On the Hosoya index of unicyclic graphs with a given diameter*

Shuchao Li[a], Zhongxun, Zhu[b,†]

[a]Faculty of Mathematics and Statistics, Central China Normal University, Wuhan 430079, P.R. China

[b]Department of Computer Science, South Central University for Nationalities, Wuhan 430074, P.R. China

Abstract. The Hosoya index of a graph is defined as the total number of the matchings of the graph. In this paper, we determine the lower bounds for the Hosoya index of unicyclic graph with a given diameter. The corresponding extremal graphs are characterized.

Keywords: Hosoya index; Unicyclic graph; Diameter; Pendent vertex

AMS subject classification: 05C69, 05C05

1. Introduction

Let G be a graph on 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 k-matching of G. For convenience, we regard the empty edge set as a matching. Then $z(G,0)=1$ for any graph G. The *Hosoya index* of G, denoted by $z(G)$, is defined as

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

Obviously, $z(G)$ is equal to the total number of matchings of G.

The Hosoya index of a graph was introduced by Hosoya [9] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [10, 16]. Since then, many authors have investigated the Hosoya index (e.g., see [2, 3, 5, 6, 7, 10, 16]). An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. In [4], Gutman showed that linear

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†Corresponding author.

Email addresses: lscmath@mail.ccnu.edu.cn (S. Li), zzxun73@163.com (Z. Zhu)

hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. In [20], Zhang showed that the zig-zag hexagonal chain is the unique chain with maximal Hosoya index among all hexagonal chains. In [21], Zhang and Tian determined the graphs with minimal and second minimal Hosoya indices among catacondensed systems. As for n-vertex trees, it has been shown that the path has the maximal Hosoya index and the star has the minimal Hosoya index (see [8]). Recently, Hou [11] characterized the trees with a given size of matching and having minimal and second minimal Hosoya index, respectively. In [18], Yu and Tian studied the graphs with given edge-independence number and cyclomatic number and having the minimal Hosoya indices. In [17], Yan and Ye characterized the trees having many pendent vertices with the maximal Hosoya index. Yu and Lv characterize the trees with k pendent vertices having minimal Hosoya index in [19]. In [12], Li and the present authors order the unicyclic graphs according to their Hosoya indices. For many more results on this topic, the reader is referred to [22-29]. In this paper, we determine the unicyclic graph with a given diameter having minimal Hosoya index.

In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to Bondy and Murty [1]. We only consider finite, undirected and simple graphs. For a vertex v of a graph G, we denote $N(v) = \{u|uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$. A *pendent vertex* is a vertex of degree 1. For two vertices x and y ($x \neq y$), the *distance* between x and y is the number of edges in a shortest path joining x and y. The *diameter* of a graph G is the maximum distance between any two vertices of G. A *unicyclic graph* is a connected graph with n vertices and n edges, we shall by $\mathcal{U}_{n,d}$ denote the set of all unicyclic graphs on n vertices with diameter d.

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. Similarly, if $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. We denote by P_n, C_n and $K_{1,n-1}$ the path, the cycle and the star, each with n vertices. We use $VL(G)$ to denote the vertex set $\{v : v \in V(G)$ and $d(v) = 1\}$.

In order to formulate our results, some unicyclic graphs need to be defined. Let $U_p^{c,j}$ denote a unicyclic graph on n vertices with diameter d created from a path $P_{d+1} = u_1u_2 \ldots u_j \ldots u_{d+1}$ by attaching a cycle C_c and p pendent vertices $v_1, v_2, \ldots, v_p$ to u_j on P_{d+1} such that $c + p + d = n$; see Figure 1.

Let $B_{d,m}^{g,k}$ denote the unicyclic graph with diameter d created from a cycle $C_g = w_1w_2 \ldots w_t \ldots w_k \ldots w_h \ldots w_g w_1$ by joining the vertices w_1 (respectively, w_k) of C_g to an end vertex of P_{m-1} (respectively, $P_{d-m-k+2}$), where $k \leqslant \frac{1}{2}g$; see Figure 1. Note that h and t are used throughout to stand for arbitrary (not fixed) integers with $1 \leqslant t \leqslant k < h \leqslant g$. Since $B_{d,m}^{g,k}$ is a unicyclic graph on $d+g-k+1$ vertices; hence, for convenience, we might relabel the vertices of $B_{d,m}^{g,k}$ as $u_1, u_2, \ldots, u_{d+1}, u_{d+2}, \ldots, u_{d+g-k+1}$. Let $Q_{n-d-g+k-1,m}^{g,i}$ be a unicyclic graph on n vertices with diameter d cre-

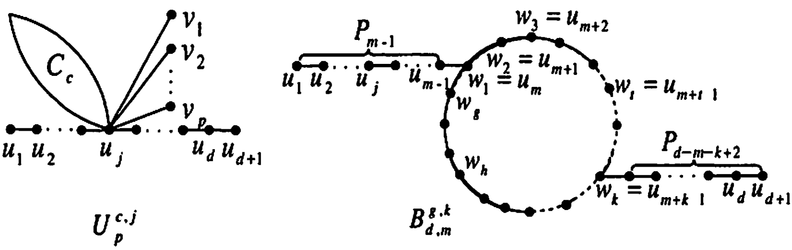

Figure 1: Graphs $U_p^{c,j}$ and $B_{d,m}^{g,k}$.

ated from $B_{d,m}^{g,k}$ by attaching $n-d-g+k-1$ pendent vertices $v_1, v_2, \ldots, v_{n-d-g+k-1}$ to a non-pendent vertex u_i in $V(U_{d,m}^{g,k})$.

