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The extremal graph with the largest Merrifield-Simmons index of $(n, n+2)$-graphs

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Abstract—The Merrifield-Simmons index of a graph G is defined as the total number of its independent sets. A $(n, n+2)$-graph is a connected simple graph with n vertices and $n+2$ edges. In this paper we characterize the $(n, n+2)$-graph with the largest Merrifield-Simmons index. We show that its Merrifield-Simmons index i.e. the upper bound of the Merrifield-Simmons index of the $(n, n+2)$-graphs is $9 \times 2^{n-5} + 1$ for $n \geq 5$.

Keywords—Merrifield-Simmons index, (n,n+2)-graph.

I. INTRODUCTION

THE Merrifield-Simmons index of a graph G is a prominent example of topological indices which are interested in combinatorial Chemistry. It is defined as the total number of independent vertex subsets. The Merrifield-Simmons index was introduced by Merrifield and Simmons [8], [11] and it was shown that it is correlated with the boiling points of hydrocarbons.

Several papers deal with the characterization of the extremal graphs with respect to this index in some especial graphs. Usually, trees, unicyclic graphs and certain structures involving pentagonal and hexagonal cycles are some of major interest[7], [9].

For instance, it was observed [10], [6], [4], [5] that the star S_n and the path P_n have the largest and smallest Merrifield-Simmons index among all trees with n vertices, respectively. [9], [1] gave upper and lower bounds of this index in unicyclic graphs and characterized the extremal graphs. [2] determined the extremal graph with the largest Merrifield-Simmons index among all $(n, n+1)$-graphs. In this paper, we use the classification of $(n, n+2)$-graphs, i.e. the simple connected graphs with n vertices and $n+2$ edges given in [3] and characterize the extremal graph with the largest Merrifield-Simmons index among all.

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $v \in V$, $N_G(v)$ denotes the neighbors of v, $d_G(v) = |N(v)|$ is the degree of v and $N_G[v] = \{v\} \cup \{u | uv \in E(G)\}$. A leaf is a vertex of degree one.

If $E' \subseteq E(G)$ and $W \subseteq V(G)$,then $G - E'$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of E' and the vertices of W,respectively. We denote by P_n the path on n vertices, C_n the cycle on n vertices and S_n the star consisting of one central vertex which is adjacent to $n-1$ leaves. $i(G)$ represents the Merrifield-Simmons index of graph G. The following basic result will be used [2].

(i). If v is a vertex of G, then

$$i(G) = i(G - \{v\}) + i(G - N_G[v])$$

(ii). If G is a graph with components $G_1, G_2, ..., G_k$, then

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

(iii). $i(S_n) = 2^{n-1} + 1$, $i(P_n) = f(n+2)$ for $n \in N$; and $i(C_n) = f(n-1) + f(n+1)$ for $n \geq 3$ where $f(0) = 0$, $f(1) = 1$ and $f(n) = f(n-1) + f(n-2)$ for $n \geq 2$ denotes the sequence of Fibonacci numbers.

(iv). If u and v are not adjacent in G, then $i(G) = i(G - \{u, v\}) + i(G - \{u\} \cup N_G[v]) + i(G - \{v\} \cup N_G[u]) + i(G - N_G[u] \cup N_G[v])$.

(v). If u and v are adjacent in G, then

$$i(G) = i(G - \{u, v\}) + i(G - N_G[u]) + i(G - N_G[v]).$$

II. INCREASING THE MERRIFIELD-SIMMONS INDEX

In this chapter, we give some transformation and lemmas in order to increase the Merrifield-Simmons index of graphs.

Transformation C.

Assume G is a graph includes subgraph G_0 and an interior path $W : x_1x_2x_3$ in which $d_G(x_2) = 2$ and vertices x_1 and x_3 are not adjacent. Let G' be obtained from G by deleting x_2x_3 and adding x_1x_3 i.e.

$$G' = (G - \{x_2x_3\}) + \{x_1x_3\}.$$

Lemma 2.1. Let G' be obtained from G by transformation C, then

$$i(G') \geq i(G).$$

Proof.
By constructing an injective mapping ξ from $I(G)$ to $I(G')$, We can show that $i(G) \leq i(G')$ as follows. ($I(G)$ and $I(G')$ are the sets of independent sets of G and G',respectively.)(see Fig. 1).

