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Unicycle graphs with **extremal** Merrifield–Simmons Index

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The Merrifield–Simmons index $f(G)$ of a (molecular) graph G is defined as the number of subsets of the vertex set, in which any two vertices are non-adjacent, i.e., the number of independent-vertex sets of G. By $\mathcal{U}(n, k)$ we denote the set of unicycle graphs in which the length of its unique cycle is k. In this paper, we investigate the Merrifield–Simmons index $f(G)$ for an unicycle graph G in $\mathcal{U}(n, k)$. Unicycle graphs with the largest or smallest Merrifield–Simmons index are uniquely determined.

KEY WORDS: unicycle graph, Merrifield–Simmons index, girth

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 $N(v)$. By $n(G)$, we denote the number of vertices of G. All graphs considered here are both finite and simple. We denote, respectively, by S_n, P_n, and C_n the star, path, and cycle with n vertices.

Let (G_1, v_1) and (G_2, v_2) be two graphs rooted at v_1 and v_2, respectively, then $G = (G_1, v_1) \bowtie (G_1, v_2)$ denote the graph obtained by identifying v_1 with v_2 as one common vertex. Let $\mathcal{U}_n$ denote the set of all unicycle graphs of order n. By $\mathcal{U}(n, k)$ we denote the set of unicycle graphs in which the length of its cycle is k. For any graph G in $\mathcal{U}(n, k)$, we denote the unique cycle of length k in G as C_k. Other notations and terminology not defined here will conform to those in [1].

For any given graph G, its Merrifield–Simmons index, simply denoted as $f(G)$, is defined to be the 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. We take the cycle $C_4 =$

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$v_0v_1v_2v_3$ for instance. The independent-vertex subsets of $V(C_4)$ of all size are as follows: $\emptyset, \{v_0\}, \{v_1\}, \{v_2\}, \{v_3\}, \{v_0, v_2\}, \{v_1, v_3\}$, and then $f(C_4) = 7$. As for the path P_n, $f(G)$ is exactly equal to the Fibonacci number F_{n+2}. This is perhaps why some researchers call the Merrifield–Simmons index "Fibonacci number." The above-mentioned 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], Li et al. gave its other properties and applications. For progress along these lines (see [5–15]).

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

In this paper, we investigate the Merrifield–Simmons index for unicycle graphs in $\mathcal{U}(n, k)$. We determine the unique unicycle graphs with the largest or smallest Merrifield–Simmons index.

For any graph G in $\mathcal{U}(n, k)$ with $n = k$, its Merrifield–Simmons index $f(G)$ can be easily calculated. So we'll always assume that $n \geqslant k + 1$ throughout this paper.

2. Some lemmas

The following lemmas 2.1–2.4 can be found from [2, 5].

Lemma 2.1. Let T be a tree. Then $F_{n+2} \leqslant f(T) \leqslant 2^{n-1} + 1$ and $f(T) = F_{n+2}$ if and only if $T \cong P_n$ and $f(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$.

Lemma 2.2. Let G be a graph with m components $G_1, G_2, \ldots, G_m$. Then $f(G) = \prod_{i=1}^{m} f(G_i)$.

Lemma 2.3. For any graph G with any $v \in V(G)$, we have

$$f(G) = f(G - v) + f(G - [v]),$$

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

Lemma 2.4. Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$be two graphs. If $V(G_1) = V(G_2)$ and $E(G_1) \subset E(G_2)$, then $f(G_1) > f(G_2)$.

The following corollary follows immediately from lemma 2.4.

Corollary 2.5. Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs. If $V(G_1) = V(G_2)$ and $E(G_1) \subseteq E(G_2)$, then $f(G_1) \geqslant f(G_2)$ with equality holds if and only if $G_1 \cong G_2$.

3. Unicycle graphs with extremal Merrifield–Simmons index

For any graph G and $u, v \in V(G)$, set $[u, v] = [u] \bigcup [v]$, then we have

Lemma 3.1. For any graph G, we have $f(G - xy) = f(G) + f(G - [x, y])$ and $f(G + yz) = f(G) - f(G - [y, z])$ for any $xy \in E(G)$ and $yz \notin E(G)$.

