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Research article

The extremal unicyclic graphs with given diameter and minimum edge revised Szeged index

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Abstract: Let H be a connected graph. The edge revised Szeged index of H is defined as $Sz_e^*(H) = \sum\limits_{e=uv\in E_H}(m_u(e|H) + \frac{m_0(e|H)}{2})(m_v(e|H) + \frac{m_0(e|H)}{2})$, where $m_u(e|H)$ (resp., $m_v(e|H)$) is the number of edges whose distance to vertex u (resp., v) is smaller than to vertex v (resp., u), and $m_0(e|H)$ is the number of edges equidistant from u and v. In this paper, the extremal unicyclic graphs with given diameter and minimum edge revised Szeged index are characterized.

Keywords: unicyclic graph; diameter; edge revised Szeged index; edge Szeged index
Mathematics Subject Classification: 05C12, 05C90

1. Introduction

Let $H = (V_H, E_H)$ be a simple and connected graph, where V_H and E_H be the vertex set and the edge set of H, respectively. For $u \in V_H$, the *degree* of u in H, denoted by $deg_H(u)$, is the number of edges which connected to u in H. If $deg_H(u) = 1$, then, u is a *pendant vertex*. For an edge $e = xy \in E_H$, e is a *pendant edge* of H if $deg_H(x) = 1$ or $deg_H(y) = 1$. For any $u, v \in V_H$, $d_H(u, v)$ denote the distance between u and v in H. The diameter of a graph H is the maximum distance between any vertex pair in H. Denote by P_n, C_n and S_n the path, the cycle and the star with n vertices, respectively. For integers $i \le j$, $[i, j]$ denote the set $\{k \in \mathbb{Z}, i \le k \le j\}$. One can refer to [1] for other notations and terminologies undefined throughout this paper.

The topological indices can be used in theoretical chemistry for understanding the physicochemical properties of chemical compounds. The atoms and bonds of molecules can be represented by the vertices and edges of graphs, respectively. The first and most well-known topological index, named Wiener index, was introduced by the famous chemist Harry Wiener for investigating boiling points of alkanes [21]. The Wiener index and its deformation were studied extensively by many researchers [9, 10, 12, 16]. The edge version of the Wiener index, named edge Wiener index [3], of a graph H is defined as follows:

$$W_e(H) = \sum_{\{f_1,f_2\}\subseteq E_H} d_H(f_1, f_2).$$

If $e = xy$ and f are two edges of H and w is a vertex of H, the distance between e and w is defined as $d_H(e,w) = \min\{d_H(x,w), d_H(y,w)\}$, and the distance between e and f is defined as $d_H(e, f) = \min\{d_H(x, f), d_H(y, f)\}$. For an edge $e = xy$ of H, the edge set E_H can be partitioned into three sets as follows:

$$\begin{aligned} M_x(e|H) &= \{f \in E_H : d_H(x, f) < d_H(y, f)\}, \\ M_y(e|H) &= \{f \in E_H : d_H(y, f) < d_H(x, f)\}, \\ M_0(e|H) &= \{f \in E_H : d_H(x, f) = d_H(y, f)\}. \end{aligned}$$

Set $m_x(e|H) = |M_x(e|H)|$, $m_y(e|H) = |M_y(e|H)|$ and $m_0(e|H) = |M_0(e|H)|$. The edge Szeged index of a graph H was introduced by Gutman and Ashrafi [5], and defined as

$$Sz_e(H) = \sum_{e=xy\in E_H} m_x(e|H)m_y(e|H).$$

The edge Szeged index does not consider the edges with equal distances from the endpoints of an edge. A modified version of the edge Szeged index, named edge revised Szeged index [4], of a graph H is defined as:

$$Sz_e^*(H) = \sum_{e=xy\in E_H} (m_x(e|H) + \frac{m_0(e|H)}{2})(m_y(e|H) + \frac{m_0(e|H)}{2}).$$

In recently, the study on the topological indices of the unicyclic graphs with given diameter received more and more attention. The minimum Wiener index of the unicyclic graphs with given diameter was investigated independently in [18] and [17]. Liu et al. [14] studied the minimum Szeged index of the unicyclic graphs with given diameter. Wang et al. [19] characterized the minimum edge Szeged index and corresponding extremal graphs among all the unicyclic graphs with given order and diameter. Yu et al. [22] identified the unicyclic graphs with given diameter having minimum revised Szeged index. For other results on topological indices, one can refer to [2, 8, 11, 13, 15]. Before presenting our main results, we introduce some definitions firstly.

Let $P_n = v_1v_2\cdots v_n$ be an n-vertex path, $C_g = u_1u_2\cdots u_gu_1$ be a g-vertex cycle and T_i be a tree with root vertex w_i for $i \in [1, g]$. Denote by $TP^s_{n,k}$ the tree formed by attaching s pendant vertices to v_k, (see Figure 1). Let $U^g_{T_1,T_2,\cdots,T_g}$ be the unicyclic graph obtained from the cycle $C_g = u_1u_2\cdots u_gu_1$ by identifying the root vertex w_i of T_i with u_i for $i \in [1, g]$. Obviously, $TP^0_{n,k} \cong P_n$, $TP^{n-2}_{3,2} \cong S_{n+1}$, $TP^s_{n,k} \cong TP^s_{n,n+1-k}$ and $U^g_{S_1,S_1,\cdots,S_1} \cong C_g$, and any unicyclic graph can be represented in the form of $U^g_{T_1,T_2,\cdots,T_g}$.

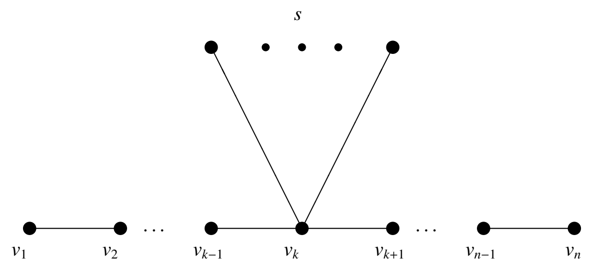

Figure 1. The tree $TP^s_{n,k}$.

Let H be an unicyclic graph with diameter d and order n. It can be checked that $H \cong C_3$ if $d = 1$; $H \in \{C_4, U^3_{P_2,S_1,S_1}\}$ if $d = 2$ and $n = 4$; $H \in \{C_5, C^3_{S_3,S_1,S_1}\}$ if $d = 2$ and $n = 5$; $H \cong U^3_{S_{n-2},S_1,S_1}$ for $d = 2$ and $n \geq 6$. Thus, it is trivial to determine the minimum edge revised Szeged index of the unicyclic graphs with diameter $1 \leq d \leq 2$. Let $\mathcal{UC}^d_n$ be the set of n-vertex unicyclic graphs with diameter d ($d \in [3, n-2]$). Recently, Wang and Liu [20] established the lower bound of edge revised Szeged index of unicyclic graphs with given diameter and characterized the corresponding extremal graphs. But there is a flaw in their proof as the cases of $d = n-2$ and $d = n-3$ have not been discussed. In this paper, by using a completely different approach with Wang and Liu [20], the extremal graphs in $\mathcal{UC}^d_n$ with minimum edge revised Szeged index are characterized. The following Theorem 1.1 is our main result.

Theorem 1.1. *Let $H \in \mathcal{UC}^d_n$ ($n > 15$ and $3 \leq d \leq n-2$) be the unicyclic graph with minimum edge revised Szeged index.*

(i) If $d = n-2$, then $H \cong U^3_{P_{\lfloor \frac{d-1}{2} \rfloor+1}, P_{\lceil \frac{d-1}{2} \rceil+1}, S_1}$;

(ii) If $d = n-3$, then $H \cong U^3_{TP^0_{d+1,\lfloor \frac{d}{2} \rfloor+1}, S_1, S_1}$;

(iii) If $7 \leq d \leq n-4$, then $H \cong U^4_{TP^{n-d-4}_{d+1,\lfloor \frac{d}{2} \rfloor+1}, S_1, S_1, S_1}$;

(iv) If $3 \leq d \leq 6$, then $H \cong U^4_{TP^{n-d-2}_{d-1,d-1}, S_1, S_1, S_1}$.

Some properties of the edge revised Szeged index of graphs are represented in Section 3, and we prove that the cycle length of the graphs in $\mathcal{UC}^d_n$ with minimum edge revised Szeged index is 3 or 4. Moreover, the extremal unicyclic graphs in $\mathcal{UC}^d_n$ with minimum edge revised Szeged index and cycle length 3 (resp., 4) are identified in Section 4 (resp., Section 5). Furthermore, the Theorem 1.1 is proved in Section 6.

2. Lemmas

For an integer g, define

$$\tau(g) = \begin{cases} 1, & \text{if } g \text{ is odd ;} \\ 0, & \text{if } g \text{ is even.} \end{cases}$$

Let H be a connected graph. For any edge $e = xy \in E_H$, define

$$m_H(e) = m_x(e|H) m_y(e|H)$$

and

$$m^*_H(e) = [m_x(e|H) + \frac{m_0(e|H)}{2}][m_y(e|H) + \frac{m_0(e|H)}{2}].$$

Lemma 2.1. *Let $H = U^g_{T_1,T_2,\cdots,T_g}$ be an unicyclic graph with $|V_H| = n$. Then,*

$$Sz_e^*(H) = Sz_e(H) + \frac{1}{4}n(2n-1) + \frac{1}{4}(2n-3)g + \tau(g)[\frac{1}{4}g(5-4n) + \frac{n^2-n}{2} - \frac{1}{4}\sum_{i=1}^{g}|E_{T_i}|^2].$$

Proof. We divide the edges of H into two types:

(a) the edges belonging to the tree T_i for $i = 1, 2, \cdots, g$;

(b) the edges belonging to the unique cycle C_g of H.

