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Some Graphs with Minimum Hosoya Index and Maximum Merrifield-Simmons Index

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Abstract

The Hosoya index of a graph is defined as the total number of the matchings of the graph and the Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph. In this paper, we obtain the graphs with minimum Hosoya index among the trees with n vertices and diameter d. The extremal graphs is the same as ones given by X. Li *et al* with maximum Merrifield-Simmons index among such a class of graphs. Also, we give the graphs with both minimum Hosoya index and maximum Merrifield-Simmons index among the trees with n vertices and r pendant vertices.

1 Introduction and Results

It is well known that a topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. There are more than hundred topological indices available in the literature [1]. Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds [2]. The Hosoya index is one of the topological indices. It was introduced by Hosoya in 1971 [3] and

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was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures (see [4,5]). Since 1971, many authors have investigated the Hosoya index and many results are obtained (see [5-13]). Similar to the Hosoya index, the Merrifield and Simmons index is also a topological index whose correlation with the boiling points is shown in [4]. Its mathematical properties were studied in some details [2, 13–26]. In particular, Li, Zhao and Gutman [2] gave the graphs with maximum Merrifield-Simmons index among the trees with order n and diameter d.

Recently, finding the graphs with both minimum Hosoya index and maximum Merrified-Simmons index attracted the attention of a few researchers and some results are achieved. Among these results, Gutman [27] pointed out the linear hexagonal chain is the unique hexagonal chain with minimum Hosoya index and maximum Merrifield-Simmons index among all the hexagonal chains with n hexagons. Zhang [13] noticed that the graph with minimum Hosoya index is also the graph with maximum Merrifield-Simmons index in some classes of graphs, such as hexagonal chains and catacondensed systems. Yu and Tian [28] characterized the graphs with minimum Hosoya index and maximum Merrified-Simmons index among the connected graphs with the given cyclomatic number and edge-independence number.

In this paper, we give two classes of graphs, i.e. trees of n vertices with diameter d and trees of n vertices with r pendant vertices, in each of which the graph with minimum Hosoya index is also the graph with maximum Merrifield-Simmons index.

All graphs considered here are finite and simple. Undefined terminology and notation may refer to [29]. Let $G = (V, E)$ be a graph of n vertices. Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $z(G, k)$ the number of the k-matchings of G. For convenience, let $z(G, 0) = 1$ for any graph G. Hosoya index of G, denoted by $z(G)$, is defined as $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G, k)$. Obviously, $z(G)$ is equal to the total number of the matchings of the graph G. Similarly, two vertices of G are said to be independent if they are not adjacent in G. A k-independent set of G is a set of k mutually independent vertices. Denote by $\sigma(G, k)$ the number of the k-independent sets of G. For convenience, let $\sigma(G, 0) = 1$ for any graph G. Merrifield-Simmons index of G, denoted by $\sigma(G)$, is defined as $\sigma(G) = \sum_{k=0}^{n} \sigma(G, k)$. So $\sigma(G)$ is equal to the total number of the independent sets of the graph G.

Denoted by $n(G)$ and $D(G)$ the total number of vertices in G and the diameter of G, respectively. For a vertex v of G, we denote the degree of v by $d(v)$, and define $N_v = \{v\} \cup \{u|uv \in E(G)\}$. Let $V' \subset V$, we will use $G - V'$ to denote the graph obtained from G by deleting the vertices in V' together with their incident edges. If $V' = \{v\}$, we write $G - v$ for $G - \{v\}$. A pendant vertex is a vertex of degree 1 and a pendant edge is an edge incident to a pendant vertex. Denoted by $PV(G)$ the total number of pendant vertices in G. Let $\mathscr{T}_{n,d} = \{T : T$ is a tree with n vertices and diameter d $\}$ and $\mathscr{T}_r^n = \{T : T$ is a tree with n vertices and r pendant vertices$\}$. Let $S_{p,q}$ (See Fig 1.) denote the tree obtained from stars S_{p+1} and S_q by identifying a pendant vertex of S_{p+1} with the center of S_q. Let $P_{n-d,d}$ (see Fig. 1) denote the tree created from path P_d by adding $n - d$ pendant edges to an end vertex of P_d.

