On the extremal Merrifield-Simmons index of quasi-unicyclic graphs

Shan Duan, Zhongxun Zhu*

Faculty of Mathematics and Statistics, South Central University for Nationalities, Wuhan 430074, P.R. China

Abstract. The Merrifield-Simmons index $i(G)$ of a graph G is defined as the total number of the independent sets of G. A connected graph $G = (V, E)$ is called a quasi-unicyclic graph if there is a vertex $u_0 \in V$ such that $G - u_0$ is a unicyclic graph. Denote by $\mathscr{U}(n, d_0)$ the set of quasi-unicyclic graphs of order n with $G - u_0$ being a unicyclic graph and $d_G(u_0) = d_0$. In this paper, we characterize the quasi-unicyclic graphs with the smallest, the second-smallest, the largest and the second-largest Merrifield-Simmons indices, respectively, in $\mathscr{U}(n, d_0)$.

Keywords: independent set; Merrifield-Simmons index; quasi-unicyclic graph

AMS subject classification: 05C69, 05C05

1. Introduction

Let $G = (V, E)$ be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. If $m = n-1+c$, then G is called a *c-cyclic graph*. If $c = 0, 1$ and 2, then G is a tree, unicyclic graph, and bicyclic graph, respectively. A connected graph $G = (V, E)$ is called a quasi-c-cyclic graph if there is a vertex $u_0 \in V$ such that $G - u_0$ is a c-cyclic graph. If $c = 0$ and 1, then G is a *quasi-tree* and *qasi-unicyclic graph*, respectively. Let $\mathscr{U}(n, d_0)$ denote the set of quasi-unicyclic graphs of order n with $G - u_0$ being a unicyclic graph and $d_G(u_0) = d_0$. We denote by K_n, P_n, C_n and S_n the complete graph, the path, the cycle and the star on n vertices, respectively.

Let $d_G(v)$ be the degree of the vertex v of G. let $N(v) = \{u|uv \in E(G)\}$, $N[v] = N(v) \cup \{v\}$. Two vertices of G are said to be independent if they are not adjacent in G. An independent k-set is a set of k vertices, no two of which are adjacent. Denote by $i(G, k)$ the number of k-independent sets of G. For convenience, we regard the empty set(denote by $\emptyset$) as an

The Project was Supported by the Special Fund for Basic Scientic Research of Central Colleges, South-Central University for Nationalities(ZZZ10005). * Corresponding author (E-mail: zzxun73@mail.scuec.edu.cn)

independent set. Then $i(G, 0) = 1$ for any graph G. The *Merrifield-Simmons index*, denoted by $i(G)$, is defined to be the total number of independent sets of G, that is, $i(G) = \sum_{k=0}^{n} i(G, k)$. It was introduced in 1982 in a paper of Prodinger and Tichy [9], although it is called Fibonacci number of a graph there.

Since then, many researchers have investigated this graph invariant. An important direction is to determine the graphs with maximal or minimal indices in a given class of graphs. As for n-vertex general graphs, the complete graph is the one that has the smallest Merrifield-Simmons index. Generally, it is clear that removing edges increases the Merrifield-Simmons index. Things become more interesting but more difficult if one imposes further restrictions. As for n-vertex trees, Prodinger and Tichy [9] showed that the path P_n has the minimal Merrifield-Simmons index and the star S_n has the maximal Merrifield-Simmons index, respectively. In [10], Liu et al. studied trees with a prescribed diameter with respect to the Merrifield-Simmons index. As for n-vertex unicyclic graphs, Li and Zhu [6] attained the upper bounds for the Merrifield-Simmons index of unicyclic graphs with a given diameter. For n-vertex bicyclic graphs, Deng and coauthors [3, 4] obtained the lower and the upper bounds for the Merrifield-Simmons index.

