On Maximum Merrifield-Simmons Index of Unicyclic Graphs with Prescribed Pendent Vertices

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Abstract

The Merrifield-Simmons index $\sigma(G)$ of a (molecular) graph G is defined as the number of independent-vertex sets of G. By $G(n,l,k)$ we denote the set of unicyclic graphs with girth and the number of pendent vertices being l and k respectively. Let S_n^l be the graph obtained by identifying the center of the star S_{n-l+1} with any vertex of C_l. By $S_n^{l,k}$ we denote the graph obtained by identifying one pendent vertex of the path $P_{n-l-k+1}$ with one pendent vertex of S_{l+k}^l. In this paper, we first investigate the Merrifield-Simmons index for all unicyclic graphs in $G(n,l,k)$ and $S_n^{l,k}$ is shown to be the unique unicyclic graph with maximum Merrifield-Simmons index among all unicyclic graphs in $G(n,l,k)$ for fixed l and k. Moreover, we proved that:

- When $k = n-3$, $S_n^{3,k}$ has the maximum Merrifield-Simmons index among all graphs in $G(n,k)$; When $k = 1, n-4$, $S_n^{4,k}$ or $S_n^{n-k,k}$ has the maximum Merrifield-Simmons index among all graphs in $G(n,k)$.
- When $2 \leq k \leq n-5$, $S_n^{n-k,k}$ and $S_n^{4,k}$ are resp. unicyclic graphs having maximum and second-maximum Merrifield-Simmons indices among all unicyclic graphs in $G(n,k)$, where $G(n,k)$ denotes the set of unicyclic graphs with n vertices and k pendent vertices.

Key words: Unicyclic graph; Merrifield-Simmons index; Pendent vertex.

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MSC(2000): 05C90, 05C69.

1 Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of v as $N_G(v)$.

For any given graph G, its Merrifield-Simmons index, simply denoted as $\sigma(G)$, is defined to be the total number of subsets of the vertex set, in which any two vertices are non-adjacent, i.e., in graph-theoretical terminology, the number of independent-vertex subsets of G, including the empty set. As for the $n-$vertex path P_n, $\sigma(G)$ is exactly equal to the Fibonacci number F_{n+2}. So some researchers call the Merrifield-Simmons index *Fibonacci number*. It is significant to determine the graph with extremal Merrifield-Simmons index. The concept of a (molecular) graph is introduced in [2], and discussed later in [3]. The Merrifield-Simmons index for a molecular graph was extensively investigated in [4], where its chemical applications were demonstrated. In [5], X. Li et al gave its other properties and applications. Wang et al [16] gave sharp lower and upper bounds for Merrifield-Simmons index among all unicyclic graphs. More recently, Yu et al [17] determined the unique trees with maximum Merrifield-Simmons index among all trees with k pendent vertices. There have been many literature studying the Merrifield-Simmons index. For further details along this line, see [5-15] and the cited references therein.

In this paper, we investigate the Merrifield-Simmons index for unicyclic graph with given pendent vertices. We first determined the unique unicyclic graph with maximum Merrifield-Simmons index among all unicyclic graphs with prescribed girth l and number of pendent vertices k. Moreover, we determined, for all possible values of k, the unicyclic graphs having maximum Merrifield-Simmons indices among all unicyclic graphs with given number of pendent vertices k.

2 Results

All graphs considered in this paper are connected and simple. By S_n, C_n, and P_n we denote respectively the star, the cycle and the path with n vertices. Let $G(n,l,k)$ denote the set of all unicyclic graphs on n vertices with girth and the number of pendent vertices being resp. l and k. Let S_n^l be the graph obtained by identifying the center of S_{n-l+1} with any vertex of C_l. By $S_n^{l,k}$ we denote the graph obtained by identifying one pendent vertex of the path $P_{n-l-k+1}$ with one pendent vertex of S_{l+k}^l. S_n^l and $S_n^{l,k}$ are graphs shown as in Fig.s 1 and 2, respectively.

Let $V_1(G)$ denote the set of pendent vertices in G and $d_G(x, y)$ denote the length of the shortest path connecting x and y, namely, the distance between x and y. Let $d_G(x,C_l) = min\{d_G(x,y)|y \in V(C_l)\ and\ x \notin V(C_l)\}$.

