The Second Largest Hosoya Index of Unicyclic Graphs

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Abstract
Let \( m(G, k) \) be the number of the \( k \)-matching of a graph \( G \), \( z(G) \) denotes the Hosoya index of the graph \( G \), then the Hosoya index of \( G \) is \( z(G) = \left\lfloor \frac{n^2}{2} \right\rfloor \sum_{k=0}^{m(G, k)} \), where \( n \) denote the number of vertex of \( G \).
In this paper, the second largest Hosoya index of unicyclic graphs is determined.

1 Introduction

Let \( G = (V, E) \) be a simple connected graph with the vertex set \( V(G) \) and the edge set \( E(G) \). For any \( v \in V \), \( N(v) \) denotes the neighbors of \( v \), and

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$N_G[v] = \{v\} \cup \{u| uv \in E(G)\}$, $d_G(v) = |N(v)|$ is the degree of $v$. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf, leaves and their stems consisting all pendent edges. The girth of a graph is the smallest cycle length of the graph, if the graph contains no cycle, the girth is defined as $\infty$. If $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of $G$ obtained by deleting the edges of $E'$. If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. If $G$ has components $G_1, G_2, \cdots, G_t$, then $G$ is denoted by $\bigcup_{i=1}^{t} G_i$. We denote the sequence of fibonacci numbers by $F(n)$, i.e. $F(0) = 0$, $F(1) = 1$, and for $n \geq 2$, the fibonacci number has the recursion formula: $F(n) = F(n - 1) + F(n - 2)$. The related reviews referred as [2-4].

The Hosoya index $z(G)$ of a graph, proposed by Hosoya in [1], defined as the total number of its matching, namely

$$z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k)$$

where $\lfloor \frac{n}{2} \rfloor$ stands for the integer part of $\frac{n}{2}$ and $m(G, k)$ is the number of $k$-matching of $G$. A $k$-matching of graph $G$ is a subset $S$ of its edge set such that $|S| = k$ and that no two different edges of $S$ enjoy a common vertex. It is convenient to see $m(G, 0) = 1$ and $m(G, 1) = m$, the number of edges of graph $G$. When $k > \frac{n}{2}$, we have $m(G, k) = 0$. The Hosoya index is well correlated with the boiling points, entropies, calculated bond orders, and for the coding of chemical structures [2,3]. Since then, many authors have investigated the Hosoya index. It was established long ago that the $n$-vertex path $P_n$ has maximal Hosoya index, which equal to the $(n+1)$th Fibonacci number $F(n + 1)$ and the star $S_n$ has the minimal Hosoya index. In recent, Hou [5] characterized the acyclic graphs that have the first and the second minimal Hosoya indices. Gutman [6] showed that the linear chain
is the unique chain with minimal Hosoya index among all hexagonal chain.
Zhang [7] determined the unique graphs with minimal and second minimal
Hosoya index among all catacondensed systems. Ou [8] characterized the
unicyclic molecular graphs with the smallest Hosoya index. Deng and Chen
[9] characterized the extremal Hosoya index of unicyclic graphs, and Deng
[10] got the smallest Hosoya index of bicyclic graphs.

Let $P_n$, $C_n$ and $S_n$ (i.e., $K_{1,n-1}$) be the path, cycle and the star on $n$
vertices.

A graph is called unicyclic if it is connected and contains exactly one
cycle. A graph is unicyclic if and only if it is connected and has size equal
to its order.

Let $U_n$ denote the set of the unicyclic graphs with $n$ vertices.

Let $U^g_n$ denote the set of the unicyclic graphs with $n$ vertices and girth $g$.

$H_{n,g}$ be the unicyclic graph that results from identifying one vertex $u$ of
$C_g$ with the vertex $v_0$ of a simple path $v_0v_1 \cdots v_{n-g}$ of length $n - g$.

In this paper, we shall determine the second largest Hosoya index of
unicyclic graphs.

The related graph notations and terminologies undefined will conform
to [11].

2 Preliminaries

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

(i) If $G$ is a graph with components $G_1, G_2, \cdots, G_k$, then $z(G) = \prod_{i=1}^{k} z(G_i)$.

(ii) If $e = uv$ is an edge of $G$, then $z(G) = z(G - uv) + z(G - \{u, v\})$.

(iii) If $v$ is a vertex of $G$, then $z(G) = z(G - v) + \sum_{x \in N_G(v)} z(G - \{v, x\})$.

(iv) $z(P_0) = 0$, $z(P_1) = 1$ and $z(P_n) = F(n + 1)$ for $n \geq 2$;
$z(C_n) = F(n - 1) + F(n + 1)$, $z(K_{1,n-1}) = n$. 

From above, if $uv$ be an edge of $G$, then we have $z(G) > z(G - uv)$; moreover if $G$ is a graph with at least one edge, then $z(G) > z(G - v)$.

For convenience, we introduce two transformations.

**Transformation A.** Let $G \neq P_1$ be a simple connected graph, $u \in V(G)$. $G_1$ be the graph that results from identifying $u$ with the vertex $v_k$ ($1 < k < n$) of the simple path $v_1v_2\cdots v_n$; $G_2$ is obtained from $G_1$ by deleting the edge $v_{k-1}v_k$ and adding the edge $v_{k-1}v_n$ (see Fig 1.).

