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On the number of independent sets in cycle-separated tricyclic graphs

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ABSTRACT

A cycle-separated tricyclic graph (CSTC graph) is a connected simple graph with n vertices and $n+2$ edges whose subgraph induced by its cycles consists of three disjoint cycles. In this paper we investigate the number of independent sets in CSTC graphs. We show that the tight upper bound for the number of independent sets in the n-vertex CSTC graphs is $48 \times 2^{n-9} + 9$ (for $n \geq 9$); we also characterize the extremal graph with respect to the aforementioned bound.

1. Introduction and preliminaries

A cycle-separated tricyclic graph (CSTC graph) is a connected simple graph with n vertices and $n+2$ edges whose subgraph induced by its cycles consists of three disjoint cycles. We denote the number of independent sets in a graph G by $i(G)$. This is called the Fibonacci number or Merrifield–Simmons index of G, too. It is an important example of the topological indices which are of interest in combinatorial chemistry. It was introduced in [1,2]. The characterizations of the extremal graphs with respect to this quantity have been presented for several graph classes with fixed order and size. For instance, it was observed in [2] that the star S_n and the path P_n have the maximal and the minimal number of independent sets amongst all trees with n vertices, respectively; $i(S_n) = 2^{n-1} + 1$ and $i(P_n) = f(n+2)$, where $f(n)$ is the nth Fibonacci number. In [3,4] the upper and lower bounds of the number of independent sets in unicyclic graphs in terms of order were given and the extremal graphs were characterized. In [5] the sharp upper bound for the number of independent sets in all $(n, n+1)$-graphs was determined and the extremal graph was characterized. The reader is referred to some other papers (cf., e.g., [6–16]), particularly a recent review [17] and references therein, for more information about this quantity and the number of matchings in some prescribed classes of graphs. In this paper, we shall show that $48 \times 2^{n-9} + 9$ is the tight upper bound for the number of independent sets in n-vertex CSTC graphs, where $n \geq 9$. We also characterize the extremal n-vertex CSTC graph with respect to the bound mentioned above.

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For any $v \in V(G)$, $N_G(v) = \{u | uv \in E(G)\}$ denotes the neighbors of v, and by $N_G[v]$ we mean $N_G(v) \cup \{v\}$. The degree of v is denoted by $d_G(v)$ and it is defined as $d_G(v) = |N_G(v)|$. A pendant vertex is a vertex of degree 1. A pendant edge is incident with a pendant vertex. If $F \subseteq E(G)$ and $W \subseteq V(G)$, then $G - F$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of F and the vertices of W, respectively. If x and y are two nonadjacent vertices of a graph G, the graph obtained from G by adding edge xy is denoted by $G + xy$. We denote by P_n the path on n vertices, by C_n the cycle on n vertices, and by S_n the star consisting of one central vertex adjacent to $n-1$ pendant vertices. Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs such that $V(G) \cap V(H) = \emptyset$. If $u \in V(G)$ and $v \in V(H)$ by $G^u.H^v$ we mean the graph obtained from identifying the vertices u and v. In this case, we refer to this common vertex either as u or as v. By $I(G)$ we mean the family of independent sets of G.

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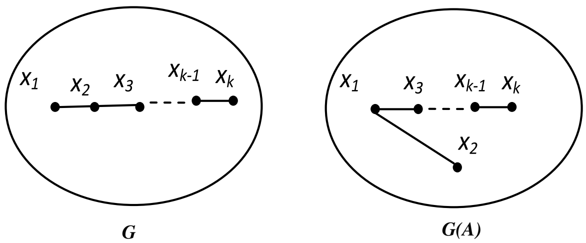


Fig. 1. Transformation A.

The following basic results will be used and can be found in the references cited.

- (i) If G is a graph with connected components $G_1, G_2, \ldots, G_k$, then $i(G) = \prod_{i=1}^{k} i(G_i)$.
- (ii) If v is a vertex of G, then $i(G) = i(G - \{v\}) + i(G - N_G[v])$.
- (iii) If u and v are not adjacent in G, then $i(G) = i(G - \{u, v\}) + i(G - \{u\} \cup N_G[v]) + i(G - \{v\} \cup N_G[u]) + i(G - N_G[u] \cup N_G[v])$.
- (iv) If u and v are adjacent in G, then $i(G) = i(G - \{u, v\}) + i(G - N_G[u]) + i(G - N_G[v])$.

