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On ABS index of unicyclic graphs with fixed diameter

Yuan Zhang[a], Haiying Wang[a,*], Shaohui Wang[b]

[a]School of Science, China University of Geosciences, Beijing, Beijing 100083, China
[b]Department of Mathematics, Louisiana Christian University, Pineville, LA 71359, USA

Abstract. Given a simple connected graph $G = (V(G), E(G))$, the atom-bond sum-connectivity (ABS) index is defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u) + d(v)}} = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d(u) + d(v)}},$$

where $d(u)$ and $d(v)$ are the degrees of $u, v \in V(G)$, respectively. In this paper, let $\mathcal{U}_{n,\alpha}$ be a set of all unicyclic graphs of order n with diameter α. Firstly, we present the minimum ABS index of $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 2$. We also determine the maximum ABS index of $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 4$. Finally, the corresponding extremal graphs with the sharp upper and lower bounds have been characterized, respectively.

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $x \in V(G)$, we use $d_G(x)$ and $N_G(x)$ to denote the degree of x and the set of neighbors of x in G, respectively. In particular, x is called a pendant vertex when $d_G(x) = 1$. Let $PV(G)$ be a set of all pendant vertices in G. We call an edge uv is a pendant edge of G if either $d_G(u) = 1$ or $d_G(v) = 1$.

A path P is denoted by $P = u_0u_1 \cdots u_k = P_{k+1}$, and we call P a path from u_0 to u_k, or briefly by u_0-u_k path. The distance $d(u, v)$ of two vertices u and v is the length of the shortest u-v path. The longest distance between any two vertices in G is the diameter of G, denoted by $\alpha(G)$. The longest path P^α is called a diametral path of G. A unicyclic graph is a connected graph with n vertices and n edges. Let C_n denote the cycle on n vertices. $G - u$ is obtained from G by deleting a vertex u and its incident edges. Let $G + uv$ and $G - uv$ be obtained from G by adding an edge $uv \notin E(G)$ and deleting an edge $uv \in E(G)$, respectively. We drop G from the notations $d_G(v), N_G(v)$ and $\alpha(G)$ if there is no confusion.

Topological indices are a class of molecular descriptors, which are of great significance in the fields of biology and physical chemistry, especially in the study of the structural properties of molecules[7, 14, 15,

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* Corresponding author: Haiying Wang
Email addresses: 2019220014@email.cugb.edu.cn (Yuan Zhang), whycht@126.com (Haiying Wang), shaohuiwang@yahoo.com (Shaohui Wang)
ORCID iDs: https://orcid.org/0009-0005-6262-9108 (Yuan Zhang), https://orcid.org/0000-0002-2058-5443 (Haiying Wang), https://orcid.org/0000-0001-6941-3194 (Shaohui Wang)

17, 21]. So far, there have been a lot of invariants based on the degree of vertices, and they are hot research topics to explore the extremal values of these invariants among all classes of graphs for a fixed condition. Numerous topological indices exhibit interrelations with one another.

In fact, the atom-bond sum-connectivity (ABS) index of a graph is a variant from three famous chemical topological indices, which are the Randić index, the sum-connectivity index and the atom-bond connectivity index. The *Randić index* of G is the first chemical index introduced by the famous chemist Randić [16], which was defined by

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

One modified version of the Randić index of G is the *sum-bond connectivity index* proposed by Zhou and Trinajstić [18] as

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

And the *atom-bond connectivity index* of G is another modified version of the Randić index defined by Estrada et al. [6] as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}.$$

According to the main idea of the sum-bond connectivity index, Ali, Furtula, Redžepović and Gutman [2] put forward the *atom-bond sum-connectivity (ABS) index* of a graph G, which was denoted as

$$ABS(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}} = \sum_{uv\in E(G)} \sqrt{1-\frac{2}{d(u)+d(v)}}.$$

The ABS index is a crucial topological index widely employed to quantify and characterize molecular structures. The primary significance of the ABS index lies in its ability to simplify and mathematically process molecular structures, providing a powerful tool for predicting and interpreting molecular physicochemical properties, reactivity, and biological activity. While traditional physicochemical methods accurately measure molecular properties, they often struggle to deliver rapid conclusions in complex systems. As a topological index, the ABS index offers preliminary estimates of molecular properties through relatively simple calculations [1, 12].

The aim of studying the ABS index is to explore its potential applications across various fields, particularly in the property prediction and molecular design of organic compounds. The accuracy and generalizability of the ABS index in predicting molecular properties are further validated through comparisons with other topological indices.

For example, among the Randić index, the sum-connectivity index, the atom-bond connectivity index and the ABS index, Ali, Gutman and Redžepović found some conclusions referring to [1]. In the case of octane isomers, it can be concluded from the values of some correlation coefficients that the ABS index is as effective as the other three indices in predicting molecular properties. Additionally, they indicated that the ABS index predicts molecular properties as well as other connectivity indices and, in some cases, performs even better. Notably, the ABS index outperforms the ABC index in specific predictions of physicochemical properties. Consequently, investigating the correlation properties of the ABS index holds significant importance.

Up to now, Ali et al. determined the largest, second largest, smallest and second smallest ABS index values for the class of unicyclic graphs in [1], respectively. As above, we cite the maximum and minimum ABS index values for a class of unicyclic graphs as lemmas below. The extremal problems on the ABS indices among all trees with given order has been studied by Ali et al. in [2]. Besides, Alraqad et al. obtained the smallest ABS index values among all trees with a given number of pendant vertices in [4]. Further, Maitreyi et al. investigated the largest ABS index values among all trees with a given number of pendant vertices in [11]. The maximum *ABS* index of trees with fixed number of leaves was proposed by Noureen and Ali in [13]. In addition, Nithya et al. in [12] characterized the extremal graphs with respect to the *ABS* index among all unicyclic graphs with given girth recently.

Lemma 1.1. *[1] Among all unicyclic graphs of order $n \geq 4$, the graph S_n^+ has the maximum ABS index, equal to*

$$(n-3)\sqrt{\frac{n-2}{n}} + 2\sqrt{\frac{n-1}{n+1}} + \frac{1}{\sqrt{2}}.$$

In chemical graph theory, a family of unicyclic graphs is one of the most common molecular structures. In this paper, we discuss the minimum *ABS* index of $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 2$. Moreover, the maximum *ABS* index of $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 4$ is determined. Finally, we characterize the graphs with minimum and maximum *ABS* indices among the n-vertex unicyclic graphs with given diameter α, respectively.

2. The minimum *ABS* index of unicyclic graphs with fixed diameter

In this section, we discuss the minimum *ABS* index of unicyclic graphs with given diameter $\alpha \geq 2$ and characterize the corresponding minimal graphs. To facilitate the narrative, we introduce some lemmas and notations below.

Assume that T is a tree with order $n \geq 4$ and $e = uv$ is a non-pendant edge of T. Let T' be the new tree obtained from T by contracting the edge $e = uv$ into a new vertex w and adding a new pendant edge to w. We say that T' is obtained from T by *e.g.t.* the edge uv (see Figure 1).

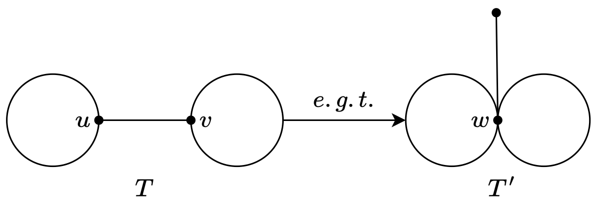

Figure 1. Two trees T and T' for *e.g.t.*.

Denote $\mathcal{U}_{n,\alpha} = \{G \mid G$ is a unicyclic graph with order n and diameter $\alpha\}$.

Next, we construct a new unicyclic graph and denote by U_1 in Figure 2. Then $U_1 \in \mathcal{U}_{n,\alpha}$.

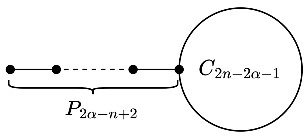

Figure 2. U_1.

Lemma 2.1. *[22] Let*

$$f(x) = \sqrt{\frac{x-a}{x-a+2}} - \sqrt{\frac{x-b}{x-b+2}}$$

with $x \geq b \geq a \geq 0$. Then $f(x) \geq 0$ with equality if and only if $a = b$ and $f(x)$ is a decreasing function in $(b, +\infty)$.

Lemma 2.2. *Let $G \in \mathcal{U}_{n,\alpha}$ be a unicyclic graph and let P^α be a diametral path of G. If there is a pendant vertex v such that $v \notin V(P^\alpha)$, then there exists a unicyclic subgraph G' of G such that $ABS(G) > ABS(G')$ with $v \notin V(G')$ and $\alpha(G) = \alpha(G')$.*

Proof. Let u be the endpoint of the shortest path among all u-v paths with $d_G(u) \geq 3$. Let G' be a graph obtained from G by deleting the u-v path while containing the vertex u. Then $V(G') \subset V(G)$. Let x be adjacent to u and on the u-v path (If u-v path has exactly one edge, then $v = x$). It is easy to see that G' is a unicyclic graph and $\alpha(G') = \alpha(G)$.