Proof. It's not difficult to see that when deleting any edge xy from $E(G)$, the Merrifield–Simmons index of G will increase, while adding the edge yz into $E(G)$ will decrease the Merrifield–Simmons index of G. Obviously $f(G - xy) - f(G)$ is equal to the number of independent sets containing both x any y in G, i.e., the number of independent sets of the graph $G - [x, y]$, which is equal to $f(G - [x, y])$. Similarly, $f(G) - f(G + yz)$ should be equal to the number of independent sets containing both y and z in G. It's exactly equal to $f(G - [y, z])$. So the result follows. □

Let $(C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ denote the graph obtained by identifying any vertex v_i of C_k with the center v_i of S_{n-k+1} and $(C_k, v_i) \bowtie (P_{n-k+1}, v_i)$ the graph obtained by identifying any vertex v_i of C_k with one end-vertex v_i of P_{n-k+1}.

For convenience, we simply denote $(C_k, v_i) \bowtie (S_{n-k+1}, v_i)$ and $(C_k, v_i) \bowtie (P_{n-k+1}, v_i)$ as (C_k, S_{n-k+1}) and (C_k, P_{n-k+1}), respectively.

The next lemma follows directly for lemma 2.3 by an elementary calculating, so we omit its proof here.

Lemma 3.2. Let $G_1 \cong (C_k, S_{n-k+1})$ and $G_2 \cong (C_k, P_{n-k+1})$, then $f(G_1) = 2^{n-k} F_{k+1} + F_{k-1}$ and $f(G_2) = F_{k-1} F_{n-k+1} + F_{k+1} F_{n-k+2}$.

Before introducing the next lemma, we give the following definitions.

Set $S = \{v_i \in V(C_k) : d(v_i) \geqslant 3\}$.

Let v_i be any vertex in C_k. By $T(v_i)$ we denote the connected component containing v_i of the graph $G - \{v_{i-1}, v_{i+1}\}$.

Theorem 3.3. Let G be a unicycle graph in $\mathcal{U}(n, k)$ such that $f(G)$ is as large or small as possible, then each $T(v_i)$ is a star or path of order $n(T(v_i))$ resp., where v_i is any vertex of S.

Proof. Let G be a graph in $\mathcal{U}(n, k)$. Since $n \geqslant k + 1$, then $S \neq \emptyset$. Let v_k be any vertex in S. By lemma 2.3, we must have

$$\begin{aligned} f(G) &= f(G - v_k) + f(G - [v_k]) \\ &= f(G_1) \prod_{i=1}^{l} f(T_i) + f(G_2) \prod_{j=1}^{m} f(T_j), \end{aligned}$$

where T_i and T_j denote, respectively, the subtrees of $T(v_k)$ in the graphs $G - v_k$ and $G - [v_k]$ while G_1 and G_2 denote, respectively, the graphs $G - \bigcup_{i=1}^{l} T_i - v_k$ and $G - \bigcup_{j=1}^{m} T_j - [v_k]$. It's not difficult to see that $G_2 = G_1 - \{v_{k-1}, v_{k+1}\}$.

From lemma 2.3 it follows that

$$\begin{aligned} f(G_2) &= f(G_1 - v_{k-1} - v_{k+1}) \\ &= f(G_1) - f(G_1 - [v_{k-1}]) - f(G_1 - v_{k-1} - [v_{k+1}]). \end{aligned}$$

Set $A = \prod_{i=1}^{l} f(T_i)$ and $B = \prod_{j=1}^{m} f(T_j)$, then

$$\begin{aligned} f(G) &= Af(G_1) + Bf(G_2) \\ &= Af(G_1) + B[f(G_1) - f(G_1 - [v_{k-1}]) - f(G_1 - v_{k-1} - [v_{k+1}])] \\ &= (A + B)f(G_1) - B[f(G_1 - [v_{k-1}]) + f(G_1 - v_{k-1} - [v_{k+1}])] \qquad (1) \end{aligned}$$