Firstly, we consider the edges of type (a). For each edge $e = xy$ of T_i ($i \in [1, g]$), it can be checked that $m_x(e|H) + m_y(e|H) = n-1$ and $m_0(e|H) = 1$. Let μ be the contributions to $Sz_e^*(H)$ of the edges of type (a). Then,

$$\begin{aligned}
\mu &= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}}[m_x(e|H) + \frac{m_0(e|H)}{2}][m_y(e|H) + \frac{m_0(e|H)}{2}] \\
&= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}} m_H(e) + \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}}[\frac{m_0(e|H)}{2}(m_x(e|H) + m_y(e|H)) + \frac{(m_0(e|H))^2}{4}] \\
&= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}} m_H(e) + \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}}[\frac{1}{2}(n-1) + \frac{1}{4}] \\
&= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}} m_H(e) + (n-g)[\frac{1}{2}(n-1) + \frac{1}{4}] \\
&= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}} m_H(e) + \frac{1}{4}(2n-1)(n-g).
\end{aligned}$$

Now, we consider the edges of type (b). We divide this problem into two cases according to the parity of g.

Case 1. g is even.

For each edge $e = xy \in E_{C_g}$, it can be checked that $m_x(e|H) + m_y(e|H) = n-2$ and $m_0(e|H) = 2$. Let λ_1 be the contributions to $Sz_e^*(H)$ of the edges of type (b). Then,

$$\begin{aligned}
\lambda_1 &= \sum_{e=xy\in E_{C_g}}[m_x(e|H) + \frac{m_0(e|H)}{2}][m_y(e|H) + \frac{m_0(e|H)}{2}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \sum_{e=xy\in E_{C_g}}[\frac{m_0(e|H)}{2}(m_x(e|H) + m_y(e|H)) + \frac{(m_0(e|H))^2}{4}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \sum_{e=xy\in E_{C_g}}[\frac{2}{2}(n-2) + \frac{4}{4}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + g(n-1).
\end{aligned}$$

By the definition of edge revised Szeged index, we have

$$Sz_e^*(H) = \mu + \lambda_1$$

$$= \sum_{i=1}^{g}\sum_{e=xy\in E_{T_i}} m_H(e) + \frac{1}{4}(2n-1)(n-g) + \sum_{e=xy\in E_{C_g}} m_H(e) + g(n-1)$$
$$= Sz_e(H) + \frac{1}{4}(2n-1)n + \frac{1}{4}(2n-3)g.$$

Case 2. g is odd.

Let λ_2 be the contributions to $Sz_e^*(H)$ of the edges of type (b). It can be checked that

$$\begin{aligned}
\lambda_2 &= \sum_{e=xy\in E_{C_g}} [m_x(e|H) + \frac{m_0(e|H)}{2}][m_y(e|H) + \frac{m_0(e|H)}{2}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \sum_{e=xy\in E_{C_g}} [\frac{m_0(e|H)}{2}(m_x(e|H) + m_y(e|H)) + \frac{(m_0(e|H))^2}{4}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \sum_{i=1}^{g}[\frac{|E_{T_i}|+1}{2}(n-|E_{T_i}|-1) + \frac{(|E_{T_i}|+1)^2}{4}] \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \frac{n^2}{2} - \sum_{i=1}^{g}\frac{|E_{T_i}|^2}{4} - \sum_{i=1}^{g}\frac{|E_{T_i}|}{2} - \frac{1}{4}g \\
&= \sum_{e=xy\in E_{C_g}} m_H(e) + \frac{n^2}{2} - \sum_{i=1}^{g}\frac{|E_{T_i}|^2}{4} - \frac{n-g}{2} - \frac{1}{4}g.
\end{aligned}$$

By the definition of edge revised Szeged index, we have

$$\begin{aligned}
Sz_e^*(H) &= \mu + \lambda_2 \\
&= Sz_e(H) + \frac{1}{4}(4n-3)n - \frac{1}{2}(n-1)g - \sum_{i=1}^{g}\frac{|E_{T_i}|^2}{4}.
\end{aligned}$$

The proof is completed. □

Lemma 2.2. [6] *Let $H = U^g_{T_1,T_2,\cdots,T_g}$ be an unicyclic graph with $|V_H| = n$ and $C_g = v_1v_2\cdots v_gv_1$ be the unique cycle of H. Let*

$$S = \sum_{e\in E_{C_g}} m_H(e).$$

Then,

$$\begin{aligned}
S &= g(\lceil\frac{g-2}{2}\rceil)^2 + \lceil\frac{g-2}{2}\rceil g(n-g) - \tau(g)\lceil\frac{g-2}{2}\rceil(n-g) \\
&\quad + \sum_{i=1}^{g}\sum_{j=1}^{g}|E_{T_i}||E_{T_j}|d_{C_g}(v_i,v_j) - \tau(g)\sum_{i<j}|E_{T_i}||E_{T_j}|.
\end{aligned}$$

Lemma 2.3. [7] *Let H and H' be the graphs shown as in Figure 2, where H consists of H_0 and H_1 with a common vertex u, and H' consists of H_0 and H_2 with a common vertex u. If $|E_{H_1}| = |E_{H_2}|$, then,*

$$\sum_{e\in E_{H_0}} m_H(e) = \sum_{e\in E_{H_0}} m_{H'}(e).$$

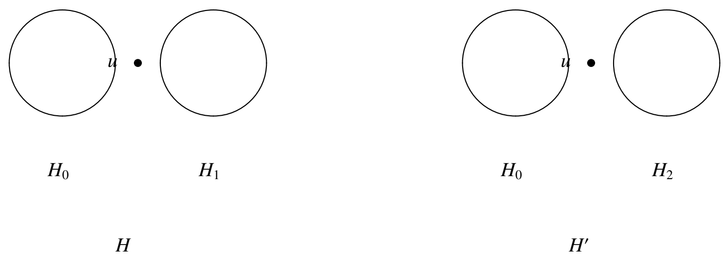

Figure 2. H and H' in Lemma 2.3.

By similar proof process of Lemma 2.3, the following corollary holds directly.

Corollary 2.4. *Let H_0, H_1, H_2, H and H' be the graphs defined in Lemma 2.3. If $|E_{H_1}| = |E_{H_2}|$, then,*

$$\sum_{e\in E_{H_0}} m^*_H(e) = \sum_{e\in E_{H_0}} m^*_{H'}(e).$$

3. Properties of the edge revised Szeged index of graphs

Fact 1: Let $i \in [0, n]$ be an integer. Then $(i + \frac{1}{2})(n - i + \frac{1}{2}) \geq \frac{1}{2}(n + \frac{1}{2})$ with equality holds if and only if $i = 0$ or n.

Lemma 3.1. *Let H_0 be a connected graph with a vertex u and T be a tree. Let H (resp., H') be the graph obtained by identifying u (resp., u) with a vertex of T (resp., the root vertex of $|V_T|$-vertex star $S_{|V_T|}$), (see Figure 3). Then,*

$$Sz_e(H) \geq Sz_e(H')$$

and

$$Sz^*_e(H) \geq Sz^*_e(H')$$

with equalities hold if and only if $H \cong H'$.

Figure 3. H and H' in Lemma 3.1.

Proof. By Lemma 2.3 and Corollary 2.4, one has

$$Sz_e(H) - Sz_e(H') = \sum_{e\in E_T} m_H(e) - \sum_{e\in E_{S_{|V_T|}}} m_{H'}(e)$$

and

$$Sz^*_e(H) - Sz^*_e(H') = \sum_{e\in E_T} m^*_H(e) - \sum_{e\in E_{S_{|V_T|}}} m^*_{H'}(e).$$

By the fact that pendant edges make no contributions to the edge Szeged index and Fact 1, the results hold. □

Corollary 3.2. *Let $H \in \mathcal{UC}_d^n$ with minimum edge revised Szeged index. Let C_g be the unique cycle of H and $\mathcal{P}_H^d$ be a longest path in H. If an edge $e \in E_H \setminus \{E_{C_g} \cup E_{\mathcal{P}_H^d}\}$, then e is a pendant edge.*

Lemma 3.3. *Let H_1 and H_2 be two connected graphs which connected by an edge $e = uv$, H_0 be a connected graph with a vertex w. Let H (resp., H') be a graph obtained by identifying w with u (resp., v), (see Figure 4). If $|E_{H_2}| \geq |E_{H_1}|$, then,*

$$Sz_e(H) \geq Sz_e(H')$$

and

$$Sz_e^*(H) \geq Sz_e^*(H')$$

with equalities hold if and only if $|E_{H_0}| = 0$ or $|E_{H_1}| = |E_{H_2}|$.

Figure 4. H and H' in Lemma 3.3.

Proof. Let $|E_{H_i}| = m_i$ for $i = 0, 1, 2$. By Lemma 2.3 and Corollary 2.4, one has

$$\begin{aligned} Sz_e(H) - Sz_e(H') &= m_H(e) - m_{H'}(e) \\ &= (m_1 + m_0)m_2 - m_1(m_0 + m_2) \\ &= m_0(m_2 - m_1) \end{aligned}$$

and

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= m_H^*(e) - m_{H'}^*(e) \\ &= (m_1 + m_0 + \frac{1}{2})(m_2 + \frac{1}{2}) - (m_1 + \frac{1}{2})(m_0 + m_2 + \frac{1}{2}) \\ &= m_0(m_2 - m_1). \end{aligned}$$

Thus, the results hold. □

Corollary 3.4. *Let $H = U^g_{T_1,T_2,T_3,\cdots,T_{g-1},T_g} \in \mathcal{UC}_d^n$ with minimum edge revised Szeged index. Let $C_g = u_1u_2\cdots u_gu_1$ be the unique cycle of H and $\mathcal{P}_H^d$ be a longest path in H.*

(i) If $V_{C_g} \cap V_{\mathcal{P}_H^d} = \{u_i\}$, then $T_i \cong TP^{|E_{T_i}|-d}_{d+1,\lfloor \frac{d}{2} \rfloor+1}$ and $T_j \cong S_{|V_{T_j}|}$ for $j \neq i$.

(ii) If $V_{C_g} \cap V_{\mathcal{P}_H^d} = \{u_i, u_{i+1}, \cdots, u_j\}$ and $|E_{\mathcal{P}_H^d} \cap E_{T_i}| = l_1 \leq l_2 = |E_{\mathcal{P}_H^d} \cap E_{T_j}|$, then $T_k \cong S_{|V_{T_k}|}$ for $k \notin \{i, j\}$, $T_i \cong TP^{|E_{T_i}|-l_1}_{l_1+1,l_1+1}$ and $T_j \cong TP^{|E_{T_j}|-l_2}_{l_2+1,s}$ for some $s \in [1, l_2 + 1]$.