For $1 \leq i \leq d_G(u) - 1$, let $w_i \in N_G(u)\backslash\{x\}$ and $w_i \in N_{G'}(u)$. Then we have $d_G(u) = d_{G'}(u) + 1 = d(u)$, $d_G(w_i) = d_{G'}(w_i) = d(w_i)$ and the following holds.

$$\begin{aligned}
&ABS(G) - ABS(G') \\
&\geq \sqrt{\frac{d_G(u)-1}{d_G(u)+1}} + \sum_{w_i \in N_G(u)\backslash\{x\}} \sqrt{\frac{d_G(u)+d_G(w_i)-2}{d_G(u)+d_G(w_i)}} - \sum_{w_i \in N_{G'}(u)} \sqrt{\frac{d_{G'}(u)+d_{G'}(w_i)-2}{d_{G'}(u)+d_{G'}(w_i)}} \\
&= \sqrt{\frac{d(u)-1}{d(u)+1}} + \sum_{w_i \in N_G(u)\backslash\{x\}} \left(\sqrt{\frac{d(u)+d(w_i)-2}{d(u)+d(w_i)}} - \sqrt{\frac{d(u)+d(w_i)-3}{d(u)+d(w_i)-1}} \right) \\
&> 0,
\end{aligned}$$

which implies that $ABS(G) > ABS(G')$. Thus, Lemma 2.2 holds immediately. □

Lemma 2.3. *[1] For every fixed integer $n \geq 3$, among all unicyclic graphs of order n, the cycle C_n is the only graph possessing the minimum ABS index, equal to $n/\sqrt{2}$.*

Remark 2.4. *Let G be a unicyclic graph and let $|PV(G)|$ be the number of pendant vertices of G. By Lemmma 2.3, if $|PV(G)| = 0$, then $G \cong C_n$ and C_n is the only graph possessing the minimum ABS index. Therefore, we will consider $|PV(G)| \geq 1$ in the remaining part of the paper.*

Theorem 2.5. *Let $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 3$ and $\alpha + 2 \leq n \leq 2\alpha$. Then we have*

$$ABS(G) \geq ABS(U_1) = (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.$$

Proof. Let $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \geq 3$ and $\alpha + 2 \leq n \leq 2\alpha$. Since we have $|PV(G)| \geq 1$ from Remark 2.4, it suffices to discuss three cases below from the view of pendant vertices.

Case 1. $|PV(G)| = 1$.

Since $G \in \mathcal{U}_{n,\alpha}$ and $|PV(G)| = 1$, G contains a path P of length $m \geq 1$ and a cycle C_l with order $l \geq 3$, where $n = m + l$. Then P and C_l of G have a common vertex denoted by u_1 and $d(u_1) = 3$. As above, we obtain $ABS(G)$ by the following equation.

$$ABS(G) = ABS(C_l) + ABS(P). \tag{1}$$

Case 1.1. $m \geq 2$ and $l \geq 4$.

In this subcase, it is easy to calculate that

$$ABS(P) = (m-2)\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3}$$

and

$$ABS(C_l) = (l-2)\sqrt{\frac{2}{2+2}} + 2\sqrt{\frac{3}{3+2}} = (l-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5}.$$

We substitute the values of $ABS(C_l)$ and $ABS(P)$ above into Equation (1). Then

$$ABS(G) = ABS(C_l) + ABS(P) = (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3} = ABS(U_1).$$

Case 1.2. $m = 1$ and $l \geq 4$.

By $m = 1$, we know $ABS(P) = \frac{\sqrt{2}}{2}$. Combined with Equation (1), that is,

$$\begin{aligned} ABS(G) &= (l-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{2}}{2} \\ &\geq (n-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} \\ &\geq ABS(U_1). \end{aligned}$$

Case 1.3. $l = 3$ and $m \geq 2$.

In this subcase, we have $ABS(C_l) = \frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5}$. According to Equation (1), it holds that

$$ABS(G) = (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3} = ABS(U_1).$$

Case 2. $|PV(G)| = 2$.

Since $G \in \mathcal{U}_{n,\alpha}$ and $|PV(G)| = 2$, there exists two paths and exactly one cycle in G, denoted by P of length m_1, P' of length m_2 and C_l of order l, respectively. Thus there are three structures a, b and c in all, of which the structure a is divided into three seed structures a_1, a_2 and a_3 in Figure 3, the structure b is divided into three seed structures b_1 and b_2 in Figure 4 and the structure c is divided into four seed structures c_1, c_2, c_3 and c_4 in Figure 5.

Without loss of generality, we assume that $V(C_l) \cap V(P) = u_1$ and $V(C_l) \cap V(P') = u_2$ in Figure 3. Denote $V(P) \cap V(P') = u_2$ if $V(C_l) \cap V(P) = u_1$ and $V(P) \cap V(P') = u_1$ if $V(C_l) \cap V(P') = u_2$ in Figure 4 and 6. Then $d(u_1), d(u_2) \in \{3, 4\}$ and $n = l + m_1 + m_2$. Hence,

$$ABS(G) = ABS(C_l) + ABS(P) + ABS(P'). \tag{2}$$

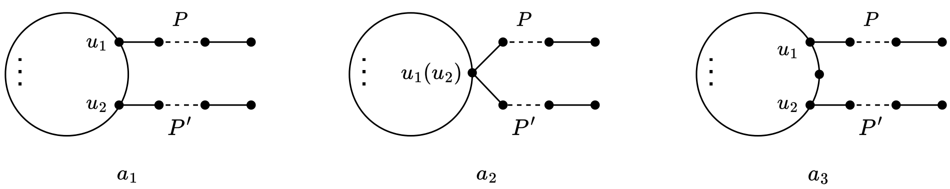

Figure 3. Attaching two paths P and P' to the unique cycle C_l.

Case 2.1. $V(P) \cap V(P') = \emptyset$.

Case 2.1.1. $l \geq 4$ and $m_1, m_2 \geq 2$.

Firstly, if $l \geq 4$ and $m_1, m_2 \geq 2$, then we obtain

$$ABS(P) = (m_1 - 2)\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3} \tag{3}$$

and

$$ABS(P') = (m_2 - 2)\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \tag{4}$$

If we attach P and P' to two non-adjacent vertices of C_l referring to a_3 in Figure 3, then

$$ABS(C_l) = (l-4)\frac{\sqrt{2}}{2} + \frac{4\sqrt{15}}{5}. \tag{5}$$

If we attach P and P' to two adjacent vertices of C_l referring to a_1 in Figure 3, then

$$ABS\,(C_l) = (l-3)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3}. \tag{6}$$

Combined with the condition that Equation (6) is smaller than Equation (5) about values, as we consider the lower bound of the ABS index by Theorem 2.5. Hence we just have to think about whether the Theorem 2.5 holds if we substitute Equations (3), (4) and (6) into Equation (2). As a result, we conclude that

$$\begin{aligned} ABS(G) &\geq (l+m_1+m_2-7)\,\frac{\sqrt{2}}{2} + \frac{4\sqrt{15}}{5} + \frac{2\sqrt{3}}{3} + \frac{\sqrt{6}}{3} \\ &\geq (n-7)\frac{\sqrt{2}}{2} + \frac{4\sqrt{15}}{5} + \frac{2\sqrt{3}}{3} + \frac{\sqrt{6}}{3} \\ &\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \end{aligned}$$

Case 2.1.2. $l \geq 4$ and $m_1 = 1, m_2 \geq 2$.

In this subcase, we know $ABS(P) = \frac{\sqrt{2}}{2}$ and $ABS\,(P') = (m_2-2)\,\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3}$. By substituting Equation (6) and the above two equations into Equation (2), we have

$$\begin{aligned} ABS(G) &\geq (l+m_2-5)\,\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} + \frac{\sqrt{2}}{2} \\ &\geq (n-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} \\ &\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \end{aligned}$$

Case 2.1.3. $l \geq 4$ and $m_1 = m_2 = 1$.

Since $ABS(P) + ABS\,(P') = \sqrt{2}$ and combining with Equations (2) and (6), we obtain

$$\begin{aligned} ABS(G) &\geq (l-3)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3} + \sqrt{2} \\ &\geq (n-5)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3} + \sqrt{2} \\ &\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \end{aligned}$$

Case 2.1.4. $l = 3$ and $m_1, m_2 \geq 2$.

Note that $ABS\,(C_l) = \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3}$, then combined Equations (2), (3) and (4), it holds that

$$\begin{aligned} ABS(G) &= (m_1+m_2-4)\,\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + \frac{2\sqrt{3}}{3} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3} \\ &\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \end{aligned}$$

Case 2.1.5. $l = 3$ and $m_1 = 1, m_2 \geq 2$.

In this subcase, we have $ABS\,(C_l) = \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3}$ and $ABS(P) = \frac{\sqrt{2}}{2}$. According to Equations (2) and (4), the following holds.

$$\begin{aligned} ABS(G) &= (m_2-2)\,\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3} + \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3} \\ &\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}. \end{aligned}$$

Case 2.1.6. $l = 3$ and $m_1 = m_2 = 1$.

Since $ABS(C_l) = \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3}$ and $ABS(P) = ABS(P') = \frac{\sqrt{2}}{2}$, we substitute these two equations into Equation (2). Then

$$ABS(G) = \frac{2\sqrt{15}}{5} + \frac{\sqrt{6}}{3} + \sqrt{2} \geq \frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.$$

Case 2.2. $V(P) \cap V(P') \neq \emptyset$ and P^α contains both pendant vertices of G.

Case 2.2.1. Attaching both pendant vertices of P and P' to exactly one vertex of C_l.