Let F_n denote the n^{th} Fibonacci number, we have $F_n + F_{n+1} = F_{n+2}$ with initial conditions $F_1 = F_2 = 1$.

Other notations and terminology not defined here will follow that of [1].

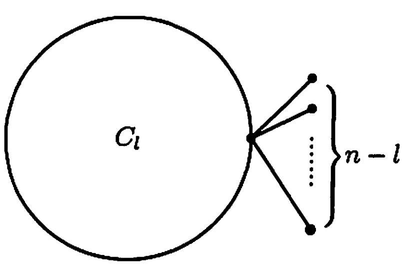

Fig.1. The graph S_n^l

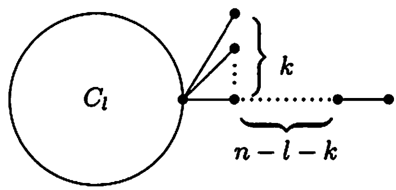

Fig.2. The graph $S_n^{l,k}$

It is necessary to introduce several important lemmas reported in [2, 5] which will be helpful to the proofs of our main results.

Lemma 1 *Let G be a graph with m components G_1, G_2, $\cdots G_m$. Then $\sigma(G) = \prod_{i=1}^{m} \sigma(G_i)$.*

Lemma 2 *Let G be a graph and v any vertex in $V(G)$, then*

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

where $[v] = N_G(v) \bigcup \{v\}$.

Lemma 3 *Let T be a tree. Then $F_{n+2} \leq \sigma(T) \leq 2^{n-1} + 1$ and $\sigma(T) = F_{n+2}$ if and only if $T \cong P_n$ and $\sigma(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$.*

Lemma 4 *Let G and G' be any two graphs. If G' is a proper spanning subgraph of G, then $\sigma(G') > \sigma(G)$.*

Proof. Let $xy \in E(G)$, then $\sigma(G - xy) - \sigma(G)$ equals to the number of independent vertex sets containing both x and y. Thus the result follows immediately. □

By $G(n,\ l)$ we denote the set of unicyclic graphs with n vertices and the length of its unique cycle being l. More recently, H. Wang and H. Hua reported the following result in [16].

Lemma 5 *Let $G \in G(n,\ l)$ with $l \geq 3$, then $\sigma(G) \leq \sigma(S_n^l)$ with equality holding if and only if $G \cong S_n^l$.*

The following theorem determined the unique graphs with maximum Merrifield-Simmons index among all graphs in $G(n,l,k)$ for given l and k.

Theorem 6 *Let $G \in G(n,l,k)$ with $3 \leq l \leq n-k$ and $1 \leq k \leq n-3$. If $G \ncong S_n^{l,\ k}$, then $\sigma(G) < \sigma(S_n^{l,\ k})$. (Referring to Fig.2. for $S_n^{l,\ k}$)*

Proof. For any $G \in G(n,l,k)$, let $q(G)$ denote the subset of $V(G)$ not including all pendent vertices as well as all vertices in $V(C_l)$. For fixed l, we have $|V(G)|+|V_1(G)| = (l+|q(G)|+|V_1(G)|)+|V_1(G)| \geq l+2|V_1(G)| = l+2k \geq l+2$, where $|V(G)|$, $|V_1(G)|$ and $|q(G)|$ are respectively the number of vertices in $V(G), V_1(G)$ and $q(G)$.

We shall complete the proof by induction on $|V(G)| + |V_1(G)|$. When $|V(G)| + |V_1(G)| = l + 2$, $G \cong S_n^{n-1,1} = S_n^{n-1}$ and the theorem follows immediately due to the fact that $S_n^{n-1,1}$ is the unique element in $G(n,n-1,1)$.

When $|q(G)| = 0$, it can be seen that the statement of theorem is true by Lemma 5. When $k = 1$, $G(n,l,1)$ contains a single element $S_n^{l,1}$, and the theorem holds clearly.

Let $q = |q(G)| \geq 1$, $k \geq 2$ and suppose the statement of theorem is true for all graphs G with $|V(G)| + |V_1(G)| < l + q + 2k$. Now suppose that G

is a graph in $G(n,l,k)$ with $|V(G)|+|V_1(G)|=l+q+2k$.