In this paper, we show that $Q_{n-d-2,2}^{4,2}$ (e.g., see Figure 2) is the unique graph in $\mathcal{U}_{n,d}$ with minimal Hosoya index.

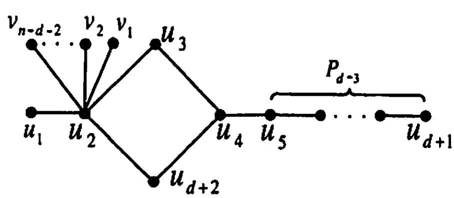

Figure 2: Graph $Q_{n-d-2,2}^{4,2}$

We list some lemmas that will be used in this paper.

Lemma 1.1 ([8]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G - uv) + z(G - \{u, v\})$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G - v) + \sum_{u \in N(v)} z(G - \{u, v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$.

Lemma 1.2 ([13]). *Let $n = 4s + r$, where n, s and r are integers with $0 \le r \le 3$.*

(i) *If $r \in \{0, 1\}$, then*

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} \\ &> F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1}; \end{aligned}$$

(ii) *If $r \in \{2, 3\}$, then*

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} \\ &> F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}. \end{aligned}$$

Lemma 1.3 ([14]). *Let H, X, Y be three connected graphs pairwise disjoint. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'; see Figure 3. Then*

$$z(G_1^*) < z(G) \quad or \quad z(G_2^*) < z(G).$$

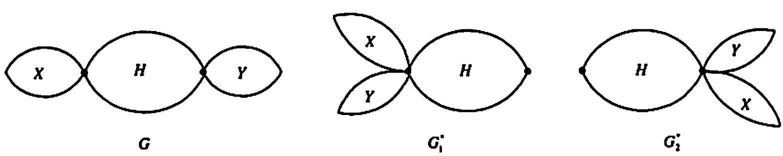

Figure 3: Graphs G, G_1^* and G_2^*.

Let H_1, H_2 be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let $G = H_1vH_2$ be a graph defined by $V(G) = V(H_1) \cup V(H_2)$ and $E(G) = E(H_1) \cup E(H_2)$.

Lemma 1.4 ([15]). *Let H be a connected graph and T_l be a tree of order $l+1$ with $V(H) \cap T_l = \{v\}$. Then $z(HvT_l) \ge z(HvK_{1,l})$, the equality holds if and only if $HvT_l \cong HvK_{1,l}$, where v is identified with the center of the star $K_{1,l}$ in $HvK_{1,l}$.*

2. Lemmas and main results

According to the definition of the Hosoya index of a graph, by Lemma 1.1, if v is a vertex of G, then $z(G) > z(G-v)$. In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $z(G) = z(G-v)+z(G-\{u,v\})$. So it is easy to see that $z(P_0) = 1, z(P_1) = 1$ and $z(P_n) = z(P_{n-1}) + z(P_{n-2})$ for $n \geqslant 2$. Recall that the nth Fibonacci number F_n satisfying recursive relation $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. We have

$$z(P_n) = F_n = \frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1}\right].$$

Note that $F_{n+m} = F_nF_m + F_{n-1}F_{m-1}$. For convenience, we let $F_n = 0$, if $n < 0$. By Lemma 1.1, we obtain the following results.

Lemma 2.1. *For the graph $U_p^{c,j}$, we have*

$$z(U_p^{c,j}) = pF_{j-1}F_{c-1}F_{d+1-j} + 2F_{j-1}F_{c-2}F_{d+1-j} + F_{c-1}F_{d+1}.$$

Proof. By Lemma 1.1,

$$\begin{aligned}
z(U_p^{c,j}) &= z(U_p^{c,j}) - v_1) + \sum_{v\in N(v_1)} (z(U_p^{c,j}) - \{v, v_1\}) \\
&= z(U_{p-1}^{c,j}) + z(P_{j-1} \cup P_{c-1} \cup P_{d+1-j} \cup \{v_2, \dots, v_p\}) \\
&= z(U_{p-1}^{c,j}) + F_{j-1}F_{c-1}F_{d+1-j} \\
&= \cdots \\
&= z(U_0^{c,j}) + pF_{j-1}F_{c-1}F_{d+1-j} \\
&= z(U_0^{c,j} - u_j) + \sum_{u\in N(u_j)} z(U_0^{c,j} - \{u, u_j\}) + pF_{j-1}F_{c-1}F_{d+1-j} \\
&= z(P_{c-1} \cup P_{j-1} \cup P_{d+1-j}) + z(P_{c-1} \cup P_{j-2} \cup P_{d+1-j}) \\
&\quad +2z(P_{c-2} \cup P_{j-1} \cup P_{d+1-j}) + z(P_{c-1} \cup P_{j-1} \cup P_{d-j}) \\
&\quad +pF_{j-1}F_{c-1}F_{d+1-j} \\
&= pF_{j-1}F_{c-1}F_{d+1-j} + 2F_{j-1}F_{c-2}F_{d+1-j} + F_{c-1}F_{j-1}F_{d+1-j} \\
&\quad +F_{c-1}F_{j-2}F_{d+1-j} + F_{c-1}F_{j-1}F_{d-j} \\
&= pF_{j-1}F_{c-1}F_{d+1-j} + 2F_{j-1}F_{c-2}F_{d+1-j} + F_{c-1}F_{d+1}.
\end{aligned}$$

This completes the proof of Lemma 2.1. □

Lemma 2.2. *For positive integers g, k, if $g - k \geqslant 2$, then*

(i) $z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) < z(Q^{g,m+k-1}_{n+k-d-g-1,m})$.