Let u_1 be the common vertex of P, P' and C_l. Then $d(u_1) = 4$ referring to a_2 in Figure 3. If u_1 is not adjacent to a pendant vertex of P^α, then $l \geq 3$ and $m_1, m_2 \geq 2$ as $V(P^\alpha)$ is a subset of $V(P) \cup V(P')$. According to Equation (2), we obtain

$$\begin{aligned}
ABS(G) &= ABS(C_l) + ABS(P) + ABS(P') \\
&= (l-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3} + (m_1 - 2)\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3} + \frac{\sqrt{3}}{3} \\
&\quad + (m_2 - 2)\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3} + \frac{\sqrt{3}}{3} \\
&= (n-6)\frac{\sqrt{2}}{2} + \frac{4\sqrt{6}}{3} + \frac{2\sqrt{3}}{3} \\
&\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

If u_1 is adjacent to one pendant vertex of P^α (Without loss of generality, we assume that u_1 is adjacent to another endpoint of P), then $l = 3$, $m_1 = 1$ and $m_2 \geq 2$ as $V(P^\alpha)$ is a subset of $V(P) \cup V(P')$. Since $ABS(C_l) = \frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3}$, $ABS(P) = \frac{\sqrt{15}}{5}$ and from Equations (2) and (4), the following holds.

$$\begin{aligned}
ABS(G) &= (m_2 - 2)\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3} + \frac{\sqrt{3}}{3} + \frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3} + \frac{\sqrt{15}}{5} \\
&\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

If u_1 is adjacent to two pendant vertices of P^α, i.e., u_1 is adjacent to both end vertices of P and P', then $l = 3$ and $m_1 = m_2 = 1$. We consider $ABS(C_l) = \frac{2\sqrt{6}}{3} + \frac{\sqrt{2}}{2}$, $ABS(P) = ABS(P') = \frac{\sqrt{15}}{5}$ and substitute these two equations into Equation (2). Then

$$ABS(G) = \frac{2\sqrt{15}}{5} + \frac{2\sqrt{6}}{3} + \frac{\sqrt{2}}{2} \geq \frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.$$

Case 2.2.2. Attaching a pendant vertex of P' (P) to an inner vertex of P (P').

There are two conditions in this subcase and we characterize them in Figure 4. Below, we just consider the condition b_1 and the proof of condition b_2 is similar.

Let u_2 be the common vertex of P and P' and let v_1, v_2 be the another endpoint of P' and P, respectively. Then $d(u_2) = 3$. Note that $V(P^\alpha)$ is a subset of $V(P) \cup V(P')$, one has $t_1 + t_2 \geq \max\left\{m_1 + \left\lfloor \frac{l}{2} \right\rfloor, m_2 + \left\lfloor \frac{l}{2} \right\rfloor\right\}$, where t_1 and t_2 are the number of edges of u_2-v_1 path and u_2-v_2 path, respectively. We are able to deduce that the vertex u_2 is not adjacent to a pendant vertex of P^α (otherwise the diametral path P^α has only one pendant vertex). Then

$$\begin{aligned}
ABS(G) &= ABS\left(C_l\right) + ABS(P) + ABS\left(P'\right)\\
&= (l-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{15}}{5} + (m_1-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5}\\
&\quad + \frac{\sqrt{3}}{3} + (m_1-2)\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3}\\
&= (n-8)\frac{\sqrt{2}}{2} + \frac{2\sqrt{3}}{3} + \frac{6\sqrt{15}}{5}\\
&\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

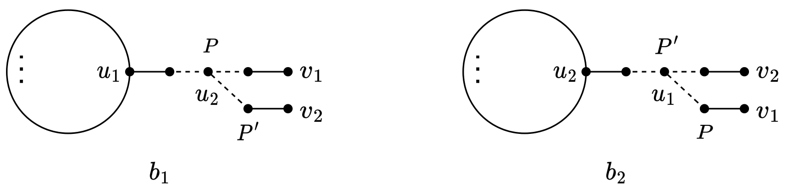

Figure 4. Attaching a pendant vertex of $P(P')$ to an inner vertex of $P'(P)$.

Case 2.2.3. Attaching a pendant vertex of P' (P) to a pendant vertex of P (P').

Let v_1, v_2 be the another pendant vertex of P and P', respectively. If u_1 is adjacent to a pendant vertex of P^α, then $l = 3$ and $m_1, m_2 \geq 1$ (see c_1 in Figure 5). Then $ABS\left(C_l\right) = \frac{2\sqrt{6}}{3} + \frac{\sqrt{2}}{2}$ and substitute it into Equation (2). As a result, we have

$$\begin{aligned}
ABS(G) &= \frac{2\sqrt{6}}{3} + \frac{\sqrt{2}}{2} + (m_1+m_2-3)\frac{\sqrt{2}}{2} + \frac{\sqrt{15}}{5} + \frac{\sqrt{6}}{3} + \frac{\sqrt{3}}{3}\\
&= (n-5)\frac{\sqrt{2}}{2} + \sqrt{6} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3}\\
&\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

If u_1 is not adjacent to a pendant vertex of P^α, then $m_1 + m_2 \geq \max\left\{s_1 + \left\lfloor \frac{l}{2} \right\rfloor, m_2 + s_2 + \left\lfloor \frac{l}{2} \right\rfloor\right\}$, where $s_1 = d(u_1, v_2)$ and $s_2 = d(u_1, u_2)$ (see c_3 in Figure 5). Then we calculate that

$$\begin{aligned}
ABS(G) &= ABS\left(C_l\right) + ABS(P) + ABS\left(P'\right)\\
&= (l-2)\frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3} + (m_1+m_2-4)\frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3} + \frac{2\sqrt{3}}{3}\\
&= (n-6)\frac{\sqrt{2}}{2} + \frac{4\sqrt{6}}{3} + \frac{2\sqrt{3}}{3}\\
&\geq (n-4)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}.
\end{aligned}$$

The condition c_2 and c_4 is similar to c_1 and c_2, respectively.

Case 2.3. $V(P) \cap V(P') \neq \emptyset$ and P^α contains one pendant vertex of G.

Given the one pendant vertex belonging to P^α denoted by w_1. If w_2 is another pendant vertex of G and $w_2 \notin PV(P^\alpha)$, then there exists a unicyclic subgraph G' satisfying $V(G') \subset V(G)$ from Lemma 2.2. As above,

G' contains exactly one pendant vertex w_1 such that $\alpha(G) = \alpha(G')$ and $ABS(G) > ABS(G')$. According to Case 1, this leads to the fact

$$ABS(G) \geq ABS(G') \geq ABS(U_1).$$

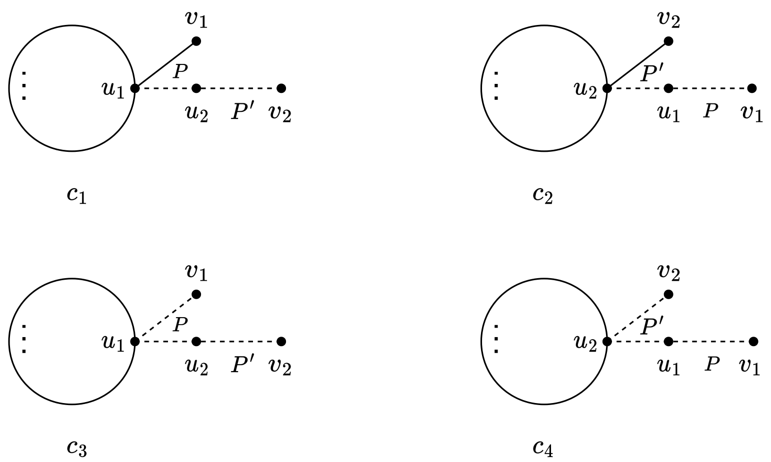

Figure 5. Attaching a pendant vertex of $P(P')$ to a pendant vertex of $P'(P)$.

Case 3. $|PV(G)| \geq 3$.

For $|PV(G)| \geq 3$, we obtain that the diametral path P^{α} contains at most two pendant vertices denoted by u_1 and u_2 of G. If $|PV(G)| \geq 3$, then there are at least $|PV(G)| - 2$ pendant vertices $u_3, u_4, \cdots, u_{|PV(G)|}$ not in P^{α}. Further, by Lemma 2.2, there exists a unicyclic subgraph G' of G such that G' contains at most two pendant vertices of P^{α} satisfying $V(G') \subset V(G)$, $\alpha(G) = \alpha(G')$ and $ABS(G) > ABS(G')$. If P^{α} has exactly one pendant vertex, then from Case 1 and we have

$$ABS(G) \geq ABS(G') \geq ABS(U_1).$$

On the other hand, if P^{α} has two pendant vertices, then by Case 2 one has

$$ABS(G) \geq ABS(G') \geq ABS(U_1).$$

Therefore, the result holds. □

Theorem 2.6. *Let $G \in \mathcal{U}_{n,\alpha}$ with $\alpha = 2$, then $ABS(G) \geq 2\sqrt{2}$.*

Proof. Given a graph $G \in \mathcal{U}_{n,\alpha}$ for $\alpha = 2$, there are three structures as follows. If $G = C_4$ or $G = C_5$, then $ABS(G) = 2\sqrt{2}$ and $ABS(G) = \dfrac{5\sqrt{2}}{2}$, respectively. Further, we may assume that G is obtained by attaching at least one pendant vertex to one vertex of C_3.

Let $V(C_3) = \{v_1, v_2, v_3\}$ and let $u_1, u_2, \cdots, u_k$ be pendant vertices adjacent to v_1. Then $v_2v_1u_1$ is a diametral path of G. Note that there exists a unicyclic subgraph G' satisfying $V(G') \subset V(G)$ and containing the unique pendant vertex u_1 from Lemma 2.2. Hence, it is clear that $\alpha(G) = \alpha(G')$ and $ABS(G) > ABS(G')$. Therefore, $ABS(G') = \sqrt{2} + \frac{2\sqrt{15}}{5}$, which implies that $ABS(G) \geq 2\sqrt{2}$. □

3. The maximum *ABS* index of unicyclic graphs with fixed diameter

In this section, we obtain the maximum *ABS* index among all unicyclic graphs with given diameter $\alpha \geq 2$ and characterize the corressponding maximal graphs. Let

$$\mathcal{U}_{n,\alpha}^{\max} = \{G \mid G \text{ is a graph in } \mathcal{U}_{n,\alpha} \text{ with the maximum } ABS \text{ index }\}.$$

For every $4 \leq \alpha \leq n-2$, we construct a new unicyclic graph $U_n^\alpha \in \mathcal{U}_{n,\alpha}$ (see Figure 6). Therefore,

$$ABS\,(U_n^\alpha) = (n-\alpha-1)\sqrt{\frac{n-\alpha}{n-\alpha+2}} + 2\sqrt{\frac{n-\alpha+1}{n-\alpha+3}} + A_1,$$

where $A_1 = \frac{2\sqrt{15}}{5} + \frac{\sqrt{2}}{2}$ if $\alpha = 4$ and $A_1 = (\alpha-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}$ if $\alpha \geq 5$.