In light of the information available for Merrifield-Simmons index on trees, unicyclic graphs and bicyclic graphs, it is natural that the quasi-tree graphs are an other reasonable starting point for such an investigation. In [7], Li et al. studied the lower and the upper bounds for the Merrifield-Simmons index of n-vertex quasi-tree graphs. In this paper, we characterize the quasi-unicyclic graphs with the smallest, the second-smallest, the largest and the second-largest Merrifield-Simmons index, respectively, in $\mathscr{U}(n, d_0)$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1]. If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E \subset E(G)$, 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. For any two graphs G_1 and G_2, let $G_1 \cup G_2$ denote the disjoint union of G_1 and G_2, and for any nonnegative integer s, let sG stand for the disjoint union of s copies of G. We obtain the join $G + H$ from $G \cup H$ by adding all edges between G and H. If H_1, H_2 are graphs with $V(H_1) \cap V(H_2) = v$, then $G = H_1 v H_2$ is defined as a new graph with $V(G) = V(H_1) \cup V(H_2)$ and $E(G) = E(H_1) \cup E(H_2)$. We always assume that in graph GvS_l, v is identified with the center of the star S_l in GvS_l.

Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}, n \geq 2$ with initial conditions $F_0 = F_1 = 1$. Then $i(P_n) = F_{n+1}, z(P_n) = F_n$. Note that $F_{n+m} = F_nF_m + F_{n-1}F_{m-1}$. For convenience, we let $F_n = 0$ for $n < 0$.

Now we give some lemmas that will be used in the proof of our main results.

Lemma 1.1 ([5]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G - uv) - i(G - \{N[u] \cup N[v]\}))$;*
(ii) *If $v \in V(G)$, then $i(G) = i(G - v) + i(G - N[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

Lemma 1.2 ([5]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G - uv) + z(G - \{u, v\}))$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G - v) + \sum_{u \in N(v)} z(G - \{u, v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

Lemma 1.3 ([10]). *Let G be a connected graph and T_l be a tree of order $l + 1$ with $V(G) \cap V(T_l) = \{v\}$. Then $i(GvT_l) \leq i(GvS_{l+1})$.*

Lemma 1.4 ([11]). *Let H, X, Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'. Then*

$$i(G_1^*) > i(G) \qquad or \qquad i(G_2^*) > i(G).$$

Lemma 1.5 ([8]). *Let $n = 4s + r$, where n, s and r are integers with $0 \leq r \leq 3$.*

(i) *If $r \in \{0, 1\}$, then $F_0F_n > F_2F_{n-2} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} > F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1}$;*
(ii) *If $r \in \{2, 3\}$, then $F_0F_n > F_2F_{n-2} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} > F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}$.*

Lemma 1.6. *[2] Among all unicyclic graphs of order n, the maximum of the Merrifield-Simmons index (which is $3 \cdot 2^{n-3} + 1$) is attained for* *the graph G_n^0 that results from attaching $n-3$ leaves to a triangle (the only exception being $n = 4$, in which case the cycle C_4 also maximizes the Merrifield-Simmons index). On the other hand, the minimum of the Merrifield-Simmons index ($F_n + F_{n-2}$) is attained for the cycle C_n and the graph Δ_n that results from attaching a path to a triangle.*

2. The Merrifield-Simmons index of quasi- unicyclic graphs

Lemma 2.1. *Let G be a graph of order n. Then*

(i) *[7] $i(G) \leq 2^n$, the equality holds if and only if $G \cong nP_1$.*
(ii) *If $G \ncong nP_1$, $i(G) \leq 3 \cdot 2^{n-2}$, the equality holds if and only if $G \cong (n-2)P_1 \cup P_2$.*

Proof. By Lemma 1.1(i), we have $i(G-uv) = i(G)+i(G-\{N[u] \cup N[v]\})) > i(G)$. Then $i(G) < i(G-e_1) < \cdots < i(G-e_1-e_2-\cdots-e_{m-1}) = i((n-2)P_1 \cup P_2) < i(G-e_1-e_2-\cdots-e_m) = i(nP_1)$. This complete the proof. □

Let G_1^*, G_2^* and G^{**} be the graphs as shown in Figure 1, where $G_1^* = K_1+C_{n-1}$, $G_2^* = K_1+\Delta_{n-1}$ and G^{**} is obtained by attaching $n-4$ pendent vertices to one of the two vertices of degree 3 of the unique 4-vertex bicyclic graph.