The rest of this paper is organized as follows. In Section 2 we present some results for increasing the number of independent sets in a graph without changing its order and size. The tight upper bound for the number of independent sets of n-vertex CSTC graphs is determined in Section 3. The extremal graph amongst all CSTC graphs is also characterized in the same section.

2. The increasing transformation

In this section, we present some useful results for increasing the number of independent sets in the graphs without changing their order and size. First let us introduce an important transformation.

Transformation A: Let $W = x_1x_2 \ldots x_k$ be a path of length $k - 1$ $(k \geq 3)$ in a graph $G = (V(G), E(G))$ for which $N_G(x_1) \setminus N_G(x_3) \neq \emptyset, d_G(x_2) = 2$, and $x_1x_3 \notin E(G)$. The new graph $G(A)$ is obtained from G as follows: $G(A) = (G - \{x_2x_3\}) + \{x_1x_3\}$ (see Fig. 1).

By the following proposition we show that Transformation A is an increasing transformation.

Proposition 2.1. *Let G_t be a graph which is obtained from G by recursively applying Transformation A. Then $i(G_t) > i(G)$.*

Proof. It is sufficient to show that in Transformation A, $i(G) < i(G(A))$. To this end, we construct an injective but non-surjective mapping $\phi : I(G) \mapsto I(G(A))$ as follows:

$$\phi(S) = \begin{cases} (S \setminus \{x_1\}) \cup \{x_2\} & x_1, x_3 \in S \\ S & \text{otherwise.} \end{cases}$$

It is easy to show that the mapping is injective. Let u be an arbitrary vertex in $N_G(x_1) \setminus N_G(x_3)$. There is no $S \in I(G)$ with $\phi(S) = \{x_2, x_3, u\}$. Therefore the mapping is not surjective. That means that $|I(G(A))| > |I(G)|$ or $i(G(A)) > i(G)$. $\square$

If w is a vertex such that $i(G - w) \geq i(G - v)$ for all vertices v we call it a *max-touch-vertex*. In finding the extremal CSTC graphs with respect to the number of independent sets, the max-touch-vertices play an important role. Let u be a vertex of a nontrivial graph G. We denote the graph obtained from attaching k pendant edges at vertex u by $G_k(u)$. Obviously, $i(G_k(u) - u) = 2^k i(G - u)$; therefore, if u and v are two distinct vertices of a graph G and $i(G - u) > i(G - v)$ then $i(G_k(u) - u) > i(G_k(v) - v)$ for all $k = 1, 2, \ldots$. This fact will be generalized in Lemma 2.6.

Lemma 2.2. *If u be an arbitrary vertex of G; then the number of independent sets of $G_k(u)$ is $i(G_k(u)) = i(G) + (2^k - 1)i(G - u)$.*

Proof. We prove the assertion by induction on k. If $k = 0$ then the assertion is readily satisfied. Now, suppose that the assertion is satisfied for all $k - 1$ $(k \geq 1)$. Assume that w does not belong to the vertex set of $G_{k-1}(u)$. For constructing $G_k(u)$ we add vertex w and edge wu to $G_{k-1}(u)$, and therefore,

$$i(G_k(u)) = i(G_k(u) - w) + i(G_k(u) - N_{G_k(u)}[w]). \quad \text{or,}$$
$$i(G_k(u)) = i(G_{k-1}(u)) + 2^{k-1} i(G - u).$$

Now, by the induction hypothesis we have

$$i(G_k(u)) = (i(G) + (2^{k-1} - 1)i(G - u)) + 2^{k-1} i(G - u) \quad \text{thus,}$$
$$i(G_k(u)) = i(G) + (2^k - 1)i(G - u). \quad \square$$

Corollary 2.3. *Suppose that u and v are two distinct vertices of a graph G, If $i(G - u) > i(G - v)$ then $i(G_k(u)) > i(G_k(v))$.*

Now, let u be a max-touch-vertex of a graph G. If w is an arbitrary vertex of G then

$$i(G_1(u) - u) = 2i(G - u) > i(G - w) + i(G - u - w) = i(G_1(u) - w).$$

So, by an induction argument we have the following lemma. The lemma says: by attaching k ($k \geq 0$) pendant edges to a max-touch-vertex it remains a max-touch-vertex in the new graph.

