AUSTRALASIAN JOURNAL OF COMBINATORICS
Volume **50** (2011), Pages 87–95

On Merrifield-Simmons index of unicyclic graphs with given girth and prescribed pendent vertices*

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Abstract

For a graph G, the Merrifield-Simmons index $i(G)$ is defined as the total number of independent sets of the graph G. Let $G(n, l, k)$ be the class of unicyclic graphs on n vertices with girth and pendent vertices being resp. l and k. In this paper, we characterize the unique unicyclic graph possessing prescribed girth and pendent vertices with the maximal Merrifield-Simmons index among all graphs in $G(n, l, k)$.

1 Introduction

All graphs considered in this paper are finite, undirected and simple. Let $G = (V, E)$ be a graph on n vertices. 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. It follows directly from the definition that $\emptyset$ is an 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

* The project was supported by the Special Fund for Basic Scientific Research of Central Colleges, South-Central University for Nationalities (CZY10010).

in 1982 in a paper of Prodinger and Tichy [15], although it is called the Fibonacci number of a graph there.

The *Merrifield-Simmons index* is an important example of the topological indices which are of interest in combinatorial chemistry, which was extensively studied in a monograph [13]. There Merrifield and Simmons showed the correlation between this index and boiling points. Since then, many authors have investigated this graph invariant. In [15], Prodinger and Tichy showed that the path P_n has the minimal Merrifield-Simmons index and the star S_n has the maximal Merrifield-Simmons index for all trees with n vertices. In [4, 14], The authors studied the Merrifield-Simmons index of the unicyclic graphs. Li and one of the present authors [9] studied bound for the Merrifield-Simmons index of unicyclic graphs with a given diameter. Wang and Hua [17] characterized the extremal (maximal and minimal) Merrifield-Simmons index of unicyclic graphs with a given girth. In [2, 3], Deng et al characterized the bicyclic graphs with the maximal and smallest Merrifield-Simmons index. In [20], Li, Zhu and Tan studied tricyclic graphs with maximal Merrifield-Simmons index. Gutman [5], Zhang and Tian [19] studied the Merrifield-Simmons index of hexagonal chains and catacondensed systems, respectively. For further details, We refer readers to survey papers [8, 10], especially, a recent paper by S. Wagner and I. Gutman [18], which is a wonderful survey on this topic, and the cited references therein.

The *Hosoya index* [6], denoted by $z(G)$, is defined as the total number of matchings of G. As the authors of [18] say, in spite of the fact that there is a substantial amount of literature on the topic of maximizing or minimizing the Merrifield-Simmons index and the Hosoya index, there are still many interesting open questions for further study, for example, little is also known about the case that two restrictions are imposed at the same time, so this might be another worthwhile problem to study. A *unicyclic graph* is a connected graph with n vertices and n edges. The *girth* $g(G)$ of a graph G is the length of the shortest cycle in G. Let $G(n, l, k)$ be the class of unicyclic graphs on n vertices with girth and pendent vertices being resp. l and k. In [7], Hua characterized the unique unicyclic graph with minimal *Hosoya index* among all graphs in $G(n, l, k)$. It is natural to consider the *Merrifield-Simmons index* in $G(n, l, k)$. In this paper, we characterize the unique unicyclic graph possessing prescribed girth and pendent vertices with the maximal Merrifield-Simmons index among all graphs in $G(n, l, k)$.

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. We denote by P_n, C_n and S_n the path, the cycle and the star on n vertices, respectively. If H_1, H_2 are graphs with $V(H_1) \cap V(H_2) = v$, then $G = H_1vH_2$ 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. Set $N(v) = \{u|uv \in E(G)\}$, $N[v] = N(v) \cup \{v\}$. Let $d_G(u, v)$ be the distance between vertices u and v in G, and

$d_G(u, G_1) = \min\{d_G(u, v)|v \in V(G_1), u \notin V(G_1), G_1 \subset G\}$.