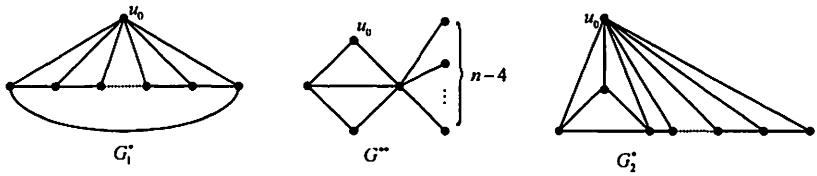

Figure 1: The graphs G_1^*, G^{**} and G_2^*

Lemma 2.2. *Let $G \in \mathscr{U}(n, d_0)$ with $d_0 \geq 2$, then $F_{n-1} + F_{n-3} + 1 \leq i(G) \leq 5 \cdot 2^{n-4} + 1$. The equality holds on the left if and only if $G \cong G_1^*$ or G_2^*. The equality holds on the right if and only if $G \cong G^{**}$.*

Proof. By Lemma 1.1 and Lemma 1.6, we have

$$i(G) = i(G-u_0) + i(G-N[u_0]) \geq F_{n-1} + F_{n-3} + 1,$$

the equality holds if and only if $G - u_0 \cong C_{n-1}$ or Δ_{n-1}, $G - N[u_0] = \emptyset$, which implies that u_0 is adjacent to each vertex of C_{n-1} or Δ_{n-1}. Then the equality holds if and only if $G \cong G_1^*$ or G_2^*.

For any $G \in \mathscr{U}(n, d_0)$ with $d_0 \geq 2$, $G - u_0$ is a unicyclic graph and $|V(G - N[u_0])| \leq n - 3$. By Lemma 1.1 and Lemma 1.6, we have

$$i(G) \;=\; i(G - u_0) + i(G - N[u_0]) \leq i(G_{n-1}^0) + i((n-3)P_1),$$

the equality holds if and only if $G - u_0 \cong G_{n-1}^0$ and $G - N[u_0] = (n-3)P_1$. Then the right equality holds if and only if $G \cong G^{**}$. By direct calculation, $i(G_{n-1}^0) = 3 \cdot 2^{n-4} + 1$ and $i((n-3)P_1) = 2^{n-3}$, then $i(G) \leq 5 \cdot 2^{n-4} + 1$. This complete the proof. □

By Lemma 1.6 and Lemma 2.2, the following result is immediate.

Theorem 2.3. *Let $G \in \mathscr{U}(n, d_0)$ with $d_0 \geq 1$ then $F_{n-1} + F_{n-3} + 1 \leq i(G) \leq 3 \cdot 2^{n-3} + 1$. The equality holds on the left if and only if $G \cong G_1^*$ or G_2^*. The equality holds on the right if and only if $G \cong G_n^0$.*

To obtain the graphs in $\mathscr{U}(n, d_0)$ with the second-smallest Merrifield-Simmons index, we first recall two transformations that decrease the Merrifield-Simmons index.

Transformation I[12, 3] Let $G \ncong P_1$ be a connected graph and choose $u \in V(G)$, G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $P_n : v_1 - v_2 - \cdots - v_n$, $1 < k < n$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding v_1v_n. Then $i(G_1) > i(G_2)$.

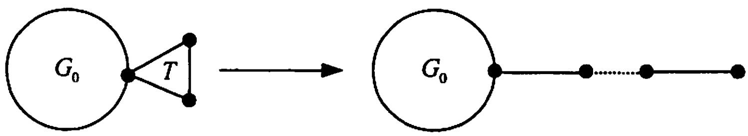

Figure 2: The graphs in remark 1

Remark 1: By repeating Transformation I, any tree T attached to a graph G_0 can be changed iteratively into a path (as shown in Figure 2). The Merrifield-Simmons index decreases at each iteration.

Transformation II[3] Let $P = uu_1u_2, \cdots, u_tv$ be an internal path in G, the degrees of $u_1, u_2, \cdots, u_t$ in G are 2 and $G \ncong P$, let A_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $P_k : v_1 - v_2 - \cdots - v_k$ and identifying v with the vertex v_{k+1} of a simple path $P_{n-k} : v_{k+1} - v_{k+2} - \cdots - v_n$, $1 < k < n-1$; A_2 is obtained from A_1 by deleting $v_{k-1}v_k$ and adding v_1v_n, A_3 is obtained from A_1 by deleting $v_{k+1}v_{k+2}$ and adding v_1v_n. Then $i(A_1) > i(A_2)$ or $i(A_1) > i(A_3)$.