Lemma 2.4. *Let u and v be two distinct vertices of a graph G such that $i(G - u) > i(G - v)$; then $i(G_k(u) - u) > i(G_k(u) - v)$.*

The following theorem plays an important role in constructing the extremal CSTC graph with the maximum number of independent sets.

Theorem 2.5. *Suppose that u and v are two distinct vertices of a graph $G = (V(G), E(G))$ such that $i(G - u) > i(G - v)$. Let w be an arbitrary vertex of a tree $H = (V(H), E(H))$ which is isomorphic to S_{n+1}. If $V(G) \cap V(H) = \emptyset$, $G' = G^u.H^w$, and $G'' = G^v.H^w$, then $i(G') > i(G'')$.*

Proof. Suppose that c is the center vertex of H. If $w \neq c$, then $i(G') = i(G' - c) + i(G' - N_{G'}[c]) = 2^{n-1}i(G) + i(G - u)$. On the other hand, $i(G'') = i(G'' - c) + i(G'' - N_{G''}[c]) = 2^{n-1}i(G) + i(G - v)$. Therefore, in this case, we conclude that $i(G') > i(G'')$. Now, suppose that $w = c$. In this case, $G' = G_n(u)$ and $G'' = G_n(v)$ and by Corollary 2.3 the assertion follows. □

Lemma 2.6. *Let G_1 and G_2 be two graphs that have no vertex in common with a graph H. Suppose that $u \in V(G_1)$ and $v \in V(G_2)$ such that $i(G_1 - u) > i(G_2 - v)$. If $w \in V(H)$ and $G' = G_1^u.H^w$ and $G'' = G_2^v.H^w$ then $i(G' - u) > i(G'' - v)$.*

Proof. Since $i(G' - u) = i(G_1 - u)i(H - w)$ and $i(G'' - v) = i(G_2 - v)i(H - w)$ the assertion immediately follows. □

In the following we generalize Theorem 2.5. However, Theorem 2.5 is sufficient for obtaining the CSTC graph with the maximum number of independent sets.

Theorem 2.7. *Let u and v be two distinct vertices of a graph G such that $i(G - u) > i(G - v)$. Suppose that w is a vertex of a nontrivial tree T and $V(G) \cap V(T) = \emptyset$. If $G' = G^u.T^w$ and $G'' = G^v.T^w$ then $i(G') > i(G'')$.*

Proof. We prove the theorem by induction on degree of w. Suppose that $k = d_T(w)$; in this case, if $k = 1$ then w is a pendant vertex of the tree. Assume in this case that x is the vertex of T that is adjacent to w. Then $i(G') = i(G' - x) + i(G' - N_{G'}[x])$ which means that

$$i(G') = i(G)\frac{i(T - x)}{2} + i(G - u)i(T - N_T[x]) \tag{1}$$

and $i(G'') = i(G'' - x) + i(G'' - N_{G''}[x])$ which means that

$$i(G'') = i(G)\frac{i(T - x)}{2} + i(G - v)i(T - N_T[x]). \tag{2}$$

By (1) and (2) we conclude that $i(G') > i(G'')$. Now, assume by the induction hypothesis that the assertion for $k - 1$ ($k \geq 2$) is proved. Suppose that w is of degree k and x is one of the vertices of T that are adjacent to w. Assume that

$$S = \{v \in V(T) : \text{ There is a path } P \text{ from } x \text{ to } v, \text{ such that } w \text{does not belong } P\}.$$