Lemma 3.5. *Let $l_1 \geq 0$ and $g \geq 5$ be two integers. Let $H = U^g_{T_1,T_2,T_3,\cdots,T_{g-1},T_g}$ and $H' = U^{g-2}_{T'_1,T_3,\cdots,T_{g-1}}$ be two unicyclic graphs with $|E_H| = |E_{H'}| = n$ as shown in Figure 5, where T_1 consists of an l_1-length path and a tree T_0 with a common vertex, T'_1 consists of a pendant edge, an (l_1+1)-length path and the three trees T_0, T_2 and T_g with a common vertex. Let $C_g = u_1u_2\cdots u_gu_1$ and $C'_{g-2} = u_1u_3\cdots u_{g-1}u_1$ be the unique cycle of H and H', respectively. If $\sum_{j=3}^{g-1}|E_{T_j}| \geq l_1$, then $Sz_e(H') < Sz_e(H)$ and $Sz^*_e(H') < Sz^*_e(H)$.*

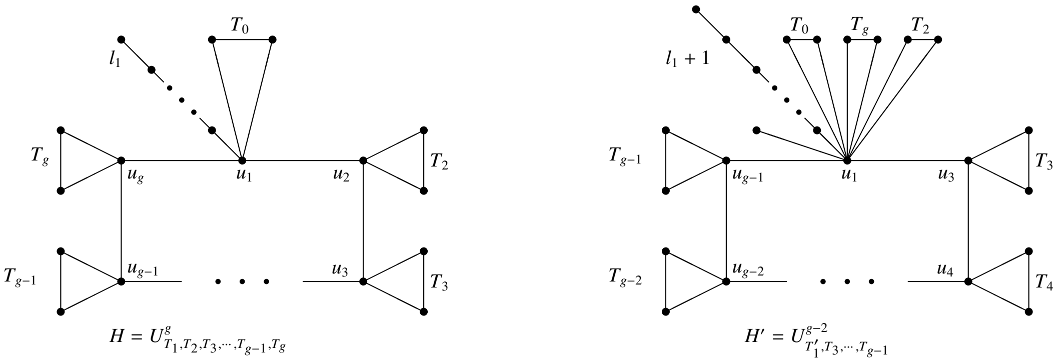

Figure 5. H and H' in Lemma 3.5.

Proof. Let $m_p = |E_{T_p}|$ and $d_{p,q} = d_H(u_p,u_q)$ for each $p,q \in [1,g]$. Let $d'_{i,j} = d_{H'}(u_i,u_j)$ for $i,j \in \{1,3,4,\cdots,g-1\}$ and $m'_1 = |E_{T'_1}|$. It can be checked that $n = \sum_{i=1}^{g} m_i + g$ and $m'_1 = m_1 + m_2 + m_g + 2$.

From Lemma 2.3, one has

$$\sum_{e\in E_H\setminus E_{C_g}} m(e|H) = \sum_{e\in E_{H'}\setminus E_{C'_{g-2}}} m(e|H') - l_1(n-1-l_1).$$

By Lemma 2.2, we have

$$\begin{aligned}\sum_{e\in E_{C_g}} m(e|H) &= g(\lceil\frac{g-2}{2}\rceil)^2 + \lceil\frac{g-2}{2}\rceil g(n-g) - \tau(g)\lceil\frac{g-2}{2}\rceil(n-g)\\ &\quad + \sum_{i=1}^{g}\sum_{j=1}^{g} m_im_jd_{i,j} - \tau(g)\sum_{1\leq i<j\leq g} m_im_j\end{aligned}$$

and

$$\begin{aligned}\sum_{e\in E_{C'_{g-2}}} m(e|H') &= (g-2)(\lceil\frac{g-4}{2}\rceil)^2 + \lceil\frac{g-4}{2}\rceil(g-2)(n-g+2) - \tau(g)\lceil\frac{g-4}{2}\rceil(n-g+2)\\ &\quad + \sum_{i=3}^{g-1}\sum_{i=3}^{g-1} m_im_jd'_{i,j} + 2\sum_{j=3}^{g-1} m'_1m_jd'_{i,j} - \tau(g)[\sum_{3\leq i<j\leq g-1} m_im_j + \sum_{j=3}^{g-1} m'_1m_j].\end{aligned}$$

Thus,

$$Sz_e(H) - Sz_e(H') \geq \Lambda_1 + 2\Lambda_2 - \Lambda_3 - \tau(g)\Lambda_4,$$

where

$$\Lambda_1 = g(\lceil\frac{g-2}{2}\rceil)^2 + \lceil\frac{g-2}{2}\rceil g(n-g) - \tau(g)\lceil\frac{g-2}{2}\rceil(n-g)$$

$$
\begin{aligned}
& -(g-2)(\lceil\frac{g-4}{2}\rceil)^2-\lceil\frac{g-4}{2}\rceil(n-g+2)(g-2)+\tau(g)\lceil\frac{g-4}{2}\rceil(n-g+2),\\
\Lambda_2 &= \sum_{j=3}^{g-1} m_1m_jd_{1,j}-\sum_{j=3}^{g-1} m_1'm_jd_{1,j}'+\sum_{j=3}^{g-1} m_2m_jd_{2,j}+\sum_{j=3}^{g-1} m_gm_jd_{g,j}\\
& +m_1m_2d_{1,2}+m_1m_gd_{1,g}+m_2m_gd_{2,g},\\
\Lambda_3 &= l_1(n-1-l_1),\\
\Lambda_4 &= \sum_{j=2}^{g} m_1m_j-\sum_{j=3}^{g-1} m_1'm_j+\sum_{j=3}^{g-1} m_2m_j+\sum_{j=3}^{g-1} m_gm_j+m_2m_g\\
&= m_1m_2+m_1m_g+m_2m_g-2\sum_{j=3}^{g-1} m_j.
\end{aligned}
$$

In the following, the lower bounds of Λ_1 and Λ_2 and the upper bound of Λ_3 are investigated by Claims 1–3, respectively.

Claim 1. $\Lambda_1 > \sum_{j=3}^{g-1} m_j[g+2\lceil\frac{g-2}{2}\rceil-2-\tau(g)]+g(m_1+m_2+m_g+1)$.

Proof of Claim 1: Let $\lceil\frac{g-2}{2}\rceil = x$. Then,

$$\Lambda_1 = g(n-g+1)+2(x-1)(n-g+2)-\tau(g)(n-g+2-2x)+2(x-1)^2.$$

As $n-g=\sum_{j=1}^{g} m_j$ and $x-1>0$, one has

$$g(n-g+1) \geq g\sum_{j=3}^{g-1} m_j+g(m_1+m_2+m_g+1),$$

$$2(x-1)(n-g+2) \geq \sum_{j=3}^{g-1} m_j(2x-2)+m_1+m_2+m_g$$

and

$$\tau(g)(n-g+2-2x) \leq \tau(g)(n-g) = \tau(g)\sum_{j=1}^{g} m_j.$$

Hence,

$$\Lambda_1 > \sum_{j=3}^{g-1} m_j[g+2x-2-\tau(g)]+g(m_1+m_2+m_g+1).$$

This completes the proof of Claim 1.

Claim 2. $\Lambda_2 \geq \sum_{j=3}^{g-1} m_j(m_1-2d_{1,j}')+m_1m_2+m_1m_g+2m_2m_g$.

Proof of Claim 2: From the fact $d_{1,j}'=d_{1,j}-1$ for $j\in[3,g-1]$, we have

$$\Lambda_2 = \sum_{j=3}^{g-1} m_1m_jd_{1,j}-\sum_{j=3}^{g-1} m_1'm_j(d_{1,j}-1)+\sum_{j=3}^{g-1} m_2m_jd_{2,j}+\sum_{j=3}^{g-1} m_gm_jd_{g,j}$$

$$
\begin{aligned}
&+m_1m_2d_{1,2}+m_1m_gd_{1,g}+m_2m_gd_{2,g}\\
= &\sum_{j=3}^{g-1} m_j[m_2(d_{2,j}-d_{1,j}+1)+m_g(d_{g,j}-d_{1,j}+1)+m_1-2d'_{1,j}]\\
&+m_1m_2+m_1m_g+2m_2m_g.
\end{aligned}
$$

As $d_{2,j}+1\geq d_{1,j}$ and $d_{g,j}+1\geq d_{1,j}$, $\sum\limits_{j=3}^{g-1} m_j[m_2(d_{2,j}-d_{1,j}+1)+m_g(d_{g,j}-d_{1,j}+1)]\geq 0$.

This completes the proof of Claim 2.

Claim 3. $\Lambda_3\leq 2m_1\sum\limits_{j=3}^{g-1} m_j+m_1m_2+m_1m_g+m_1(g-1)$.

Proof of Claim 3: It can be checked that

$$\Lambda_3=l_1(n-1-l_1)=l_1(\sum_{j=1}^{g} m_j+g-1-l_1)=l_1\sum_{j=2}^{g} m_j+l_1m_1+l_1(g-1)-l_1^2.$$

By $l_1\leq m_1$ and $l_1\leq \sum_{j=3}^{g-1} m_j$, we have

$$
\begin{aligned}
\Lambda_3 &= l_1\sum_{j=3}^{g-1} m_j+l_1m_1+l_1m_2+l_1m_g+l_1(g-1)-l_1^2\\
&\leq m_1\sum_{j=3}^{g-1} m_j+m_1\sum_{j=3}^{g-1} m_j+m_1m_2+m_1m_g+l_1(g-1)-l_1^2\\
&\leq 2m_1\sum_{j=3}^{g-1} m_j+m_1m_2+m_1m_g+l_1(g-1)\\
&\leq 2m_1\sum_{j=3}^{g-1} m_j+m_1m_2+m_1m_g+m_1(g-1).
\end{aligned}
$$

Claim 4. $\sum\limits_{j=3}^{g-1} m_j[g+2\lceil\frac{g-2}{2}\rceil-2-4d'_{1,j}+\tau(g)]\geq 4\tau(g)\sum\limits_{j=3}^{g-1} m_j$.