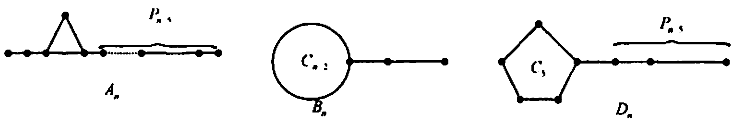

Figure 3: The graphs A_n, B_n and D_n

Lemma 2.4. *Let G be a connected unicyclic graph of order n and $G \ncong C_n, \Delta_n$,*

(i) if $n = 5$, $i(G) > 3F_{n-2} + 2F_{n-4}$;

(ii) if $n \geq 6$, $i(G) \geq 3F_{n-2} + 2F_{n-4}$, the equality holds if and only if $G \cong A_n, B_n$ or D_n (as shown in Figure 3).

Proof. Since $G \ncong C_n, \Delta_n$, then $n \geq 5$. For any unicyclic graph G, it can be obtained from a cycle by planting trees to some vertices of the cycle. Let k be the length of the unique cycle in G.

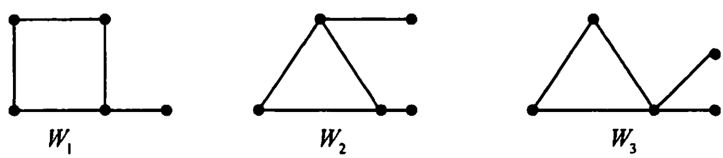

Figure 4: The unicyclic graphs of order 5 except C_5, Δ_5

(i) if $n = 5$, by direct calculation, we have $i(W_1) = i(W_2) = 12, i(W_3) = 13$. Then $i(G) > 3F_{5-2} + 2F_{5-4} = 11$.

(ii) $n \geq 6$.

Case 1. $k \geq 4$.

Let G_1 be the graph obtained by replacing each planted subtree of G by a pendant path of same order. By *Remark 1*, we have that $i(G) \geq i(G_1)$. Repeatedly by Transformation II, we can obtained a graph G_2 that results from attaching a path P_{n-k+1} to a vertex of the cycle C_k and $i(G) \geq i(G_1) \geq i(G_2)$. The equality holds if and only if $G \cong G_1 \cong G_2$. By Lemma 1.1, we have

$$i(G_2) \quad = \quad F_kF_{n-k+1} + F_{k-2}F_{n-k} = F_{n+1} - F_{k-3}F_{n-k}.$$

Since $G \not\cong C_n$, then $4 \le k \le n-1$. By Lemma 1.5, we have $F_2F_{(n-3)-2} \ge F_{k-3}F_{n-k}$, then $i(G_2) \ge F_{n+1} - F_2F_{(n-3)-2} = 3F_{n-2} + 2F_{n-4}$. The equality holds if and only if $k-3=2$ or $n-k=2$, that is, $G_2 \cong B_n$ or D_n.

Case 2. $k = 3$. Let $C_3 = v_1v_2v_3$.

If at least two of $d_G(v_1), d_G(v_2)$ and $d_G(v_3)$ are larger than 3, replacing each tree by a pendant path $P_i = v_iu_1^iu_2^i \cdots u_{l_i}^i (i = 1,2,3)$ of the same order gives the graph G_1, by Remark 1, $i(G) \ge i(G_1)$. If all of l_1, l_2, l_3 are larger than 1, let G_1' be the graph which is obtained from G_1 by deleting $v_1u_1^1$ and adding $u_{l_2}^2u_1^1$ or by deleting $v_2u_1^2$ and adding $u_{l_1}^1u_1^2$. By Transformation II, we have $i(G) \ge i(G_1) \ge i(G_1')$. Let one of the pendant paths of G_1' be P_l. By Lemma 1.1, we have

$$i(G_1') = F_n + F_lF_{n-1-l}.$$

Then $i(G) \ge F_n + F_lF_{n-1-l} \ge F_n + F_3F_{n-4} = 3F_{n-2} + 2F_{n-4} > F_n + F_1F_{n-2}$ since $G \not\cong \Delta_n$, the second equality holds if and only if $G \cong A_n$.

If only one of $d_G(v_1), d_G(v_2)$ and $d_G(v_3)$ is larger than 3, without loss of generality, let $d_G(v_3) \ge 3$.