(ii) $z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) < z(Q^{g,h}_{n+k-d-g-1,m})$.

(iii) $z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) < z(Q^{g,t}_{n+k-d-g-1,m})$.

(iv) $z(U^{g-k+1,m+k-1}_{n-d-g'+k'-1}) < z(Q^{g,j}_{n+k-d-g-1,m})$ *for* $j > m+k-1$.

Proof. (i) By Lemma 2.1, we have

$$\begin{aligned} z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) &= (n-d-g+k-1)F_{m+k-2}F_{g-k}F_{d+2-m-k} \\ &\quad +2F_{m+k-2}F_{g-k-1}F_{d+2-m-k} \\ &\quad +F_{g-k}F_{m+k-2}(F_{d+2-m-k}+F_{d+1-m-k}) \\ &\quad +F_{g-k}F_{m+k-3}F_{d+2-m-k}. \end{aligned}$$

On the other hand, it is easy to see that $P_m w_1 C_g$ is a subgraph of $B^{g,k}_{d,m}$. Let $T_0 = P_m w_1 C_g - w_k$, then repeatedly using Lemma 1.1,

$$\begin{aligned} & z(Q^{g,m+k-1}_{n+k-d-g-1,m}) \\ =\; & z(Q^{g,m+k-1}_{n+k-d-g-1,m} - v_1 w_k) + z(Q^{g,m+k-1}_{n+k-d-g-1,m} - \{v_1, w_k\}) \\ =\; & z(Q^{g,m+k-1}_{0,m}) + (n-d-g+k-1)F_{d+2-m-k}z(T_0) \\ =\; & (n-d-g+k-1)F_{d+2-m-k}(F_{m-1}F_{g-1}+F_{m-2}F_{g-k}F_{k-2}) \\ & +F_{d+3-m-k}F_{m-1}F_{g-1}+F_{d+3-m-k}F_{m-2}F_{k-2}F_{g-k} \\ & +F_{d+2-m-k}F_{m-1}F_g + F_{d+2-m-k}F_{m-2}F_{g-k}F_{k-1}. \end{aligned}$$

Therefore,

$$\begin{aligned} & z(Q^{g,m+k-1}_{n+k-d-g-1,m}) - z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) \\ =\; & (n-d-g+k-1)F_{d+2-m-k}(F_{m-1}F_{g-1}+F_{m-2}F_{g-k}F_{k-2}) \\ & +F_{d+3-m-k}F_{m-1}F_{g-1}+F_{d+3-m-k}F_{m-2}F_{k-2}F_{g-k} \\ & +F_{d+2-m-k}F_{m-1}F_g + F_{d+2-m-k}F_{m-2}F_{g-k}F_{k-1} \\ & -\{(n-d-g+k-1)F_{m+k-2}F_{g-k}F_{d+2-m-k} \\ & +2F_{m+k-2}F_{g-k-1}F_{d+2-m-k}+F_{g-k}F_{m+k-2}F_{d+2-m-k} \\ & +F_{g-k}F_{m+k-3}F_{d+2-m-k}+F_{g-k}F_{m+k-2}F_{d+1-m-k}\} \\ =\; & (n-d-g+k-1)F_{d+2-m-k}F_{k-2}F_{m-1}F_{g-k-1} \\ & +F_{d+2-m-k}F_{m-1}F_{g-k-2}F_{k-1}+F_{d+2-m-k}F_{k-2}(F_{m-2}F_{g-k-2} \\ & +F_{m-3}F_{g-k-1})+F_{d+1-m-k}F_{m-1}F_{g-k-1}F_{k-2} \\ \geq\; & F_{d+2-m-k}F_{m-1}F_{g-k-2}F_{k-1} > 0. \end{aligned}$$

Hence,

$$z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) < z(Q^{g,m+k-1}_{n+k-d-g-1,m}).$$

(ii) Let $P_{x_1} = w_k w_{k+1} \dots w_h, P_{x_2} = w_h w_{h+1} \dots w_1, T_0 = P_m w_1 C_g - w_k, T_1 = Q_{0,m}^{g,h} - w_h, T_2 = T_1 - P_{x_1} - P_{d-m-k+2}$ and $T_2' = T_2 - w_{k-1}$.

$$
\begin{aligned}
& z(Q_{n-d-g+k-1,m}^{g,h}) \\
= \; & z(Q_{n-d-g+k-1,m}^{g,h} - v_1 w_h) + z(Q_{n-d-g+k-1,m}^{g,h} - \{v_1, w_h\}) \\
= \; & z(Q_{n-d-g+k-2,m}^{g,h}) + z(T_1 \cup \{v_2, \dots, v_{n-d-g+k-1}\}) \\
= \; & \cdots \\
= \; & z(Q_{0,m}^{g,h}) + (n-d-g+k-1) z(T_1).
\end{aligned}
$$

By (i), we have

$$
z(Q_{n-d-g+k-1,m}^{g,m+k-1}) = z(Q_{0,m}^{g,m+k-1}) + (n-d-g+k-1) F_{d-m-k+2} z(T_0).
$$

Therefore,

$$
\begin{aligned}
z(Q_{n-d-g+k-1,m}^{g,h}) - z(Q_{n-d-g+k-1,m}^{g,m+k-1}) \; = \; & (n-d-g+k-1)(z(T_1) \\
& - F_{d-m-k+2} z(T_0)).
\end{aligned}
$$