Proof of Claim 4: If g is even, then $d'_{1,j}\leq\frac{g-2}{2}$ and $\tau(g)=0$. Thus,

$$\sum_{j=3}^{g-1} m_j[g+2\lceil\frac{g-2}{2}\rceil-2-4d'_{1,j}-3\tau(g)]\geq\sum_{j=3}^{g-1} m_j[g+2\cdot\frac{g-2}{2}-2-4\cdot\frac{g-2}{2}]=0.$$

If g is odd, then $d'_{1,j}\leq\frac{g-3}{2}$, $\lceil\frac{g-2}{2}\rceil=\frac{g-1}{2}$ and $\tau(g)=1$. Thus,

$$
\begin{aligned}
\sum_{j=3}^{g-1} m_j[g+2\lceil\frac{g-2}{2}\rceil-2-4d'_{1,j}-3\tau(g)] &\geq \sum_{j=3}^{g-1} m_j[g+2\cdot\frac{g-1}{2}-2-4\cdot\frac{g-3}{2}+1]\\
&= 4\sum_{j=3}^{g-1} m_j.
\end{aligned}
$$

This completes the proof of Claim 4.

By Claims 1–4, one has that

$$\begin{aligned}
\Lambda_1 + 2\Lambda_2 - \Lambda_3 - \tau(g)\Lambda_4 &> \sum_{j=3}^{g-1} m_j[g + 2\lceil\frac{g-2}{2}\rceil - 2 - \tau(g)] + g(m_1 + m_2 + m_3 + 1) \\
&\quad +2\sum_{j=3}^{g-1} m_j(m_1 - 2d'_{1,j}) + 2m_1m_2 + 2m_1m_g + 2m_2m_g \\
&\quad -2m_1\sum_{j=3}^{g-1} m_j - m_1m_2 - m_1m_g - m_1(g-1) \\
&\quad +2\tau(g)\sum_{j=3}^{g-1} m_j - m_1m_2 - m_1m_g - m_2m_g \\
&\geq \sum_{j=3}^{g-1} m_j[g + 2\lceil\frac{g-2}{2}\rceil - 2 - 4d'_{1,j} + \tau(g) + 2m_1 - 2m_1] \\
&\quad +g(m_2 + m_3 + 1) + m_1 \\
&\geq 4\tau(g)\sum_{j=3}^{g-1} m_j + m_1 + g(m_2 + m_g + 1) \\
&\geq \tau(g)\sum_{j=3}^{g-1} m_j + m_1 + m_2 + m_g + g \\
&\geq \tau(g)n.
\end{aligned}$$

Thus, $Sz_e(H) > Sz_e(H')$.

Since $|E_{T'_1}| = |E_{T_1}| + |E_{T_2}| + |E_{T_g}| + 2$, $|E_{T'_1}|^2 \geq |E_{T_1}|^2 + |E_{T_2}|^2 + |E_{T_g}|^2 + 4$. From Lemma 2.1, one has

$$\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') + \frac{2}{4}\cdot(2n-3) \\
&\quad +\frac{1}{4}\tau(g)[2\cdot(5-4n) - |E_{T_1}|^2 - |E_{T_2}|^2 - |E_{T_g}|^2 + |E_{T'_1}|^2] \\
&\geq Sz_e(H) - Sz_e(H') + n - \frac{3}{2} - \tau(g)(2n - \frac{5}{2}) \\
&> \tau(g)n + n - \frac{3}{2} - 2\tau(g)n + \tau(g)\frac{5}{2} \\
&> 0.
\end{aligned}$$

This completes the proof. □

The Lemma 3.5 shows the fact that one can decrease the cycle length and edge revised Szeged index of an unicyclic graph simultaneously keeping the diameter of the unicyclic graph.

Let $H = U^g_{T_1,T_2,T_3,\cdots,T_{g-1},T_g} \in \mathcal{UC}^d_n$ ($g \geq 5$) with $C_g = v_1v_2\cdots v_gv_1$ be the unique cycle of H and $\mathcal{P}^d_H$ be a longest path in H.

(i) If $|E_{C_g} \cap E_{\mathcal{P}^d_H}| \geq 2$, Lemma 3.5 can be used directly.

(ii) If $|E_{C_g} \cap E_{\mathcal{P}_H^d}| = 1$, the operations can be refer to Figure 6 and set $l_1 = 0$ in Lemma 3.5, regard v_{g-1} in Figure 6 as u_1 in Lemma 3.5.

(iii) If $|E_{C_g} \cap E_{\mathcal{P}_H^d}| = 0$, the operations can be refer to Figure 7 and set $l_1 = 0$ in Lemma 3.5, regard v_k ($k = \lceil \frac{g}{2} \rceil$) in Figure 7 as u_1 in Lemma 3.5.

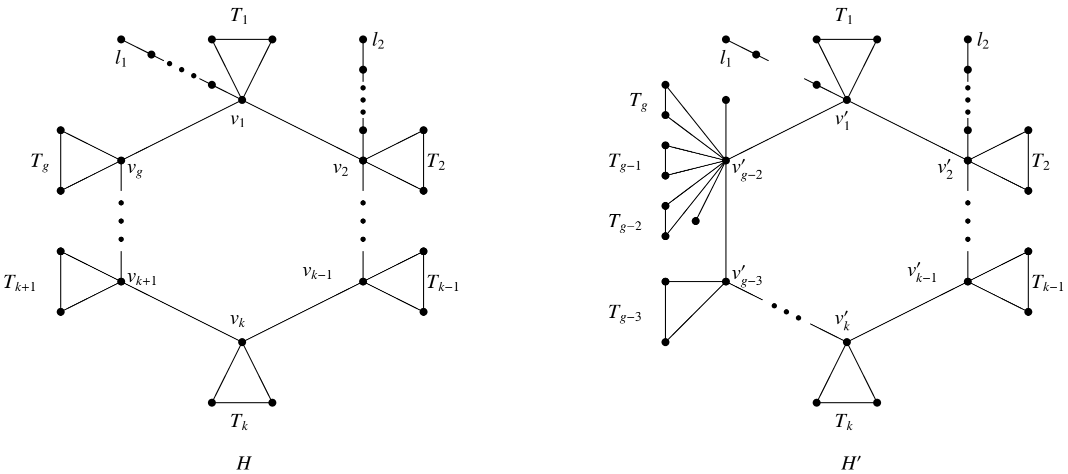

Figure 6. The case of $|E_{C_g} \cap E_{\mathcal{P}_H^d}| = 1$.

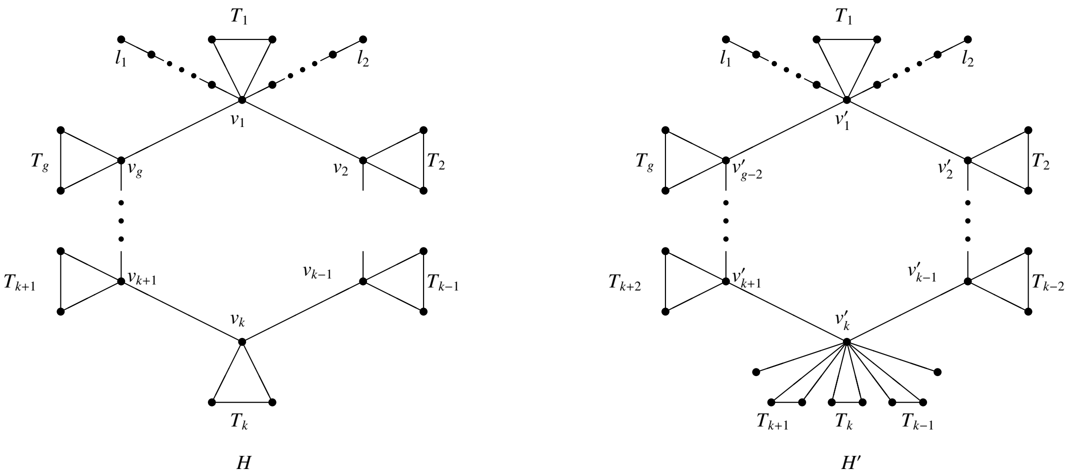

Figure 7. The case of $|E_{C_g} \cap E_{\mathcal{P}_H^d}| = 0$.

Corollary 3.6. *Let $H \in \mathcal{UC}_d^n$ with minimum edge revised Szeged index. Then the length of the unique cycle of H is* 3 *or* 4.

From Corollaries 3.2, 3.4 and 3.6, one has that the unicyclic graph with given diameter and minimum edge revised Szeged index must be one of the following five types in Figure 8.

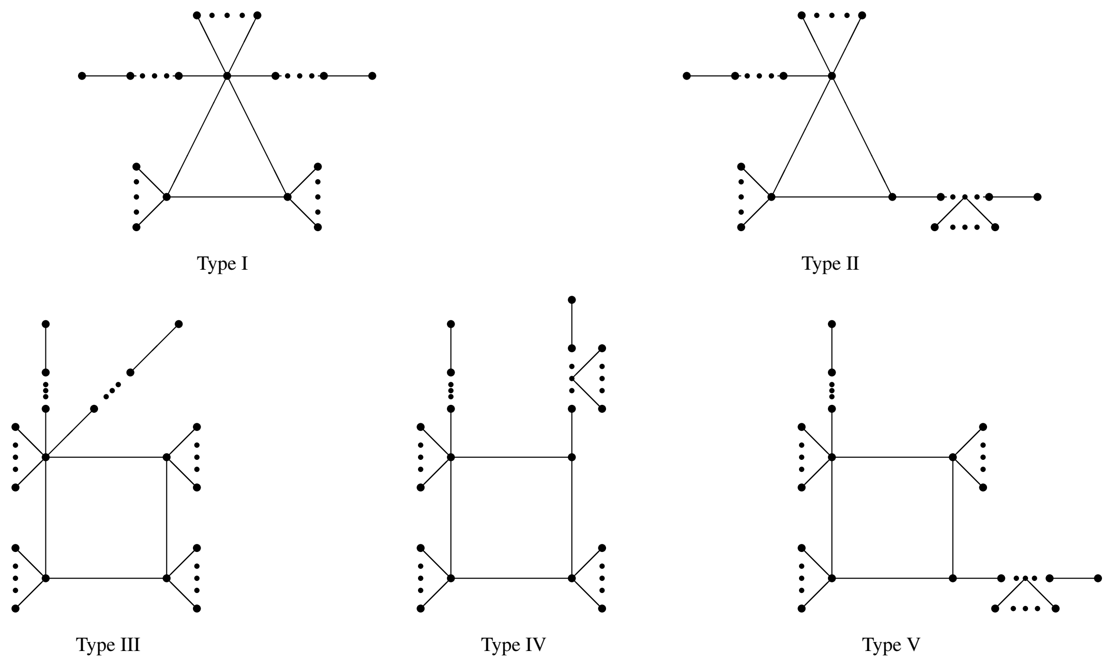

Figure 8. The five types unicyclic graphs.