If $d_G(v_3) \ge 4$, let G_2 be the graph obtained by attaching two pendant paths to v_3, by Remark 1 and Transformation II, $i(G) \ge i(G_2)$. Let one of the pendant paths be P_l. By Lemma 1.1, we have

$$i(G_2) = F_{n-1} + 2F_lF_{n-1-l}.$$

Then $i(G) \ge F_{n-1} + 2F_lF_{n-1-l} \ge F_{n-1} + 2F_3F_{n-4} > 3F_{n-2} + 2F_{n-4} > F_{n-1} + 2F_1F_{n-2}$ since $G \not\cong \Delta_n$.

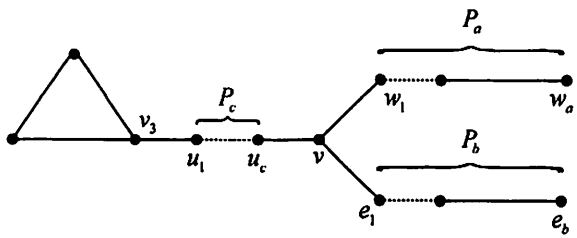

Figure 5: The graph G_2'

If $d_G(v_3) = 3$, then there exists a vertex $v \ne v_3$ and $d_G(v) \ge 3$ since $G \not\cong \Delta_n$. Let G_2' be the graph as shown in Figure 5, where a, b are the lengths of the two pendant paths attaching at v, respectively. By Remark

1 and Transformation II, $i(G) \geq i(G'_2)$. By Lemma 1.1, we have

$$\begin{aligned} i(G'_2) &= 3F_{a+1}F_{b+1}F_{n-3-a-b} + F_aF_bF_{n-4-a-b} + \\ & F_{a+1}F_{b+1}F_{n-4-a-b} + F_aF_bF_{n-5-a-b}. \end{aligned}$$

But

$$\begin{aligned} i(G'_2) - (3F_{n-2} + 2F_{n-4}) &= F_{a+1}F_{b+1}F_{n-4-a-b} + \\ & 3F_{a+1}F_{b+1}F_{n-5-a-b} + F_aF_bF_{n-4-a-b} \\ & -2F_aF_bF_{n-5-a-b} - 2F_{a-1}F_{b-1}F_{n-5-a-b} \\ &> F_{a+1}F_{b+1}F_{n-4-a-b} > 0. \end{aligned}$$

Hence $i(G) \geq 3F_{n-2} + 2F_{n-4}$, the equality holds if and only if $G \cong A_n, B_n$ or D_n. □

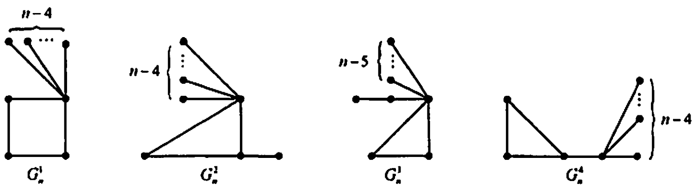

Figure 6: The graphs G_n^1, G_n^2, G_n^3 and G_n^4

Lemma 2.5. *Let G be a connected unicyclic graph of order n. If $G \not\cong G_n^0$, then $i(G) \leq 5 \cdot 2^{n-4} + 2$, the equality holds if and only if $G \cong G_n^1$ or G_n^2.*

Proof. By direct calculation, $i(G_n^1) = i(G_n^2) = 5 \cdot 2^{n-4} + 2$. For any unicyclic graph G, it can be obtained from a cycle by planting trees to some vertices of the cycle. Let k be the length of the unique cycle in G.

Case 1. $k \geq 4$.

Replacing each tree of G by a star of the same order gives the graph H_1, by Lemma 1.3, $i(G) \leq i(H_1)$. Repeatedly by Lemma 1.4, we can attained a graph H_2 which is obtained by attaching a star S_{n-k+1} to a vertex of the cycle C_k, and $i(G) \leq i(H_1) \leq i(H_2)$, the equality holds on the right if and only if $G \cong H_1 \cong H_2$. By Lemma 1.1, we have

$$i(H_2) = 2^{n-k}F_k + F_{k-2} = f(k),$$

but for $k \geq 5$, we have

$$\begin{aligned} f(k-1) - f(k) &= 2^{n-k+1}F_{k-1} + F_{k-3} - (2^{n-k}F_k + F_{k-2}) \\ &= 2^{n-k}F_{k-3} - F_{k-4} > 0, \end{aligned}$$

So $i(G) \leq i(G_n^1) < i(G_n^0)$, the equality holds on the right if and only if $G \cong G_n^1$.

