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Research article

On the maximum atom-bond sum-connectivity index of unicyclic graphs with given diameter

Zhen Wang[1,2] **and Kai Zhou**[1,2,*]

[1] School of Big Data and Artificial Intelligence, Chizhou University, Chizhou 247000, China
[2] Applied Mathematics Research Center, Chizhou University, Chizhou 247000, China

* **Correspondence:** Email: zk1984@163.com.

Abstract: Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The atom-bond sum-connectivity (ABS) index was proposed recently and is defined as $ABS(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)+d_G(v)}}$, where $d_G(u)$ represents the degree of vertex $u \in V(G)$. A connected graph G is called a unicyclic graph if $|V(G)| = |E(G)|$. In this paper, we determine the maximum ABS index of unicyclic graphs with given diameter. In addition, the corresponding extremal graphs are characterized.

Keywords: atom-bond sum-connectivity index; unicyclic graph; diameter; pendent vertex
Mathematics Subject Classification: 05C12, 05C35

1. Introduction

Throughout this paper, we take into consideration simple connected graphs. For a graph G, denote the set of all vertices and edges of G by $V(G)$ and $E(G)$, respectively. For $u \in V(G)$, denote the set of vertices adjacent to u by $N_G(u)$. The degree of vertex $u \in V(G)$ is denoted by $d_G(u)$ and $d_G(u) = |N_G(u)|$. A vertex of degree 1 is called a pendent vertex. Let $\mathcal{P}(G) \triangleq \{v \in V(G) : v \text{ is a pendent vertex of } G\}$. Denote by $G - v$ the graph obtained from G by deleting the vertex $v \in V(G)$ and the edges incident with v. If $S \subseteq E(G)$, denote by $G - S$ the graph obtained from G by removing all the edges in S. The complement of a graph G, denoted by $\overline{G}$, has the same vertices with G, but two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G. If $S \subseteq E(\overline{G})$, denote by $G + S$ the graph obtained from G by adding all the edges in S. The distance between u and v of G is the number of edges in a shortest path connecting u and v. The maximum distance between any two vertices of a graph G is called the diameter of G. A diametral path is a shortest path between two vertices with a distance equal to the diameter. A connected graph G is called a unicyclic graph if $|V(G)| = |E(G)|$. As usual, denote by P_n, C_n, and S_n the path, the cycle, and the star with n vertices, respectively.

In chemical graph theory, a molecule is usually modeled as a graph. Topological indices, also called the graph invariants, are introduced to predict some physico-chemical properties of the corresponding molecular graph. A topological index maps the set of molecular graphs into the set of real numbers, which is invariant under the graph isomorphism.

In 1998, Estrada et al. [7] put forward the atom-bond connectivity (ABC) index, defined as

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

The atom-bond connectivity index has demonstrated its ability to accurately describe the heat of formation of alkanes. For more chemical applications and mathematical properties of the atom-bond connectivity index, we refer to [8–10, 15] and the references cited therein.

In 2009, Zhou and Trinajstić [18] proposed the sum-connectivity (SC) index, defined as

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

The sum-connectivity index has shown a strong correlation with the π electronic energy of benzenoid hydrocarbons. For more results on the sum-connectivity index, we refer to [6, 16] and the references cited therein.

Based on the atom-bond connectivity index and the sum-connectivity index, Ali et al. [2], introduced a new topological index, named the atom-bond sum-connectivity (ABS) index, defined as

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

The minimum and the maximum ABS index of trees with given pendent vertices were determined in [5, 14], respectively. In [17], Zhang et al. obtained the extremal values of trees with given matching number or domination number with respect to the ABS index. Nithya et al. [12] presented the minimum ABS index among unicyclic graphs with given girth. Zuo et al. [19] characterized the extremal chemical graphs with respect to the ABS index. In [3], Ali et al. gave the extremal values on the ABS index of unicyclic graphs and investigated the possible applications of the ABS index. For more results on the ABS index, we refer to [1, 4, 11, 13]. Motivated by these, we explore the maximum ABS index of unicyclic graphs with given diameter. In addition, the corresponding extremal graphs are characterized.