Definition Let $\alpha(G) = (r, s, t)$, where r is the number of pendent vertices, s the number of non-pendent vertices outside the unique cycle and t the number of vertices of G, respectively. If $r_1 \leq r_2$ or $s_1 \leq s_2$ and $t_1 \leq t_2$, then we write $(r_1, s_1, t_1) \leq (r_2, s_2, t_2)$. Moreover, $(r_1, s_1, t_1) = (r_2, s_2, t_2)$ if and only if $r_1 = r_2$, $s_1 = s_2$ and $t_1 = t_2$.

If $(r_1, s_1, t_1) \leq (r_2, s_2, t_2)$ but $(r_1, s_1, t_1) \neq (r_2, s_2, t_2)$, then we write $(r_1, s_1, t_1) < (r_2, s_2, t_2)$. Set $\alpha(G_i) = (r_i, s_i, t_i)$ for $i = 1, 2$. If $(r_1, s_1, t_1) < (r_2, s_2, t_2)$, then we write $\alpha(G_1) < \alpha(G_2)$.

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 $i(P_n) = F_{n+1}$. 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. [11] *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 1.3. [12] *Let H, X, Y be three connected graphs pairwise disjoint. 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 $i(G_1^*) > i(G)$ or $i(G_2^*) > i(G)$.*

2 The graph with maximal Merrifield-Simmons index

In this section, we investigate the maximal Merrifield-Simmons index for graphs in $G(n, l, k)$. As shown in Figure 1, let S_n^l be the graph obtained by identifying the center of star S_{n-l+1} with any vertex of C_l; by $R_n^{l,k}$ 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.

Lemma 2.1. [14] *Let G be a connected n-vertex unicyclic graph. If $g(G) = l$, then $i(G) \leq 2^{n-l} + F_{l-2}$, with the equality holding if and only if $G \cong S_n^l$.*

Lemma 2.2. $i(R_n^{l,k}) = 2^{k-1}F_lF_{n-l-k+2} + F_{l-2}F_{n-l-k+1}$.

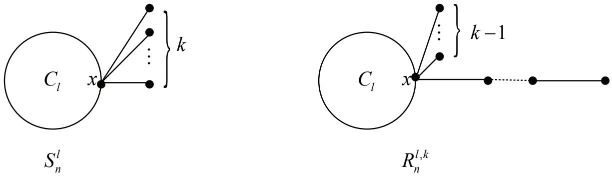

Figure 1: The graphs S_n^l and $R_n^{l,k}$

Proof. By Lemma 1.1, we have

$$\begin{aligned} i(R_n^{l,k}) &= i(R_n^{l,k} - x) + i(R_n^{l,k} - N[x]) \\ &= i((k-1)P_1 \cup P_{l-1} \cup P_{n-l-k+1}) + i(P_{l-3} \cup P_{n-l-k}) \\ &= 2^{k-1} F_l F_{n-l-k+2} + F_{l-2} F_{n-l-k+1}. \end{aligned}$$

□

For any $G \in G(n, l, k)$, G can be obtained from C_l by planting trees to some vertices of C_l. Let t be the number of vertices in $V(G)$ other than all pendent vertices as well as all vertices in $V(C_l)$. Obviously, $n = l + k + t, t \geq 0$. Let $V_1(G)$ be the set of pendent vertices in G. Let $d_{max} = \max\{d_G(x, C_l) | x \in V_1(G)\}$ and $V_d = \{v | v \in V_1(G), d_G(v, C_l) = d_{max}\}$.