Case 2. $k = 3$, let $C_k = v_1v_2v_3$.

If at least two of $d_G(v_1), d_G(v_2)$ and $d_G(v_3)$ are larger than 3, let H_1 be the graph obtained by replacing each tree of G by a star of the same order, by Lemma 1.3, $i(G) \leq i(H_1)$. By Lemma 1.4, we can obtain the graph G_n^2, and $i(G) \leq i(H_1) \leq i(G_n^2) < i(G_n^0)$, the equality holds if and only if $G \cong H_1 \cong G_n^2$.

If only one of $d_G(v_1), d_G(v_2)$ and $d_G(v_3)$ is larger than 3, without loss of generality, let $d_G(v_3) \geq 3$.

If $d_G(v_3) \geq 4$, repeatedly by Lemma 1.3 and Lemma 1.4, we can obtain the graph G_n^3. By Lemma 1.1, we have

$$i(G_n^3) = 9 \cdot 2^{n-5} + 2 < 5 \cdot 2^{n-4} + 2.$$

If $d_G(v_3) = 3$, similar to the procedure of the case of $d_G(v_3) \geq 4$, we can obtain the graph G_n^4. By direct calculation, we have

$$i(G_n^4) = 4 \cdot 2^{n-4} + 2 < 5 \cdot 2^{n-4} + 2.$$

Hence $i(G) \leq 5 \cdot 2^{n-4} + 2$, the equality holds if and only if $G \cong G_n^1$ or G_n^2.

□

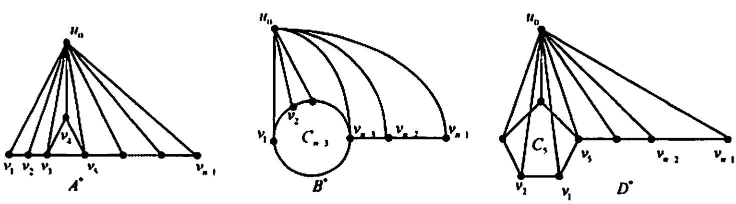

Figure 7: The graphs A^*, B^* and D^*

Let A be the graph obtained by attaching a pendant path P_3 at v_3 and P_{n-5} at v_5 of $C_3 = v_3v_4v_5$, respectively. By $C_{n-1,k}$ denote the graph constructed by identifying a vertex of C_k with one of the end vertex of P_{n-k}. Let A^*, B^*, D^*, E_n and $G_{1,j}^*, G_{2,j}^*$ be the graphs as shown in Figure 7 and Figure 8, where $A^* = K_1 + A, B^* = K_1 + C_{n-1,n-3}, D^* = K_1 + C_{n-1,5}$ and $G_{1,j}^* = G_1^* - u_0v_j, G_{2,j}^* = G_2^* - u_0v_j$.

Lemma 2.6. *Let $G \in \mathscr{U}(n, d_0)$ with $n \geq 7, d_0 \geq 2$, if $G \ncong G_1^*, G_2^*, G^{**}$.*

