Discrete Applied Mathematics 159 (2011) 971–980

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

Graphs with given number of cut vertices and extremal Merrifield–Simmons index[☆]

Hongbo Hua[a,b,*], Shenggui Zhang[a]

[a] *Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, PR China*

[b] *Faculty of Mathematics and Physics, Huaiyin Institute of Technology, Huai'an, Jiangsu 223003, PR China*

ARTICLE INFO

Article history:
Received 26 March 2010
Received in revised form 28 January 2011
Accepted 3 March 2011
Available online 3 April 2011

Keywords:
Merrifield–Simmons index
Independent sets
Cut vertex
Bound
Extremal graph

ABSTRACT

The Merrifield–Simmons index of a graph is defined as the total number of its independent sets, including the empty set. Denote by $\mathcal{G}(n, k)$ the set of connected graphs with n vertices and k cut vertices. In this paper, we characterize the graphs with the maximum and minimum Merrifield–Simmons index, respectively, among all graphs in $\mathcal{G}(n, k)$ for all possible k values.

1. Introduction

In this paper we consider only simple graphs without loops and multiple edges. We use [2] for terminology and notation not defined here.

Let G be a graph. A subset S of $V(G)$ is called an *independent set* of G if the subgraph induced by S has no edges. The *Merrifield–Simmons index* of G is defined as

$$i(G) = \sum_{k \geq 0} i(G; k),$$

where $i(G; k)$ denotes the number of k-membered independent sets of G for $k \geq 1$ and $i(G; 0) = 1$.

Since, for the n-vertex path P_n, $i(P_n)$ is exactly equal to the Fibonacci number F_{n+1} the Merrifield–Simmons index of a graph is also called its *Fibonacci number* (see [1,17,19]). In mathematical chemistry, the Merrifield–Simmons index originated from [17]. This index is one of the most popular topological indices in chemistry. It has been extensively studied, as can be seen in the monograph [14]. During the past decades, many results on the Merrifield–Simmons index of graphs have been obtained. The characterization of graphs with the extremal Merrifield–Simmons index within given classes of graphs has been one of the most popular tendencies. For instance, see [10,19] for trees, [5,12,16] for trees with a given diameter, [18] for trees with a given number of pendent vertices, [3] for trees with a given stability number, [15] for unicyclic graphs, [13] for unicyclic graphs with a given diameter, [11] for cacti, [9] for quasi-tree graphs, [4] for general graphs and connected graphs with a given stability number, [8] for connected graphs, [1] for maximal outerplanar graphs, and so on.

☆ Supported by NSFC (No. 10871158), SRF of HIT (HGA1010) and Qing Lan Project of Jiangsu Province, PR China.

* Corresponding author at: Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, PR China.
E-mail addresses: hongbo.hua@gmail.com, hhb.hyit@gmail.com (H. Hua).

0166-218X/$ – see front matter
doi:10.1016/j.dam.2011.03.008

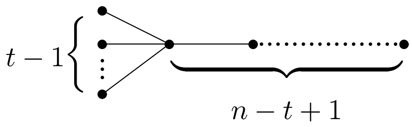

Fig. 1. The graph $SP_{n,t}$.

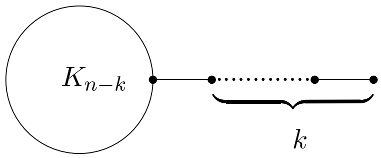

Fig. 2. The graph $KP_{n,k}$.

More recently, Hua [7] characterized the graphs having maximum Merrifield–Simmons index among all connected graphs with k cut edges for all possible k values. In this paper we continue this study by characterizing graphs with the maximum and minimum Merrifield–Simmons index, respectively, among all graphs in $\mathcal{G}(n, k)$, the set of connected graphs with n vertices and k cut vertices, for all possible k values.

Before proceeding, we introduce some notation and terminology. For any $v \in V(G)$, we let $N_G(v)$ be the set of neighbors of v, and let $N_G[v] = N_G(v) \cup \{v\}$. The degree of a vertex v in G, denoted by $d_G(v)$, or simply $d(v)$, is the number of vertices in $N_G(v)$. If $d(v) = 1$ for a vertex v, then v is said to be a *pendent vertex*. A *cut vertex* of a graph is any vertex that when removed increases the number of connected components of this graph. By the definition of cut vertex, if a graph G has k cut vertices, then $0 \le k \le n-2$. Denote, as usual, by P_n, S_n, C_n and K_n the path, star, cycle and complete graph on n vertices, respectively. Let $K_{s,t}$ denote a complete bipartite graph with one partition set having s vertices and the other one having t vertices. We use mG to denote the union of m copies of a graph G. A *block* is a connected graph that has no cut vertices, and a block of a graph G is a subgraph of G that is itself a block and maximal with respect to this property. A *clique* of graph G is a subset S of $V(G)$ such that $G[S]$, the subgraph induced by S, is a complete graph (in some cases, the term clique may also refer to the subgraph). Suppose $P = v_1v_2\cdots v_k$ $(k \ge 2)$ is a path lying within a graph G. If $d(v_1) \ge 3$, $d(v_k) = 1$ and $d(v_j) = 2 (1 < j < k)$, we call P a *pendant path* of G. Let $SP_{n,t}$ be a tree obtained from the path P_{n-t+1} by attaching to one of its end-vertices $t-1$ pendent vertices and $KP_{n,k}$ denote a graph obtained by connecting an edge between one pendent vertex of P_k and one vertex of the complete graph K_{n-k}, respectively. For the sake of brevity, we shall, in the following, write $G - [x]$ instead of $G - N_G[x]$.

2. Main results

In this section, we present our main results of this paper. More precisely, we have the following two results.