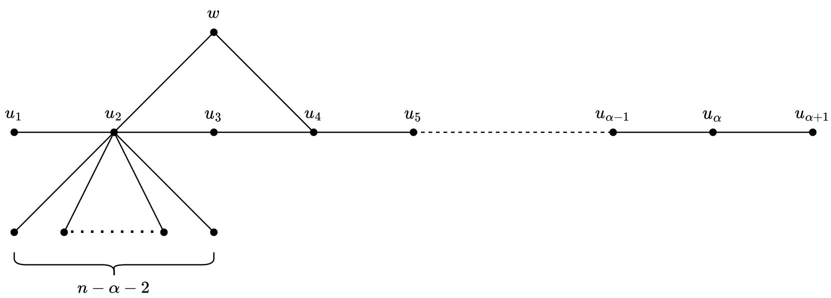

Figure 6. U_n^α

Lemma 3.1. *[22] Let*

$$f(x) = (x-a)\sqrt{\frac{x-a}{x-a+2}} - (x-b)\sqrt{\frac{x-b}{x-b+2}}$$

with $x \geq b \geq a \geq 0$. Then $f(x) \geq 0$ with equality if and only if $a = b$ and $f(x)$ is an increasing function in $(b, +\infty)$.

Theorem 3.2. *Let $G \in \mathcal{U}_{n,\alpha}$ with diameter $\alpha = 2$ and $n \geq 4$. Then we have $ABS(G) \leq 2\sqrt{\frac{n-1}{n+1}} + (n-3)\sqrt{\frac{n-2}{n}} + \frac{\sqrt{2}}{2}$.*

Proof. According the proof of Theorem 2.6, there are three structures such that $G \in \mathcal{U}_{n,\alpha}$ for $\alpha = 2$. If $G = C_4$ or $G = C_5$, then $ABS(C_4) = 2\sqrt{2}$ and $ABS(C_5) = \dfrac{5\sqrt{2}}{2}$, respectively. Further, if G is obtained by attaching $n-3$ pendant vertices to one vertex of C_3, then it is clearly that $ABS(G) = 2\sqrt{\frac{n-1}{n+1}} + (n-3)\sqrt{\frac{n-2}{n}} + \frac{\sqrt{2}}{2}$. Above all, the result holds. □

Theorem 3.3. *Let $G \in \mathcal{U}_{n,\alpha}$ with diameter $\alpha = 3$ and $n \geq 5$. Then we have $ABS(G) \leq 2\sqrt{\frac{n-1}{n+1}} + (n-3)\sqrt{\frac{n-2}{n}} + \frac{\sqrt{2}}{2}$.*

Proof. By Lemma 1.1, we know the graph S_n^+ has the maximum ABS index in the class of all unicyclic graphs. When $n_1,\ n_2 \geq 1$ and $n_3 \geq 0$, we obtain $\alpha(S_n^+) = 3$ and $n = n_1 + n_2 + n_3 + 3 \geq 5$. Thus, the result is true. □

Theorem 3.4. *Let $G \in \mathcal{U}_{n,\alpha}$ with diameter $\alpha \geq 4$ and $n = \alpha + 2$. Then $ABS(G) \leq ABS(U_{\alpha+2}^\alpha)$, where the equality holds if and only if $G \cong U_{\alpha+2}^\alpha$.*

Proof. Let $G^+ \in \mathcal{U}_{n,\alpha}^{max}$ with $n = \alpha + 2$. Let $P^\alpha = u_1u_2\cdots u_\alpha u_{\alpha+1}$ be a diametral path and C_l be the unique cycle of G^+. Then there exists a vertex $w \notin V(P^\alpha)$ such that C_l is denoted by $C_l = u_iu_{i+1}wu_i$ or $C_l = u_iu_{i+1}u_{i+2}wu_i$ (otherwise, if $l \geq 5$, then it contradicts P^α).

Claim 1. *$u_1 \notin V(C_l)$ and $u_{\alpha+1} \notin V(C_l)$.*

Seeking a contradiction, we assume that $u_1 \in V(C_l)$ or $u_{\alpha+1} \in V(C_l)$.
Case 1. $C_l = u_1u_2wu_1$.

Let $G^{++} = G^{+} - \{u_1w\} + \{u_3w\}$. Then $G^{++} \in \mathcal{U}_{\alpha+2,\alpha}$ and

$$ABS\,(G^{+}) - ABS\,(G^{++}) = 2\sqrt{\frac{2}{2+2}} - \sqrt{\frac{2}{3+1}} - \sqrt{\frac{4}{3+3}} < 0.$$

Case 2. $C_l = u_1u_2u_3wu_1$.

Let $G^{++} = G^{+} - \{u_1w\} + \{u_2w\}$. Then $G^{++} \in \mathcal{U}_{\alpha+2,\alpha}$ and

$$ABS\,(G^{+}) - ABS\,(G^{++}) = 2\sqrt{\frac{2}{2+2}} - \sqrt{\frac{2}{3+1}} - \sqrt{\frac{4}{3+3}} < 0.$$

Note that these two cases are both contradicted with $G^{+} \in \mathcal{U}_{n,\alpha}^{max}$, and hence $u_1 \notin V(C_l)$. Similarly, we also have $u_{\alpha+1} \notin V(C_l)$.

Claim 2. $l = 4$.

By contradiction, we may assume $l \geq 5$, which contradicts to the fact the diametral path $P^{\alpha} = u_1u_2 \ldots u_{\alpha}u_{\alpha+1}$. In what follows, we consider $l = 3$ or $l = 4$. If $l = 3$, then $C_l = u_iu_{i+1}wu_i$. According to Claim 1, it is clear that $2 \leq i \leq \alpha - 1$ and $u_{i-1} \notin PV\,(G^{+})$ or $u_{i+2} \notin PV\,(G^{+})$ (otherwise, the diameter $\alpha = 3$). Without loss of generality, we assume that $u_{i-1} \notin PV\,(G^{+})$. Thus $d_{G^{+}}\,(u_{i-2}) = 1$ or 2.

Let $G^{++} = G^{+} - \{u_iw\} + \{u_{i-1}w\}$. Then $G^{++} \in \mathcal{U}_{\alpha+2,\alpha}$. By Lemma 2.1, it holds that

$$\begin{aligned}
&ABS\,(G^{+}) - ABS\,(G^{++})\\
&= \sqrt{\frac{d_{G^{+}}\,(u_{i-2})}{d_{G^{+}}\,(u_{i-2})+2}} - \sqrt{\frac{d_{G^{+}}\,(u_{i-2})+1}{d_{G^{+}}\,(u_{i-2})+3}} - \sqrt{\frac{4}{3+3}} - \sqrt{\frac{3}{2+3}}\\
&\leq \sqrt{\frac{1}{1+2}} - \sqrt{\frac{2}{1+3}} - \sqrt{\frac{4}{3+3}} - \sqrt{\frac{3}{2+3}} < 0,
\end{aligned}$$

which contradicts $G^{+} \in \mathcal{U}_{n,\alpha}^{max}$. Hence we obtain that $l = 4$ and $2 \leq i \leq \alpha - 2$. Above all, if $2 < i < \alpha - 2$, then

$$ABS\,(G^{+}) - ABS\left(U_{\alpha+2}^{\alpha}\right) = \sqrt{\frac{3}{2+3}} + \sqrt{\frac{1}{1+2}} - \sqrt{\frac{2}{1+3}} - \sqrt{\frac{2}{2+2}} < 0,$$

which also contradicts $G^{+} \in \mathcal{U}_{n,\alpha}^{max}$. Therefore whether $i = 2$ or $i = \alpha - 2$, i.e., $G^{+} \cong U_{\alpha+2}^{\alpha}$. □

The case of $n = \alpha + 2$ has discussed in Theorem 3.4, we discuss the case of $n \geq \alpha + 3$ in the remainder of the article. To simplify the proof, we present three lemmas as follows.

Lemma 3.5. *Let $G^{+} \in \mathcal{U}_{n,\alpha}^{\max}$ with $3 \leq \alpha \leq n-3$ and $P^{\alpha} = u_1u_2 \cdots u_{\alpha}u_{\alpha+1}$ be a diametral path. If $u \in PV(G^{+})$ and either $uu_2 \in E(G^{+})$ or $uu_{\alpha} \in E(G^{+})$, then $|V(C_l) \cap V(P^{\alpha})| \geq 2$.*

Proof. In the following proof, we suppose that $|V(C_l) \cap V(P^{\alpha})| \leq 1$ seeking a contradiction.

Case 1. $|V(C_l) \cap V(P^{\alpha})| = 0$.

If $|V(C_l) \cap V(P^{\alpha})| = 0$, then there exists a path $u_iw_1w_2 \cdots w_k$ attaching cycle C_l and path P^{α}. Hence $u_{i-1} \notin PV\,(G^{+})$ and $u_{i+1} \notin PV\,(G^{+})$ with $3 \leq i \leq \alpha - 1$, that is, $d_{G^{+}}(u_{i-1}) \geq 2$ and $d_{G^{+}}(u_{i+1}) \geq 2$.