If $T_1 = T - S$, $G_1 = G^u.T_1^w$ and $G_2 = G^v.T_1^w$ then according to the induction hypothesis

$$i(G_1) > i(G_2) \tag{3}$$

because $d_{T_1}(w) = k - 1$. Suppose that T_2 is the subgraph of T induced on $S \cup \{w\}$. Obviously, $d_{T_2}(w) = 1$, $G' = G_1^u.T_2^w$ and $G'' = G_2^v.T_2^w$. Assume that y is the vertex that is adjacent to w in T_2. So $i(G') = i(G' - y) + i(G' - N_{G'}[y])$ which means that

$$i(G') = i(G_1)\frac{i(T_2 - y)}{2} + i(G_1 - u)i(T_2 - N_{T_2}[y]) \tag{4}$$

and $i(G'') = i(G'' - y) + i(G'' - N_{G''}[y])$ which means that

$$i(G'') = i(G_2)\frac{i(T_2 - y)}{2} + i(G_2 - v)i(T_2 - N_{T_2}[y]). \tag{5}$$

On the other hand, by Lemma 2.6 $i(G_1 - u) > i(G_2 - v)$. By this fact, and the relations (3)–(5) we conclude that $i(G') > i(G'')$. □

3. Constructing the extremal CSTC graph

In this section, we use the results of the previous section to formulate the main results of the paper. That means that we find the tight upper bound for the number of independent sets in n-vertex CSTC graphs and we also characterize the graph with respect to the aforementioned bound. Note that the subgraph induced on the edges of the cycles in a CSTC graph

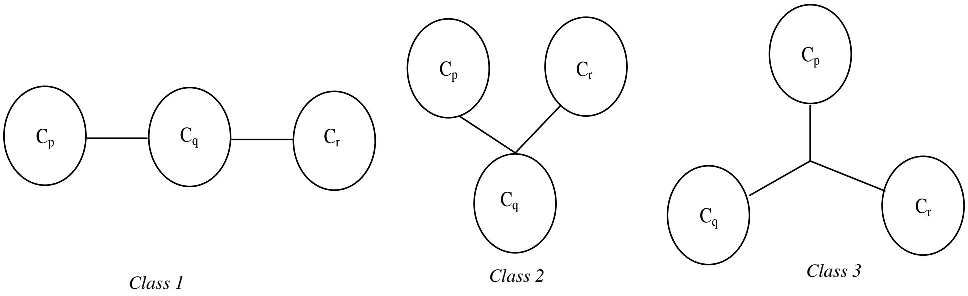


Fig. 2. The classes of the CSTC graph after deleting the pendant paths.

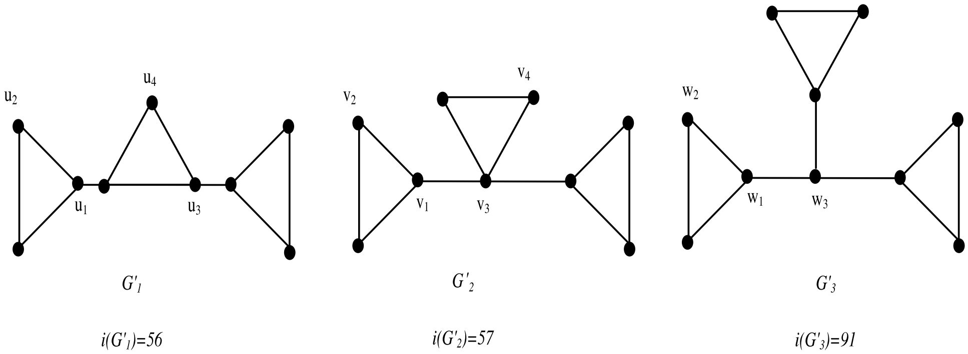


Fig. 3. The reduced graphs achieved after Step 3 of the algorithm and their numbers of independent sets.

consists of three disjoint cycles. These cycles can be connected to each other by some paths. If we delete the pendant paths of CSTC graphs the remaining graphs can be divided into three classes (see Fig. 2). Note that if we apply Transformation A on a path in a cycle of length more than 3 in which the vertex corresponding to x_1 in the transformation is the vertex of degree more than 2, then a pendant edge is created. The length of the cycle is also decreased. Applying the transformation decreases the lengths of the other paths (not belonging the cycles) and increases the number of independent sets.