Furthermore,

$$
\begin{aligned}
& z(T_1) - F_{d-m-k+2} z(T_0) \\
= \; & z(T_1 - w_k) + \sum_{u \in N(w_k)} z(T_1 - \{u, w_k\}) - F_{d-m-k+2} z(T_0) \\
= \; & z(T_2 \cup P_{x_1-1} \cup P_{d-m-k+2}) + z(T_2 \cup P_{x_1-2} \cup P_{d-m-k+2}) \\
& + z(T_2 \cup P_{x_1-1} \cup P_{d-m-k+1}) + z(T_2' \cup P_{x_1-1} \cup P_{d-m-k+2}) \\
& - F_{d-m-k+2} z(T_0) \\
= \; & z(T_2)(F_{x_1-1} F_{d-m-k+2} + F_{x_1-2} F_{d-m-k+2} + F_{x_1-1} F_{d-m-k+1}) \\
& + z(T_2') F_{x_1-1} F_{d-m-k+2} - F_{d-m-k+2} z(T_0) \\
= \; & (F_{m-1} F_{g-x_1} + F_{m-2} F_{k-2} F_{g-k-x_1+1}) F_{x_1-1} F_{d-m-k+2} \\
& + (F_{m-1} F_{g-x_1} + F_{m-2} F_{k-2} F_{g-k-x_1+1}) F_{x_1-2} F_{d-m-k+2} \\
& + (F_{m-1} F_{g-x_1} + F_{m-2} F_{k-2} F_{g-k-x_1+1}) F_{x_1-1} F_{d-m-k+1} \\
& + (F_{m-1} F_{g-x_1-1} + F_{m-2} F_{k-3} F_{g-k-x_1+1}) F_{x_1-1} F_{d-m-k+2} \\
& - F_{d-m-k+2}(F_{m-1} F_{g-1} + F_{m-2} F_{g-k} F_{k-2}) \\
= \; & F_{d-m-k+2}(F_{x_1-2} F_{m-1} F_{g-x_1-2} + F_{x_1-1} F_{m-1} F_{g-x_1-1} \\
& + F_{x_1-1} F_{m-2} F_{k-3} F_{g-k-x_1+1} + F_{x_1-2} F_{m-2} F_{k-2} F_{g-k-x_1-1}) + \\
& F_{d-m-k+1} F_{x_1-1}(F_{m-1} F_{g-x_1} + F_{m-2} F_{k-2} F_{g-k-x_1+1}) \\
\geq \; & F_{d-m-k+2} F_{x_1-1} F_{m-1} F_{g-x_1-1} > 0.
\end{aligned}
$$

Hence,

$$
z(Q_{n-d-g+k-1,m}^{g,h}) > z(Q_{n-d-g+k-1,m}^{g,m+k-1}).
$$

By (i), we have

$$z(U^{g-k+1,m+k-1}_{n-d-g+k-1}) < z(Q^{g,h}_{n+k-d-g-1,m}).$$

Similarly, we can show that (iii) and (iv) hold. □

Use a similar method as in Lemma 2.2, we can also prove the following lemma, we will not repeat the procedure here.

Lemma 2.3. *For positive integers g, k, if $g-k \geqslant 2$, then*

(i) $z(U^{g-k+1,m}_{n-d-g+k-1}) < z(Q^{g,m}_{n+k-d-g-1,m})$.
(ii) $z(U^{g-k+1,m}_{n-d-g+k-1}) < z(Q^{g,h}_{n+k-d-g-1,m})$.
(iii) $z(U^{g-k+1,m}_{n-d-g+k-1}) < z(Q^{g,t}_{n+k-d-g-1,m})$.
(iv) $z(U^{g-k+1,m}_{n-d-g+k-1}) < z(Q^{g,i}_{n+k-d-g-1,m})$ *for* $1 < i < m$.

Lemma 2.4. $z(U^{g-k,j}_{n+k-d-g}) < z(U^{g-k+1,j}_{n+k-d-g-1})$ *for* $g-k \geqslant 3$.

Proof. By Lemma 2.1, we have

$$\begin{aligned}
& z(U^{g-k+1,j}_{n+k-d-g-1}) - z(U^{g-k,j}_{n+k-d-g}) \\
= \ & (n+k-d-g)F_{j-1}F_{g-k-2}F_{d+1-j} - F_{j-1}F_{d+1-j}(F_{g-k} + 2F_{g-k-3}) \\
& +F_{g-k-2}F_{j-1}F_{d+1-j} + F_{j-2}F_{g-k-2}F_{d+1-j} + F_{j-1}F_{g-k-2}F_{d-j} \\
\geq \ & F_{j-1}F_{g-k-2}F_{d+1-j} - F_{j-1}F_{g-k-1}F_{d+1-j} + 2F_{j-1}F_{g-k-3}F_{d+1-j} \\
& +F_{j-2}F_{g-k-2}F_{d+1-j} + F_{j-1}F_{g-k-2}F_{d-j} \\
= \ & F_{j-1}F_{g-k-3}F_{d+1-j} + F_{g-k-2}F_{j-2}F_{d+1-j} + F_{j-1}F_{g-k-2}F_{d-j} \\
\geq \ & F_{j-1}F_{g-k-3}F_{d+1-j} > 0.
\end{aligned}$$

Hence, we have $z(U^{g-k,j}_{n+k-d-g}) < z(U^{g-k+1,j}_{n+k-d-g-1})$. □

Corollary 2.5. $z(U^{3,j}_{n-d-3}) < z(U^{4,j}_{n-d-4}) < \cdots < z(U^{n-d,j}_{0})$.