Case 1.1. $k = 1$.

Let G^{++} be the graph obtained from G^{+} by *e.g.t.* edge u_iw_1. Then $G^{++} \in \mathcal{U}_{n,\alpha}$. As $d_{G^{+}}\,(u_{i-1}) = d_{G^{++}}\,(u_{i-1})$ and $d_{G^{+}}(u_{i+1}) = d_{G^{++}}(u_{i+1})$, the following holds from Lemma 2.1.

$$\begin{aligned}
&ABS\,(G^{+}) - ABS\,(G^{++})\\
&= \left(\sqrt{\frac{d_{G^{+}}\,(u_{i-1})+1}{d_{G^{+}}\,(u_{i-1})+3}} - \sqrt{\frac{d_{G^{++}}\,(u_{i-1})+3}{d_{G^{++}}\,(u_{i-1})+5}}\right) + 2\sqrt{\frac{3}{2+3}} + \sqrt{\frac{4}{3+3}}\\
&\quad + \left(\sqrt{\frac{d_{G^{+}}(u_{i+1})+1}{d_{G^{+}}(u_{i+1})+3}} - \sqrt{\frac{d_{G^{++}}(u_{i+1})+3}{d_{G^{++}}(u_{i+1})+5}}\right) - 2\sqrt{\frac{5}{2+5}} - \sqrt{\frac{4}{1+5}}\\
&< 0.
\end{aligned}$$

Case 1.2. $k = 2$.

We consider $G^{++} = G^{+} - \{w_1w_2\} + \{u_iw_2\}$, then $G^{++} \in \mathcal{U}_{n,\alpha}$. Since $d_{G^+}(u_{i-1}) = d_{G^{++}}(u_{i-1})$ and $d_{G^+}(u_{i+1}) = d_{G^{++}}(u_{i+1})$, by Lemma 2.1, we obtain that

$$\begin{aligned}
&ABS\,(G^+) - ABS\,(G^{++})\\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1})+1}{d_{G^+}(u_{i-1})+3}} - \sqrt{\frac{d_{G^{++}}(u_{i-1})+2}{d_{G^{++}}(u_{i-1})+4}}\right) + 2\sqrt{\frac{3}{2+3}} - \sqrt{\frac{5}{3+4}}\\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i+1})+1}{d_{G^+}(u_{i+1})+3}} - \sqrt{\frac{d_{G^{++}}(u_{i+1})+2}{d_{G^{++}}(u_{i+1})+4}}\right) - \sqrt{\frac{3}{1+4}}\\
&< 0.
\end{aligned}$$

Case 1.3. $k \geq 3$.

We denote $G^{++} = G^{+} - \{w_1w_2\} + \{u_iw_2\}$. One can easily find that $G^{++} \in \mathcal{U}_{n,\alpha}$, $d_{G^+}(u_{i-1}) = d_{G^{++}}(u_{i-1})$ and $d_{G^+}(u_{i+1}) = d_{G^{++}}(u_{i+1})$. On the basis of Lemma 2.1, then

$$\begin{aligned}
&ABS\,(G^+) - ABS\,(G^{++})\\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1})+1}{d_{G^+}(u_{i-1})+3}} - \sqrt{\frac{d_{G^{++}}(u_{i-1})+2}{d_{G^{++}}(u_{i-1})+4}}\right) + \sqrt{\frac{3}{2+3}}\\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i+1})+1}{d_{G^+}(u_{i+1})+3}} - \sqrt{\frac{d_{G^{++}}(u_{i+1})+2}{d_{G^{++}}(u_{i+1})+4}}\right) - \sqrt{\frac{4}{2+4}}\\
&< 0.
\end{aligned}$$

Case 2. $|V(C_l) \cap V(P^\alpha)| = 1$.

Let $C_l = v_1v_2v_3\cdots v_lv_1$ and let v_1 be the common vertex of C_l and P^α, where $u_i = v_1$. Note that $\alpha \geq 4$, one has $d_{G^+}(u_{i-1}) \geq 2$ or $d_{G^+}(u_{i+1}) \geq 2$ for $2 \leq i \leq \alpha$. Without loss of generality, we assume that $d_{G^+}(u_{i+1}) \geq 2$, and hence $d_{G^+}(u_i) \geq 4$ and $d_{G^+}(u_{i+2}) \geq 1$.

Case 2.1. $l = 3$.

Let $G^{++} = G^{+} - \{v_2v_3\} + \{v_2u_{i+1}\}$. Then $G^{++} \in \mathcal{U}_{n,\alpha}$ and by Lemma 2.1, we have

$$\begin{aligned}
&ABS\,(G^+) - ABS\,(G^{++})\\
&= \sqrt{\frac{d_{G^+}(u_i)}{d_{G^+}(u_i)+2}} - \sqrt{\frac{d_{G^+}(u_i)-1}{d_{G^+}(u_i)+1}} + \sqrt{\frac{2}{2+2}} - \sqrt{\frac{d_{G^+}(u_{i+1})+1}{d_{G^+}(u_{i+1})+1+2}}\\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_i)+d_{G^+}(u_{i+1})-2}{d_{G^+}(u_i)+d_{G^+}(u_{i+1})}} - \sqrt{\frac{d_{G^+}(u_i)+d_{G^+}(u_{i+1})-1}{d_{G^+}(u_i)+d_{G^+}(u_{i+1})+1}}\right)\\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_i)+d_{G^+}(u_{i+2})-2}{d_{G^+}(u_i)+d_{G^+}(u_{i+2})}} - \sqrt{\frac{d_{G^+}(u_i)+d_{G^+}(u_{i+2})-1}{d_{G^+}(u_i)+1+d_{G^+}(u_{i+2})}}\right)\\
&< \sqrt{\frac{4}{4+2}} - \sqrt{\frac{3}{4+1}} + \sqrt{\frac{2}{2+2}} - \sqrt{\frac{3}{2+1+2}} < 0.
\end{aligned}$$

Case 2.2. $l \geq 4$.

For $l \geq 4$ and $3 \leq i \leq \alpha - 1$, we define $G^{++} = G^{+} - \{v_2v_3\} + \{u_iv_3\}$. Thus we know $G^{++} \in \mathcal{U}_{n,\alpha}$. According to Lemma 2.1, the following holds.

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1}) + 2}{d_{G^+}(u_{i-1}) + 4}} - \sqrt{\frac{d_{G^+}(u_{i-1}) + 3}{d_{G^+}(u_{i-1}) + 5}} \right) + \sqrt{\frac{2}{2+2}} - \sqrt{\frac{4}{1+5}} \\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i+1}) + 2}{d_{G^+}(u_{i+1}) + 4}} - \sqrt{\frac{d_{G^+}(u_{i+1}) + 3}{d_{G^+}(u_{i+1}) + 5}} \right) + 2\left(\sqrt{\frac{4}{2+4}} - \sqrt{\frac{5}{2+5}} \right) \\
&< \frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{3} < 0.
\end{aligned}
$$

Above all cases contradict to $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$, and hence $|V(C_l) \cap V(P^\alpha)| \geq 2$ is feasible. □

Lemma 3.6. *Let $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$ with $3 \leq \alpha \leq n-3$. Then there must exist a vertex $u_0 \in PV(G^+)$ such that $G^+ - u_0 \in \mathcal{U}_{n-1,\alpha}$.*

Proof. Based on Lemma 2.2, we just prove the existence of vertex u_0. By contradiction, we suppose that $G^+ - u \in \mathcal{U}_{n-1,\alpha-1}$ for each $u \in PV(G^+)$. Let $P^\alpha = u_1u_2\cdots u_\alpha u_{\alpha+1}$ be a diametral path of G^+ and $u_1 \in PV(G^+)$. Then $u = u_1$ or $u = u_{\alpha+1}$. Combined with Lemma 3.5, we claim that $|V(C_l) \cap V(P^\alpha)| \geq 2$. Let $C_l = u_iu_{i+1}\cdots u_{i+j}v_kv_{k-1}\cdots v_3v_2v_1(u_i)$ for $j \geq 1$. Then $j \leq k$ (otherwise it contradicts the diametral path P^α) and $k \geq 2$ as $n \geq \alpha + 3$. Note that $d_{G^+}(u_{i-1}) \geq 1, d_{G^+}(u_i) = 3$ and $d_{G^+}(v_2) = d_{G^+}(v_3) = 2$.

Case 1. $j = k \geq 3$.

Let $G^{++} = G^+ - \{u_iv_2\} - \{v_2v_3\} + \{u_{i+1}v_2\} + \{u_{i+1}v_3\}$. Then $d_{G^{++}}(u_{i-1}) = d_{G^+}(u_{i-1}) \geq 1$ and we conclude that $G^{++} \in \mathcal{U}_{n,\alpha}$. As a result, we have

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1}) + 1}{d_{G^+}(u_{i-1}) + 3}} - \sqrt{\frac{d_{G^{++}}(u_{i-1}) + 1}{d_{G^{++}}(u_{i-1}) + 2}} \right) + 2\left(\sqrt{\frac{2}{2+2}} + \sqrt{\frac{3}{2+3}} \right) \\
&\quad - 3\sqrt{\frac{4}{2+4}} - \sqrt{\frac{3}{1+4}}.
\end{aligned}
$$

Case 1.1. $d_{G^+}(u_{i-1}) = 1$.

Using Lemma 2.1, it holds that

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{2}{1+3}} - \sqrt{\frac{1}{1+2}} \right) + \sqrt{2} + \frac{\sqrt{15}}{5} - \sqrt{6} \\
&= \frac{3\sqrt{2}}{2} - \frac{\sqrt{3}}{3} - \sqrt{6} + \frac{\sqrt{15}}{5} < 0.
\end{aligned}
$$

Case 1.2. $d_{G^+}(u_{i-1}) \geq 2$.