Theorem 1. *Let G be a graph in $\mathcal{G}(n, k)$ with $n \ge 4$. Then*

$$i(G) \le \begin{cases} 2^{n-2}+3, & k = 0; \quad (1) \\ 2^{n-k-1}F_{k+1} + F_k, & k \ge 1. \quad (2) \end{cases}$$

Equality holds in (1) *if and only if $G \cong K_{2,n-2}$ or C_5, and in* (2) *if and only if $G \cong SP_{n,n-k}$, respectively (see Fig. 1 for $SP_{n,n-k}$ by setting $t = n-k$).*

Theorem 2. *Let G be a graph in $\mathcal{G}(n, k)$ with $n \ge 4$. Then $i(G) \ge (n-k)F_{k+1} + F_k$, with equality if and only if $G \cong KP_{n,k}$ (see Fig. 2 for $KP_{n,k}$).*

Note 1. When $k = 0$, if $n = 2$, then $\mathcal{G}(n, k)$ contains only P_2, and if $n = 3$, then $\mathcal{G}(n, k)$ contains only K_3; When $k \ge 1$, we must have $n \ge 3$. Also, if $k \ge 1$ and $n = 3$, then $\mathcal{G}(n, k)$ contains only P_3. So we have assumed that $n \ge 4$ in the above two theorems.

3. Some preliminary results

We first give some lemmas that will be used in the proof of our main results.

Lemma 1 ([6]). *Let G be a graph with m components $G_1, G_2, \ldots, G_m$. Then*

$$i(G) = \prod_{i=1}^{m} i(G_i).$$

Lemma 2. *Let G be a graph.*

(i) [6] *If* u *is a vertex in* G, *then* $i(G) = i(G - u) + i(G - [u])$;
(ii) [6] *If* vw *is an edge in* G, *then* $i(G) = i(G - vw) - i(G - \{[v] \cup [w]\})$;
(iii) *If* vw *is an edge in* G, *then* $i(G) = i(G - v - w) + i(G - [v]) + i(G - [w])$.

In fact, (iii) follows from (i). Lemma 2(ii) implies the following result.

Lemma 3. *Let* G_1 *and* G_2 *be two graphs. If* G_1 *can be obtained from* G_2 *by deleting some edges, then* $i(G_2) < i(G_1)$.

Prodinger and Tichy [17] gave an upper bound for the Merrifield–Simmons index of trees, and later Lin and Lin [10] characterized the unique tree attaining this upper bound. Their result is summarized as follows:

Theorem 3. *Let* T *be a tree on* n *vertices. Then* $i(T) \le 2^{n-1} + 1$, *with equality if and only if* $T \cong S_n$.

In fact, the upper bound in Theorem 3 applies to any connected graph.

Corollary 1. *Let* G *be a connected graph on* n *vertices. Then* $i(G) \le 2^{n-1} + 1$, *with equality if and only if* $G \cong S_n$.

Proof. Let G be a connected graph on n vertices and $T(G)$ denote a spanning tree of G. By Lemma 3 and Theorem 3, we obtain

$$i(G) \le i(T(G)) \le 2^{n-1} + 1,$$

with the equality if and only if $G \cong S_n$. □

Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = F_1 = 1$. Thus for $n \ge 1$,

$$i(P_n) = F_{n+1} = \frac{\sqrt{5}}{5}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+2} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+2}\right],$$

while for $n < 0$, it is conventional and convenient to set $i(P_n) = i(\emptyset) = 1$.

Yu and Lv proved the following result.

Theorem 4 ([18]). *Let* T *be a tree with* n *vertices and* k *pendent vertices. Then* $i(T) \le 2^{k-1}F_{n-k+1} + F_{n-k}$, *with equality if and only if* $T \cong SP_{n,k}$ *(see Fig. 1).*

More recently, Hua obtained the following result.

Theorem 5 ([7]). *Let* G *be a connected graph with* $n \ge 4$ *vertices and without cut edges. Then* $i(G) \le 2^{n-2} + 3$, *with equality if and only if* $G \cong K_{2,n-2}$ *or* C_5.

4. The proof of main results

Let $\mathcal{C}(G)$ be the set of cut vertices in G, and let $d_G(x, y)$ be the distance between two vertices x and y in G. At first, we give some useful definitions used later in the proof of our main results.

Definition 1. Let G be a graph with at least two distinct cut vertices. Two cut vertices u and v of G are said to be *close cut vertices*, if there exists no cut vertex $x \in \mathcal{C}(G) \setminus \{u, v\}$ such that $d_G(u, x) < d_G(u, v)$ and $d_G(v, x) < d_G(u, v)$.

Definition 2. Let G be a graph with at least two distinct cut vertices, say u and v. The *subgraph induced by two close cut vertices* u and v of G, denoted by $CCVS(G; u, v)$, is the subgraph of G with vertex set consisting of the vertices u, v, and all vertices $w \in V(G) \setminus \mathcal{C}(G)$ with

$$d_{G-v}(w, u) < d_{G-v}(w, x)$$

and

$$d_{G-u}(w, v) < d_{G-u}(w, x)$$

for all $x \in \mathcal{C}(G) \setminus \{u, v\}$; and with edge set consisting of the edges $z_1z_2 \in E(G)$ where both z_1 and z_2 are vertices of $CCVS(G; u, v)$.

Definition 3. Let G be a graph with at least two distinct cut vertices. The *close cut vertex graph* of G, denoted by $CCVG(G)$, is the graph with the set of cut vertices of G being its vertex set, and two vertices x and y of $CCVG(G)$ are connected by an edge only if x and y are close cut vertices of G.