4. The graphs with cycle length 3 and minimum edge revised Szeged index in $\mathcal{UC}_n^d$

In this section, the graphs with cycle length 3 and minimum edge revised Szeged index in $\mathcal{UC}_n^d$ are identified by comparing with the edge revised Szeged indices of the graphs of Type I and Type II in Figure 8.

Lemma 4.1. *Let $H = U^3_{T_1,S_{b+1},S_{c+1}}$ and $H' = U^3_{T_1',S_1,S_1}$ be two unicyclic graphs, where $T_1 \cong TP^a_{l_1+l_2+1,l_1+1}$ and $T_1' \cong TP^{a+b+c}_{l_1+l_2+1,l_1+1}$, (see Figure 9). Then, $Sz_e^*(H) \geq Sz_e^*(H')$ with equality holds if and only if $b = c = 0$.*

Figure 9. H and H' in Lemma 4.1.

Proof. By Corollary 2.4, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= \sum_{e \in E_{C_3}} m_H^*(e) - \sum_{e \in E_{C_3'}} m_{H'}^*(e) \\ &= (c + 1 + \frac{l_1 + l_2 + a + 1}{2})(b + 1 + \frac{l_1 + l_2 + a + 1}{2}) \end{aligned}$$

$$
\begin{aligned}
&+(l_1+l_2+a+1+\frac{c+1}{2})(b+1+\frac{c+1}{2})\\
&+(l_1+l_2+a+1+\frac{b+1}{2})(c+1+\frac{b+1}{2})\\
&-2(l_1+l_2+a+b+c+1+\frac{1}{2})(1+\frac{1}{2})\\
&-(1+\frac{l_1+l_2+a+b+c+1}{2})(1+\frac{l_1+l_2+a+b+c+1}{2})\\
= \;& \frac{3}{2}[bc+(b+c)(a+l_1+l_2)]\\
\geq \;& 0.
\end{aligned}
$$

□

Lemma 4.2. *Let $H = U^3_{T_1,T_2,S_{c+1}}$ and $H' = U^3_{T_1',T_2',S_{c+1}}$ be two unicyclic graphs, where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T_1' \cong TP^a_{l_1+2,l_1+2}$, $T_2 \cong TP^b_{l_2+1,i}$ and $T_2' \cong TP^b_{l_2,i}$ for some $i \in [1, l_2]$, (see Figure 10). If $l_1 + 2 \leq l_2$, then $Sz^*_e(H) > Sz^*_e(H')$.*

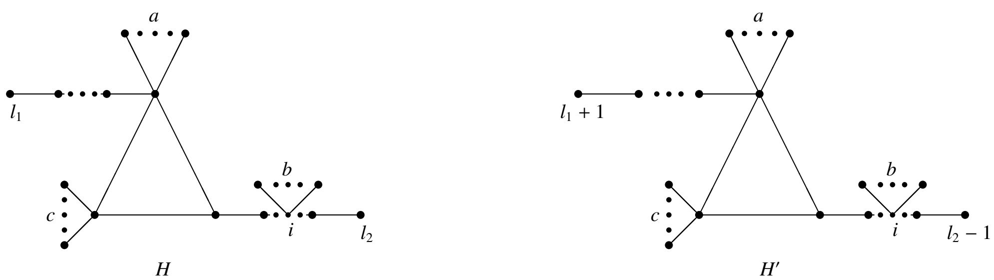

Figure 10. H and H' in Lemma 4.2.

Proof. By Corollary 2.4, one has

$$
\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') \;=\;& \sum_{e\in E_{C_3}} m^*_H(e) + (l_2-1+b+\frac{1}{2})(a+c+l_1+3+\frac{1}{2})\\
&-\sum_{e\in E_{C_3}} m^*_{H'}(e) - (l_1+\frac{1}{2})(a+b+c+l_2-1+3+\frac{1}{2})\\
=\;& (c+1+\frac{l_1+a+1}{2})(b+l_2+1+\frac{l_1+a+1}{2})\\
&+(l_1+a+1+\frac{c+1}{2})(b+l_2+1+\frac{c+1}{2})\\
&+(l_1+a+1+\frac{l_2+b+1}{2})(c+1+\frac{l_2+b+1}{2})\\
&+(l_2-1+b+\frac{1}{2})(a+c+l_1+3+\frac{1}{2})\\
&-(c+1+\frac{l_1+1+a+1}{2})(b+l_2-1+1+\frac{l_1+1+a+1}{2})\\
&-(l_1+1+a+1+\frac{c+1}{2})(b+l_2-1+1+\frac{c+1}{2})
\end{aligned}
$$

$$
\begin{aligned}
& -(l_1+1+a+1+\frac{l_2-1+b+1}{2})(c+1+\frac{l_2-1+b+1}{2}) \\
& -(l_1+\frac{1}{2})(a+b+c+l_2-1+3+\frac{1}{2}) \\
= \;& \frac{1}{2}(l_2+b-l_1-1)(3+2c+2a)+\frac{3}{2}a \\
> \;& 0.
\end{aligned}
$$

□

From Lemmas 3.3 and 4.2, the following corollary can be obtained.

Corollary 4.3. *Let $H = U^3_{T_1,T_2,S_{c+1}}$ be an unicyclic graph, where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T_2 \cong TP^b_{l_2+1,i}$ for some $i \in [1, l_2]$, (see Figure 11). Then, there exists an unicyclic graph $H' = U^3_{T'_1,T'_2,S_{c+1}}$ with $T'_1 \cong TP^a_{l_1+l_2-k+1,l_1+l_2-k+1}$ and $T'_2 \cong TP^b_{k+1,k+1}$ and $k \le l_2$ such that $Sz^*_e(H) \ge Sz^*_e(H')$.*

Figure 11. H and H' in Corollary 4.3.

Proof. If $l_2 \le l_1+1$, one has that the edge revised Szeged index decrease when i increased until $i = l_2+1$ by Lemma 3.3, that is

$$Sz^*_e(U^3_{T_1,TP^b_{l_2+1,i},S_{c+1}}) \ge Sz^*_e(U^3_{T_1,TP^b_{l_2+1,i+1},S_{c+1}}) \ge \cdots \ge Sz^*_e(U^3_{T_1,TP^b_{l_2+1,l_2+1},S_{c+1}}).$$

Then, $k = l_2$ and $H' = U^3_{T_1,TP^b_{l_2+1,l_2+1},S_{c+1}}$.

If $l_2-(l_2+1-i) \ge l_1+2+(l_2+1-i)$, the result holds by Lemma 4.2.

If $l_2 \ge l_1+2$ and $l_2-(l_2+1-i) \le l_1+1+(l_2+1-i)$, by Lemmas 4.2 and 3.3, one has

$$
\begin{aligned}
Sz^*_e(U^3_{TP^a_{l_1+1,l_1+1},TP^b_{l_2+1,i},S_{c+1}}) \;&>\; Sz^*_e(U^3_{TP^a_{l_1+1+s,l_1+1+s},TP^b_{l_2+1-s,i},S_{c+1}}) \\
&\ge\; Sz^*_e(U^3_{TP^a_{l_1+1+s,l_1+1+s},TP^b_{l_2+1-s,i+1},S_{c+1}}) \\
&\ge\; \cdots \\
&\ge\; Sz^*_e(U^3_{TP^a_{l_1+1+s,l_1+1+s},TP^b_{l_2+1-s,l_2+1-s},S_{c+1}}),
\end{aligned}
$$

where $s = \lfloor \frac{l_2-l_1-2}{2} \rfloor$ and $k = l_2 - s$.

This completes the proof. □

Lemma 4.4. *Let $H = U^3_{T_1,T_2,S_{c+1}}$ and $H' = U^3_{T'_1,T'_2,S_1}$ be two unicyclic graphs, where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T'_1 \cong P_{l_1+1}$, $T_2 \cong TP^b_{l_2+1,l_2+1}$ and $T'_2 \cong TP^{a+b+c}_{l_2+1,l_2+1}$, (see Figure 12). If $0 < l_1 \le l_2$, then $Sz^*_e(H) \ge Sz^*_e(H')$ with equality holds if and only if $c = a = 0$, or $c = 0$ and $b + l_2 - l_1 = 0$.*

Figure 12. H and H' in Lemma 4.4.

Proof. By Corollary 2.4, one has

$$\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= \sum_{e\in E_{C_3}} m_H^*(e) - \sum_{e\in E_{C_3'}} m_{H'}^*(e)\\
&= (c+1+\frac{l_1+a+1}{2})(b+l_2+1+\frac{l_1+a+1}{2})\\
&\quad +(l_1+a+1+\frac{c+1}{2})(b+l_2+1+\frac{c+1}{2})\\
&\quad +(l_1+a+1+\frac{l_2+b+1}{2})(c+1+\frac{l_2+b+1}{2})\\
&\quad -(1+\frac{l_2+a+b+c+1}{2})(l_1+1+\frac{l_2+a+b+c+1}{2})\\
&\quad -(l_1+1+\frac{1}{2})(l_2+a+b+c+1+\frac{1}{2})\\
&\quad -(1+\frac{l_1+1}{2})(l_2+a+b+c+1+\frac{l_1+1}{2})\\
&= \frac{3}{2}[ab+ac+bc+cl_2+a(l_2-l_1)]\\
&\geq 0.
\end{aligned}$$

□

Lemma 4.5. *Let $H = U^3_{T_1,T_2,S_1}$ and $H' = U^3_{T_1',S_1,S_1}$ be two unicyclic graphs, where $T_1 \cong P_{l_1+1}$, $T_2 \cong TP^a_{l_2+1,l_2+1}$ and $T_1' \cong TP^{a-1}_{l_1+l_2+1,l_1+2}$, (see Figure 13). If $a \geq 1$, $l_2 \geq l_1 > 0$ and $l_2 + a > 4$, then $Sz_e^*(H) > Sz_e^*(H')$.*

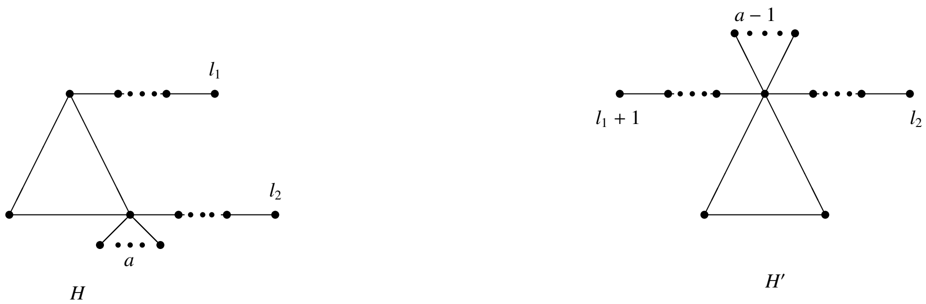

Figure 13. H and H' in Lemma 4.5.