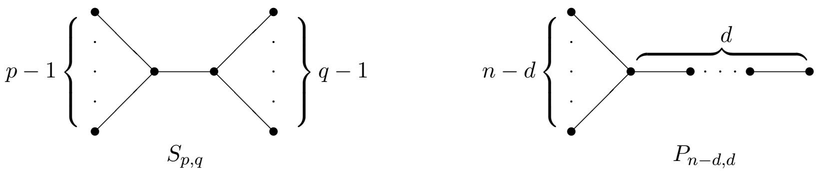

Fig. 1

Our main results are stated in the following three theorems.

Theorem 1. If $T \in \mathscr{T}_{n,d}$, then

$$z(T) \geq (n - d + 1)F_{d-1} + F_{d-2}$$

and the equality holds if and only if $T \cong P_{n-d,d}$.

Theorem 2. If $T \in \mathscr{T}_r^n$, then

$$z(T) \geq rF_{n-r} + F_{n-r-1}$$

and the equality holds if and only if $T \cong P_{r-1,n-r+1}$.

Theorem 3. If $T \in \mathscr{T}_r^n$, then

$$\sigma(T) \leq 2^{r-1}F_{n-r+1} + F_{n-r}$$

and the equality holds if and only if $T \cong P_{r-1,n-r+1}$.

Here, F_n is the n-th Fibonacci number which satisfies $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$.

The proofs of the above theorems are given in section 2.

2 Proofs

We only give the proof of Theorem 2. Proofs of Theorems 1 and 3 are similar to that of Theorem 2, so we omitted them here. We use some techniques in [2]. First we give some lemmas.

Lemma 1 [10]. Let v be a vertex of G. Then

(i) $z(G) = z(G-v) + \sum_u z(G - \{u,v\})$, where the summation extends over all vertices adjacent to v.

(ii) $\sigma(G) = \sigma(G-v) + \sigma(G - N_v)$.

Lemma 2 [10]. If $G_1, G_2, \ldots, G_t$ are the components of a graph G, then

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

(ii) $\sigma(G) = \prod_{i=1}^{t} \sigma(G_i)$.

Proof of Theorem 2. It is not difficult to check that $z(P_{r-1,n-r+1}) = rF_{n-r}+F_{n-r-1}$ by Lemma 1 and $z(P_n) = F_n$. Now we prove if $T \in \mathscr{T}_r^n$, then $z(T) \geq rF_{n-r} + F_{n-r-1}$ with equality only if $T \cong P_{r-1,n-r+1}$.

Since $T \in \mathscr{T}_r^n$, we have that $PV(T) = r$ and $n \geq r+1$. We prove the theorem by double induction on r and n.

If $r = 2$, then $T \cong P_n \cong P_{1,n-1}$ and the theorem holds obviously for $r = 2$.

If T is a tree with $PV(T) = r$ and $n(T) = r+1$, then $T \cong S_{r+1} \cong P_{n-2,2}$ and hence there is nothing to prove. If T is a tree with $PV(T) = r$ and $n(T) = r+2$, then $T \cong S_{p,q}$ with $p + q = r+2$, and $z(S_{p,q}) = pq + 1 \geq 2r + 1$ with equality only if $T \cong P_{r-1,3}$. Thus the theorem holds for $PV(T) = r$ and $n(T) = r+2$.

In the following, we assume $r \geq 3$ and $n \geq r+3$. Suppose that the theorem holds for $PV(T) \leq r-1$ and $n(T) \geq r+1$, and for $PV(T) = r$ and $r+2 \leq n(T) \leq n-1$. When $PV(T) = r$ and $n(T) = n$, we distinguish the following two cases.

Case 1. There is at least one maximal path $u_1u_2u_3 \ldots u_du_{d+1}$ in T, such that $d(u_2) = 2$ or $d(u_d) = 2$. Without loss of generality, assume $d(u_2) = 2$. From Lemma 1, we have

$$z(T) = z(T-u_1) + z(T - \{u_1, u_2\}). \tag{1}$$

Now, $n(T-u_1) = n-1$ and $n(T - \{u_1,u_2\}) = n-2$. In addition, $PV(T-u_1) = r$ and

$r-1 \leq PV(T-\{u_1,u_2\}) \leq r$.

By the induction hypothesis, we have

$$z(T-u_1) \geq z(P_{r-1,n-r}) = rF_{n-r-1} + F_{n-r-2} \tag{2}$$

with equality only if $T-u_1 \cong P_{r-1,n-r}$.