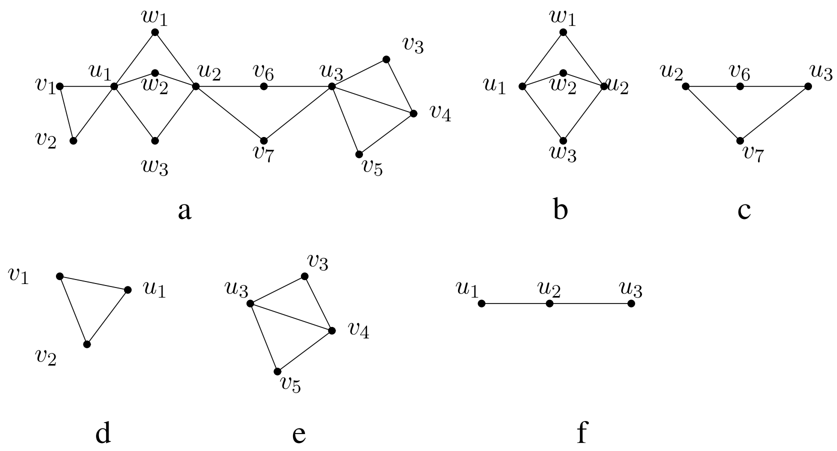

Fig. 3. (a) A connected graph G with three cut vertices; (b–c). Two subgraphs induced by close cut vertices of G; (d–e). Two terminal blocks of G; (f). A close cut vertex graph of G.

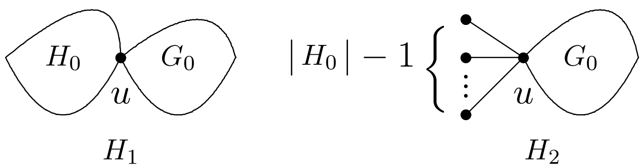

Fig. 4. Operation I: $H_1 \Rightarrow H_2$.

Definition 4. Let G be a graph with at least one cut vertex. Suppose that v is a cut vertex of G, and that $G - v = \bigcup_{j=1}^{m} G_j$ ($m \geq 2$). If some G_j has no cut vertices, then we say that $G[V(G_j) \cup \{v\}]$ is a *terminal block* of G with respect to v, or, simply, the *terminal block* of G.

From the above definition about the terminal block, we know that a graph G may have more than one terminal block with respect to a given cut vertex.

About the cut vertex, we have the following observation.

Observation 1. If v is a cut vertex of a graph G, H is a component of $G - v$, and $w \in V(H)$ is a cut vertex of G, then w is also a cut vertex of H.

In the following, we give an example to illustrate these new concepts, please see Fig. 3.

4.1. The proof of Theorem 1

Before we give the proof of Theorem 1, we first introduce two kinds of graph transformations that will increase the Merrifield–Simmons index of the graphs under consideration.

Lemma 4. *Given a graph H_1, a vertex u of H_1 and a $\{u\}$-component $H_0 - u$ of H_1, let H_2 denote the graph obtained from $H_1 - (H_0 - u)$ by adding $|H_0| - 1$ fresh vertices and joining each fresh vertex by an edge to u. Then $i(H_2) > i(H_1)$, unless $H_2 \cong H_1$ (see Fig. 4).*

Proof. According to Lemmas 1 and 2(i), we have

$$i(H_1) = i(H_0 - u)i(G_0 - u) + i(H_0 - [u])i(G_0 - [u])$$

and

$$i(H_2) = 2^{|H_0|-1} i(G_0 - u) + i(G_0 - [u]).$$

If $H_2 \ncong H_1$, then

$$\begin{aligned} i(H_2) - i(H_1) &= \left(2^{|H_0|-1} - i(H_0 - u)\right) i(G_0 - u) + (1 - i(H_0 - [u]))\, i(G_0 - [u]) \\ &> \left(2^{|H_0|-1} - i(H_0 - u) - i(H_0 - [u]) + 1\right) \cdot i(G_0 - [u]) \\ &= (2^{|H_0|-1} + 1 - i(H_0))i(G_0 - [u]) \geq 0, \end{aligned}$$

where $2^{|H_0|-1} + 1 \geq i(H_0)$ holds due to Corollary 1. Therefore, we are done. □

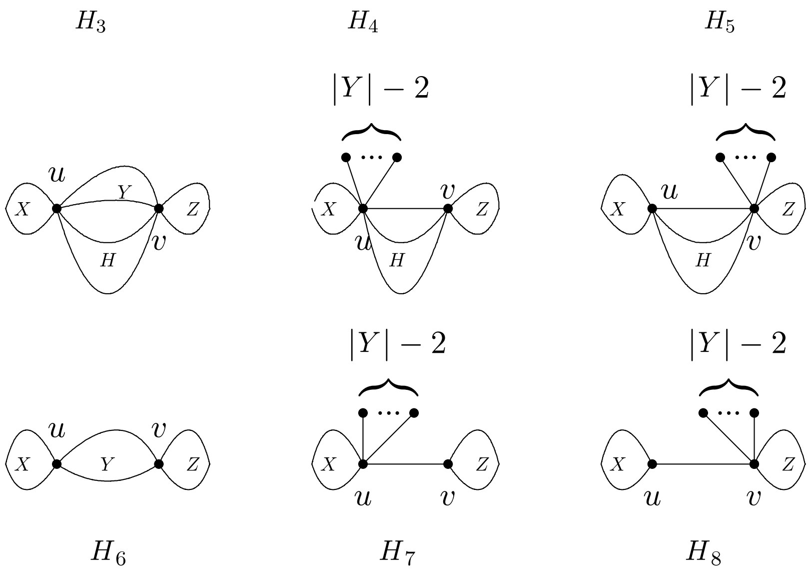

Fig. 5. Operation II: $H_3 \Rightarrow H_4$, or $H_3 \Rightarrow H_5$; Operation II′: $H_6 \Rightarrow H_7$, or $H_6 \Rightarrow H_8$.