Lemma 2.6. *Let $d = 4s + r$, where n, s and r are integers with $0 \leqslant r \leqslant 3$.*

(i) *For $r \in \{0, 1\}$, we have*

$$\begin{aligned}
z(U^{g-k+1,2}_{n-d-g+k-1}) < z(U^{g-k+1,4}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,2s}_{n-d-g+k-1}) \\
< z(U^{g-k+1,2s-1}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,1}_{n-d-g+k-1}).
\end{aligned}$$

(ii) *For $r \in \{2, 3\}$, we have*

$$\begin{aligned}
z(U^{g-k+1,2}_{n-d-g+k-1}) < z(U^{g-k+1,4}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,2s}_{n-d-g+k-1}) \\
< z(U^{g-k+1,2s+1}_{n-d-g+k-1}) < z(U^{g-k+1,2s-1}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,1}_{n-d-g+k-1}).
\end{aligned}$$

Proof. (i) By Lemma 2.1,

$$\begin{aligned} z(U^{g-k+1,j}_{n-d-g+k-1}) &= (n-d-g+k-1)F_{j-1}F_{g-k}F_{d+1-j} \\ &\quad +2F_{j-1}F_{g-k-1}F_{d+1-j} + F_{g-k}F_{d+1}. \end{aligned} \tag{2.1}$$

For $r \in \{0, 1\}$, by Lemma 1.2 (i),

$$\begin{aligned} F_0F_d > F_2F_{d-2} > F_4F_{d-4} > \cdots > F_{2s}F_{2s+r} \\ > F_{2s-1}F_{2s+r+1} > \cdots > F_1F_{d-1}. \end{aligned}$$

Together with (2.1), we have

$$\begin{aligned} z(U^{g-k+1,2}_{n-d-g+k-1}) < z(U^{g-k+1,4}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,2s}_{n-d-g+k-1}) \\ < z(U^{g-k+1,2s-1}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,1}_{n-d-g+k-1}). \end{aligned}$$

(ii) For $r \in \{2, 3\}$, by Lemma 1.2 (ii),

$$\begin{aligned} F_0F_d > F_2F_{d-2} > F_4F_{d-4} > \cdots > F_{2s}F_{2s+r} \\ > F_{2s+1}F_{2s+r-1} > F_{2s-1}F_{2s+r+1} > \cdots > F_1F_{d-1}. \end{aligned}$$

Together with (2.1), we get

$$\begin{aligned} z(U^{g-k+1,2}_{n-d-g+k-1}) < z(U^{g-k+1,4}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,2s}_{n-d-g+k-1}) \\ < z(U^{g-k+1,2s+1}_{n-d-g+k-1}) < z(U^{g-k+1,2s-1}_{n-d-g+k-1}) < \cdots < z(U^{g-k+1,1}_{n-d-g+k-1}). \end{aligned}$$

This completes the proof of Lemma 2.6. □

By Lemma 2.6, the following corollary is obvious.

Corollary 2.7. $z(U^{3,2}_{n-d-3}) < z(U^{3,4}_{n-d-3}) < \cdots < z(U^{3,2s}_{n-d-3}) < U^{3,2s-1}_{n-d-3} < \cdots < z(U^{3,3}_{n-d-3})$.

Let $\mathcal{U}_{n,d} = \mathcal{U}^1_{n,d} \bigcup \mathcal{U}^2_{n,d}$, where $\mathcal{U}^1_{n,d} = \{U : U \in \mathcal{U}_{n,d}$, there exist C_g and P_{d+1} in U such that $g - |V(C_g) \cap V(P_{d+1})| \geqslant 2\}$, $\mathcal{U}^2_{n,d} = \{U : U \in \mathcal{U}_{n,d}$, there exist C_g and P_{d+1} in U such that $g - |V(C_g) \cap V(P_{d+1})| = 1\}$.

Theorem 2.8. *If $G \in \mathcal{U}^1_{n,d}$, then $z(G) \geq 2(n-d-2)F_{d-1} + 2F_{d+1}$, the equality holds if and only if $G \cong U^{3,2}_{n-d-3}$.*

Proof. By Lemma 2.1, we have

$$z(U^{3,2}_{n-d-3}) = 2(n-d-2)F_{d-1} + 2F_{d+1}. \tag{2.2}$$

Note that $G \in \mathcal{U}_{n,d}$, we choose a path P of length d in G.

Case 1. $P \cap C_g \neq \emptyset$. Without loss of generality, we assume that P and C_g have exactly k vertices in common, $k \leqslant \frac{g}{2}$. Then the arrangement of P and C_g in G is the same as $B_{d,m}^{g,k}$ in Figure 1.

Let $V^*(G)$ be the set of all the vertices chosen from a subgraph of G that is isomorphic to $B_{d,m}^{g,k}$, each of which has pendent tree attached. Assume that $|V^*(G)| = t$, then relabel the vertices in $V^*(G)$ as $x_1, x_2, \ldots, x_t$. For each $x_i \in V^*(G), i = 1, \ldots, t$, let T_i be a subtree of $G - E(B_{d,m}^{g,k})$ which contains x_i and $|V(T_i)| = p_i + 1$, denote

$$H = B_{d,m}^{g,k} \cup \left(\bigcup_{1 \leqslant j \leqslant t, j \neq i} T_j \right),$$

then $G = Hx_iT_i$. By Lemma 1.4, we have $z(Hx_iT_i) \geq z(Hx_iK_{1,p_i})$. Thus repeatedly using Lemma 1.4,