Similarly, the following holds from Lemma 2.1.

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&\leq \left(\sqrt{\frac{3}{2+3}} - \sqrt{\frac{2}{2+2}} \right) + 2\left(\sqrt{\frac{2}{2+2}} + \sqrt{\frac{3}{2+3}} \right) - 3\sqrt{\frac{4}{2+4}} - \sqrt{\frac{3}{1+4}} \\
&= \frac{\sqrt{2}}{2} - \sqrt{6} + \frac{2\sqrt{15}}{5} < 0.
\end{aligned}
$$

Case 2. $k > j$.

If $k > j$, then $G^{++} = G^{+} - \{v_2v_3\} + \{u_iv_3\}$, in which we obtain $G^{++} \in \mathcal{U}_{n,\alpha}$ and the following is true by Lemma 2.1.

$$\begin{aligned}
&ABS(G^{+}) - ABS(G^{++})\\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1})+1}{d_{G^+}(u_{i-1})+3}} - \sqrt{\frac{d_{G^+}(u_{i-1})+2}{d_{G^+}(u_{i-1})+4}}\right) + \left(\sqrt{\frac{2}{2+2}} + \sqrt{\frac{3}{2+3}}\right)\\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i+1})+1}{d_{G^+}(u_{i+1})+3}} - \sqrt{\frac{d_{G^+}(u_{i+1})+2}{d_{G^+}(u_{i+1})+4}}\right) - \left(\sqrt{\frac{4}{2+4}} + \sqrt{\frac{3}{1+4}}\right)\\
&< \frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{3} < 0.
\end{aligned}$$

Both of these two cases are contradicted with $G^{+} \in \mathcal{U}_{n,\alpha}^{\max}$, in which there must exist a vertex $u_0 \in PV(G^{+})$ such that $G^{+} - u_0 \in \mathcal{U}_{n-1,\alpha}$. □

Lemma 3.7. *Let $G^{+} \in \mathcal{U}_{n,\alpha}^{\max}$ with $4 \le \alpha \le n-3$ and $V_1 = \{u \in PV(G^{+}) \mid G^{+} - u \in \mathcal{U}_{n-1,\alpha}\}$. Let $v \in \bigcup_{u\in V_1} N_{G^+}(u)$ and $R_{G^+}(v) = \{w \in N_{G^+}(v) \mid d_{G^+}(w) \ge 2\}$, where $|R_{G^+}(v)| \ge 1$. Then there must exist a vertex $u_0 \in PV(G^{+})$ such that $u_0 \in V_1$ and $|R_{G^+}(N_{G^+}(u_0))| \ge 2$.*

Proof. In this proof, we know $V_1 \ne \emptyset$ by Lemma 3.6. On the contrary, we suppose $|R_{G^+}(v)| = 1$ for all $v \in \bigcup_{u\in V_1} N_{G^+}(u)$ since $|R_{G^+}(v)| \ge 1$. Let $C_l = v_1v_2\cdots v_lv_1$ be a cycle and let $P^{\alpha} = u_1u_2\cdots u_{\alpha}u_{\alpha+1}$ be a diametral path of G^{+}.

Claim 1. $V_1 \subseteq N_{G^+}(u_2) \bigcup N_{G^+}(u_{\alpha})$.

If $V_1 \subseteq N_{G^+}(u_2) \bigcup N_{G^+}(u_{\alpha})$, then there exists a vertex $u \in N_{G^+}(u_2) \bigcup N_{G^+}(u_{\alpha})$, while $u \notin V_1$. Seeking a contradiction, we may assume that $u \in V_1$, but $u \notin N_{G^+}(u_2) \bigcup N_{G^+}(u_{\alpha})$. Denote $N_{G^+}(u) = v$, and hence $v \notin \{u_2, u_{\alpha}\}$ and $v \notin \{u_1, u_{\alpha+1}\}$ (otherwise, the diameter α will change). Since $|R_{G^+}(v)| = 1$ for all $v \in \bigcup_{u\in V_1} N_{G^+}(u)$, we know $v \notin V(P^{\alpha}) \bigcup V(C_l)$. Let $w \in N_{G^+}(v)$ with $d_{G^+}(w) = t+1 \ge 2$ and $N_{G^+}(w) = \{v, x_1, x_2, \cdots, x_t\}$.

Let $G^{++} = G^{+} - \bigcup_{1\le i\le t}\{x_iw\} + \bigcup_{1\le i\le t}\{x_iv\}$. Observe that $G^{++} \in \mathcal{U}_{n,\alpha}$ and the following holds from Lemma 2.1.

$$\begin{aligned}
&ABS(G^{+}) - ABS(G^{++})\\
&= \sum_{i=1}^{t}\left(\sqrt{\frac{d_{G^+}(x_i)+t-1}{d_{G^+}(x_i)+(t+1)}} - \sqrt{\frac{d_{G^+}(x_i)+d_{G^+}(v)+t-2}{d_{G^+}(x_i)+(d_{G^+}(v)+t)}}\right)\\
&\quad + (d_{G^+}(v)-1)\left(\sqrt{\frac{d_{G^+}(v)-1}{d_{G^+}(v)+1}} - \sqrt{\frac{d_{G^+}(v)+t-1}{(d_{G^+}(v)+t)+1}}\right)\\
&\quad + \left(\sqrt{\frac{d_{G^+}(v)+t-1}{d_{G^+}(v)+(t+1)}} - \sqrt{\frac{d_{G^+}(v)+t-1}{(d_{G^+}(v)+t)+1}}\right)\\
&< 0,
\end{aligned}$$

which is a contradiction with $G^{+} \in \mathcal{U}_{n,\alpha}^{\max}$. Thus the Claim 1 holds.

As $V_1 \ne \emptyset$ and $V_1 \subseteq N_{G^+}(u_2) \cup N_{G^+}(u_{\alpha})$, there exists $u \in V_1$ such that $u \in N_{G^+}(u_2)$ and $|R_{G^+}(u_2)| = 1$. Then u_1, $u_2 \notin C_l$, $d_{G^+}(u_2) \ge 3$ and $d_{G^+}(u_{i-1}) \ge 1$. By Lemma 3.5, then $|V(C_l) \cap V(P^{\alpha})| \ge 2$. Let $C_l = u_iu_{i+1}\ldots u_{i+j}v_kv_{k-1}\cdots v_3v_2v_1\,(u_i)$ for $j \ge 1$. Then $j \le k$.

Claim 2. $|V(C_l)\backslash V(P^{\alpha})| = 1$.

By contradiction, we may assume $|V(C_l)\backslash V(P^\alpha)| \geq 2$, which implies $k \geq 2$. Thus it suffices to only consider the following two cases.

Case 1. $k = j$.

Let $G^{++} = G^+ - \{u_iv_2\} - \{v_2v_3\} + \{u_{i+1}v_2\} + \{u_{i+1}v_3\}$. Then $G^{++} \in \mathcal{U}_{n,\alpha}$ and we conclude the following holds by Lemma 2.1.

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{d_{G^+}(u_{i+2})}{d_{G^+}(u_{i+2})+2}} - \sqrt{\frac{d_{G^+}(u_{i+2})+2}{d_{G^+}(u_{i+2})+4}}\right) + 2\left(\sqrt{\frac{3}{3+2}} - \sqrt{\frac{4}{2+4}}\right) \\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i-1})+1}{d_{G^+}(u_{i-1})+3}} - \sqrt{\frac{d_{G^+}(u_{i-1})}{d_{G^+}(u_{i-1})+2}}\right) + \left(\sqrt{\frac{2}{2+2}} - \sqrt{\frac{3}{1+4}}\right) \\
&< 2\left(\frac{\sqrt{15}}{5} - \frac{\sqrt{6}}{3}\right) + \sqrt{\frac{2}{1+3}} - \sqrt{\frac{1}{1+2}} + \frac{\sqrt{2}}{2} - \frac{\sqrt{15}}{5} < 0.
\end{aligned}
$$

Case 2. $k > j$.

We denote $G^{++} = G^+ - \{v_2v_3\} + \{u_iv_3\}$. Then $G^{++} \in \mathcal{U}_{n,\alpha}$ and by Lemma 2.1, we have

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{d_{G^+}(u_{i-1})+1}{d_{G^+}(u_{i-1})+3}} - \sqrt{\frac{d_{G^+}(u_{i-1})+2}{d_{G^+}(u_{i-1})+4}}\right) + \sqrt{\frac{3}{3+2}} + \sqrt{\frac{2}{2+2}} \\
&\quad + \left(\sqrt{\frac{d_{G^+}(u_{i+1})+1}{d_{G^+}(u_{i+1})+3}} - \sqrt{\frac{d_{G^+}(u_{i+1})+2}{d_{G^+}(u_{i+1})+4}}\right) - \sqrt{\frac{2}{2+4}} - \sqrt{\frac{3}{1+4}} \\
&< \frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{3} < 0,
\end{aligned}
$$

which is a contradiction with $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$. Therefore, the Claim 2 holds.

Claim 3. $d_{G^+}(u_{\alpha+1}) = 1$.

It suffices to prove that $d_{G^+}(u_{\alpha+1}) \geq 2$ not holds. If $d_{G^+}(u_{\alpha+1}) \geq 3$, then the diametral path P^α will be changed. Hence we obtain $d_{G^+}(u_{\alpha+1}) = 2$. For all $v \in \bigcup_{u\in V_1} N_{G^+}(u)$, we suppose $|R_{G^+}(v)| = 1$, then u_α is non-adjacent to a pendant vertex. As $\alpha \geq 4$, it is clear that $d_{G^+}(u_{\alpha-2}) \geq 2$. Further, we have $|V(C_l)\backslash V(P^\alpha)| = 1$ by Claim 2, i.e., $|V(C_l)| = 3$ or 4 .