Lemma 2.3. *If $\alpha(G) = (1, t, n)$, then $G \cong R_n^{l,1}$.*

Lemma 2.4. *If $\alpha(G) = (k, 0, n)$, then $i(G) \leq i(R_n^{l,k})$, with the equality holding if and only if $G \cong R_n^{l,k}$.*

Proof. If $\alpha(G) = (k, 0, n)$, then G can be obtained from C_l by attaching some pendent edges to some vertices of C_l. By repeated application of Lemma 1.3, we can attach all the pendent edges to one vertex of C_l, and the Merrifield-Simmons index increases. Obviously, the resulting graph is S_n^l, and $S_n^l \cong R_n^{l,k}$, where $k = n - l$. Hence the result holds. □

Lemma 2.5. *If $\alpha(G) = (k, 1, n)$, then $i(G) \leq i(R_n^{l,k})$, with the equality holding if and only if $G \cong R_n^{l,k}$.*

Proof. Since $t = 1$, then $d(v, C_l) = 2$ for any $v \in V_d$. Let u be the unique neighbor of v.

Case 1 $d(u) = 2$. By Lemma 1.1, we have

$$i(G) = i(G - v) + i(G - v - u), \tag{2.1}$$

where $G - v \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k-1)$. In this case, we clearly have $R_{n-1}^{l,k} (\cong S_{n-1}^l) \in G(n-1, l, k)$ and $R_{n-2}^{l,k} (\cong S_{n-2}^l) \in G(n-2, l, k-1)$, by Lemma 2.1, we have

$$i(G - v) \leq i(R_{n-1}^{l,k}), \quad i(G - v - u) \leq i(R_{n-2}^{l,k-1}),$$

then

$$i(G) \leq i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k-1}) = i(R_n^{l,k}).$$

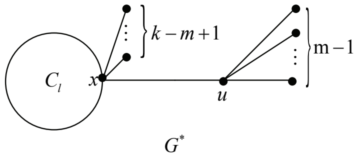

Figure 2: The graph G^*

Case 2 $d(u) = m \geq 3$. Let the pendent vertices in $N(u)$ be $v_1, \dots, v_{m-1}$. Then G can be obtained from C_l by attaching some pendent edges to some vertices of C_l and identifying a vertex of C_l with a pendent vertex of star S_{m+1}. By repeated application of Lemma 1.3, we can move all the pendent edges and the star S_{m+1} to a vertex of C_l, denoted it by G^*, as shown in Figure 2, and the Merrifield-Simmons index increases, that is, $i(G) \leq i(G^*)$. By Lemma 1.1, we have

$$\begin{aligned} i(G^*) &= 2^k F_l + 2^{k-m+1} F_l + 2^{m-1} F_{l-2} \\ i(R_n^{l,k}) &= 3 \cdot 2^{k-1} F_l + 2F_{l-2}, \end{aligned}$$

hence

$$\begin{aligned} i(R_n^{l,k}) - i(G^*) &= 3 \cdot 2^{k-1} F_l + 2F_{l-2} - [2^k F_l + 2^{k-m+1} F_l + 2^{m-1} F_{l-2}] \\ &= (3 \cdot 2^{k-1} - 2^k - 2^{k-m+1}) F_l - (2^{m-1} - 2) F_{l-2} \\ &= 2^{k-m+1}(2^{m-2} - 1) F_l - 2(2^{m-2} - 1) F_{l-2} \\ &= (2^{m-2} - 1)[2^{k-m+1} F_l - 2F_{l-2}] \\ &\geq (2^{m-2} - 1)[F_l - 2F_{l-2}] \\ &= (2^{m-2} - 1) F_{l-3} \geq F_{l-3} > 0. \end{aligned}$$

Hence $i(G) \leq i(R_n^{l,k})$, and the equality holds if and only if $G \cong G^* \cong R_n^{l,k}$. □

Lemma 2.6. *If $\alpha(G) = (k, t, n)$ with $k, t \geq 2$, then $i(G) \leq i(R_n^{l,k})$, with the equality holding if and only if $G \cong R_n^{l,k}$.*

Proof. Note that $d_G(v, C_l) \geq 2$ for any $v \in V_d$, let u be the unique neighbor of v. We proceed by induction on $\alpha(G)$. Suppose that the result holds for all unicyclic graphs G' with $\alpha(G') < \alpha(G)$.