$$\xi : I(G) \longrightarrow I(G')$$

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$\forall B \in I(G)$,

$$\xi(B) = \begin{cases} (B - \{x_1, x_3\}) \cup \{x_2, x_3\} & x_1, x_3 \in B\,, \\ B & otherwise. \end{cases}$$

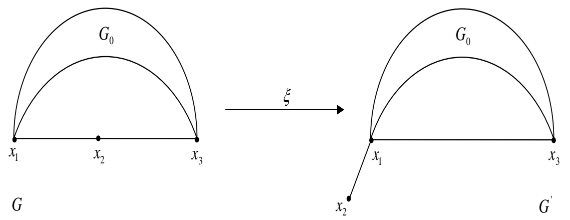

Fig. 1. Transformation C

Lemma 2.2. Let subgraph G_0 and cycle C_p have a common path start and end at u and u'(it is possible that $u = u'$) and the vertex v of the cycle C_p. Let G_1 be a graph in which the pendant edges $ux_1, ux_2, ..., ux_k$ are attached to the vertex u and G_2 be a graph in which the pendant edges $vx_1, vx_2, ..., vx_k$ are attached to the vertex v. (see Fig.2). Then $i(G_1) \geq i(G_2)$.

Proof.
(i). If $d(u, u') = m - 1$, $d(u, v) = k - 1$ and $k > 2$

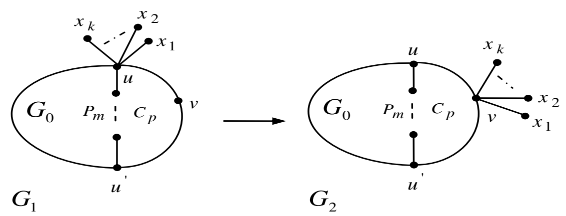

Fig. 2. Lemma2.2

(If u and v are not adjacent), then

$$\begin{aligned} i(G_1) &= i(G_1 - \{u, v\}) + i(G_1 - \{v\} \cup N_{G_1}[u]) \\ &\quad + i(G_1 - \{u\} \cup N_{G_1}[v]) \\ &\quad + i(G_1 - N_{G_1}[u] \cup N_{G_1}[v]) \\ i(G_2) &= i(G_2 - \{u, v\}) + i(G_2 - \{v\} \cup N_{G_2}[u]) \\ &\quad + i(G_2 - \{u\} \cup N_{G_2}[v]) \\ &\quad + i(G_2 - N_{G_2}[u] \cup N_{G_2}[v]) \end{aligned}$$

$$\begin{aligned} & i(G_1) - i(G_2) = \\ & i(P_{k-3})i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m-k+1}) \\ & +2^r i(P_{k-3})i(G_0 - \{u\}, P_{m-1}, P_{p-m-k}) \\ & -2^r i(P_{k-3})i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m-k+1}) \\ & -i(P_{k-3})i(G_0 - \{u\}, P_{m-1}, P_{p-m-k}) \\ & = (2^r - 1)i(P_{k-3})i(G_0 - \{u\}, P_{m-1}, P_{p-m-k}) \\ & -(2^r - 1)i(P_{k-3})i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m-k+1}) \\ & = (2^r - 1)i(P_{k-3})(i(G_0 - \{u\}, P_{m-1}, P_{p-m-k}) \\ & -i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m-k+1})) \geq 0 \end{aligned}$$

(ii). If $d(u, u') = m - 1$, $d(u, v) = 1$ and (If u and v are adjacent), then

$$\begin{aligned} & i(G_1) = i(G_1 - \{u, v\}) + i(G_1 - N_{G_1}[u]) + \\ & i(G_1 - N_{G_1}[v]) \\ & i(G_2) = i(G_2 - \{u, v\}) + i(G_2 - N_{G_2}[u]) + \\ & i(G_2 - N_{G_2}[v]) \end{aligned}$$

$$\begin{aligned} & i(G_1) - i(G_2) = \\ & i(G_1 - N_{G_1}[u]) + i(G_1 - N_{G_1}[v]) \\ & -i(G_2 - N_{G_2}[u]) - i(G_2 - N_{G_2}[v]) \\ & = i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m}) \\ & +2^r i(G_0 - \{u\}, P_{m-1}, P_{p-m-1}) \\ & -2^r i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m}) \\ & -i(G_0 - \{u\}, P_{m-1}, P_{p-m-1}) \\ & = (2^r - 1)i(G_0 - \{u\}, P_{m-1}, P_{p-m-1}) \\ & -(2^r - 1)i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m}) \\ & = (2^r - 1)(i(G_0 - \{u\}, P_{m-1}, P_{p-m-1}) \\ & -i(G_0 - N_{G_0}[u], P_{m-2}, P_{p-m})) \geq 0 \end{aligned}$$