Proof. By Corollary 2.4, one has

$$
\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= \sum_{e\in E_{C_3}} m_H^*(e) + \frac{1}{2}(l_1 + l_2 + 3 + a - 1 + \frac{1}{2}) \\
&\quad - \sum_{e\in E_{C_3'}} m_{H'}^*(e) - (l_1 + \frac{1}{2})(l_2 + 3 + a - 1 + \frac{1}{2}) \\
&= \frac{1}{2}(l_1 + l_2 + 3 + a - 1 + \frac{1}{2}) + (l_1 + 1 + \frac{1}{2})(l_2 + a + 1 + \frac{1}{2}) \\
&\quad + (l_1 + 1 + \frac{l_2 + a + 1}{2})(1 + \frac{l_2 + a + 1}{2}) \\
&\quad + (1 + \frac{l_1 + 1}{2})(l_2 + a + 1 + \frac{l_1 + 1}{2}) \\
&\quad - (l_1 + \frac{1}{2})(l_2 + 3 + a - 1 + \frac{1}{2}) - 2(1 + \frac{1}{2})(l_1 + l_2 + a + 1 + \frac{1}{2}) \\
&\quad - (1 + \frac{l_1 + l_2 + a + 1}{2})(1 + \frac{l_1 + l_2 + a + 1}{2}) \\
&= \frac{1}{2} l_1(l_2 + a - 4) \\
&> 0.
\end{aligned}
$$

□

Theorem 4.6. *Let $H \in \mathcal{UC}_n^d$ ($n > 15$) be an unicyclic graph with cycle length 3 and minimum edge revised Szeged index.*

(i) If $d = n - 2$, then $H \cong U^3_{P_{\lfloor \frac{d}{2} \rfloor+1}, P_{\lceil \frac{d}{2} \rceil+1}, S_1}$.

(ii) If $3 \le d \le n - 3$, then $H \cong U^3_{T_1, S_1, S_1}$ with $T_1 \cong TP^{n-d-3}_{d+1, \lfloor \frac{d}{2} \rfloor+1}$.

Proof. (i) If $d = n - 2$, then $H \cong U^3_{P_{p+1}, P_{q+1}, S_1}$ for some p, q with $p + q + 1 = d$. By Lemma 4.2, one has $|p - q| \le 1$, i.e., $H \cong U^3_{P_{\lfloor \frac{d}{2} \rfloor+1}, P_{\lceil \frac{d}{2} \rceil+1}, S_1}$.

(ii) If $3 \le d \le n - 3$, from Corollaries 3.2, 3.4 and 3.6, H must be Type I or Type II in Figure 8 in Section 3. If H is Type II, then there exists at least three pendant edges in H. From Corollary 4.3 and Lemmas 4.4 and 4.5, there exists an unicycle graph of Type I whose edge revised Szeged index smaller strictly than H. Thus H must be Type I. By Lemma 4.1 and Corollary 3.4, one has $H \cong U^3_{T_1, S_1, S_1}$ with $T_1 \cong TP^{n-d-3}_{d+1, \lfloor \frac{d}{2} \rfloor+1}$. □

5. The graphs with cycle length 4 and minimum edge revised Szeged index in $\mathcal{UC}_n^d$

From Section 3, the unicyclic graphs with cycle length 4 and given diameter and minimum edge revised Szeged index must be one of the graphs of Type III, Type IV and Type V in Figure 8. In this section, the properties of the graphs with cycle length 4 and minimum edge revised Szeged index in $\mathcal{UC}_n^d$ are characterized.

Lemma 5.1. *Let $H = U^4_{T_1,S_{b+1},S_{c+1},S_{d+1}}$ and $H' = U^4_{T_1',S_1,S_1,S_1}$ be two unicyclic graphs of Type III in Figure 8, where $T_1 \cong TP^a_{l_1+l_2+1,l_1+1}$, $|E_{T_1}| > 0$ and $T_1' \cong TP^{a+b+c+d}_{l_1+l_2+1,l_1+1}$. Then $Sz_e^*(H) \geq Sz_e^*(H')$ with equality holds if and only if $b = c = d = 0$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\
&= \sum_{e\in E_{C_4}} m_H(e) - \sum_{e\in E_{C_4'}} m_{H'}(e) \\
&= 2(l_1 + l_2 + a + b + 1)(c + d + 1) + 2(l_1 + l_2 + a + d + 1)(b + c + 1) \\
&\quad -4(l_1 + l_2 + a + b + c + d + 1) \\
&= 2(l_1 + l_2 + a + b)(c + d) + 2(l_1 + l_2 + a + d)(b + c) \\
&\geq 0.
\end{aligned}$$

□

Lemma 5.2. *Let $H = U^4_{T_1,T_2,S_{c+1},S_{d+1}}$ and $H' = U^4_{T_1',T_2,S_1,S_1}$ be two unicyclic graphs of Type IV in Figure 8, where $T_1 \cong TP^a_{l_1+1,l_1+1}$, $|E_{T_1}| > 0$ and $T_1' \cong TP^{a+c+d}_{l_1+1,l_1+1}$, $T_2 \cong TP^b_{l_2+1,i}$ for some $i \in [1, l_2 + 1]$. Then $Sz_e^*(H) \geq Sz_e^*(H')$ with equality holds if and only if $c = d = 0$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\
&= \sum_{e\in E_{C_4}} m_H(e) - \sum_{e\in E_{C_4'}} m_{H'}(e) \\
&= 2(l_1 + l_2 + a + b + 1)(c + d + 1) + 2(l_1 + a + d + 1)(l_2 + b + c + 1) \\
&\quad -2(l_1 + l_2 + a + b + c + d + 1) - 2(l_1 + a + c + d + 1)(l_2 + b + 1) \\
&= 4c(l_1 + a) + 2d(l_1 + l_2 + a + b + c) \\
&\geq 0.
\end{aligned}$$

□

Lemma 5.3. *Let $H = U^4_{T_1,T_2,S_1,S_1}$ and $H' = U^4_{T_1',T_2',S_1,S_1}$ be two unicyclic graphs of Type IV in Figure 8, where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T_1' \cong TP^a_{l_1+2,l_1+2}$, $T_2 \cong TP^b_{l_2+1,i}$ and $T_2' \cong TP^b_{l_2,i}$ for some $i \in [1, l_2]$. If $l_1 + 2 \leq l_2$, then $Sz_e^*(H) > Sz_e^*(H')$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned}
Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\
&= \sum_{e\in E_{C_4}} m_H(e) + (l_2 + b - 1)(l_1 + a + 4) \\
&\quad - \sum_{e\in E_{C_4'}} m_{H'}(e) - l_1(l_2 - 1 + b + a + 4) \\
&= 2(l_1 + a + 1)(l_2 + b + 1) + (l_2 + b - 1)(l_1 + a + 4)
\end{aligned}$$

$$
\begin{aligned}
& -2(l_1+1+a+1)(l_2-1+b+1)-l_1(l_2-1+b+a+4) \\
= & \ 2(l_2-l_1-1)+a(b+l_2+1-l_1)+2b \\
> & \ 0.
\end{aligned}
$$

□

By Lemmas 3.3 and 5.3 and similar proof method with Corollary 4.3, the following Corollary 5.4 derived.

Corollary 5.4. *Let $H = U^4_{T_1,T_2,S_1,S_1}$ be an unicyclic graph, where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T_2 \cong TP^b_{l_2+1,i}$ for some $i \in [1, l_2]$. Then, there exists an unicyclic graph $H' = U^4_{T'_1,T'_2,S_1,S_1}$ with $T'_1 \cong TP^a_{l_1+l_2-k+1,l_1+l_2-k+1}$ and $T'_2 \cong TP^b_{k+1,k+1}$ and $k \le l_2$ such that $Sz^*_e(H) \ge Sz^*_e(H')$.*

Lemma 5.5. *Let $H = U^4_{T_1,T_2,S_1,S_1}$ and $H' = U^4_{T'_1,S_1,S_1,S_1}$ be two unicyclic graphs of Type IV and Type III in Figure 8, respectively. Where $T_1 \cong TP^a_{l_1+1,l_1+1}$, $T_2 \cong TP^b_{l_2+1,l_2+1}$ and $T'_1 \cong TP^{a+b-1}_{l_1+l_2+2,l_1+2}$. If $a+b \ge 1$, $l_2 \ge l_1 \ge 1$ and $l_1+l_2+a+b+4 > 15$, then $Sz^*_e(H) > Sz^*_e(H')$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$
\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= Sz_e(H) - Sz_e(H') \\
&= \sum_{e\in E_{C_4}} m_H(e) - \sum_{e\in E_{C'_4}} m_{H'}(e) - l_1(l_2+b+a-1+4) \\
&= 2(l_1+a+1)(l_2+b+1) - 2(l_1+l_2+a+b+1) - l_1(l_2+b+a+3) \\
&= a(l_2-l_1) + l_1l_2 + al_2 + 2ab + l_1b - 3l_1 \\
&> 0.
\end{aligned}
$$