Case 1 $d_G(v, C_l) = 2$. Obviously, $G \ncong R_n^{l,k}$.

Case 1.1 $d(u) = 2$.

$G-v \in G(n-1,l,k)$ and $G-v-u \in G(n-2,l,k-1)$. Obviously, $\alpha(G-v) = (k,t-1,n-1) < (k,t,n) = \alpha(G)$, and $\alpha(G-v-u) = (k,t-1,n-2) < (k,t,n) = \alpha(G)$. Then by the induction hypothesis, we have

$$i(G-v) \le i(R_{n-1}^{l,k}), i(G-v-u) \le i(R_{n-2}^{l,k-1}),$$

and then

$$i(G) \le i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k-1}).$$

Since $t \ge 2$, we have

$$i(R_n^{l,k}) = i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k}). \tag{2.2}$$

If $(n-2)-l-k = 0$, by Lemma 2.1, we have $i(R_{n-2}^{l,k-1}) < i(R_{n-2}^{l,k})$.

If $(n-2)-l-k \ge 1$, by Lemma 2.2, we have

$$\begin{aligned} & i(R_{n-2}^{l,k}) - i(R_{n-2}^{l,k-1}) \\ &= 2^{k-1}F_lF_{n-l-k} + F_{l-2}F_{n-l-k-1} - [2^{k-2}F_lF_{n-l-k+1} + F_{l-2}F_{n-l-k}] \\ &= (2^{k-2}F_l - F_{l-2})(F_{n-l-k} - F_{n-l-k-1}) > 0, \end{aligned} \tag{2.3}$$

so $i(R_{n-2}^{l,k-1}) < i(R_{n-2}^{l,k})$. Then

$$\begin{aligned} i(G) &= i(G-v) + i(G-v-u) \le i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k-1}) \\ &< i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k}) = i(R_n^{l,k}). \end{aligned}$$

Case 1.2 $d(u) = m \ge 3$.

Obviously, all vertices but one in $N(u)$ are pendent vertices. By Lemma 1.1, we have

$$i(G) = i(G-v) + 2^{m-2} i(G_1),$$

where G_1 denotes the subgraph containing C_l of $G-v-u$. Then $G-v \in G(n-1,l,k-1)$ and $G_1 \in G(n-m,l,k-m+1)$. Note that $\alpha(G-v) = (k-1,t,n-1) < (k,t,n) = \alpha(G)$ and $\alpha(G_1) = (k-m+1,t-1,n-m) < (k,t,n) = \alpha(G)$. Then by the induction hypothesis, we have

$$i(G-v) \le i(R_{n-1}^{l,k-1}), \quad i(G_1) \le i(R_{n-m}^{l,k-m+1}).$$

Furthermore, by Lemma 2.2, we have

$$\begin{aligned} i(G) &\le i(R_{n-1}^{l,k-1}) + 2^{m-2} i(R_{n-m}^{l,k-m+1}) \\ &\le 2^{k-2}F_lF_{n-l-k+2} + F_{l-2}F_{n-l-k+1} + 2^{k-2}F_lF_{n-l-k+1} + 2^{m-2}F_{l-2}F_{n-l-k}. \end{aligned}$$

Let $A = 2^{k-2}F_lF_{n-l-k+2} + F_{l-2}F_{n-l-k+1} + 2^{k-2}F_lF_{n-l-k+1} + 2^{m-2}F_{l-2}F_{n-l-k}$.

$$\begin{aligned} i(R_n^{l,k}) - A &= 2^{k-1}F_lF_{n-l-k+2} + F_{l-2}F_{n-l-k+1} - A \\ &= F_{n-l-k}[2^{k-2}F_l - 2^{m-2}F_{l-2}] > 0, \end{aligned}$$

so $i(G) < i(R_n^{l,k})$.

Case 2 $d_G(v, C_l) > 2$. There is exactly one vertex, say w, in $N(u)$ with $d(w) \geq 2$.