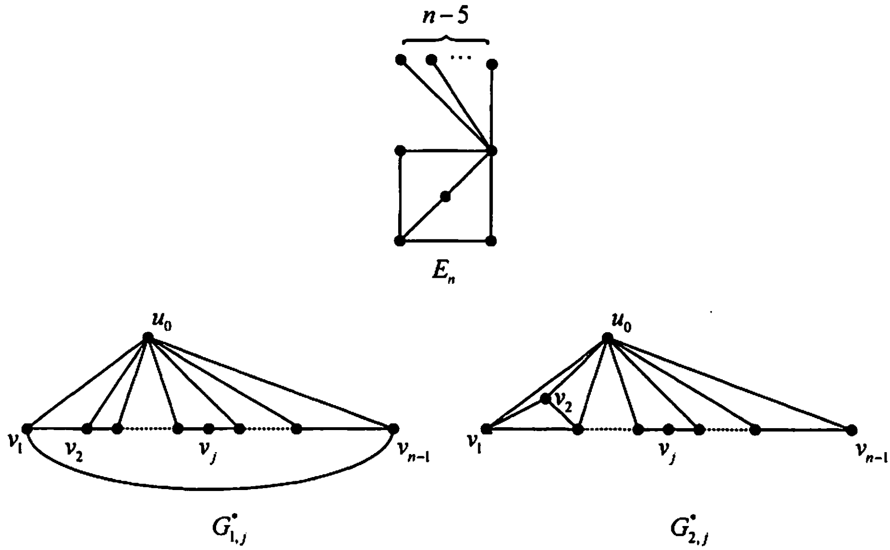

Figure 8: The graphs $E_n, G^*_{1,j}$ and $G^*_{2,j}$

(i) *If* $n = 7, 8$, $F_{n-1} + F_{n-3} + 2 \leq i(G) \leq 9 \cdot 2^{n-5} + 2$. *The equality on the left holds if and only if* $G \cong A^*$ *or* $B^*, D^*, G^*_{1,j}, G^*_{2,j}, j = 1, \cdots, n-1$. *The equality holds on the right if and only if* $G \cong E_n$.

(ii) *If* $n \geq 9$, $F_{n-1} + F_{n-3} + 2 \leq i(G) \leq 9 \cdot 2^{n-5} + 2$. *The equality on the left holds if and only if* $G \cong G^*_{1,j}$ *or* $G^*_{2,j}, j = 1, \cdots, n-1$. *The equality holds on the right if and only if* $G \cong E_n$.

Proof. By Lemma 1.1, we have

$$i(G) = i(G - u_0) + i(G - N[u_0]),$$

Case 1. Both $i(G - u_0)$ and $i(G - N[u_0])$ attain the smallest values, that is, $G - u_0 \cong C_{n-1}$ or Δ_{n-1}, and $G - N[u_0] = \emptyset$. Then $G \cong G^*_1$ or G^*_2, it is impossible.

Case 2. $i(G - u_0)$ achieves its smallest value, while $i(G - N[u_0])$ reaches its second-smallest value. Then $G - u_0 \cong C_{n-1}$ or Δ_{n-1}, and $G - N[u_0] = P_1$. So we have

$$i(G) = i(G - u_0) + i(G - N[u_0]) \geq F_{n-1} + F_{n-3} + 2,$$

the equality holds if and only if $G - u_0 \cong C_{n-1}$ or Δ_{n-1}, and $G - N[u_0] = P_1$, that is, $G \cong G^*_{1,j}$ or $G^*_{2,j}, j = 1, \cdots, n-1$.

Case 3. $i(G-N[u_0])$ reaches its smallest value, while $i(G-u_0)$ attains its second-smallest value. By Lemma 2.5, $G-u_0 \cong A_{n-1}, B_{n-1}$ or D_{n-1}, and $G-N[u_0]=\emptyset$. So we have

$$i(G) \;=\; i(G-u_0)+i(G-N[u_0]) \geq 3F_{n-3}+2F_{n-5}+1,$$

the equality holds if and only if $G-u_0 \cong A_{n-1}, B_{n-1}$ or D_{n-1}, and $G-N[u_0]=\emptyset$, that is, $G \cong A^*, B^*$ or D^*.

But

$$3F_{n-3}+2F_{n-5}+1-(F_{n-1}+F_{n-3}+2)=F_{n-5}-F_{n-6}-1,$$

then we have the following results:

(i) If $n=7,8$, $i(G) \geq F_{n-1}+F_{n-3}+2=3F_{n-3}+2F_{n-5}+1$. The equality holds if and only if $G \cong A^*$ or $B^*, D^*, G^*_{1,j}, G^*_{2,j}, j=1,\cdots,n-1$.

(ii) If $n \geq 9$, $3F_{n-3}+2F_{n-5}+1 > F_{n-1}+F_{n-3}+2$ and $i(G) \geq F_{n-1}+F_{n-3}+2$. The equality holds if and only if $G \cong G^*_{1,j}$ or $G^*_{2,j}, j=1,\cdots,n-1$.

Now, we consider the right inequality. Note that, for any $G \in \mathscr{U}(n,d_0)$ with $d_0 \geq 2$, $G-u_0$ is a unicyclic graph and $|V(G-N[u_0])| \leq n-3$.

Case 1. Both $i(G-u_0)$ and $i(G-N[u_0])$ attain the largest values, that is, $G-u_0 \cong G^0_{n-1}$, and $G-N[u_0]=(n-3)P_1$. Then $G \cong G^{**}$, it is impossible.