Let G be a connected graph with at least two cut vertices. Suppose that u and v are two close cut vertices of G and that $Y = CCVS(G; u, v)$. Let $X - u$ denote the union of $\{u\}$-components of G not containing v and $Z - v$ denote the union of $\{v\}$-components of G not containing u. Then $|X| \geq 2$ and $|Z| \geq 2$, since X contains u and Z contains v.

If there exist other cut vertices, apart from u and v, in G and they belong neither to $X - u$ nor to $Z - v$, then each of these cut vertices must lie on a cycle, containing u and v, of the close cut vertex graph of G. If not so, then we can always choose a cut vertex $w \in \mathcal{C}(G) \setminus ((X - u) \cup (Z - v))$ such that w is the close cut vertex of u (or v) and the path connecting v (or u) and w in G passing through u (or v). But then, we conclude that w belongs to a $\{u\}$-component of G not containing v (or, $\{v\}$-component of G not containing u), that is, $w \in X - u$ (or $w \in Z - v$), a contradiction. Now, we write $H = G[(V(G) \setminus (V(X) \cup V(Y) \cup V(Z))) \cup \{u, v\}] - uv$ (here, we mean that if $uv \in E(G)$, then $uv \in E(Y)$, that is, Y and H are edge-disjoint subgraphs of G). Thus, G can be viewed the graph H_3 as shown in Fig. 5.

Now, we delete all edges of $E(Y)$ in G, connect u and v by an edge, and add edges between u (or v) and each of the remaining $|Y| - 2$ isolated vertices. Then we obtain the graph H_4 (or H_5). We call the graph transformation from H_3 to H_4 (or H_5) **Operation II**.

If all other cut vertices, apart from u and v, in G belong either to $X - u$ or to $Z - v$, then G can be viewed the graph H_6 as shown in Fig. 5. Now, we delete all edges of $E(Y)$ in G, connect u and v by an edge, and add edges between u (or v) and each of the remaining $|Y| - 2$ isolated vertices. Then we obtain the graph H_7 (or H_8). We call the graph transformation from H_6 to H_7 (or H_8) **Operation II** ′.

When $|Y| = 2$, it is easy to see that $uv \in E(H_j)$ ($j = 3$ or 6), as u and v are close cut vertices. But then, we have $H_3 = H_4 = H_5$ and $H_6 = H_7 = H_8$. So we will assume that $|Y| \geq 3$ in the following lemma.

Lemma 5. *Let $H_3, H_4, H_5, H_6, H_7, H_8$ be graphs as shown in Fig. 5 with u and v being two close cut vertices.*

(i) *If $H_3 \ncong H_4, H_5$, then $i(H_4) > i(H_3)$, or $i(H_5) > i(H_3)$;*
(ii) *If $H_6 \ncong H_7, H_8$, then $i(H_7) > i(H_6)$, or $i(H_8) > i(H_6)$.*

Proof. Here, we only prove (i). By a similar way, we can prove (ii) holds.

Note that $H_3 \ncong H_4, H_5$; then $|Y| \geq 3$ by our previous analysis. Also, $|X| \geq 2$ and $|Z| \geq 2$.

We first assume that $uv \notin E(Y)$.

Let

$$A = i(X - u)i(Z - v)i(H - u - v),$$
$$A_v = i(X - u)i(Z - [v])i(H - u - [v]),$$
$$A_u = i(X - [u])i(Z - v)i(H - [u] - v),$$
$$A_{uv} = i(X - [u])i(Z - [v])i(H - \{[u] \cup [v]\}).$$

According to Lemmas 1 and 2(i), we have

$$i(H_3) = i(Y - u - v)A + i(Y - u - [v])A_v + i(Y - [u] - v)A_u + i(Y - \{[u] \cup [v]\})A_{uv}$$

and

$$i(H_4) = 2^{|Y|-2}A + 2^{|Y|-2}A_v + A_u + A_{uv}.$$

Then

$$\begin{aligned} i(H_4) - i(H_3) = &\left(2^{|Y|-2} - i(Y-u-v)\right)A + (2^{|Y|-2} - i(Y-u-[v]))A_v \\ &+ (1 - i(Y-[u]-v))\,A_u + (1 - i(Y - \{[u] \cup [v]\}))\,A_{uv}. \end{aligned}$$

Note that $H - [u] - v = H - v - [u], H - [v] - u = H - u - [v]$. By symmetry, we obtain

$$\begin{aligned} i(H_5) - i(H_3) = &\left(2^{|Y|-2} - i(Y-v-u)\right)A + (2^{|Y|-2} - i(Y-v-[u]))A_u \\ &+ (1 - i(Y-[v]-u))\,A_v + (1 - i(Y - \{[v] \cup [u]\}))\,A_{uv}. \end{aligned}$$

Since

$$\begin{aligned} &2^{|Y|-2} - i(Y-u-[v]) > 2^{|Y|-2} - i(Y-u-v), \\ &1 - i(Y - \{[u] \cup [v]\}) > 1 - i(Y-[u]-v), \\ &2^{|Y|-2} - i(Y-v-[u]) > 2^{|Y|-2} - i(Y-v-u), \\ &1 - i(Y - \{[v] \cup [u]\}) > 1 - i(Y-[v]-u), \end{aligned}$$

we have

$$i(H_4) - i(H_3) > \left(2^{|Y|-2} - i(Y-u-v)\right)(A + A_v) + (1 - i(Y-[u]-v))(A_u + A_{uv})$$

and

$$i(H_5) - i(H_3) > \left(2^{|Y|-2} - i(Y-v-u)\right)(A + A_u) + (1 - i(Y-[v]-u))(A_v + A_{uv}).$$

By the definitions of $A,\ A_u,\ A_v,\ A_{uv}$ and Lemma 2, we have

$$\begin{aligned} &A + A_v > i(X-u)i(Z-[v])i(H-u), \\ &A + A_u > i(Z-v)i(X-[u])i(H-v), \\ &A_u + A_{uv} < i(X-[u])i(Z-v)i(H-[u]), \\ &A_v + A_{uv} < i(Z-[v])i(X-u)i(H-[v]). \end{aligned}$$