When $f(G)$ is large enough, since $f(G_1) > 0$ and $f(G_1 - [v_{k-1}]) + f(G_1 - v_{k-1} - [v_{k+1}])] > 0$, we must get that $A + B$ is large enough while B is small enough. It implies that $A = (A + B) + (-B)$ is large enough. It's easy to see that $A = \prod_{i=1}^{l} f(T_i) \leqslant 2^{\sum_{i=1}^{l} n(T_i)}$, where the equality holds if and only if each T_i is an isolated vertex. It follows that $T(v_k)$ is a star. Since v_k is arbitrarily chosen, then each $T(v_k)$ is a star of order $n(T(v_k))$.

When $f(G)$ is small enough, $A = (A + B) + (-B)$ must be small enough by (1). From lemmas 2.1, 2.2 and corollary 2.5 follows that

$$A = \prod_{i=1}^{l} f(T_i) \geqslant \prod_{i=1}^{l} f(P_{n(T_i)}) = f\left(\bigcup_{i=1}^{l} P_{n(T_i)}\right) \geqslant f\left(P_{\sum_{i=1}^{l} n(T_i)}\right).$$

It's easy to see that the above equality holds if and only if $T(v_k)$ is a path of order $n(T(v_k))$. Therefore proof of theorem 3.3 is completed. □

Lemma 3.4. If G is a unicycle graph in $\mathcal{U}(n,k)$ such that $f(G)$ achieves the maximum cardinality, then $G \cong (C_k, S_{n-k+1})$.

Proof. Suppose G is a graph in $\mathcal{U}(n,k)$ with $f(G)$ taking the maximum value. For convenience, we call such a graph G to be maximum unicycle graph. By theorem 3.3, we know that each $T(x)$ is a star of order $n(T(x))$ for any $x \in S$.

If $|S| = 1$, then $G \cong (C_k, S_{n-k+1})$ and the result holds. So we may assume that $|S| \geqslant 2$. We will complete the proof by distinguishing the following two cases:

Case 1. For any $v \in S$, $d(v) = 3$.

Let $S = \{v_{i1}, v_{i2}, \ldots, v_{is}\} (s \geqslant 2)$ and $N(v_{ij}) - V(C_k) = \{x_j\}$ where $j = 1, 2, \ldots, s$.

Set $G' = G - v_{i2}x_2 - \cdots - v_{is}x_s + v_{i1}x_2 + \cdots + v_{i1}x_s$. We will show that $f(G') > f(G)$ by induction on n, namely, the order of the graph G.

Assume that $f(G^{'}) > f(G)$ for any maximum unicycle graph G in $\mathcal{U}(n, k)$ with $|S| \geqslant 2$ and order $n^{'} < n$.

When $n^{'} = n$, by lemma 2.3, we have

$$f(G^{'}) = f(G^{'} - x_1) + f(G^{'} - [x_1]).$$

By induction hypothesis, we have $f(G^{'} - x_1) \geqslant f(G - x_1)$ with equality holding only if $|S| = 2$.

Moreover, $f(G^{'} - [x_1]) = 2^{s-1} f(G^{''})$ where $G^{''}$ denote the graph $G^{'} - \{v_{i1}, x_1, \ldots, x_s\}$. Since $V(G^{'} - [x_1]) = V(G - [x_1])$ and $E(G^{'} - [x_1]) \subset E(G - [x_1])$, then $f(G^{'} - [x_1]) = 2^{s-1} f(G^{''}) > f(G - [x_1])$ by lemma 2.4. Hence $f(G^{'}) > f(G)$ when $n^{'} = n$.

By the principle of mathematical induction, we know that $f(G^{'}) > f(G)$ for any maximum unicycle graph G in $\mathcal{U}(n, k)$ with $|S| \geqslant 2$. It's a contradiction to the maximality of $f(G)$.