The proof is completed. □

III. Main result

In this chapter, we characterize the extermal graph with the largest Merrifield-Simmons index of $(n, n+2)$-graphs, i.e. connected simple graph with n vertices and $n+2$ edges. To this end, we use two increasing transformations A and B which have been given in [2] and increasing transformation C described in previous chapter. By using and repeating these transformations we increase the Merrifield-Simmons index of $(n, n+2)$-graphs as follows. Let $G(n, n+2)$ be the set of simple connected graphs with n vertices and $n+2$ edges. Initially, with repeated the transformation A, any graph G in $G(n, n+2)$ can be changed into a graph G' in which the edges not on the cycles are pendant edges. In the second step, by using transformation B, we reach a graph in which the pendant edges have been attached to a single vertex. Then we apply the transformation C to minimize the length of the cycles. Transformation C is repeated till it is possible. This step, reduces the cycles to C_3 or C_4. Now, we have a graph that all its pendant edges are attached to a finite set of vertices. Once again, applying the transformation B, we reach a graph in which all pendant edges are attached to a single vertex. By using the Lemma 2.2, we surrender some cases in final graphs (those their pendant edges are attached to a vertex of degree 2 of cycles). Eventually, the Merrifield-Simmons index of final graphs is calculated.

Now We consider all nineteen classes of $G(n, n+2)$ given in [3](see Fig.3). All classes have been shown in the second column of table. The third column represents the final graph(s) obtained by using the above process in each class as described. The fourth column represents the largest Merrifield-Simmons index in each class. Note that the final graph(s) with the largest Merrifield-Simmons index in each class has been highlighted by solid lines in third column. By comparing the largest Merrifield-Simmons index in 19 classes we find the largest Merrifield-Simmons index of $G(n, n+2)$ which is $9 \times 2^{n-5} + 1$ and is related to the class 10.

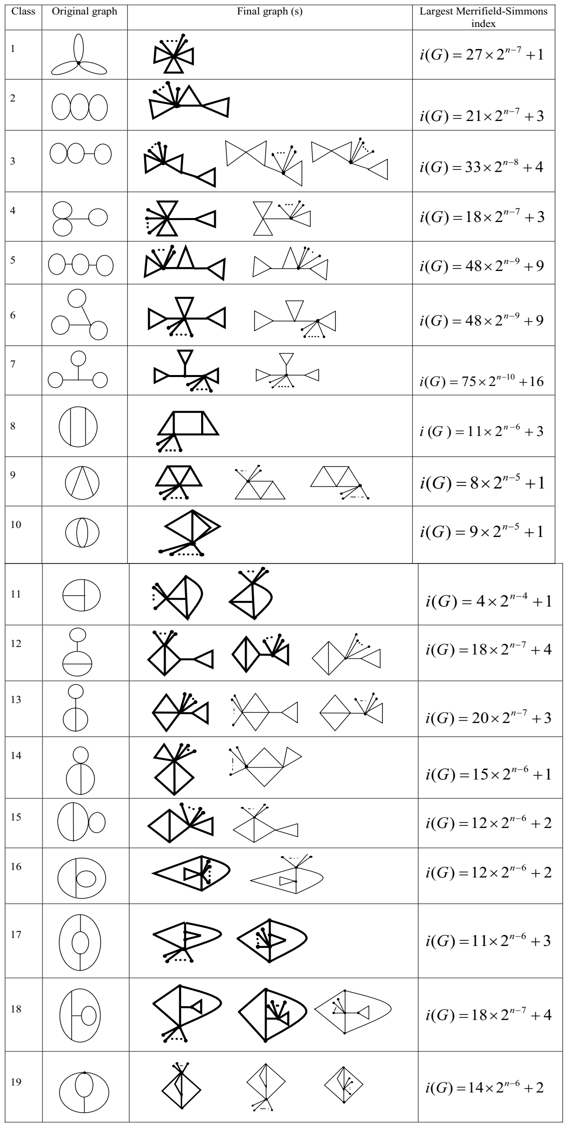

Fig. 3. Original graph, Final graph(s) and the largest Merrifield-Simmons index in 19 classes.

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