \cap V_0(T_j) \neq \emptyset$. If $T_j \ncong P_{s_j+l_j}$, then $d_T(v) \geq 3$.*

Proof of Fact 2. Otherwise, we assume that $P_t^0 = v_0v_1 \cdots v_t$ ($t \geq 2$) is the pendent chain of T_j for some j ($1 \leq j \leq m$) with $v_0 \in V_0(T)$. Let w_1 be the only vertex that belongs to the (w, v_t)-path with $w_1v_t \in E(G)$. Set $G' = G - \{w_1v_t, v_0v_1\} + \{w_1v_1, v_0v_t\}$. Then $G' \in \mathscr{U}_{n,k}$. By Lemma 2.7, we have $\sigma(G') > \sigma(G)$, a contradiction with our choice. ■

Fact 3. If $T_j \ncong P_{s_j+l_j}$, then $T_j \cong S_{s_j,l_j}$ and w is the tail of T_j, $1 \leq j \leq m$.

Proof of Fact 3. Assume that there exists some j ($1 \leq j \leq m$) such that $T_j \ncong S_{s_j,l_j}$. Then there are two vertices $u, v \in V(T_j) \setminus \{w\}$ such that $N_{T_j}(u) \cap V_0(T_j) \neq \emptyset$ and $N_{T_j}(v) \cap V_0(T_j) \neq \emptyset$. Denote $N_{T_j}(u) \cap V_0(T_j) = \{u_1, \cdots, u_t\}$, $t \geq 1$ and $N_{T_j}(v) \cap V_0(T_j) = \{v_1, \cdots, v_s\}$, $s \geq 1$. Note that if $t = d_G(u) - 1$, $s = d_G(v) - 1$, then $s, t \geq 2$ by Fact 2. Set $G_1 = G - \{uu_1, \ldots, uu_{t'}\} + \{vu_1, \cdots, vu_{t'}\}$ and $G_2 = G - \{vv_1, \cdots, vv_{s'}\} + \{uv_1, \cdots, uv_{s'}\}$, where $t' = t - 1$ (or $s' = s - 1$, resp.) if $t = d_G(u) - 1$ (or $s = d_G(v) - 1$, resp.); otherwise $t' = t$ ($s' = s$, resp.). Then $G_1, G_2 \in \mathscr{U}_{n,k}$. By Lemma 2.6, we have $\sigma(G_1) > \sigma(G)$ or $\sigma(G_2) > \sigma(G)$, a contradiction with our choice. ■

Fact 4. $T_j \cong K_{1,l_j}$, $1 \leq j \leq m$.

Proof of Fact 4. Assume that $T_j \ncong K_{1,l_j}$ for some j, $1 \leq j \leq m$. Then $s_j \geq 2$. Set $H = \bigcup_{1 \leq l \leq m, j \neq l} T_l$. Then by Lemma 2.5, we have $\sigma(H(q, s_j, l_j)) > \sigma(H(q + s_j - 1, 1, l_j))$. Note that $H(q, s_j, l_j) \cong G$ by Fact 3, and hence we get a contradiction with our choice. ■

Therefore the proof of the theorem is complete.

Lemma 3.2. *Suppose that* $0 \leq k \leq n-4$ *and* $n \geq 5$. *Then*

(i) $\sigma(U_n^{k+1}) > \sigma(U_n^k)$;

(ii) $z(U_n^{k+1}) < z(U_n^k)$.

Proof. (i) By Lemma 2.4(i), we have

$$\begin{aligned} \sigma(U_n^{k+1}) - \sigma(U_n^k) &= 2^{k+1}F_{n-k-1} + F_{n-k-3} - 2^k F_{n-k} - F_{n-k-2} \\ &= 2^k F_{n-k-3} - F_{n-k-4} > 0. \end{aligned}$$

Therefore, $\sigma(U_n^{k+1}) > \sigma(U_n^k)$ for $0 \leq k \leq n-4$ and $n \geq 5$.

(ii) By Lemma 2.4(ii), we have

$$\begin{aligned} z(U_n^{k+1}) - z(U_n^k) &= 2F_{n-k-1} + kF_{n-k-2} - 2F_{n-k} - (k-1)F_{n-k-1} \\ &= -F_{n-k-2} - (k-1)F_{n-k-3} < 0. \end{aligned}$$

■

From Lemma 3.2 and Theorem 3.1, we have the following:

Corollary 3.3. *Let G be a unicyclic graph with $n (n \geq 5)$ vertices. Then*

$$\sigma(G) \leq 3 \cdot 2^{n-3} + 1 \qquad \textit{and} \qquad z(G) \geq 2n - 2.$$

Moreover, the equality holds if and only if $G \cong U_n^{n-3}$.

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