If

$$\frac{i(X-u)}{i(X-[u])} \geq \frac{i(Z-v)}{i(Z-[v])},$$

then

$$\begin{aligned} A + A_v &> i(X-u)i(Z-[v])i(H-u) \\ &> i(X-[u])i(Z-v)i(H-[u]) \\ &> A_u + A_{uv}, \end{aligned}$$

since $i(H-u) > i(H-[u])$.
Otherwise, we have

$$\frac{i(X-u)}{i(X-[u])} < \frac{i(Z-v)}{i(Z-[v])}.$$

Thus

$$\begin{aligned} A + A_u &> i(Z-v)i(X-[u])i(H-v) \\ &> i(Z-[v])i(X-u)i(H-[v]) \\ &> A_v + A_{uv}, \end{aligned}$$

since $i(H-v) > i(H-[v])$.
Since $uv \notin E(Y)$, we have

$$i(Y-u-v) + i(Y-[u]-v) = i(Y-v-u) + i(Y-v-[u]) = i(Y-v).$$

We claim that $Y - v$ is connected for $|Y| \geq 3$. Note that Y is the subgraph of H_3 induced by close cut vertices u and v; then by our definition of close cut vertices, every vertex in $Y - \{u,\ v\}$ is connected by a path to the vertex u in $Y - v$. When $|Y| = 3$, $Y - v$ is already connected by the statement above. When $|Y| \geq 4$, for any two vertices x and y in $Y - \{u,\ v\}$, there exists a path connecting x and y in $Y - v$. So $Y - v$ is connected for $|Y| \geq 3$.

Similarly, we can prove that $Y - u$ is connected for $|Y| \geq 3$.

Because $Y - v$ is a connected graph having $|Y| - 1$ vertices, by Corollary 1, we get

$$(2^{|Y|-2} - i(Y - u - v)) - (i(Y - [u] - v) - 1) = 2^{|Y|-2} + 1 - i(Y - v) \geq 0.$$

Similarly, we have

$$(2^{|Y|-2} - i(Y - v - u)) - (i(Y - [v] - u) - 1) = 2^{|Y|-2} + 1 - i(Y - u) \geq 0.$$

By the above arguments, if

$$\frac{i(X - u)}{i(X - [u])} \geq \frac{i(Z - v)}{i(Z - [v])},$$

then $i(H_4) > i(H_3)$; if

$$\frac{i(X - u)}{i(X - [u])} < \frac{i(Z - v)}{i(Z - [v])},$$

then $i(H_5) > i(H_3)$.

When $uv \in E(Y)$, the result can be obtained by the same reasoning.

This completes the proof. □

Remark 1. It can be concluded from Fig. 5 that $\mathcal{C}(H_3) = \mathcal{C}(H_4) = \mathcal{C}(H_5)$ and $\mathcal{C}(H_6) = \mathcal{C}(H_7) = \mathcal{C}(H_8)$. If it is not so, we may suppose without loss of generality that $\mathcal{C}(H_3) \neq \mathcal{C}(H_4)$, that is, $\mathcal{C}(H_3) - \mathcal{C}(H_4) \neq \emptyset$ or $\mathcal{C}(H_4) - \mathcal{C}(H_3) \neq \emptyset$. Assume without loss of generality that $\mathcal{C}(H_3) - \mathcal{C}(H_4) \neq \emptyset$ and $x \in \mathcal{C}(H_3) - \mathcal{C}(H_4)$. Clearly, $x \neq u, v$. Thus, $x \in X - u$ (or $Z - v$, or $H - u - v$). By Observation 1, x is also a cut vertex of $X - u$ (or $Z - v$, or $H - u - v$). But then, x is a cut vertex of H_4, a contradiction. So, $\mathcal{C}(H_3) = \mathcal{C}(H_4) = \mathcal{C}(H_5)$ and $\mathcal{C}(H_6) = \mathcal{C}(H_7) = \mathcal{C}(H_8)$, that is, $|\mathcal{C}(H_3)| = |\mathcal{C}(H_4)| = |\mathcal{C}(H_5)|$ and $|\mathcal{C}(H_6)| = |\mathcal{C}(H_7)| = |\mathcal{C}(H_8)|$. Hence, both Operation II and Operation II′ will not change the number of cut vertices of the graphs under consideration. This property also holds for Operation III and Operation IV introduced in the next subsection of this paper.

Now, we turn to the proof of Theorem 1.

Proof. If G contains no cut vertices, i.e., $k = 0$, then G contains no cut edges, and thus by Theorem 5, we have $i(G) \leq 2^{n-2}+3$, with equality if and only if $G \cong K_{2,\,n-2}$ or C_5.

If G contains precisely one cut vertex, then by Corollary 1, we have $i(G) \leq i(S_n) = 2^{n-1} + 1 = 2^{n-2}F_2 + F_1$, with equality if and only if $G \cong S_n = SP_{n,\,n-1}$. So, we may suppose that $k \geq 2$ in the following.

Now, let G_{max} be the graph chosen from $\mathcal{G}(n, k)$ such that $i(G_{max}) \geq i(G)$ for any G in $\mathcal{G}(n, k) \setminus \{G_{max}\}$. Next, we shall prove that $G_{max} \cong SP_{n,\,n-k}$.

If G_{max} is a tree, the statement of the theorem is evident from Theorem 4, since G_{max} has $n - k$ pendent vertices. So we may suppose that G_{max} is a connected graph with at least one cycle and at least two cut vertices.