$$z(G) \geq z(B_{d,m}^{g,k}(p_1, p_2, \ldots, p_i, \ldots, p_t)),$$

where $B_{d,m}^{g,k}(p_1, p_2, \ldots, p_i, \ldots, p_t)$ is a unicyclic graph of order n with diameter d created from $B_{d,m}^{g,k}$ by attaching p_i pendent vertices to $x_i \in V^*(G), 1 \leqslant i \leqslant t$, respectively. Corresponding to $x_i, x_j \in V^*(G)$, let

$$X = K_{1,p_i}, Y = K_{1,p_j}, \text{ and } H' = G - VL(K_{1,p_i}) - VL(K_{1,p_j}),$$

then $B_{d,m}^{g,k}(p_1, p_2, \ldots, p_t) = Xx_iH'x_jY$. By Lemma 1.3, we have either

$$\begin{aligned} z(G) &\geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_t)) \\ &> z(B_{d,m}^{g,k}(p_1, \ldots, p_i + p_j, \ldots, 0, \ldots, p_t)), \end{aligned}$$

or

$$\begin{aligned} z(G) &\geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_t)) \\ &> z(B_{d,m}^{g,k}(p_1, \ldots, 0, \ldots, p_i + p_j, \ldots, p_t)). \end{aligned}$$

Repeatedly using above step, we obtain either

$$z(G) \geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_t)) > \ldots$$
$$> z(Q_{n+k-d-g-1,m}^{g,k}), \tag{2.3}$$
$$z(G) \geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_t)) > \ldots$$
$$> z(Q_{n+k-d-g-1,m}^{g,h}), \tag{2.4}$$
$$z(G) \geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_t)) > \ldots$$
$$> z(Q_{n+k-d-g-1,m}^{g,t}), \tag{2.5}$$

or

$$z(G) \geq z(B_{d,m}^{g,k}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_m)) > \ldots$$
$$> z(Q_{n+k-d-g-1,m}^{g,j}). \tag{2.6}$$

Together with (2.3)–(2.6) and Lemma 2.3, we obtain that

$$z(G) > z(U_{n-d-g+k-1}^{g-k+1,m+k-1}).$$

Similarly, we have

$$z(G) > z(U_{n-d-g+k-1}^{g-k+1,m}).$$

By Corollaries 2.5 and 2.7, we obtain

$$z(U_{n-d-g+k-1}^{g-k+1,m+k-1}) > z(U_{n-d-3}^{3,m+k-1}) > z(U_{n-d-3}^{3,2}),$$

and

$$z(U_{n-d-g+k-1}^{g-k+1,m}) > z(U_{n-d-3}^{3,m}) > z(U_{n-d-3}^{3,2}).$$

Therefore, $z(G) > z(U_{n-d-3}^{3,2}) = 2(n-d-2)F_{d-1} + 2F_{d+1}$.

Case 2. $P \cap C_g = \emptyset$. Then cycle C_g connects P by a path of length at least 1. By Lemma 1.3, we can obtain a unicyclic graph $G' \in B_{d,m}^{g,k}$ such that $z(G) > z(G')$ and the cycle C_g and P in G' have exactly one vertex in common. By Case 1, $z(G) > z(G') \geq 2(n-d-2)F_{d-1} + 2F_{d+1}$.

By Cases 1 and 2, we obtain that if $G \in \mathcal{U}_{n,d}^1$, then $z(G) \geq 2(n-d-2)F_{d-1} + 2F_{d+1}$, the equality holds if and only if $G \cong U_{n-d-3}^{3,2}$. □

Corollary 2.9. *$U^{3,2}_{n-d-3}$ is the graph with the minimal Hosoya index in $\mathcal{U}^1_{n,d}$.*

In the following we shall determine the graph G in $\mathcal{U}^2_{n,d}$ with minimal Hosoya index. It is straightforward to check that in this case the length of the cycle in G is either 3 or 4. The arrangement of the longest path and the cycle contained in G is G_1 or G_2, which were depicted in Figure 4.

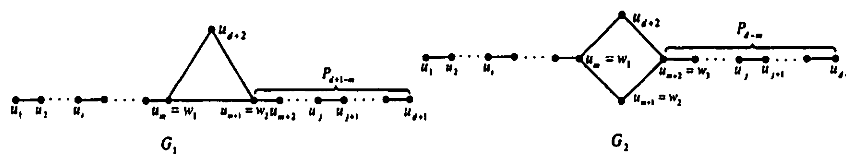

Figure 4: Graphs G_1 and G_2.

By definition, $Q^{3,i}_{n-d-2,m}$ (respectively, $Q^{3,m}_{n-d-2,m}, Q^{3,m+1}_{n-d-2,m}, Q^{3,d+2}_{n-d-2,m}, Q^{3,j}_{n-d-2,m}$) is the unicyclic graph with diameter d created from G_1 by attaching $n-d-2$ pendent vertices to the vertex u_i (respectively, $u_m, u_{m+1}, u_{d+2}, u_j$). Similarly, $Q^{4,i}_{n-d-2,m}$ (respectively, $Q^{4,m}_{n-d-2,m}, Q^{4,m+2}_{n-d-2,m}, Q^{4,d+2}_{n-d-2,m}, Q^{4,j}_{n-d-2,m}$) is the unicyclic graph with diameter d created from G_2 by attaching $n-d-3$ pendent vertices to the vertex u_i (respectively, $u_m, u_{m+2}, u_{d+2}, u_j$).