**Lemma 1** ([9,10]). Let $G_1$ and $G_2$ be the graphs depicted above. Then $z(G_2) > z(G_1)$.

**Remark 1.** Repeating transformation A, an arbitrary tree $T_i$ in $G$ can be changed into the graph $P_i$ (see Fig.2), and the Hosoya index increasing after transformation.

**Transformation B.** Let $P = uu_1u_2\cdots u_tv$ be a path in $G$, and $G \neq P$. Let $G$ is obtained from identifying $u$ with the vertex $v_k$ of $P_1 = v_1v_2\cdots v_{k}$, and identifying $v$ with the vertex $v_{k+1}$ of $P_2 = v_{k+1}v_{k+2}\cdots v_n$; $G_1$ is obtained from $G$ by deleting the edge $v_{k-1}v_k$ and adding the edge $v_{n}v_{k-1}$; $G_2$ is obtained from $G$ by deleting the edge $v_{k+1}v_{k+2}$ and adding the edge $v_{1}v_{k+2}$ (see Fig.3).
Lemma 2 ([9,10]). Let $G_1$ and $G_2$ be the graphs depicted in Fig 3, then $z(G_1) > z(G)$ or $z(G_2) > z(G)$.

Remark 2. After repeating transformation A, if we repeating transformation B, then, any arbitrary unicyclic graph with girth $g$ can be changed into the graph $H_{n,g}$, and the Hosoya index increasing.

3 The unicyclic graphs with the second largest Hosoya index

In this section we shall get the upper bounds of the unicyclic graphs with respect to their Hosoya indices.

Theorem 1 ([9]). $H_{n,g}$ has the largest Hosoya index in $U^g_n$ ($g \geq 3$).

Theorem 2 ([9]). $C_n$ (i.e.,$H_{n,n}$) is the unique graph with the largest Hosoya index among all unicyclic graphs of order $n$.

Theorem 3. $H_{n,4}$ and $H_{n,n-2}$ are the graphs with the second largest Hosoya index among all unicyclic graphs of order $n$, where $H_{n,4}$ and $H_{n,n-2}$ are shown in Fig.4.
Proof. From the theorems 1 and 2, we need only to compare the Hosoya indices of $H_{n,r}$ for $3 \leq r \leq n - 1$. By the definition of Hosoya index, it is easy to see that

$$z(H_{n,r}) = F(n + 1) + F(r - 1)F(n + 1 - r) = z(H_{n,n+2-r});$$

Let $\Delta = z(H_{n,r}) - z(H_{n,r-1})$, $\Delta' = z(H_{n,r}) - z(H_{n,r-2}).$

When $4 \leq r \leq \lfloor \frac{n}{2} \rfloor + 1$, we have

$$\Delta = F(r-1)F(n+1-r) - F(r-2)F(n+2-r)$$

$$= [F(r-2) + F(r-3)][F(n-r+2) - F(n-r)]$$

$$- F(r-2)F(n+2-r)$$

$$= -[F(r-2)F(n-r) - F(r-3)F(n+1-r)]$$

$$= \ldots$$

$$= (-1)^{r-2}[F(1)F(n+3-2r) - F(0)F(n+4-2r)]$$

$$= (-1)^{r}F(n+3-2r).$$

So,

$$z(H_{n,3}) < z(H_{n,4}) > H_{n,5}) < \cdots$$

and $z(H_{n,n-1}) < z(H_{n,n-2}) > H_{n,n-3}) < z(H_{n,n-4}) > \cdots$ since $z(H_{n,r}) = z(H_{n,n+2-r}).$

When $5 \leq r \leq \lfloor \frac{n}{2} \rfloor + 1,$

$$\Delta' = F(r-1)F(n+1-r) - F(r-2)F(n+2-r)$$

$$= [F(r-2) + F(r-3)][F(n-r+2) - F(n-r)]$$

$$- F(r-2)F(n+2-r)$$

$$= -[F(r-2)F(n-r) - F(r-3)F(n+1-r)]$$

$$= \ldots$$

$$= (-1)^{r-2}[F(1)F(n+6-2r) + F(2)F(n+5-2r)]$$

$$= (-1)^{r-1}F(n+4-2r)$$

So, we have

$$z(H_{n,3}) < z(H_{n,4}) < \cdots$$ and $z(H_{n,n-1}) < z(H_{n,n-2}) < \cdots$;

$$z(H_{n,4}) > z(H_{n,6}) > \cdots$$ and $z(H_{n,n-2}) > z(H_{n,n-4}) > \cdots$. 

Fig. 4.
We now only need to compare \( z(H_{n,4}) = z(H_{n,n-2}) \) with \( z(H(n, \frac{n}{2} + 1)) \) (\( n \) is even) or \( z(H_{n,\frac{n+1}{2}}) \) (\( n \) is odd).

Calculating immediately, \( z(H_{n,4}) > z(H(n, \frac{n}{2}+1)) \) or \( z(H_{n,4}) > z(H_{n,\frac{n+1}{2}}) \).

Therefore, \( H_{n,4} \) and \( H_{n,n-2} \) have the second largest Hosoya index among all unicyclic graphs, and \( H_{n,4} \) and \( H_{n,n-2} \) are the graphs with the second largest Hosoya index among all unicyclic graphs.

The proof of the Theorem is completed.

### References