We provide the following algorithm for finding the extremal CSTC graph.

Algorithm 3.1 (*Constructing the Extremal Graph*)**.**

Algorithm for constructing the extremal graph.
Input: A CSTC graph G in a class C.
Output: The extremal graph of the same class.

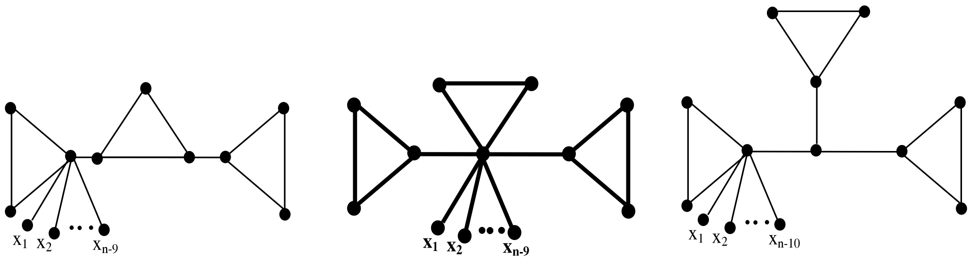
Step 1. $k := 1$
Step 2. while *there is a pendant vertex v in G*
$\quad G := G - v$
$\quad k := k + 1$
Step3. while *there is a path in G satisfying the conditions of Transformation A and $G(A)$ and v are the transformed graph and the pendant vertex created, respectively*.
$\quad G := G(A)$
$\quad G := G - v$
$\quad k := k + 1$
Step 4. *Let w be a max-touch-vertex of the graph obtained and c be the center vertex in a star tree S_k of order k*
return $(G^w.S_k^c)$

If we apply the algorithm on an arbitrary CSTC graph, after Step 3, we achieve a CSTC graph without a pendant vertex which we call the *reduced graph*. Note that the cycles of a reduced graph are of length 3. The reduced graphs for all classes of CSTC graphs are depicted in Fig. 3. The max-touch-vertices of the reduced graphs are determined in Fig. 4. Note that during the algorithm, for obtaining the reduced graphs G_1', G_2', and G_3' we delete $n-9$, $n-9$, and $n-10$ pendant vertices, respectively. Using the max-touch-vertices determined for all reduced graphs of all classes and Corollary 2.3, the extremal graphs for all classes and their number of independent sets are illustrated in Fig. 5. The extremal graph is depicted by a thick line. Consequently, we can summarize the main results of the paper in the following theorem.

graph(G) \ Vertex (x)	$\boldsymbol{u_1}$	u_2	u_3	u_4	v_1	v_2	$\boldsymbol{v_3}$	v_4	$\boldsymbol{w_1}$	w_2	w_3
G'_1	**45**	41	44	40	-	-	-	-	-	-	-
G'_2	-	-	-	-	45	42	**48**	41	-	-	-
G'_3	-	-	-	-	-	-	-	-	**75**	66	64

i(G-x)

Fig. 4. The numbers of independent sets of the reduced graphs in Fig. 3, after deleting the vertices which are candidates for being max-touch-vertices. The max-touch-vertices for each item are highlighted in bold text in the table.



$i(G_1)=45\times 2^{n-9}+11$ **$i(G_2)=48\times 2^{n-9}+9$** $i(G_3)=75\times 2^{n-10}+16$

Fig. 5. The extremal graphs for each of the classes and their numbers of independent sets. The extremal *n*-vertex CSTC graph is depicted by a thick line.

Theorem 3.2. *Suppose that G is an arbitrary n-vertex CSTC graph of order n* $(n \geq 9)$*. If* G_2 *is the graph depicted by a thick line in Fig. 5, then* $i(G) \leq i(G_2) = 48 \times 2^{n-9} + 9$*, with equality holding if and only if* $G \cong G_2$.

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