Denote by $V_d(G)$ the subset of $V_1(G)$ with the property that for any $v\in V_d(G)$, $d_G(v,C_l)=max\{d_G(x,C_l):x\in V_1(G)\}$. Take any vertex $v\in V_d(G)$ and let u be its unique neighbor.

We distinguish between two cases according to the values that $n-l-k$ assumes.

Case 1. $n-l-k=1$.

In this case, we claim that $d_G(v,C_l)=2$.

Suppose, to the contrary, that $d_G(v,C_l)\neq 2$.

If $d_G(v,C_l)=1$, then G has exactly $n-l$ pendent vertices, that is $n-l-k=0$. It is a contradiction to $n-l-k=1$. So we are left with the case that $d_G(v,C_l)\geq 3$. But then $n-l-k\geq 2$, which contradicts $n-l-k=1$ once again. So the claim follows.

Subcase 1.1 $d(u)=2$.

Since $d_G(v,C_l)=2$ and $d(u)=2$, then $G-v\in G(n-1,l,k)$ and $G-[v]\in G(n-2,l,k-1)$.

Let $v'\in V_d(S_n^{l,k})$ and u' its unique neighbor in $S_n^{l,k}$.

From Lemma 2, we have

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

and

$$\sigma(S_n^{l,k})=\sigma(S_n^{l,k}-v')+\sigma(S_n^{l,k}-v'-u').$$

Since $n-l-k=1$, then $S_n^{l,k}-v'\cong S_{n-1}^{n-1-k}\in G(n-1,l,k)$ and $S_n^{l,k}-v'-u'\cong S_{n-2}^{n-1-k}\in G(n-2,l,k-1)$.

In view of Lemma 5, we have $\sigma(G-v)\leq\sigma(S_{n-1}^{n-1-k})$ and $\sigma(G-[v])\leq\sigma(S_{n-2}^{n-1-k})$ with the equality holding if and only if $G-v\cong S_{n-1}^{n-1-k}$ and $G-v-u\cong S_{n-2}^{n-1-k}$, respectively.

Since $G\ncong S_n^{l,k}$, we have that either $\sigma(G-v)<\sigma(S_{n-1}^{n-1-k})$ or

$\sigma(G-[v]) < \sigma(S_{n-2}^{n-1-k})$. In either cases, the desired result follows.

Subcase 1.2[1] $d(u) \geq 3$.

In this case, $G-v \in G(n-1, l, k-1)$. Let $|N(u)| = m+1$. Then there're exactly m pendent vertices in $N(u)$ since $v \in V_d(G)$. Let $w \in N(u)$ such that $d(w) \geq 2$. We consider the following two subcases.

- The case when $k = m$.

From Lemma 2, we obtain

$$\begin{aligned}
\sigma(G) &= \sigma(kK_1 \bigcup C_l) + \sigma(P_{l-1}) \\
&= 2^k[\sigma(P_{l-1}) + \sigma(P_{l-3})] + \sigma(P_{l-1}) \\
&= (2^k + 1)\sigma(P_{l-1}) + 2^k\sigma(P_{l-3}),
\end{aligned}$$

$$\begin{aligned}
\sigma(S_n^{l,\,k}) &= \sigma[(k-1)K_1) \bigcup P_2 \bigcup P_{l-1}] + \sigma(K_1 \bigcup P_{l-3}) \\
&= 2^{k-1}\sigma(P_2)\sigma(P_{l-1}) + 2\sigma(P_{l-3}).
\end{aligned}$$

Bearing in mind that $\sigma(P_{l-1}) = \sigma(P_{l-2}) + \sigma(P_{l-3}) < 3\sigma(P_{l-3})$, by Lemmas 1, 3 and the above two equalities, we obtain $\sigma(G) - \sigma(S_n^{l,\,k}) = (1-2^{k-1})\sigma(P_{l-1}) + 2(2^{k-1}-1)\sigma(P_{l-3}) < 3(1-2^{k-1})\sigma(P_{l-3}) + 2(2^{k-1} - 1)\sigma(P_{l-3}) < 0$ since $k \geq 2$.