□

Lemma 5.6. *Let $H = U^4_{T_1,S_{c+1},T_2,S_{d+1}}$ and $H' = U^4_{T_1,S_{c+d+1},T_2,S_1}$ be two unicyclic graphs of Type V in Figure 8, where $T_1 \cong TP^a_{l_1+1,l_1+1}$, $T_2 \cong TP^b_{l_2+1,i}$ for some $i \in [1, l_2+1]$. Then $Sz^*_e(H) \ge Sz^*_e(H')$ with the equality holds if and only if $cd = 0$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$
\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= Sz_e(H) - Sz_e(H') \\
&= \sum_{e\in E_{C_4}} m_H(e) - \sum_{e\in E_{C'_4}} m_{H'}(e) \\
&= 2(l_1+a+c+1)(l_2+b+d+1) + 2(l_1+a+d+1)(l_2+b+c+1) \\
&\quad -2(l_1+a+c+d+1)(l_2+b+1) - 2(l_1+a+1)(l_2+b+c+d+1) \\
&= 4cd.
\end{aligned}
$$

□

Lemma 5.7. *Let $H = U^4_{T_1,S_{c+1},T_2,S_1}$ and $H' = U^4_{T'_1,T_2,S_1,S_1}$ be two unicyclic graphs of Type V and Type IV in Figure 8, respectively. Where $T_1 \cong TP^a_{l_1+1,l_1+1}$ and $T'_1 \cong TP^{a+c-1}_{l_1+2,l_1+2}$, $T_2 \cong TP^b_{l_2+1,i}$ for some $i \in [1, l_2+1]$. If $a+c \ge 1$ and $l_2 \ge l_1 \ge 1$ and $l_1+l_2+a+b+c+4 > 15$, then $Sz^*_e(H) > Sz^*_e(H')$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\ &= \sum_{e\in E_{C_4}} m_H(e) - \sum_{e\in E_{C_4'}} m_{H'}(e) - l_1(l_2+a+b+c+3) \\ &= 2(l_1+a+c+1)(l_2+b+1) + 2(l_1+a+1)(l_2+b+c+1) \\ &\quad -2(l_1+l_2+a+b+c+1) - 2(l_1+1+a+c-1+1)(l_2+b+1) \\ &\quad -l_1(l_2+a+b+c+3) \\ &= l_1(l_2+a+b+c-3) + 2a(l_2+b+c-l_1) \\ &> 0. \end{aligned}$$

□

If $a+c=0$ in the graph H mentioned in Lemma 5.7, we give the following lemmas.

Lemma 5.8. *Let $H = U^4_{P_{l_1+1},S_1,T_2,S_1}$ and $H' = U^4_{P_{l_1},S_1,T_2',S_1}$ be two unicyclic graphs of Type V in Figure 8, where $T_2 \cong TP^b_{l_2+1,i}$ and $T_2' \cong TP^b_{l_2+2,i}$ for some $i \in [1, l_2+1]$. Then $Sz_e^*(H) = Sz_e^*(H')$.*

Proof. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\ &= \sum_{e\in E_{C_4}} m_H(e) + (l_1-1)(l_2+b+4) \\ &\quad - \sum_{e\in E_{C_4'}} m_{H'}(e) - (l_1-1+4)(l_2+b) \\ &= 4(l_1+1)(l_2+b+1) + (l_1-1)(l_2+b+4) \\ &\quad -4l_1(l_2+b+2) - (l_1-1+4)(l_2+b) \\ &= 0. \end{aligned}$$

□

Note that $Sz_e^*(U^4_{P_{l_1+1},S_1,TP^b_{l_2+1,i},S_1}) = Sz_e^*(U^4_{TP^b_{l_1+l_2+1,i},S_1,S_1,S_1})$ for some $i \in [1, l_2+1]$ from Lemma 5.8. Moreover, by Lemma 3.3, if $n > 15$ and $7 \le d \le n-3$, one has $Sz_e^*(U^4_{TP^{n-d-2}_{d-1,j},S_1,S_1,S_1}) \ge Sz_e^*(U^4_{TP^{n-d-2}_{d-1,\lfloor \frac{d}{2}\rfloor+2},S_1,S_1,S_1})$ for $j \in [1, d-1]$; if $n > 15$ and $3 \le d \le 6$, one has $Sz_e^*(U^4_{TP^{n-d-2}_{d-1,j},S_1,S_1,S_1}) \ge Sz_e^*(U^4_{TP^{n-d-2}_{d-1,d-1},S_1,S_1,S_1})$ for $j \in [1, d-1]$.

Lemma 5.9. *Let $n > 15$ and $d = n-3$ be two integers. Let $H = U^4_{T_1,S_1,S_1,S_1}$ and $H' = U^4_{P_{\lfloor \frac{d-1}{2}\rfloor+1},P_{\lceil \frac{d-1}{2}\rceil+1},S_1,S_1}$ be two unicyclic graphs, where $T_1 \cong TP^1_{d-1,\lfloor \frac{d}{2}\rfloor+2}$. Then $Sz_e^*(H) > Sz_e^*(H')$.*

Proof. We divide this problem into two cases according to the parity of d.

Case 1. $d = 2k+1$ is odd.

Then, $H = U^4_{TP^1_{2k,k+2},S_1,S_1,S_1}$ and $H' = U^4_{P_{k+1},P_{k+1},S_1,S_1}$. By Lemma 2.1 and Corollary 2.4, one has

$$Sz_e^*(H) - Sz_e^*(H') = Sz_e(H) - Sz_e(H')$$

$$\begin{aligned} &= \sum_{i=0}^{k} i(2k+3-i) + \sum_{i=4}^{k+1} i(2k+3-i) + 4(2k+1) \\ &\quad -2\sum_{i=0}^{k-1} i(2k+3-i) - 2(k+1)(k+1) - 2(2k+1) \\ &= k^2 - 3k - 2 \\ &> 0. \end{aligned}$$

Case 2. $d = 2k$ is even.

Then, $H = U^4_{TP^1_{2k-1,k+2},S_1,S_1,S_1}$ and $H' = U^4_{P_k,P_{k+1},S_1,S_1}$. By Lemma 2.1 and Corollary 2.4, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\ &= \sum_{i=0}^{k} i(2k+2-i) + \sum_{i=4}^{k} i(2k+2-i) + 8k \\ &\quad - \sum_{i=0}^{k-1} i(2k+2-i) - \sum_{i=0}^{k-2} i(2k+2-i) - 2k(k+1) - 4k \\ &= k^2 - 4k - 1 \\ &> 0. \end{aligned}$$

□

Lemma 5.10. *Let $n > 15$ and $7 \le d \le n-4$ be two integers. Let $H = U^4_{T_1,S_1,S_1,S_1}$ and $H' = U^4_{T_1',S_1,S_1,S_1}$ be two unicyclic graphs, where $T_1 \cong TP^{n-d-2}_{d-1,\lfloor \frac{d}{2} \rfloor+2}$ and $T_1' \cong TP^{n-d-4}_{d+1,\lfloor \frac{d}{2} \rfloor+1}$. Then $Sz_e^*(H) > Sz_e^*(H')$.*

Proof. We divide this problem into two cases according to the parity of d.

Case 1. $d = 2k+1$ is odd.

Then, $T_1 \cong TP^{n-2k-3}_{2k,k+2}$ and $T_1' \cong TP^{n-2k-5}_{2k+2,k+1}$. By Lemma 2.1 and the definition of edge Szeged index, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\ &= \sum_{i=0}^{k} i(n-1-i) + \sum_{i=4}^{k+1} i(n-1-i) + 4(n-3) \\ &\quad - \sum_{i=0}^{k} i(n-1-i) - \sum_{i=0}^{k-1} i(n-1-i) - 4(n-3) \\ &= (2k-5)n - 2k^2 - 4k + 18 \\ &\ge (2k-5)(2k+5) - 2k^2 - 4k + 18 \\ &= 2(k-1)^2 - 5 \\ &> 0. \end{aligned}$$

Case 2. $d = 2k$ is even.

Then, $T_1 \cong TP^{n-2k-2}_{2k-1,k+2}$ and $T_1' \cong TP^{n-2k-4}_{2k+1,k+1}$. By Lemma 2.1 and the definition of edge Szeged index, one has

$$\begin{aligned} Sz_e^*(H) - Sz_e^*(H') &= Sz_e(H) - Sz_e(H') \\ &= \sum_{i=0}^{k} i(n-1-i) + \sum_{i=4}^{k} i(n-1-i) + 4(n-3) \\ &\quad -2\sum_{i=0}^{k-1} i(n-1-i) - 4(n-3) \\ &= (2k-6)n - 2k^2 - 2k + 20 \\ &\geq (2k-6)(2k+4) - 2k^2 - 2k + 20 \\ &= 2(k^2 - 3k - 2) \\ &> 0. \end{aligned}$$

□

By direct calculation, the following lemma can be obtained immediately.

Lemma 5.11. *Let $n > 15$ and $4 \leq d \leq 6$. Let $H = U^4_{TP^{n-d-2}_{d-1,d-1},S_1,S_1,S_1}$ and $H' = U^4_{TP^{n-d-4}_{d+1,\lfloor \frac{d}{2} \rfloor+1},S_1,S_1,S_1}$ be two unicyclic graphs in $\mathcal{UC}^d_n$. Then $Sz^*_e(H) < Sz^*_e(H')$.*

Theorem 5.12. *Let $H \in \mathcal{UC}^d_n$ ($n > 15$) be an unicyclic graph with cycle length 4 and minimum edge revised Szeged index.*

(i) If $d = n-2$, then $H \cong U^4_{P_{r_1+1},S_1,P_{r_2+1},S_1}$ for some nonnegative integers r_1 and r_2 with $r_1 + r_2 = n-4$.

(ii) If $d = n-3$, then $H \cong U^4_{P_{\lfloor \frac{d-1}{2} \rfloor+1},P_{\lceil \frac{d-1}{2} \rceil+1},S_1,S_1}$.

(iii) If $7 \leq d \leq n-4$, then $H \cong U^4_{TP^{n-d-4}_{d+1,\lfloor \frac{d}{2} \rfloor+1},S_1,S_1,S_1}$.

(iv) If $3 \leq d \leq 6$, then $H \cong U^4_{TP^{n-d-2}_{d-1,d-1},S_1,S_1,S_1}$.

Proof. (i) If $d = n-2$, then H must be the graph of Type V in Figure 8 in Section 3. By Lemma 5.8, (i) holds immediately.