Lemma 2.10. *For graphs $Q^{3,m}_{n-d-2,m}, Q^{3,i}_{n-d-2,m}$ and $Q^{3,d+2}_{n-d-2,m}$, we have*

(i) *$z(Q^{3,m}_{n-d-2,m}) < z(Q^{3,d+2}_{n-d-2,m})$ and $z(Q^{3,m}_{n-d-2,m}) \le z(Q^{3,i}_{n-d-2,m})$ for $1 < i \le m$, the equality holds if and only if $i = m$.*

(ii) *$z(Q^{3,m+1}_{n-d-2,m}) < z(Q^{3,d+2}_{n-d-2,m})$ and $z(Q^{3,m+1}_{n-d-2,m}) \le z(Q^{3,j}_{n-d-2,m})$ for $m+1 \le j < d+1$, the equality holds if and only if $j = m+1$.*

Proof. By Lemma 1.1, for $1 < i < m, m+1 < j < d+1$, we have

$$z(Q^{3,m}_{n-d-2,m}) = (n-d-2)F_{m-1}F_{d+2-m} + F_{m+1}F_{d+2-m}, \quad (2.7)$$

$$z(Q^{3,m+1}_{n-d-2,m}) = (n-d-2)F_{m+1}F_{d-m} + F_{m+1}F_{d+2-m}, \quad (2.8)$$

$$
\begin{aligned}
z(Q^{3,d+2}_{n-d-2,m}) &= (n-d-2)F_{d+1} + F_{m+1}F_{d+2-m},\\
z(Q^{3,i}_{n-d-2,m}) &= (n-d-2)F_{i-1}(F_{d+1-i} + F_{m-1-i}F_{d+1-m}\\
&\quad +F_{m-i}F_{d-m}) + F_{m+1}F_{d+2-m},\\
z(Q^{3,j}_{n-d-2,m}) &= (n-d-2)F_{d+1-j}(F_{j-1} + F_{m-1}F_{j-m-1}\\
&\quad +F_mF_{j-m-2}) + F_{m+1}F_{d+2-m}.
\end{aligned}
$$

Therefore,

(i)

$$z(Q^{3,d+2}_{n-d-2,m}) - z(Q^{3,m}_{n-d-2,m}) = (n-d-2)F_{m-2}F_{d+1-m}.$$

Note that $d+1 > m$ and $m \geq 2$ (otherwise, the diameter of $Q^{3,m}_{n-d-2,m}$ is $d+1$, a contradiction), therefore, $(n-d-2)F_{m-2}F_{d+1-m} > 0$, i.e., $z(Q^{3,m}_{n-d-2,m}) < z(Q^{3,d+2}_{n-d-2,m})$.

$$
\begin{aligned}
z(Q^{3,i}_{n-d-2,m}) - z(Q^{3,m}_{n-d-2,m}) &= (n-d-2)F_{m-1-i}[(F_{i-1} - F_{i-2})F_{d-m}\\
&\quad +(F_{i-1} - F_{i-2})F_{d+1-m}]
\end{aligned}
$$

Note that $d+1 > m$ and $i \geq 2$ (otherwise, the diameter of $Q^{3,i}_{n-d-2,m}$ is $d+1$, a contradiction), therefore, $(n-d-2)F_{m-1-i}(F_{i-1} - F_{i-2})(F_{d-m} + F_{d+1-m}) \geq 0$, i.e., $z(Q^{3,m}_{n-d-2,m}) \leq z(Q^{3,i}_{n-d-2,m})$.

(ii)

$$z(Q^{3,d+2}_{n-d-2,m}) - z(Q^{3,m+1}_{n-d-2,m}) = (n-d-2)F_mF_{d-1-m} > 0,$$

therefore, $z(Q^{3,m+1}_{n-d-2,m}) < z(Q^{3,d+2}_{n-d-2,m})$.

$$z(Q^{3,j}_{n-d-2,m}) - z(Q^{3,m+1}_{n-d-2,m}) = (n-d-2)F_{m+1}F_{j-m-2}F_{d-1-j} \geq 0,$$

and so, $z(Q^{3,m+1}_{n-d-2,m}) \leq z(Q^{3,j}_{n-d-2,m})$. □

Corollary 2.11. $Q^{3,2}_{n-d-2,2}$ *is the graph with the minimal Hosoya index in* $\{Q^{3,m}_{n-d-2,m} : 2 \leq m \leq d-2\} \cup \{Q^{3,m+1}_{n-d-2,m} : 2 \leq m \leq d-2\}$.

Proof. By Lemma 1.2 and Eqs.(2.7)-(2.8), we have that $Q^{3,2}_{n-d-2,2}$ is the graph with the minimal Hosoya index in $\{Q^{3,m}_{n-d-2,m} : 2 \le m \le d-2\}$ and $Q^{3,3}_{n-d-2,2}$ is the graph with the minimal Hosoya index in $\{Q^{3,m+1}_{n-d-2,m} : 2 \le m \le d-2\}$. On the other hand,

$$z(Q^{3,2}_{n-d-2,2}) - z(Q^{3,3}_{n-d-2,2}) = (n-d-2)(F_{d-3} - F_{d-2}) \le 0,$$

the equality holds if and only if $d = 3$. It is easy to see when $d = 3$, $Q^{3,2}_{n-5,2} \cong Q^{3,3}_{n-5,3}$. This completes the proof. □

Lemma 2.12. *For a fixed positive integer m, we have*

(i) $z(Q^{4,m}_{n-d-2,m}) < z(Q^{4,d+2}_{n-d-2,m})$ *and* $z(Q^{4,m}_{n-d-2,m}) \le z(Q^{4,i}_{n-d-2,m})$ *for* $1 < i \le m$, *the equality holds if and only if* $i = m$;

(ii) $z(Q^{4,m+2}_{n-d-2,m}) < z(Q^{4,d+2}_{n-d-2,m})$ *and* $z(Q^{4,m+2}_{n-d-2,m}) \le z(Q^{4,j}_{n-d-2,m})$ *for* $m+2 \le j < d+1$, *the equality holds if and only if* $j = m+2$.