Case 1. $|V(C_l)| = 3$.

There exists the unique cycle $C_l = u_\alpha u_{\alpha+1} w u_\alpha$ such that the diameter α does not change. By letting $G^{++} = G^+ - \{u_{\alpha+1}w\} + \{u_{\alpha-1}w\}$ and Lemma 2.1, it is clear that $G^{++} \in \mathcal{U}_{n,\alpha}$ and

$$
\begin{aligned}
&ABS(G^+) - ABS(G^{++}) \\
&= \left(\sqrt{\frac{d_{G^+}(u_{\alpha-2})}{d_{G^+}(u_{\alpha-2})+2}} - \sqrt{\frac{d_{G^+}(u_{\alpha-2})+1}{d_{G^+}(u_{\alpha-2})+3}}\right) + 2\sqrt{\frac{3}{3+2}} \\
&\quad + \sqrt{\frac{2}{2+2}} - \sqrt{\frac{4}{3+3}} - \sqrt{\frac{2}{1+3}} - \sqrt{\frac{3}{2+3}} \\
&< \frac{\sqrt{15}}{5} - \frac{\sqrt{6}}{3} < 0.
\end{aligned}
$$

Case 2. $|V(C_l)| = 4$.

If $|V(C_l)| = 4$, then there exists the exactly one cycle $C_l = u_{\alpha-1}u_\alpha u_{\alpha+1}wu_{\alpha-1}$ such that the diameter α does not change. Let $G^{++} = G^+ - \{u_{\alpha+1}w\} + \{u_\alpha w\}$. Then $G^{++} \in \mathcal{U}_{n,\alpha}$ and

$$ABS(G^+) - ABS(G^{++}) = 2\sqrt{\frac{2}{2+2}} - \sqrt{\frac{4}{3+3}} - \sqrt{\frac{2}{1+3}} < 0.$$

Both of these two cases are contradicted with $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$. Therefore Claim 3 is feasible.

Claim 4. $|V(C_l)| = 4$.

We assume $|V(C_l)| = 3$ by a contradiction, i.e., $C_l = u_iu_{i+1}wu_i$ $(3 \le i \le \alpha - 1)$. We have $d_{G^+}(u_2) = x \ge 3$ as $V_1 \ne \emptyset$. Thus we only consider the following two cases.

Case 1. $i = 3$.

Let $G^{++} = G^+ - \{u_3w\} + \{u_2w\}$. Then $G^{++} \in \mathcal{U}_{n,\alpha}$ and by Lemma 2.1, we have

$$\begin{aligned}
&ABS(G^+) - ABS(G^{++})\\
&= (d_{G^+}(u_2) - 1)\left(\sqrt{\frac{d_{G^+}(u_2) - 1}{d_{G^+}(u_2) + 1}} - \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 1 + 1}}\right)\\
&\quad + \sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 3}} - 2\sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 1 + 2}} + \sqrt{\frac{4}{3+3}}\\
&= (x-1)\left(\sqrt{\frac{x-1}{x+1}} - \sqrt{\frac{x}{x+1+1}}\right) + \left(\frac{\sqrt{6}}{3} - \sqrt{\frac{x+1}{x+3}}\right)\\
&< 0.
\end{aligned}$$

Case 2. $i \ge 4$.

In this case, we denote $G^{++} = G^+ - \{u_iw\} - \{u_{i+1}w\} + \{u_2w\} + \{u_4w\}$. Since $d_{G^+}(u_{i+2}) = y \ge 1$ and by Lemma 2.1, we know $G^{++} \in \mathcal{U}_{n,\alpha}$ and

$$\begin{aligned}
&ABS(G^+) - ABS(G^{++})\\
&= (d_{G^+}(u_2) - 1)\left(\sqrt{\frac{d_{G^+}(u_2) - 1}{d_{G^+}(u_2) + 1}} - \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 1 + 1}}\right) + \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 2}}\\
&\quad - 2\sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 1 + 2}} + \sqrt{\frac{d_{G^+}(u_{i+2}) + 1}{d_{G^+}(u_{i+2}) + 3}} - \sqrt{\frac{d_{G^+}(u_{i+2})}{d_{G^+}(u_{i+2}) + 2}} - \sqrt{\frac{4}{3+3}}\\
&= (x-1)\sqrt{\frac{x-1}{x+1}} - (x-2)\sqrt{\frac{x}{x+2}} - 2\sqrt{\frac{x+1}{x+3}} + \sqrt{\frac{y+1}{y+3}} - \sqrt{\frac{y}{y+2}} + \frac{\sqrt{6}}{3}.
\end{aligned}$$

We consider

$$f(x,y) = (x-1)\sqrt{\frac{x-1}{x+1}} - (x-2)\sqrt{\frac{x}{x+2}} - 2\sqrt{\frac{x+1}{x+3}} + \sqrt{\frac{y+1}{y+3}} - \sqrt{\frac{y}{y+2}} + \frac{\sqrt{6}}{3}.$$

According to Lemma 2.1, we know $f(x,y)$ is decreasing on $y \ge 1$. And for $x \ge 3$, we have

$$\frac{\partial f(x,y)}{\partial x} = \sqrt{\frac{x-1}{x+1}} + \frac{x-1}{\sqrt{\frac{x-1}{x+1}}\,(x+1)^2} - \sqrt{\frac{x}{x+2}} - \frac{x-2}{\sqrt{\frac{x}{x+2}}\,(x+2)^2} - \frac{2}{\sqrt{\frac{x+1}{x+3}}\,(x+3)^2}.$$

By Remark 3.8, the following holds.

$$f(x,y) \leq f(x,1) \leq f(3,1) = -0.047 < 0.$$

As a result, Claim 4 is true, then there exists the only one cycle $C_l = u_i u_{i+1} u_{i+2} w u_i$ with $3 \leq i \leq \alpha - 2$ such that $d_{G^+}(u_{\alpha+1}) = 1, d_{G^+}(u_2) \geq 3$ and $d_{G^+}(u_{i+3}) \geq 1$.

If $i = 3$, then $d_{G^+}(u_6) = t \geq 1$ and the following is true.

$$\begin{aligned}
&ABS\,(G^+) - ABS\,(U_n^\alpha) \\
&= (d_{G^+}(u_2) - 1)\left(\sqrt{\frac{d_{G^+}(u_2) - 1}{d_{G^+}(u_2) + 1}} - \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 1 + 1}}\right) + \sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 3}} \\
&\quad - 2\sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 1 + 2}} + \sqrt{\frac{d_{G^+}(u_6) + 1}{d_{G^+}(u_6) + 3}} - \sqrt{\frac{d_{G^+}(u_6)}{d_{G^+}(u_6) + 2}} + \sqrt{\frac{3}{2+3}}.
\end{aligned}$$

Let

$$g(x,t) = (x-1)\sqrt{\frac{x-1}{x+1}} - (x-1)\sqrt{\frac{x}{x+2}} - \sqrt{\frac{x+1}{x+3}} + \sqrt{\frac{t+1}{t+3}} - \sqrt{\frac{t}{t+2}} + \frac{\sqrt{15}}{5}.$$

By Lemma 2.1, we have $g(x,t)$ is decreasing on $t \geq 1$. And for $x \geq 3$, we have

$$\begin{aligned}
\frac{\partial g(x,t)}{\partial x} &= \sqrt{\frac{x-1}{x+1}} + \frac{x-1}{\sqrt{\frac{x-1}{x+1}}\,(x+1)^2} - \sqrt{\frac{x}{x+2}} - \frac{x-1}{\sqrt{\frac{x}{x+2}}\,(x+2)^2} - \frac{1}{\sqrt{\frac{x+1}{x+3}}\,(x+3)^2} \\
&= -\frac{A}{\sqrt{\frac{x-1}{x+1}}\,(x+1)^2\,\sqrt{\frac{x}{x+2}}\,(x+2)^2\,\sqrt{\frac{x+1}{x+3}}\,(x+3)^2} < 0,
\end{aligned}$$

where

$$\begin{aligned}
A = &\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x^6 - \sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x^6 + 11\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x^5 \\
&- 11\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x^5 + \sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x}{x+2}}x^4 + 45\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x^4 \\
&- 45\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x^4 + 6\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x}{x+2}}x^3 + 82\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x^3 \\
&- 77\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x^3 + 13\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x}{x+2}}x^2 + 59\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x^2 \\
&- 22\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x^2 + 12\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x}{x+2}}x + 3\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}}x \\
&+ 84\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}}x + 4\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x}{x+2}} - 9\sqrt{\frac{x-1}{x+1}}\sqrt{\frac{x+1}{x+3}} \\
&+ 72\sqrt{\frac{x}{x+2}}\sqrt{\frac{x+1}{x+3}} \\
> 0.&
\end{aligned}$$

Hence, the following holds.