- The case when $k \geq m+1$.

Let $G-[v] = G_0 \bigcup (m-1)K_1$, where G_0 denotes the subgraph containing C_l of $G-v-u$. Thus $G_0 \in G(n-m-1, l, k-m)$.

Note that $|V(G-v)| + |V_1(G-v)| = (n-1) + (k-1) = n+k-2 = l+2k+q-2 < l+q+2k$. Note also that $|V(G_0)| + |V_1(G_0)| = (n-m-1) + (k-m) = n-2m+k-1 = (l+q+2k) - 2m - 1 < l+q+2k$.

Then by induction assumption, we obtain $\sigma(G-v) \leq S_{n-1}^{l,\,k-1}$ and $\sigma(G_0) \leq \sigma(S_{n-m-1}^{l,\,k-m})$.

[1]Note that $n-k-l=1$ in this case . Since the method we employed here will be used later, we did not substitute the value of $n-k-l=1$ into above formulas.

From Lemma 2, we obtain

$$\sigma(S_n^{l,\,k}) = \sigma(S_{n-1}^{l,\,k-1}) + \sigma[(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}] \qquad (1)$$

and

$$\sigma(G) = \sigma(G-v) + \sigma(G-[v]) = \sigma(G-v) + \sigma[(m-1)K_1 \bigcup G_0]. \qquad (2)$$

Now, what remains is to prove that $\sigma[(m-1)K_1 \bigcup G_0] < \sigma[(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}]$. It suffices to show that $\sigma[(m-1)K_1 \bigcup S_{n-m-1}^{l,\,k-m}] < \sigma[(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}]$.

Let u_0 denote the maximum degree vertex in $S_{n-m-1}^{l,k-m}$. If we delete all $k-m-1$ pendent edges incident with u_0 as well as two edges along the cycle incident with it , we obtain $(k-m-1)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}$. So by Lemma 4, the theorem holds as expected in this case.

Case 2. $n-l-k \geq 2$.

There are two subcases we should distinguish between.

Subcases 2.1 $d_G(v, C_l) \geq 3$.

Subcases 2.1.1 $d(u) \geq 3$.

Subcases 2.1.1.1 $d(w) = 2$.

Let $G-[v] = G_0 \bigcup (m-1)K_1$, where G_0 is defined as above. Thus $G_0 \in G(n-m-1, l, k-m+1)$ and $G-v \in G(n-1, l, k-1)$.

As before, $|V(G-v)| + |V_1(G-v)| = (n-1) + (k-1) < l+q+2k$. Also, $|V(G_0)| + |V_1(G_0)| = (n-m-1) + (k-m+1) = n-2m+k = (l+q+2k) - 2m < l+q+2k$.

From induction hypothesis we deduce that $\sigma(G-v) \leq \sigma(S_{n-1}^{l,k-1})$ and $\sigma(G_0) \leq \sigma(S_{n-m-1}^{l,\,k-m+1})$.

According to Eqs. (1) and (2), we need only to prove that

$$\sigma[(m-1)K_1 \bigcup S_{n-m-1}^{l,\,k-m+1}] < \sigma[(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}].$$

One can easily see that $(m-1)K_1 \bigcup S_{n-m-1}^{l,\,k-m+1}$ contains $(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l+1}$ as its proper spanning subgraph (In fact, we can use the same operation on $S_{n-m-1}^{l,\ k-m+1}$ as that of subcase 1.2), therefore the result follows by Lemma 4.

Subcases 2.1.1.2 $d(w) \geq 3$.

Clearly, we have $k \geq m+1$ in this case. Let $G-[v] = G_0 \bigcup (m-1)K_1$, where G_0 is defined as above. It is evident that $G-v \in G(n-1, l, k-1)$ and $G_0 \in G(n-m-1, l, k-m)$. From Lemma 2, we obtain Eqs. (1) and (2) once again.

What remains is in full analogy with that of subcase 1.2, so we omit here.

Subcases 2.1.2 $d(u) = 2$.

Subcases 2.1.2.1 $d(w) = 2$.

Then $G-v \in G(n-1, l, k)$ and $G-v-u \in G(n-2, l, k)$.