Case 2. There exists some vertex $x \in S$ with $d(x) \geqslant 4$.

Let y be any other vertex in S. We denote, respectively, $N(x) - V(C_k)$ and $N(y) - V(C_k)$ as the sets $\{x_1, \ldots, x_p\}$ and $\{y_1, \ldots y_q\}$, where $p \geqslant 2$ and $q \geqslant 1$.

Set $G^{'} = G - yy_1 - \cdots - yy_q + xy_1 + \cdots + xy_q$. We will show that $f(G^{'}) > f(G)$ by induction on n, namely, the order of the graph G.

Suppose $f(G^{'}) > f(G)$ for all maximum unicycle graphs G in $\mathcal{U}(n, k)$ with order $n^{'} < n$ and $|S| \geqslant 2$.

When $n^{'} = n$, by lemma 2.3, we have

$$f(G^{'}) = f(G^{'} - x_1) + f(G^{'} - [x_1]).$$

By induction hypothesis, we have $f(G^{'} - x_1) > f(G - x_1)$.

For convenience, we denote $G_1 = G^{'} - \{x, x_1, \ldots, x_p, y_1, \ldots, y_q\}$ and $G_2 = G - \{x, x_1, \ldots, x_p\}$. Then

$$\begin{aligned} f(G^{'} - [x_1]) &= 2^{p+q-1} f(G_1) \\ &= 2^{p-1}[2^q f(G_1)] \\ &= 2^{p-1} f(G_2 - yy_1 - \cdots - yy_q). \end{aligned}$$

By lemma 3.1, $f(G_2 - yy_1 - \cdots - yy_q) = f(G_2) + f(G_2 - [y, y_1]) + \cdots + f(G_2 - yy_1 - \cdots - [y, y_q]) > f(G_2)$, so $f(G^{'} - [x_1]) > 2^{p-1} f(G_2) = f(G - [x_1])$ and then $f(G^{'}) > f(G)$ when $n^{'} = n$.

By the principle of mathematical induction, we have $f(G^{'}) > f(G)$ for any maximum unicycle graph G in $\mathcal{U}(n, k)$ with $|S| \geqslant 2$. It contradicts the choice of G once again.

From proof of cases 1 and 2, we know that $|S| = 1$ and $G \cong (C_k, S_{n-k+1})$ when $f(G)$ takes the maximum cardinality. □

Lemma 3.5. If G is a graph in $\mathcal{U}(n,k)$ such that $f(G)$ achieves the minimum cardinality, then $G \cong (C_k, P_{n-k+1})$.

Proof. Let G be a graph in $\mathcal{U}(n,k)$ with $f(G)$ taking the minimum value. For convenience, we call such a graph G minimum unicycle graph. From theorem 3.3, each $T(v_i)$ is a path of order $n(T(v_i))$ for any $v_i \in S$.

If $|S| = 1$, then $G \cong (C_k, P_{n-k+1})$ and the result holds. So we may assume that $|S| \geqslant 2$.

We'll show that the result holds by distinguishing the following two cases:

Case 1. For any $x \in S$, $T(x) \cong P_2$.

Let $S = \{v_{i1}, v_{i2}, \ldots, v_{is}\} (s \geqslant 2)$ and $N(v_{ij}) - V(C_k) = \{x_j\}$ where $j = 1, 2, \ldots, s$.

Set $G' = G - v_{i2}x_2 - \cdots - v_{is}x_s + x_1x_2 + x_2x_3 + \cdots + x_{s-1}x_s$. In the following, we will show that $f(G') < f(G)$ by induction on the order of the graph G.

Assume that $f(G') < f(G)$ for any minimum unicycle graph G in $\mathcal{U}(n,k)$ with order $n' < n$ and $|S| \geqslant 2$.

When $n' = n$, by lemma 2.3, we have

$$f(G') = f(G' - x_s) + f(G' - [x_s]).$$

By induction hypothesis, we have $f(G' - x_s) \leqslant f(G - x_s)$ with equality holding only if $|S| = 2$.