Assume first that the close cut vertex graph of G_{max}, $CCVG(G_{max})$, contains a cycle, and let $\mathcal{C}$ denote such a cycle. Suppose that $\mathcal{C} = w_{j_1}w_{j_2}\cdots w_{j_s}w_{j_1}\,(s \geq 3)$. If $|V(CCVS(G_{max};\, w_{j_t},\, w_{j_{t+1}}))| \geq 3$ for some edge $w_{j_t}w_{j_{t+1}}$ in $\mathcal{C}$, then by using Operation II on G_{max}, we shall obtain a new graph G' with precisely k cut vertices (by Remark 1), and thus $i(G_{max}) < i(G')$ by Lemma 5, a contradiction. Thus, $|V(CCVS(G_{max};\, w_{j_t},\, w_{j_{t+1}}))| = 2$ for any $w_{j_t}w_{j_{t+1}}$ (if $j_t > s$, we let $j_t \equiv j_t (\bmod s)$), and then $\mathcal{C}$ is also a cycle in G_{max}. But then, the removal of any edge from $\mathcal{C}$ will result in a new graph G'', which has the same number of cut vertices as those of G_{max}, but $i(G_{max}) < i(G'')$ by Lemma 3, a contradiction. Hence the close cut vertex graph of G_{max} contains no cycles.

Since the close cut vertex graph of G_{max} contains no cycles, we must have $|V(CCVS(G_{max};\, u, v))| = 2$ for any two close cut vertices u and v in G_{max}, for otherwise, we can use Operation II′ on G_{max} and obtain a contradiction. Now, we let w be a vertex in G_{max}. Suppose that w is not a cut vertex. Since $|V(CCVS(G_{max};\, u, v))| = 2$ for any two close cut vertices u and v, then w cannot belong to any subgraph induced by close cut vertices. So, w must be a vertex in a terminal block of G_{max}. Thus, G_{max} contain only two types of vertices: cut vertices and those vertices contained in terminal blocks.

Clearly, no terminal block of G_{max} contains a cycle. Suppose to the contrary that H_0 is a terminal block of G_{max} with respect to a cut vertex u and H_0 contains a cycle. Thus, G_{max} can be viewed the graph H_1 as shown in Fig. 4. Now, we can use Operation I on G_{max} and obtain a new graph H_2, with k cut vertices, as shown in Fig. 4. Since H_0 contains a cycle, we have $H_2 \ncong H_1 = G_{max}$. So $i(G_{max}) = i(H_1) < i(H_2)$ by Lemma 4, a contradiction.

By our definition of a terminal block, we know that there exists no edge connecting a vertex (not being cut vertex) in a terminal block of G_{max} to a vertex not belonging to this terminal block, no matter whether this vertex is a cut vertex or not. Thus, if G_{max} contains a cycle, then this cycle cannot be composed of both cut vertices and vertices in terminal blocks. Also, the cycle in G_{max} cannot be composed of cut vertices, since $CCVG(G_{max})$ contains no cycles. Therefore, G_{max} contains no cycle. This contradiction leads to the desired result. □

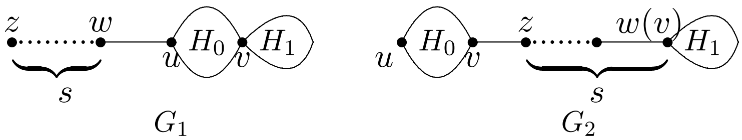

Fig. 6. Operation III: $G_1 \Rightarrow G_2$.

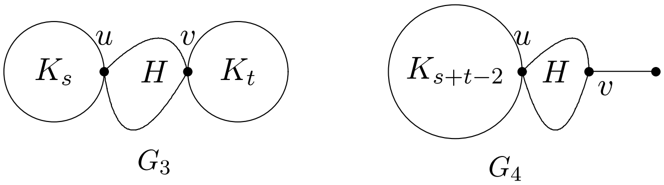

Fig. 7. Operation IV: $G_3 \Rightarrow G_4$.

4.2. The proof of Theorem 2

Before proceeding, we first introduce two kinds of graph transformations that will decrease the Merrifield–Simmons index of the graphs under consideration.

Let H_0 be a connected graph with at least two vertices and there exist two distinct vertices u and v in H_0 satisfying $N_{H_0}[u] = N_{H_0}[v]$. We attach to the vertex u a path of length $s \geq 1$ (the unique vertex in P_{s+1} adjacent to u is denoted by w and another end-vertex of this path is denoted by z for $s \geq 2$; when $s = 1$, we let $z = w$) and the vertex v a nontrivial connected graph H_1. Then the resulting graph can be viewed the graph G_1 as shown in Fig. 6. First, we delete the edge uw and the edges in H_1 incident to v. Second, we add edges between w and each vertex in $N_{H_1}(v)$ and connect the vertex v and z by an edge. Then we obtain the graph G_2 as shown in Fig. 6. By Observation 1, we conclude that G_1 and G_2 possess the same number of cut vertices. We call the graph transformation from G_1 to G_2 **Operation III**. Concerning this graph transformation, we have the following result.

Lemma 6. *Let G_1 and G_2 be graphs as shown in Fig. 6. Then $i(G_1) > i(G_2)$, unless $G_1 \cong G_2$.*

Proof. Clearly, we have $s \geq 1$ and $|H_j| \geq 2$ $(j = 0, 1)$. Since $N_{H_0}[u] = N_{H_0}[v]$, we have $uv \in E(G)$. According to Lemmas 1 and 2(iii), we obtain

$$i(G_1) = i(H_0 - u - v)i(H_1 - v)i(P_s) + i(H_0 - [u])i(H_1 - v)i(P_{s-1}) + i(H_0 - [v])i(H_1 - [v])i(P_s)$$

and

$$\begin{aligned} i(G_2) &= i(H_0 - u - v)\left(i(H_1 - w)i(P_{s-1}) + i(H_1 - [w])i(P_{s-2})\right) \\ &\quad + i(H_0 - [u])\left(i(H_1 - w)i(P_{s-1}) + i(H_1 - [w])i(P_{s-2})\right) \\ &\quad + i(H_0 - [v])\left(i(H_1 - w)i(P_{s-2}) + i(H_1 - [w])i(P_{s-3})\right). \end{aligned}$$