From Lemma 2, we obtain

$$\sigma(S_n^{l,\ k}) = \sigma(S_{n-1}^{l,\ k}) + \sigma(S_{n-2}^{l,\ k}) \tag{3}$$

and

$$\sigma(G) = \sigma(G-v) + \sigma(G-[v]). \tag{4}$$

Because $|V(G-v)| + |V_1(G-v)| = (n-1)+k = l+q+2k-1 < l+q+2k$ and $|V(G-v-u)| + |V_1(G-v-u)| = (n-2)+k < l+q+2k$, we have $\sigma(G-v) \leq \sigma(S_{n-1}^{l,k})$ and $\sigma(G-[v]) \leq \sigma(S_{n-2}^{l,\ k})$ by induction hypothesis.

The theorem holds in this case.

Subcases 2.1.2.2 $d(w) \geq 3$.

In this case, $G-v \in G(n-1, l, k)$ and $G-[v] \in G(n-2, l, k-1)$.

Once again by induction hypothesis, we have $\sigma(G-v) \leq \sigma(S_{n-1}^{l,k})$ and $\sigma(G-[v]) \leq \sigma(S_{n-2}^{l,\ k-1})$ since $|V(G-v)| + |V_1(G-v)| < l+q+2k$ and $|V(G-[v])| + |V_1(G-[v])| < l+q+2k$. Combining the above two inequalities with Eqs. (3) and (4), we need only to verify that $\sigma(S_{n-2}^{l,\ k}) > \sigma(S_{n-2}^{l,\ k-1})$.

According to Lemma 2, we obtain

$$\sigma(S_{n-2}^{l,\,k}) = \sigma(S_{n-3}^{l,\,k-1}) + \sigma[(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l-1}]$$

and

$$\sigma(S_{n-2}^{l,\,k-1}) = \sigma(S_{n-3}^{l,\,k-1}) + \sigma(S_{n-4}^{l,\,k-1}).$$

If $n-k-l=2$, then $S_{n-2}^{l,\,k} \cong S_{n-2}^{l}$. Thus the theorem holds in this case by Lemma 5.

Suppose $n-k-l \geq 3$. Using the same method as employed in subcase 1.2, we know that $(k-2)K_1 \bigcup P_{l-1} \bigcup P_{n-k-l-1}$ is a proper subgraph of $S_{n-4}^{l,\,k-1}$. From Lemma 5, the theorem follows.

Subcases 2.2 $d_G(v, C_l) = 2$.

Subcases 2.2.1 $d(u) = 2$.

Then $G - v \in G(n-1, l, k)$ and $G - [v] \in G(n-2, l, k-1)$. Similar to the proof of subcase 1.1, we omit here.

Subcases 2.2.2 $d(u) \geq 3$.

Let G_0 be defined as before and $|N(u)| = m+1$. Then $G - v \in G(n-1, l, k-1)$ and $G_0 \in G(n-m-1, l, k-m)$. What remains to do is completely similar to that of subcase 1.2.

By above arguments, the theorem follows as desired. □

Lemma 7 *For* $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$, $i \neq 3$ *and* $n \geq 6$, *we have*

$$\sigma(P_1 \bigcup P_{n-1}) > \sigma(P_3 \bigcup P_{n-3}) > \sigma(P_i \bigcup P_{n-i}). \tag{5}$$

Proof. Note from Lemmas 1, 2 and 3 that

$$F_{i+2}F_{n-i+2} - F_{i+1}F_{n-i+3} = (F_{i+1} + F_i)F_{n-i+2} - F_{i+1}(F_{n-i+2} + F_{n-i+1})$$

$$
\begin{aligned}
&= -(F_{i+1}F_{n-i+1} - F_iF_{n-i+2}) \\
&= (F_i + F_{i-1})F_{n-i+2} - F_i(F_{n-i+1} + F_{n-i}) \\
&= F_iF_{n-i} - F_{i-1}F_{n-i+1} \\
&= \cdots \\
&= (-1)^i(F_2F_{n-2i+2} - F_1F_{n-2i+3}) \\
&= (-1)^{i+1}F_{n-2i+1}.
\end{aligned}
$$

So, for any $i \geq 2$, we have $\sigma(P_1 \bigcup P_{n-1}) - \sigma(P_i \bigcup P_{n-i}) = (F_{n-3} - F_{n-5}) + (F_{n-7} - F_{n-9}) + (F_{n-11} - F_{n-13}) + \cdots > 0$. This proves the left-hand side of Eq.(5).