From lemmas 2.3 and 3.2, we obtain

$$\begin{aligned} f(G' - [x_s]) &= f(G' - [x_s] - v_{i1}) + f(G' - [x_s] - [v_{i1}]) \\ &= F_{k+1}F_{n-k} + F_{k-1}F_{n-k-1}. \end{aligned}$$

Moreover, we have

$$f(G - [x_s]) = f(T_{n-2}) \geqslant f(P_{n-2}) = F_n$$

by lemma 2.1.

Note that $F_{k+l} = F_{k+1}F_l + F_kF_{l-1}$. Thus

$$\begin{aligned} f(G - [x_s]) &\geqslant F_n \\ &= F_{k+(n-k)} \\ &= F_{k+1}F_{n-k} + F_kF_{n-k-1} \\ &> F_{k+1}F_{n-k} + F_{k-1}F_{n-k-1} \\ &= f(G' - [x_s]). \end{aligned}$$

Hence $f(G') < f(G)$ when $n' = n$.

So, by the principle of mathematical induction, we have $f(G^{'}) < f(G)$ for all minimum unicycle graphs G in $\mathcal{U}(n,k)$ with $|S| \geqslant 2$, which contradicting the choice of G.

Case 2. There exists some vertex $x_0 \in S$ with $T(x_0) \cong P_t(x_0)$ where $t \geqslant 3$. Let y_0 be any other vertex in S. Denote $P_t(x_0) = x_0x_1x_2 \ldots x_t(\ t \geqslant 2 \ )$ and $P_s(y_0) = y_0y_1 \ldots y_s(\ s \geqslant 1 \ )$.

Set $G^{'} = G - x_0x_1 + y_sx_1$, we will show that $f(G^{'}) < f(G)$ by induction on the order of G.

Suppose $f(G^{'}) < f(G)$ for all minimum unicycle graphs G in $\mathcal{U}(n,k)$ with order $n^{'} < n$ and $|S| \geqslant 2$.

When $n^{'} = n$, by lemma 2.3, we have

$$f(G^{'}) = f(G^{'} - x_t) + f(G^{'} - [x_t]).$$

By induction hypothesis, we have $f(G^{'} - x_t) \leqslant f(G - x_t)$ and $f(G^{'} - [x_t]) \leqslant f(G - [x_t])$, where the first equality holds only if $t = 1$ while the second one holds only if $t = 2$.

Hence $f(G^{'}) < f(G)$ when $n^{'} = n$.

By the principle of mathematical induction, we know $f(G^{'}) < f(G)$ for all minimum unicycle graphs G in $\mathcal{U}(n,k)$ with $|S| \geqslant 2$, a contradiction to the minimality of $f(G)$ once again.

So $|S| = 1$ and then $G \cong (C_k, P_{n-k+1})$. □

Theorem 3.6. Let G be any unicycle graph in $\mathcal{U}(n,k)$. Then $F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k+2} \leqslant f(G) \leqslant 2^{n-k}F_{k+1} + F_{k-1}$ with left equality holding if and only if $G \cong (C_k, P_{n-k+1})$ and with right equality holding if and only if $G \cong (C_k, S_{n-k+1})$.

Proof. From lemmas 3.2, 3.4, and 3.5, we can easily get

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

The proof of *if part* is trivial. The proof of *only if part* is as follows.

Suppose $f(G) = F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k+2}$ and $G \ncong (C_k, P_{n-k+1})$, then by lemma 3.5, we have

$$f(C_k, P_{n-k+1}) < f(G) = F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k+2}$$

a contradiction to (2).

Similarly, if $f(G) = 2^{n-k}F_{k+1} + F_{k-1}$ but $G \ncong (C_k, S_{n-k+1})$, then

$$f(C_k, S_{n-k+1}) > f(G) = 2^{n-k}F_{k+1} + F_{k-1}$$

by lemma 3.4, a contradiction to (2) once again.

Therefore the proof is completed. □

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