Corollary 2.13. $Q^{4,2}_{n-d-2,2}$ *is the graph with the minimal Hosoya index in* $\{Q^{4,m}_{n-d-2,m} : 2 \le m \le d-2\} \cup \{Q^{4,m+2}_{n-d-2,m} : 2 \le m \le d-2\}$.

Lemma 2.12 and Corollary 2.13 can be proved in the same way as Lemma 2.10 and Corollary 2.11, respectively. We will not repeat the procedure here.

Theorem 2.14. *If* $G \in \mathcal{U}^2_{n,d}$,

(i) *If* $d = 3$, *then*

$$z(G) \ge 3n - 6$$

with equality if and only if $G \cong Q^{3,2}_{n-5,2}$.

(ii) *If* $d \ge 4$, *then*

$$z(G) \ge \begin{cases} 24, & \text{if } n = 7, d = 5; \\ (3n-3d+4)F_{d-3} + (n-d+2)F_{d-4}, & \text{otherwise.} \end{cases} \quad (2.9, 2.10)$$

Equality in (2.9) *holds if and only if* $G \cong G^*$ *or* $G \cong G^{**}$, *where* G^*, G^{**} *are depicted in Figure* 5; *equality in* (2.10) *holds if and only if* $G \cong Q^{4,2}_{n-d-2,2}$ (*see Figure* 2).

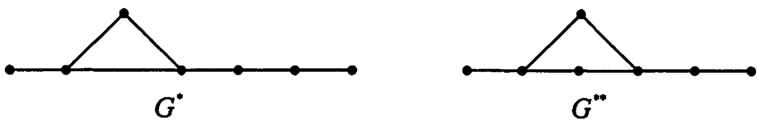

Figure 5: Graphs G^* and G^{**}.

Proof. (i) When $d = 3$, in view of Corollaries 2.11 and 2.13, we should compare the Hosoya index of $Q^{3,2}_{n-5,2}$ with that of $Q^{4,2}_{n-5,2}$. By direct computing, we have

$$z(Q^{3,2}_{n-5,2}) = 3n - 6, \quad z(Q^{4,2}_{n-5,2}) = 3n - 5.$$

Thus (i) follows immediately.

(ii) When $d \geq 4$, in view of Corollaries 2.11 and 2.13, we should compare the Hosoya index of $Q^{3,2}_{n-d-2,2}$ with that of $Q^{4,2}_{n-d-2,2}$. By an elementary calculation, we have

$$\begin{aligned} z(Q^{3,2}_{n-d-2,2}) &= 2(n-d+1)F_{d-2} + (n-d+1)F_{d-3}, \\ z(Q^{4,2}_{n-d-2,2}) &= (3n-3d+4)F_{d-3} + (n-d+2)F_{d-4}. \end{aligned}$$

Hence,

$$\begin{aligned} z(Q^{3,2}_{n-d-2,2}) - z(Q^{4,2}_{n-d-2,2}) &= (n-d)F_{d-4} - F_{d-3} \\ &\geq^* 2F_{d-4} - F_{d-3} \\ &= F_{d-4} - F_{d-5} \\ &\geq^{**} 0. \end{aligned}$$

The equality in (*) holds if and only if $n - d = 2$, and the equality in (**) holds if and only if $d = 5$. That is to say, $z(Q^{3,2}_{n-d-2,2}) = z(Q^{4,2}_{n-d-2,2})$ if and only if $n = 7$ and $d = 5$; otherwise, $z(Q^{3,2}_{n-d-2,2}) < z(Q^{4,2}_{n-d-2,2})$ Hence, (ii) holds.

This completes the proof of Theorem 2.14. □

Note that when $d \geq 4$,

$$z(Q^{4,2}_{n-d-2,2}) = (n-d-2)(F_{d-1} + F_{d-3}) + F_{d+1} + F_{d-1} + 3F_{d-3}. \quad (2.11)$$

By Eq. (2.2) and Eq.(2.11), it is easy to see that

$$z(Q^{4,2}_{n-d-2,2}) < z(U^{3,2}_{n-d-3}). \quad (2.12)$$

When $d = 3$, by (2.2) and (2.8), we have

$$z(Q^{3,2}_{n-5,2}) < z(U^{3,2}_{n-6}). \quad (2.13)$$

Summarizing Theorems 2.2 and 2.14, together with (2.12)-(2.13), we obtain our main results of this paper.

Theorem 2.15. *Let* $G \in \mathcal{U}_{n,d}$.

(i) *If* $d = 3$, *then* $z(G) \geq 3n - 6$ *with equality if and only if* $G \cong Q^{3,2}_{n-5,2}$.
(ii) *If* $d \geq 4$, *then*

$$z(G) \geq \begin{cases} 24, & \text{if } n = 7, d = 5; \\ (3n - 3d + 4)F_{d-3} + (n - d + 2)F_{d-4}, & \text{otherwise.} \end{cases} \quad (2.14, 2.15)$$

Equality in (2.14) *holds if and only if* $G \cong G^*$ *or* $G \cong G^{**}$, *where* G^*, G^{**} *are depicted in Figure* 5; *equality in* (2.15) *holds if and only if* $G \cong Q^{4,2}_{n-d-2,2}$ (*see Figure* 2).

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