Similarly, we can show that $\sigma(P_3 \bigcup P_{n-3}) > \sigma(P_i \bigcup P_{n-i})$ for all $i \geq 2$ and $i \neq 3$. This completes the proof. □

Before stating another main result of this paper, we introduce the following two lemmas:

Lemma 8 *Suppose that* $3 \leq l \leq n-k-1$, $l \neq 4$ *and* $1 \leq k \leq n-4$. *Then* $\sigma(S_n^{l,\,k}) < \sigma(S_n^{4,\,k})$.

Proof. We prove that $\sigma(S_n^{l,\,k}) < \sigma(S_n^{4,\,k})$ for any $l \geq 3$ and $l \neq 4$ by induction on k.

When $k = 1$, it derived from Lemmas 2, 4 and 7 that

$$
\begin{aligned}
\sigma(S_n^{l,\,1}) - \sigma(S_n^{4,\,1}) &= [\sigma(P_{n-1}) + \sigma(P_{l-3} \bigcup P_{n-l})] - [\sigma(P_{n-1}) \\
&\quad + \sigma(P_1 \bigcup P_{n-4})] \\
&= \sigma(P_{l-3} \bigcup P_{n-l})] - \sigma(P_1 \bigcup P_{n-4}) < 0
\end{aligned}
$$

for all $l \geq 3$ and $l \neq 4$.

Let $t \geq 2$ and assume that the result holds for $k < t$. Now, let $k = t$.

In view of Lemma 2, we have

$$\sigma(S_n^{l,\,t}) = \sigma(S_{n-1}^{l,\,t-1}) + \sigma[(t-2)K_1 \bigcup P_{l-1} \bigcup P_{n-t-l+1}]$$

and

$$\sigma(S_n^{4,\,t}) = \sigma(S_{n-1}^{4,\,t-1}) + \sigma[(t-2)K_1 \bigcup P_3 \bigcup P_{n-t-3}].$$

By induction hypothesis, we get $\sigma(S_{n-1}^{l,\,t-1}) < \sigma(S_{n-1}^{4,\,t-1})$ for all $l \geq 3$ and $l \neq 4$. Combining Lemmas 1, 3 and 7, we can get the desired result. □

Lemma 9 *Let* $1 \leq k \leq n-4$, *then* $\sigma(S_n^{4,\,k}) \leq \sigma(S_n^{n-k,\,k})$, *where the equality is attained only if* $k = 1$ *or* $k = n-4$.

Proof. When $k = n-4$, the result is immediate. When $k = 1$, we obtain $\sigma(S_n^{n-1,\,1}) = \sigma(P_{n-1}) + \sigma(P_1 \bigcup P_{n-4}) = \sigma(S_n^{4,\,1})$. So we may assume that $2 \leq k \leq n-5$ herein and we prove that $\sigma(S_n^{4,\,k}) < \sigma(S_n^{n-k,\,k})$ in what follows.

As in Lemma 8, we demonstrate the lemma by induction on k. When $k = 2$,

$$\sigma(S_n^{4,\,2}) = \sigma(S_{n-1}^{4,\,1}) + \sigma(P_3 \bigcup P_{n-5})$$

and

$$\sigma(S_n^{n-2,\,2}) = \sigma(S_{n-1}^{n-2,\,1}) + \sigma(P_1 \bigcup P_{n-3}).$$

Note that $\sigma(S_{n-1}^{4,\,1}) = \sigma(S_{n-1}^{n-2,\,1})$ and $\sigma(P_3 \bigcup P_{n-5}) < \sigma(P_1 \bigcup P_{n-3})$. Hence, the statement of lemma is true in this case.