Since $H_0 - [u] = H_0 - [v]$, $H_1 - [w] = H_1 - [v]$ and $H_1 - w = H_1 - v$, we obtain

$$\begin{aligned} i(G_1) - i(G_2) &= i(H_0 - u - v)i(H_1 - v)i(P_{s-2}) - i(H_0 - u - v)i(H_1 - [v])i(P_{s-2}) \\ &\quad - i(H_0 - [u])i(H_1 - [v])i(P_{s-2}) + 2i(H_0 - [u])i(H_1 - [v])i(P_{s-2}) \\ &\quad - i(H_0 - [u])i(H_1 - v)i(P_{s-2}) \\ &= i(P_{s-2})\left(i(H_0 - u - v) - i(H_0 - [u])\right)\left(i(H_1 - v) - i(H_1 - [v])\right). \end{aligned}$$

Obviously, $i(P_{s-2}) \geq 1$ with equality only if $s = 1$ or 2, $i(H_0 - u - v) \geq i(H_0 - [u])$ and $i(H_1 - v) > i(H_1 - [v])$.

So $i(G_1) \geq i(G_2)$, with equality if and only if $i(H_0 - u - v) = i(H_0 - [u])$, that is, $H_0 \cong P_2$ and then $G_1 \cong G_2$. This completes the proof. □

Let H denote a connected graph with at least one vertex, and let u and v be vertices in H (u and v may be a same vertex). For $s, t \geq 3$, we identify any vertex of K_s with the vertex u and identify any vertex of K_t with the vertex v. Then the resulting graph can be viewed the graph G_3 as shown in Fig. 7. Now, we replace in G_3 the clique K_s by K_{s+t-2} and the clique K_t by K_2, and we obtain a new graph G_4, as shown in Fig. 7. By Observation 1, we conclude that G_3 and G_4 possess the same number of cut vertices. We call the graph transformation from G_3 to G_4 **Operation IV**. Concerning this graph transformation, we have the following result.

Lemma 7. *Let G_3 and G_4 be graphs as shown in Fig. 7 with $s, t \geq 3$. Then $i(G_3) > i(G_4)$.*

Proof. First, we consider the case of $v \neq u$. If $uv \notin E(G)$, then by Lemmas 1 and 2(i), we have

$$i(G_3) = s\,(ti(H-u-v) + i(H-u-[v])) + ti(H-[u]-v) + i(H-[u]-[v])$$

and

$$i(G_4) = (s+t-2)\,(2i(H-u-v) + i(H-u-[v])) + 2i(H-[u]-v) + i(H-[u]-[v]).$$

Thus,

$$\begin{aligned} i(G_3) - i(G_4) &= (st-2s-2t+4)i(H-u-v) - (t-2)i(H-u-[v]) + (t-2)i(H-[u]-v) \\ &> (t-2)\,[(s-2)i(H-u-v) - i(H-u-[v])] \\ &\geq (t-2)(i(H-u-v) - i(H-u-[v])). \end{aligned}$$

Note that $i(H-u-v) > i(H-u-[v])$ and $t \geq 3$; thus $i(G_3) > i(G_4)$.
Suppose now that $uv \in E(G)$. By Lemmas 1 and 2(i), we have

$$i(G_3) = s\,(ti(H-u-v) + i(H-u-[v])) + ti(H-[u])$$

and

$$i(G_4) = (s+t-2)\,(2i(H-u-v) + i(H-u-[v])) + 2i(H-[u]).$$

Similar to the case of $uv \notin E(G)$, we can obtain $i(G_3) > i(G_4)$.
Now, we consider the case of $v = u$. In view of Lemmas 1 and 2(i), we obtain

$$i(G_3) = sti(H-u) + i(H-[u])$$

and

$$i(G_4) = 2(s+t-2)i(H-u) + i(H-[u]).$$

Since $i(H-u) > 0$, we have

$$i(G_3) - i(G_4) = (st-2s-2t+4)i(H-u) = (s-2)(t-2)i(H-u) > 0.$$

This completes the proof. □

A block of G is said to be an *internal block*, if it is not a terminal block. If a block of G is a clique of order not less than 3, we call this block *nontrivial clique* of G. A *nontrivial terminal clique* of G is a terminal block of G which is also a nontrivial clique. A *nontrivial internal clique* of G is an internal block of G which is also a nontrivial clique. If G contains a vertex induced subgraph isomorphic to $K_{1,t}$ $(t \geq 3)$, we say that G contains an *induced* $K_{1,t}$ $(t \geq 3)$.

Now, we turn to the proof of Theorem 2.

Proof. Let G_{min} be the graph chosen from $\mathcal{G}(n,k)$ such that $i(G) \geq i(G_{min})$ for any $G \in \mathcal{G}(n,k) \setminus \{G_{min}\}$. Next, we shall verify that $G_{min} \cong KP_{n,k}$.

If $k = 0$, we clearly have $G_{min} \cong K_n = KP_{n,k}$, since adding edges to a graph will decrease its Merrifield–Simmons index by Lemma 3.

If $k = n-2$, we also have $G_{min} = P_n = KP_{n,n-2}$. So we may suppose that $1 \leq k \leq n-3$ in the following.

Clearly, any block of G_{min} is a clique, for otherwise, the addition of edges to this block will lead to a new graph with k cut vertices and a smaller Merrifield–Simmons index than that of G_{min} by Lemma 3. By the same reason, we conclude that if G_{min} has terminal cliques with respect to a cut vertex, then G_{min} has exactly one terminal clique with respect to this cut vertex.