Case 2. $i(G-N[u_0])$ achieves its largest value, while $i(G-u_0)$ reaches its second-largest value. Then $G-N[u_0]=(n-3)P_1$ by Lemma 2.1, and $G-u_0 \cong G^1_{n-1}$ by Lemma 2.5. So we have

$$i(G) \;=\; i(G-u_0)+i(G-N[u_0]) \leq 5\cdot 2^{n-5}+2+2^{n-3}=9\cdot 2^{n-5}+2,$$

the equality holds if and only if $G-u_0 \cong G^1_{n-1}$, and $G-N[u_0]=(n-3)P_1$, that is, $G \cong E_n$.

Case 3. $i(G-u_0)$ reaches its largest value, while $i(G-N[u_0])$ achieves its second-largest value. Then $G-u_0 \cong G^0_{n-1}$ by Lemma 1.6, and $G-N[u_0]=(n-5)P_1 \cup P_2$ by Lemma 2.5. So we have

$$\begin{aligned} i(G) &= i(G-u_0)+i(G-N[u_0]) \leq 3\cdot 2^{n-4}+1+3\cdot 2^{n-5}=9\cdot 2^{n-5}+1 \\ &< 9\cdot 2^{n-5}+2. \end{aligned}$$

□

By Lemma 2.5 and 2.6, we have

Theorem 2.7. *Let* $G \in \mathscr{U}(n, d_0)$ *with* $n \geq 7, d_0 \geq 1$, $G \not\cong G_1^*, G_2^*, G_n^0$.

(i) *If* $n = 7, 8$, $F_{n-1} + F_{n-3} + 2 \leq i(G) \leq 5 \cdot 2^{n-4} + 2$. *The equality on the left holds if and only if* $G \cong A^*$ *or* $B^*, D^*, G_{1,j}^*, G_{2,j}^*, j = 1, \cdots, n-1$. *The equality holds on the right if and only if* $G \cong G_n^1$.

(ii) *If* $n \geq 9$, $F_{n-1} + F_{n-3} + 2 \leq i(G) \leq 5 \cdot 2^{n-4} + 2$. *The equality on the left holds if and only if* $G \cong G_{1,j}^*$ *or* $G_{2,j}^*, j = 1, \cdots, n-1$. *The equality holds on the right if and only if* $G \cong G_n^1$.

Acknowledgment. The authors are grateful to the referee for his or her valuable comments, corrections and suggestions, which led to an improved version of the original manuscript.

References

[1] B. Bollobás, Modern Graph Theory, Springer-Verlag, 1998.

[2] H. Deng, S. Chen, The extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, MATCH Commun. Math. Comput. Chem. 59 (2008) 171-190.

[3] H. Deng. The smallest Merrifield-Simmons index of $(n, n+1)$-graphs. Math. Comput. Modelling, 49(1-2)(2009) 320-326.

[4] H. Deng, S. Chen, and J. Zhang. The Merrifield-Simmons index in (n, n+1)-graphs. J. Math. Chem., 43(1)(2008) 75-91.

[5] I. Gutman, O. E. Polansky, Mathatical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[6] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, Discrete Appl. Math., 157 (2009) 1387-1395.

[7] S. Li, X. Li, W. Jing, On the extremal Merrifield-Simmons index and Hosoya index of qusi-tree graphs, Discrete Appl. Math., 157 (2009) 2877-2885.

[8] X. L. Li, H. X. Zhao, On the Fibonacci numbers of trees, Fibonacci Quart., 44 (2006) 32-38.

[9] H. Prodinger, R.F. Tichy, Fibonacci numbers of graphs, Fibonacci Quart., 20 (1982) 16-21.

[10] H. -Q. Liu, X. Yan and Z. Yan, On the Merrifield-Simmons indices and Hosoya indices of trees with a prescribed diameter, MATCH Commun. Math. Comput. Chem. 57 (2007) 371-384.

[11] H. -Q. Liu and M. Lu, A unified approach to extremal cacti for different indices, MATCH Commun. Math. Comput. Chem. 58 (2007) 193-204.

[12] S. Wagner, Extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index. MATCH Commun. Math. Comput. Chem. 57 (2007) 221-233.