(ii) If $d = n-3$, then $H \cong U^4_{TP^a_{s_1+1,s_1+1},S_{b+1},TP^c_{s_2+1,i},S_1}$ with $s_1 + s_2 = d-2$, $a+b+c = 1$ and $i \in [1, s_2+1]$; or $H \cong U^4_{P_{s_3+1},P_{s_4+1},S_1,S_1}$ with $s_3 + s_4 = d-1$.

If $a + b = 1$ and $c = 0$, by Lemmas 5.7 and 5.8, there exists a graph of Type IV with smaller edge revised Szeged index than $U^4_{TP^a_{s_1+1,s_1+1},S_{b+1},TP^c_{s_2+1,i},S_1}$; if $a + b = 0$ and $c = 1$, by Lemmas 5.9 and 5.8, there exists a graph of Type IV with smaller edge revised Szeged index than $U^4_{TP^a_{s_1+1,s_1+1},S_{b+1},TP^c_{s_2+1,i},S_1}$. Thus, $H \cong U^4_{P_{s_3+1},P_{s_4+1},S_1,S_1}$. Moreover, by Lemmas 5.3 and 5.8, one has $|s_3 - s_4| \leq 1$ and (ii) holds.

(iii) If $7 \leq d \leq n-4$, then H must be the graph of Type III, Type IV or Type V in Figure 8 in Section 3.

If H is Type V, $H \cong U^4_{TP^a_{l_1+1,l_1+1},S_{b+1},TP^c_{l_2+1,i},S_1}$ with $l_1 + l_2 = d-2$, $a+b+c \geq 2$ and $i \in [1, l_2+1]$. When $a + b \geq 1$, by Lemma 5.6, there exists a graph of Type IV with smaller edge revised Szeged index;

when $a+b=0$ and $c \geq 2$, by Lemmas 5.10 and 5.8, there exists a graph of Type III with smaller edge revised Szeged index. Thus, H can not be Type V.

Moreover, by Corollary 5.4 and Lemma 5.5, H can not be Type IV either. Thus, H is the graph of Type III and $H \cong U^4_{TP^{n-d-4}_{d+1,i},S_1,S_1,S_1}$ for some $i \in [1, d+1]$. Furthermore, by Lemma 3.3, one has $i = \lfloor \frac{d}{2} \rfloor + 1$ and (iii) holds.

(iv) If $4 \leq d \leq 6$, by Corollary 5.4 and Lemma 5.5, H can not be Type IV. From Lemma 5.11, one has $H \cong U^4_{TP^{n-d-2}_{d-1,d-1},S_1,S_1,S_1}$. If $d = 3$, by Lemma 5.1, $H \cong U^4_{TP^{n-5}_{2,2},S_1,S_1,S_1}$ and (iv) holds.

These complete the proof. □

6. The proof of Theorem 1.1

Lemma 6.1. *Let* $H = U^3_{P_{\lfloor \frac{d-1}{2} \rfloor+1},P_{\lceil \frac{d-1}{2} \rceil+1},S_1}$ *and* $H' = U^4_{P_{\lfloor \frac{d-2}{2} \rfloor+1},S_1,P_{\lceil \frac{d-2}{2} \rceil+1},S_1}$ *be two unicyclic graphs. If* $n > 15$ *and* $d = n-2$*, then* $Sz^*_e(H) < Sz^*_e(H')$.

Proof. We divide this problem into two cases according to the parity of d.

Case 1. $d = 2k$ is even.

It is routine to check that $H = U^3_{P_k,P_{k+1},S_1}$ and $H' = U^4_{P_k,S_1,P_k,S_1}$. By the definition of edge revised Szeged index, one has

$$\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= \sum_{e \in E_H} m^*_H(e) - \sum_{e \in E_{H'}} m^*_{H'}(e) \\
&= \sum_{i=0}^{k-2}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) + \sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\
&\quad +(1+\frac{k+1}{2})(k+\frac{k+1}{2}) + (k+\frac{1}{2})(k+1+\frac{1}{2}) + (1+\frac{k}{2})(k+1+\frac{k}{2}) \\
&\quad -2\sum_{i=0}^{k-2}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) - 4(k+\frac{2}{2})(k+\frac{2}{2}) \\
&= \frac{1}{4}(2k-2k^2-11) < 0.
\end{aligned}$$

Case 2. $d = 2k+1$ is odd.

Obviously, $H = U^3_{P_{k+1},P_{k+1},S_1}$ and $H' = U^4_{P_k,S_1,P_{k+1},S_1}$. By the definition of edge revised Szeged index, we have

$$\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= \sum_{e \in E_H} m^*_H(e) - \sum_{e \in E_{H'}} m^*_{H'}(e) \\
&= 2\sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) + (k+1+\frac{1}{2})(k+1+\frac{1}{2}) \\
&\quad +(1+\frac{k+1}{2})(k+1+\frac{k+1}{2}) + (1+\frac{k+1}{2})(k+1+\frac{k+1}{2}) \\
&\quad -\sum_{i=0}^{k-2}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) - \sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2})
\end{aligned}$$

$$-4(k+\frac{2}{2})(k+1+\frac{2}{2})$$
$$= \frac{1}{2}(-k^2-6) < 0.$$

Thus, the proof is completed. □

Lemma 6.2. *Let $H = U^3_{TP^0_{d+1,\lfloor \frac{d}{2} \rfloor+1}, S_1, S_1}$ and $H' = U^4_{P_{\lfloor \frac{d-1}{2} \rfloor+1}, P_{\lceil \frac{d-1}{2} \rceil+1}, S_1, S_1}$ be two unicyclic graphs. If $n > 15$ and $d = n-3$, then $Sz^*_e(H) < Sz^*_e(H')$.*

Proof. We divide this problem into two cases according to the parity of d.

Case 1. $d = 2k$ is even.

Obviously, $H = U^3_{TP^0_{2k+1,k+1}, S_1, S_1}$ and $H' = U^4_{P_k, P_{k+1}, S_1, S_1}$. By the definition of edge revised Szeged index, we have

$$\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= \sum_{e\in E_H} m^*_H(e) - \sum_{e \in E_{H'}} m^*_{H'}(e) \\
&= 2\sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) + (1+\frac{2k+1}{2})(1+\frac{2k+1}{2}) \\
&\quad +2(1+\frac{1}{2})(2k+1+\frac{1}{2}) \\
&\quad -\sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) - \sum_{i=0}^{k-2}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\
&\quad -2(k+1+\frac{2}{2})(k+\frac{2}{2}) - 2(1+\frac{2}{2})(2k+\frac{2}{2}) \\
&= -(2k+3) < 0.
\end{aligned}$$

Case 2. $d = 2k+1$ is odd.

Obviously, $H = U^3_{TP^0_{2k+2,k+1}, S_1, S_1}$ and $H' = U^4_{P_{k+1}, P_{k+1}, S_1, S_1}$. By the definition of edge revised Szeged index, we have

$$\begin{aligned}
Sz^*_e(H) - Sz^*_e(H') &= \sum_{e\in E_H} m^*_H(e) - \sum_{e \in E'_H} m^*_{H'}(e) \\
&= \sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) + \sum_{i=0}^{k}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\
&\quad +(1+\frac{2k+2}{2})(1+\frac{2k+2}{2}) + 2(1+\frac{1}{2})(2k+2+\frac{1}{2}) \\
&\quad -\sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) - \sum_{i=0}^{k-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\
&\quad -2(k+1+\frac{2}{2})(k+1+\frac{2}{2}) - 2(1+\frac{2}{2})(2k+1+\frac{2}{2}) \\
&= -\frac{1}{4}(8k+11) < 0.
\end{aligned}$$

This completes the proof. □

Lemma 6.3. *Let* $H = U^3_{TP^{n-d-3}_{d+1,\lfloor\frac{d}{2}\rfloor+1},S_1,S_1}$ *and* $H' = U^4_{TP^{n-d-4}_{d+1,\lfloor\frac{d}{2}\rfloor+1},S_1,S_1,S_1}$ *be two unicyclic graphs. If* $n > 15$ *and* $4 \le d \le n-4$*, then* $Sz^*_e(H) > Sz^*_e(H')$.

Proof. By the definition of edge revised Szeged index, one has

$$\begin{aligned} Sz^*_e(H) - Sz^*_e(H') &= \sum_{e\in E_H} m^*_H(e) - \sum_{e\in E_{H'}} m^*_{H'}(e) \\ &= \sum_{i=0}^{\lfloor\frac{d}{2}\rfloor-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) + \sum_{i=0}^{\lceil\frac{d}{2}\rceil-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\ &\quad +(n-d-3)(0+\frac{1}{2})(n-1+\frac{1}{2}) + 2(1+\frac{1}{2})(n-2+\frac{1}{2}) \\ &\quad +(1+\frac{n-2}{2})(1+\frac{n-2}{2}) \\ &\quad -\sum_{i=0}^{\lfloor\frac{d}{2}\rfloor-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) - \sum_{i=0}^{\lceil\frac{d}{2}\rceil-1}(i+\frac{1}{2})(n-1-i+\frac{1}{2}) \\ &\quad -(n-d-4)(0+\frac{1}{2})(n-1+\frac{1}{2}) - 4(1+\frac{2}{2})(n-3+\frac{2}{2}) \\ &= \frac{1}{4}(n^2-18n+45) > 0. \end{aligned}$$

Thus, the proof is completed. □

By direct calculation, the following Lemma 6.4 can be obtained.

Lemma 6.4. *If* $n > 15$ *and* $d = 3$*, then* $Sz^*_e(U^3_{TP^{n-6}_{4,2},S_1,S_1}) > Sz^*_e(U^4_{TP^{n-5}_{2,2},S_1,S_1,S_1})$.

Proof of Theorem 1.1:

(i) By Theorems 4.6 and 5.12 and Lemma 6.1, (i) holds immediately.

(ii) If $d = n-3$, by Theorems 4.6 and 5.12 and Lemma 6.2, the result holds.

(iii) If $7 \le d \le n-4$, from Theorems 4.6 and 5.12 and Lemma 6.3, the result holds.

(iv) If $4 \le d \le 6$, by Theorems 4.6 and 5.12 and Lemmas 5.11 and 6.3, the result holds. If $d = 3$, from Theorems 4.6 and 5.12 and Lemma 6.4, the result is gotten directly.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflict of interest.

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