Case 2.1 $d(u) = m = 2$ and $d(w) = 2$.

$G - v \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k)$. Note that $\alpha(G - v) = (k, t-1, n-1) < (k, t, n) = \alpha(G)$, and $\alpha(G-v-u) = (k, t-1, n-2) < (k, t, n) = \alpha(G)$. Then by the induction hypothesis, we have

$$i(G - v) \leq i(R_{n-1}^{l,k}), i(G - v - u) \leq i(R_{n-2}^{l,k}), \tag{2.4}$$

and by (2.1), (2.2) and (2.4), we have

$$i(G) = i(G - v) + i(G - v - u) \leq i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k}) = i(R_n^{l,k}).$$

Case 2.2 $d(u) = m = 2$ and $d(w) \geq 3$.

$G-v \in G(n-1, l, k)$ and $G-v-u \in G(n-2, l, k-1)$. Note that $\alpha(G-v) = (k, t-1, n-1) < (k, t, n) = \alpha(G)$, and $\alpha(G-v-u) = (k-1, t-1, n-2) < (k, t, n) = \alpha(G)$. Then by the induction hypothesis, we have

$$i(G - v) \leq i(R_{n-1}^{l,k}), i(G - v - u) \leq i(R_{n-2}^{l,k-1}), \tag{2.5}$$

and by (2.1–2.3) and (2.5), we have

$$i(G) = i(G - v) + i(G - v - u) \leq i(R_{n-1}^{l,k}) + i(R_{n-2}^{l,k-1}) < i(R_n^{l,k}).$$

Case 2.3 $d(u) = m \geq 3$ and $d(w) = 2$.

Let $G - v - u = G_1 \cup (m-2)P_1$, where G_1 denotes the subgraph containing C_l of $G - v - u$. Then $G - v \in G(n-1, l, k-1)$ and $G_1 \in G(n-m, l, k-m+2)$. Similar to Case 1.2, we have

$$\begin{aligned} i(G) &= i(G - v) + 2^{m-2} i(G_1) \\ &\leq i(R_{n-1}^{l,k-1}) + 2^{m-2} i(R_{n-m}^{l,k-m+2}) \\ &= 2^{k-2} F_l F_{n-l-k+2} + F_{l-2} F_{n-l-k+1} + 2^{k-1} F_l F_{n-l-k} + 2^{m-2} F_{l-2} F_{n-l-k-1} \end{aligned}$$

Let $B = 2^{k-2} F_l F_{n-l-k+2} + F_{l-2} F_{n-l-k+1} + 2^{k-1} F_l F_{n-l-k} + 2^{m-2} F_{l-2} F_{n-l-k-1}$,

$$\begin{aligned} i(R_n^{l,k}) - B &= 2^{k-1} F_l F_{n-l-k+2} + F_{l-2} F_{n-l-k+1} - B \\ &= F_{n-l-k-1} [2^{k-2} F_l - 2^{m-2} F_{l-2}] > 0, \end{aligned}$$

so $i(G) < i(R_n^{l,k})$.

Case 2.4 $d(u) = m \geq 3$ and $d(w) \geq 3$.

Let $G - v - u = G_1 \cup (m-2)P_1$, where G_1 denotes the subgraph containing C_l of $G - v - u$. Then $G - v \in G(n-1, l, k-1)$ and $G_1 \in G(n-m, l, k-m+1)$. Similar to Case 1.2, we have our desired result. □

Combining Lemmas 2.2–2.6, we have our main result:

Theorem 2.7. *If $G \in G(n, l, k)$, then $i(G) \leq 2^{k-1} F_l F_{n-l-k+2} + F_{l-2} F_{n-l-k+1}$, with the equality holding if and only if $G \cong R_n^{l,k}$.*

Acknowledgements

The authors are grateful to the referees for their valuable comments, corrections and suggestions, which led to an improved version of the original manuscript.

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(Received 7 July 2010; revised 7 Apr 2011)