Assume that $t \geq 3$ and suppose that the lemma is true for the case that $k < t$. When $k = t$,

$$\sigma(S_n^{4,\,t}) = \sigma(S_{n-1}^{4,\,t-1}) + \sigma[(t-2)K_1 \bigcup P_3 \bigcup P_{n-t-3}]$$

and

$$\begin{aligned} \sigma(S_n^{n-t,\,t}) &= \sigma(S_{n-1}^{n-t,\,t-1}) + \sigma[(t-1)K_1 \bigcup P_{n-t-1}] \\ &= \sigma(S_{n-1}^{n-t,\,t-1}) + \sigma[(t-2)K_1 \bigcup P_1 \bigcup P_{n-t-1}]. \end{aligned}$$

By means of Lemmas 1, 7 and induction assumption, we immediately complete the proof of this lemma. □

Summarizing Lemmas 8, 9 and Theorem 6, we arrive at:

Theorem 10 *Let $1 \leq k \leq n-3$. Then we have:*

(a). For $k = n-3$, $S_n^{3,k}$ has the maximum Merrifield-Simmons index among all graphs in $G(n,k)$; For $k = 1, n-4$, $S_n^{n-k,k}$ or $S_n^{n-4,k}$ has the maximum Merrifield-Simmons index among all graphs in $G(n,k)$.

(b). For $2 \leq k \leq n-5$, $S_n^{n-k,k}$ and $S_n^{4,k}$ have, respectively, the maximum and second-maximum Merrifield-Simmons index among all graphs in $G(n,k)$, where $G(n,k)$ is the set of unicyclic graphs with n vertices and k pendent vertices.

Acknowledgement: The author is grateful to the anonymous referee for his/her many helpful comments, which improved considerably the presentation of this paper.

References

[1] J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, North-Holland, Amsterdam, 1976 .

[2] H. Prodinger, R. F. Tichy, Fibonacci numbers of graphs, The Fibonacci Quarterly, 20(1)(1982)16-21.

[3] A. F. Alameddine, Bounds on the Fibonacci number of a maximal outerplanar graph, The Fibonacci Quarterly, 36(3)(1998)206-210.

[4] R. E. Merrifield and H. E. Simmons, Topological Methods in Chemistry, Wiley, New York,1989.

[5] X. Li, Z. Li and L. Wang, The inverse problems for some topological indices in combinatorial chemistry, J.Computational Biology 10(1) (2003)47-55.

[6] Y. Wang, X. Li and I. Gutman , More examples and couterexamples for a conjecture of Merrifield-Simmons, Publications de L'Institut Math. NS 69(83)(2001)41-50.

[7] H. Zhao, X. Li, On the Fibonacci numbers of trees, The Fibonacci Quarterly 44(1)(2006)32-38.

[8] X. Li, H. Zhao and I. Gutman, On the Merrifield-Simmons index of trees, MATCH Commun. Math. Comput. Chem. 54(2)(2005).

[9] R. E. Merrifield and H. E. Simmons, Enumeration of structure-sensitive graphical subsets: Theory, Proc. Natl. Acad. Sci. USA 78(1981)692-695.

[10] R. E. Merrifield and H. E. Simmons, Enumeration of structure-sensitive graphical subsets: Theory, Proc. Natl. Acad. Sci. USA 78(1981)1329-1332.

[11] V. Linek, Bipartite graphs can have any number of independent sets, Discr. Math. 76(1989)131-136.

[12] I. Gutman, Fragmentation formulas for the number of Kekulé structures, Hosoya and Merrifield-Simmons indices and related graph invariants, Coll.Sci.Pap.Fac.Sci.Kragujevac (11)(1990)11-18.

[13] I. Gutman, N. Kolaković, Hosoya index of the second of molecules containing a polyacene fragment, Bull. Acad. Serbe Sci. Arts (CI. Math. Natur.), 102(1990)39-46.

[14] I. Gutman, Independent vertex sets in some compound graphs, Publ. Inst. Math. (Beograd) 52(1992) 5-9.

[15] X. Li, On a conjecture of Merrifield and Simmons, Australasian J.Comb.14(1996)15-20.

[16] H. Wang and H. Hua, Unicycle graphs with extremal Merrifield-Simmons index, J.Math.Chem.(2006)Online-first, DOI: 10.1007/s10910-006-9188-4.

[17] A. Yu and X. Lv, The Merrifield -Simmons indices and Hosoya indices of trees with k pendent vertices, J. Math. Chem. 41(1)(2007)33-43.