$$g(x,t) \leq g(x,1) \leq g(3,1) = -0.047 < 0.$$

On the other hand, if $4 \le i \le \alpha - 2$, then by Lemma 2.1 and Remark 3.8 we also know

$$\begin{aligned}
&ABS\,(G^+) - ABS\,(U_n^\alpha)\\
&= (d_{G^+}(u_2) - 1)\left(\sqrt{\frac{d_{G^+}(u_2) - 1}{d_{G^+}(u_2) + 1}} - \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 1 + 1}}\right)\\
&\quad - 2\sqrt{\frac{d_{G^+}(u_2) + 1}{d_{G^+}(u_2) + 1 + 2}} + \sqrt{\frac{d_{G^+}(u_2)}{d_{G^+}(u_2) + 2}} + 2\sqrt{\frac{3}{2+3}}\\
&\quad + \sqrt{\frac{d_{G^+}\,(u_{i+3}) + 1}{d_{G^+}\,(u_{i+3}) + 3}} - \sqrt{\frac{d_{G^+}\,(u_{i+3})}{d_{G^+}\,(u_{i+3}) + 2}} - \sqrt{\frac{2}{2+2}}\\
&\le 2\left(\sqrt{\frac{2}{3+1}} - \sqrt{\frac{3}{3+1+1}}\right) - 2\sqrt{\frac{4}{4+2}} + \sqrt{\frac{3}{3+2}}\\
&\quad + \frac{2\sqrt{15}}{5} + \sqrt{\frac{2}{1+3}} - \sqrt{\frac{1}{1+2}} - \frac{\sqrt{2}}{2}\\
&= \sqrt{2} - \frac{2\sqrt{6}}{3} + \frac{\sqrt{15}}{5} - \frac{\sqrt{3}}{3} < 0.
\end{aligned}$$

Therefore, if $|R_{G^+}(v)| = 1$ for all $v \in \bigcup_{u\in V_1} N_{G^+}(u)$, then it is a contradiction to $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$. Thus, there must exist a vertex $u_0 \in PV\,(G^+)$ such that $u_0 \in V_1$ and $|R_{G^+}\,(N_{G^+}\,(u_0))| \ge 2$. The result follows. □

Remark 3.8. *For $x \ge 3$, the function $f(x) = (x-1)\sqrt{1 - \frac{2}{x+1}} - (x-2)\sqrt{1 - \frac{2}{x+2}} - 2\sqrt{1 - \frac{2}{x+3}}$ obtains its maximum value at $x = 3$. Since*

$$f'(x_0) = \sqrt{\frac{x-1}{x+1}} + \frac{x-1}{\sqrt{\frac{x-1}{x+1}}\,(x+1)^2} - \sqrt{\frac{x}{x+2}} - \frac{x-2}{\sqrt{\frac{x}{x+2}}\,(x+2)^2} - \frac{2}{\sqrt{\frac{x+1}{x+3}}\,(x+3)^2},$$

there exists a unique $6 < x_0 < 7$ such that $f'(x_0) = 0$. Further, we obtain $f'(x_0) < 0$ with $3 \le x \le x_0$ and $f'(x_0) > 0$ with $x \ge x_0$, i.e., $f(x)$ is decreasing in $[3, x_0]$ and increasing in $[x_0, +\infty)$. If $x = 3$, then $f(3) = -0.010 < 0$. If $x \to +\infty$, then $f(x) \to -1 < 0$. Hence, for $x \ge 3$, the function $f(x) \le f(3)$.

Theorem 3.9. *Let $G \in \mathcal{U}_{n,\alpha}$ with $\alpha \ge 4$ and $n \ge \alpha + 2$. Then $ABS(G) \le ABS\,(U_n^\alpha)$ with equality if and only if $G \cong U_n^\alpha$.*

Proof. We prove the theorem by induction on n. If $n = \alpha + 2$, then the result holds for Theorem 3.4. In what follows, we just consider that $4 \le \alpha \le n - 3$. For convenience, we assume the conclusion holds for $n - 1$ and let $G^+ \in \mathcal{U}_{n,\alpha}^{\max}$. According to Lemma 3.7, there exists a vertex $u \in PV\,(G^+)$ such that $G^+ - u \in \mathcal{U}_{n-1,\alpha}$.

As above, there are at least two edges $vw_1, vw_2 \in E(G^+)$, where $v = N_{G^+}(u)$ and $w_1, w_2 \notin PV(G^+)$. Let $N_{G^+}(v) = \{u, v_1, v_2, \cdots, v_{k-1}\}$. Then $|N_{G^+}(v)| = k$ and $3 \le k \le n - \alpha + 1$. Denote $d_{G^+}\,(v_i) = k_i$ for $1 \le i \le k-1$. Let

$G^{++} = G^{+} - u$. Then $G^{++} \in \mathcal{U}_{n-1,\alpha}$ with $\alpha \geq 5$. By the induction hypothesis and Remark 3.10, it is clear that

$$\begin{aligned}
&ABS\left(G^{+}\right)\\
&= ABS\left(G^{++}\right) + \sqrt{\frac{k-1}{k+1}} + \sum_{i=1}^{k-1}\left(\sqrt{\frac{k+k_i-2}{k+k_i}} - \sqrt{\frac{k+k_i-3}{k-1+k_i}}\right)\\
&\leq ABS\left(U_{n-1}^{\alpha}\right) + \sqrt{\frac{k-1}{k+1}} + 2\left(\sqrt{\frac{k}{k+2}} - \sqrt{\frac{k-1}{k-1+2}}\right)\\
&\quad + (k-3)\left(\sqrt{\frac{k-1}{k+1}} - \sqrt{\frac{k-2}{k-1+1}}\right)\\
&= (n-\alpha-2)\sqrt{\frac{n-\alpha-1}{n-\alpha+1}} + 2\sqrt{\frac{n-\alpha}{n-\alpha+2}} + (\alpha-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}\\
&\quad + (k-4)\sqrt{\frac{k-1}{k+1}} + 2\sqrt{\frac{k}{k+2}} - (k-3)\sqrt{\frac{k-2}{k}}\\
&\leq (n-\alpha-2)\sqrt{\frac{n-\alpha-1}{n-\alpha+1}} + 2\sqrt{\frac{n-\alpha}{n-\alpha+2}} + (\alpha-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}\\
&\quad + (n-\alpha-3)\sqrt{\frac{n-\alpha}{n-\alpha+2}} + 2\sqrt{\frac{n-\alpha+1}{n-\alpha+3}} - (n-\alpha-2)\sqrt{\frac{n-\alpha-1}{n-\alpha+1}}\\
&= (n-\alpha-1)\sqrt{\frac{n-\alpha}{n-\alpha+2}} + 2\sqrt{\frac{n-\alpha+1}{n-\alpha+3}} + (\alpha-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}\\
&= ABS\left(U_n^{\alpha}\right)
\end{aligned}$$

with equalities if and only if $G^{++} \cong U_{n-1}^{\alpha}$, $k = n - \alpha + 1$, exactly two vertices in $N_{G^+}(v)$ have degree 2 and the other $k-2$ vertices in $N_{G^+}(v)$ have degree 1, i.e., $G^{+} \cong U_n^{\alpha}$. If $\alpha = 4$, then we just replace $(\alpha-5)\frac{\sqrt{2}}{2} + \frac{3\sqrt{15}}{5} + \frac{\sqrt{3}}{3}$ with $\frac{2\sqrt{15}}{5} + \frac{\sqrt{2}}{2}$, and the conclusion still holds. □

Remark 3.10. *For $3 \leq k \leq n - \alpha + 1$, the function*

$$f(k) = (k-4)\sqrt{1 - \frac{2}{k+1}} + 2\sqrt{1 - \frac{2}{k+2}} - (k-3)\sqrt{1 - \frac{2}{k}}$$

is increasing. Since

$$f'(k) = \frac{k^2\left(k^2+k-3\right)\sqrt{\frac{k-2}{k}} - \left(k^2-k-3\right)(k+1)^2\sqrt{\frac{k-1}{k+1}}}{\sqrt{\frac{k-2}{k}}\sqrt{\frac{k-1}{k+1}}\,(k+1)^2 k^2}.$$

Let

$$g(k) = k^2\left(k^2+k-3\right)\sqrt{\frac{k-2}{k}} - (k+1)^2\left(k^2-k-3\right)\sqrt{\frac{k-1}{k+1}}.$$

Then for $3 \leq k \leq n - \alpha + 1$, we have

$$\begin{aligned}
g(k) = &\sqrt{\frac{k-2}{k}}k^4 - \sqrt{\frac{k-1}{k+1}}k^4 + \sqrt{\frac{k-2}{k}}k^3 - \sqrt{\frac{k-1}{k+1}}k^3\\
&- 3\sqrt{\frac{k-2}{k}}k^2 + 4\sqrt{\frac{k-1}{k+1}}k^2 + 7\sqrt{\frac{k-1}{k+1}}k + 3\sqrt{\frac{k-1}{k+1}}\\
&> 0,
\end{aligned}$$

that is, $f'(k) > 0$ and $f(k)$ is increasing on $3 \leq k \leq n - \alpha + 1$.

4. Conclusion

In this paper, we not only study the minimum *ABS* index of all unicyclic graphs of order n with diameter $\alpha \geq 2$, but also give the sharp upper bounds for the *ABS* indices of unicyclic graphs on the basis of their fixed diameter $\alpha \geq 4$. Furthermore, the corresponding extremal graphs with the sharp upper and lower bounds have been depicted, respectively.

Unicyclic graphs are quite common in molecular structure diagrams. The study of the extremal problems of the *ABS* index of unicyclic graphs with fixed diameter can be widely applied to molecular structures with a single cycle, enabling a more accurate analysis of molecular properties. Since the *ABS* index predicts better than some indices when studying physicochemical properties, investigating the extremal problems of the *ABS* index of unicyclic graphs with given diameter has significant importance.

As future work, it would be interesting and valuable to find the extremal problems of *ABS* with fixed other parameters. For example, the sharp upper bounds for the *ABS* index of unicyclic graphs with given girth represents the potential for research advancement. What's more, Jahanbani and Redžepović proposed the generalized *ABS* index of graphs in [9] recently, which also holds significant importance in the study of molecular structures and presents promising research prospects. Consequently, investigating the generalized *ABS* index with given parameters such as matching number, independence number and so on also has research significance.

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