If $T-\{u_1,u_2\} \in \mathscr{T}_{r-1}^{n-2}$, by the induction hypothesis and $n \geq r+3$, we have

$$\begin{aligned} z(T-\{u_1,u_2\}) &\geq z(P_{r-2,n-r}) = (r-1)F_{n-r-1} + F_{n-r-2} \\ &> rF_{n-r-2} + F_{n-r-3} = z(P_{r-1,n-r-1}). \end{aligned} \tag{3}$$

If $T-\{u_1,u_2\} \in \mathscr{T}_{r}^{n-2}$, by the induction hypothesis, we have

$$z(T-\{u_1,u_2\}) \geq z(P_{r-1,n-r-1}) = rF_{n-r-2} + F_{n-r-3}. \tag{4}$$

Hence, by (1)$\sim$(4), we have

$$\begin{aligned} z(T) &= z(T-u_1) + z(T-\{u_1,u_2\}) \\ &\geq z(P_{r-1,n-r}) + z(P_{r-1,n-r-1}) \\ &= rF_{n-r-1} + F_{n-r-2} + rF_{n-r-2} + F_{n-r-3} \\ &= rF_{n-r} + F_{n-r-1} \end{aligned}$$

with equality only if $T \cong P_{r-1,n-r+1}$.

Case 2. $d(u_2) \geq 3$ and $d(u_d) \geq 3$ for each longest path $u_1u_2u_3\ldots u_du_{d+1}$ in T. Suppose that $d(u_2) = t+1 \geq 3$. From Lemma 1, we have

$$z(T) = z(T-u_1) + z(T-\{u_1,u_2\}). \tag{5}$$

Now, $T-u_1$ is an $(n-1)$-vertex tree with $r-1$ pendant vertices. Then, by the induction hypothesis,

$$z(T-u_1) \geq z(P_{r-2,n-r+1}) = (r-1)F_{n-r} + F_{n-r-1} \tag{6}$$

with equality only if $T-u_1 \cong P_{r-2,n-r+1}$. On the other hand, there is a tree H such that $T-\{u_1,u_2\} = (t-1)K_1 \cup H$(otherwise, we can obtain a contradiction to that $u_1u_2u_3\ldots u_du_{d+1}$ is a longest path in T). Obviously, $2 \leq t \leq r-2$, $n(H) = n-t-1 < n$ and $r-t \leq PV(H) \leq r-t+1$.

If $PV(H) = r - t$, by the induction hypothesis, $t \leq r - 2$ and $n \geq r + 3$, then

$$\begin{aligned} z(H) &\geq z(P_{r-t-1,n-r}) = (r-t)F_{n-r-1} + F_{n-r-2} \\ &> (r-t+1)F_{n-r-2} + F_{n-r-3}. \end{aligned} \tag{7}$$

If $PV(H) = r - t + 1$, by the induction hypothesis, then

$$z(H) \geq z(P_{r-t,n-r-1}) = (r-t+1)F_{n-r-2} + F_{n-r-3} \tag{8}$$

with equality only if $H \cong P_{r-t,n-r-1}$.

By (5)∼(8), Lemma 2, $t \leq r - 2$ and $n \geq r + 3$, we have

$$\begin{aligned} z(T) &= z(T - u_1) + z(T - \{u_1, u_2\}) \\ &= z(T - u_1) + z(H) \\ &\geq (r-1)F_{n-r} + F_{n-r-1} + (r-t+1)F_{n-r-2} + F_{n-r-3} \\ &\geq (r-1)F_{n-r} + F_{n-r-1} + 3F_{n-r-2} + F_{n-r-3} \\ &= (r+1)F_{n-r} \\ &> rF_{n-r} + F_{n-r-1}. \end{aligned}$$

This completes the proof of Theorem 2. ■

3 Conclusion

By Theorem 1 in this paper and Theorem 1 in [2], $P_{n-d,d}$ has both minimum Hosoya index and maximum Merrifield-Simmons index among the trees of n vertices and diameter d. Similarly, by Theorems 2 and 3, $P_{r-1,n-r+1}$ has the two extremal indices just mentioned among the trees of n vertices with r pendant vertices.

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