When $1 \leq k \leq n-3$, G_{min} is evidently not a tree. Suppose to the contrary that G_{min} is a tree. Then G_{min} has a vertex, say v_0, of degree greater than or equal to 3. Suppose that $N(v_0) = \{v_1, \ldots, v_s\}$ $(s \geq 3)$. Now, let $G' = G_{min} + v_1v_2$. Clearly, G' has k cut vertices, but $i(G') < i(G_{min})$ by Lemma 3, a contradiction to our choice of G_{min}. Thus, G_{min} has at least one nontrivial clique.

We first claim that G_{min} has at most one nontrivial terminal clique, for otherwise, G_{min} can be viewed the graph G_3 as shown in Fig. 7. Thus, we can use Operation IV on it and obtain a new graph G_4. It is easy to conclude from Fig. 7 that all cut vertices of G_3 lie within H. So, G_4 has exactly k cut vertices, too. Then G_4 has a strictly smaller Merrifield–Simmons index than that of G_{min} by Lemma 7. It is a contradiction.

Also, G_{min} cannot contain an induced $K_{1,t}$ $(t \geq 3)$, for otherwise, adding one edge between any two pendent vertices of $K_{1,t}$ will lead to a new graph with k cut vertices and a smaller Merrifield–Simmons index than that of G_{min}. Thus, all vertices in G_{min} of degree ≥ 3 must lie in nontrivial cliques of G_{min}.

If G_{min} contains no nontrivial terminal clique, then G_{min} contains at least one nontrivial internal clique. Since G_{min} contains no nontrivial terminal clique and all vertices in G_{min} of degree ≥ 3 lie in nontrivial cliques of G_{min}, it contains pendent paths. It is obvious that no two pendent paths are attached to the same vertex of a nontrivial internal clique of G_{min}, for otherwise, G_{min} contains an induced $K_{1,t}$ $(t \geq 3)$. Since G_{min} is a finite graph, there must exist a nontrivial internal clique which is attached to either two pendent paths at distinct vertices, or to a pendent path at one vertex, say u, and to another subgraph of G_{min} at another vertex, say v. But then, we can employ Operation III on G_{min} and obtain a new graph with k cut vertices and a smaller Merrifield–Simmons index than that of G_{min} by Lemma 6.

Now, G_{min} contains exactly one nontrivial terminal clique. Suppose that G_{min} contains nontrivial internal cliques. Then there exists one nontrivial internal clique which is attached to either two pendent paths at distinct vertices, or to a pendent path at one vertex, say u, and to another subgraph of G_{min} at another vertex, say v, for otherwise, G_{min} has at least two nontrivial terminal cliques, or G_{min} contains an induced $K_{1,t}$ $(t \geq 3)$, a contradiction. Similar to above, we can use Operation III on G_{min} and obtain a contradiction once again. Thus, G_{min} contains no nontrivial internal cliques, and all vertices not in the unique nontrivial terminal clique have degree 1 or 2. So, $G_{min} \cong KP_{n,k}$. This completes the proof. □

Acknowledgements

The authors would like to express their sincere gratitude to the referees for a very careful reading of the paper and for all their insightful comments and valuable suggestions, which improve considerably the presentation of this paper.

References

[1] A.F. Alameddine, Bounds on the Fibonacci number of a maximal outerplanar graph, Fibonacci Quart 36 (1998) 206–210.
[2] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, Macmillan London and Elsevier, New York, 1976.
[3] V. Bruyère, G. Joret, H. Mélot, Trees with given stability number and minimum number of stable sets, arXiv:1002.1270v1 [math.CO], Feb 2010.
[4] V. Bruyère, H. Mélot, Fibonacci index and stability number of graphs: a polyhedral study, J. Comb. Optim. 18 (2009) 207–228.
[5] A. Frendrup, P.D. Vestergaard, A.A. Sapozhenko, A.S. Pedersen, On the structure of short trees with a minimum number of independent sets, Research Report R-2009-03, Aalborg University, 2007.
[6] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.
[7] H. Hua, A sharp upper bound for the number of stable sets in graphs with given number of cut edges, Appl. Math. Lett. 22 (2009) 1380–1385.
[8] H. Hua, S. Zhang, On the Merrifield–Simmons of connected graphs (submitted for publication).
[9] S. Li, X. Li, W. Jing, On the extremal Merrifield–Simmons index and Hosoya index of quasi-tree graphs, Discrete Appl. Math. 157 (2009) 2877–2885.
[10] S. Lin, C. Lin, Trees and forests with large and small independent indices, Chinese J. Math. 23 (1995) 199–210.
[11] H. Liu, M. Lu, A unified approach to extremal cacti for different indices, MATCH Commun. Math. Comput. Chem. 58 (2007) 193–204.
[12] X. Li, H. Zhao, I. Gutman, On the Merrifield–Simmons index of trees, MATCH Commun. Math. Comput. Chem. 54 (2005) 389–402.
[13] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, Discrete Appl. Math. 157 (2009) 1387–1395.
[14] R.E. Merrifield, H.E. Simmons, Topological Methods in Chemistry, Wiley, New York, 1989.
[15] A.S. Pedersen, P.D. Vestergaard, The number of independent sets in unicyclic graphs, Discrete Appl. Math. 152 (2005) 246–256.
[16] A.S. Pedersen, P.D. Vestergaard, An upper bound on the number of independent sets in a tree, Ars Combin. 84 (2007) 85–96.
[17] H. Prodinger, R.F. Tichy, Fibonacci numbers of graphs, Fibonacci Quart. 20 (1982) 16–21.
[18] A. Yu, X. Lv, The Merrifield–Simmons and Hosoya indices of trees with k pendent vertices, J. Math. Chem. 41 (2007) 33–43.
[19] H. Zhao, X. Li, On the Fibonacci numbers of trees, Fibonacci Quart. 44 (2006) 32–38.