Let $\mathcal{U}(n, d)$ be the set of unicyclic graphs of order n and diameter d. Obviously, $\mathcal{U}(n, 1) = \{C_3\}$. For $n_1 \geq n_2 \geq n_3 \geq 0$ and $n_1 + n_2 + n_3 = n - 3$, let $C_3(n_1, n_2, n_3)$ be a unicyclic graph obtained by attaching n_1, n_2, n_3 pendent vertices to each vertex of C_3, respectively. It is clear that $C_3(n - 3, 0, 0) \in \mathcal{U}(n, 2)$ and $C_3(n - 4, 1, 0) \in \mathcal{U}(n, 3)$ for $n \geq 5$. In [3], Ali et al. determined that $C_3(n - 3, 0, 0)$ and $C_3(n - 4, 1, 0)$ possess the maximum and second-maximum ABS indices among all unicyclic graphs, respectively. It follows that $C_3(n - 3, 0, 0)$ and $C_3(n - 4, 1, 0)$ have the maximum ABS indices among $\mathcal{U}(n, 2)$ and $\mathcal{U}(n, 3)$, respectively. So, hereafter we only consider the ABS index of graphs among $\mathcal{U}(n, d)$, where $4 \leq d \leq n - 2$.

2. Preliminary

In this section, we will present three lemmas which will be used in the proof of our main results.

Lemma 2.1. *Let uv be a non-pendent edge of graph G with $N_G(u) \bigcap N_G(v) = \emptyset$. Let $G^* = G - \{vw : w \in N_G(v) \setminus \{u\}\} + \{uw : w \in N_G(v) \setminus \{u\}\}$. We denote this transformation by $\Delta(uv)$ as shown in Figure 1. Then, $ABS(G) < ABS(G^*)$.*

Proof. We assume that $N_G(u) = \{v, u_1, u_2, \ldots, u_{t-1}\}$ and $N_G(v) = \{u, v_1, v_2, \ldots, v_{s-1}\}$. That is to say, $d_G(u) = t, d_G(v) = s$ where $t \geq 2, s \geq 2$. Then,

$$\begin{aligned} ABS(G^*) - ABS(G) = &\sum_{i=1}^{t-1} \left(\sqrt{1 - \frac{2}{d_G(u_i) + t + s - 1}} - \sqrt{1 - \frac{2}{d_G(u_i) + t}} \right) \\ &+ \sum_{j=1}^{s-1} \left(\sqrt{1 - \frac{2}{d_G(v_j) + t + s - 1}} - \sqrt{1 - \frac{2}{d_G(v_j) + s}} \right) \\ &> 0. \end{aligned}$$

The result follows. □

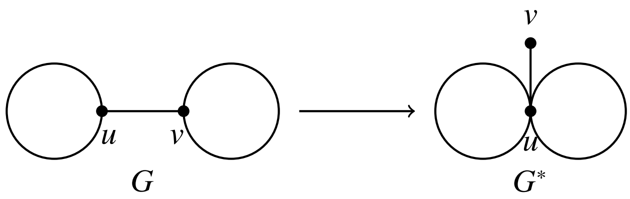

Figure 1. Transformation $\Delta(uv)$.

Lemma 2.2. *(i) Let the function $f(x) = \sqrt{1 - \frac{2}{x+1}} - \sqrt{1 - \frac{2}{x}}$ for $x \geq 3$. Then $f(x)$ is monotonously decreasing in $[3, +\infty)$.*
(ii) Let the function $g(x) = (x-1)\left(\sqrt{1 - \frac{2}{x+2}} - \sqrt{1 - \frac{2}{x+1}}\right) + \sqrt{1 - \frac{2}{x+3}}$ for $x \geq 2$. Then $g(x)$ is monotonously increasing in $[2, +\infty)$.
(iii) Let the function $\varphi(x) = 2\sqrt{1 - \frac{2}{x+2}} + (x-4)\sqrt{1 - \frac{2}{x+1}} - (x-3)\sqrt{1 - \frac{2}{x}}$ for $x \geq 3$. Then $\varphi(x)$ is monotonously increasing in $[3, +\infty)$.

Proof. (i) Let the function $f_1(x) = \sqrt{1 - \frac{2}{x}}$ for $x \geq 3$, then $f(x) = f_1(x+1) - f_1(x)$. Since $f_1''(x) = \frac{3-2x}{x^{\frac{5}{2}}(x-2)^{\frac{3}{2}}}$<0 for $x \geq 3$, we have $f'(x) = f_1'(x+1) - f_1'(x) < 0$. The result holds.

(ii) With some direct computation, we have

$$\begin{aligned} g'(x) &= \frac{x-1}{x^{\frac{1}{2}}(x+2)^{\frac{3}{2}}} - \frac{(x-1)^{\frac{1}{2}}}{(x+1)^{\frac{3}{2}}} - \frac{(x-1)^{\frac{1}{2}}}{(x+1)^{\frac{1}{2}}} + \frac{x^{\frac{1}{2}}}{(x+2)^{\frac{1}{2}}} + \frac{1}{(x+1)^{\frac{1}{2}}(x+3)^{\frac{3}{2}}} \\ &= \frac{x^2 + 3x - 1}{x^{\frac{1}{2}}(x+2)^{\frac{3}{2}}} - \frac{(x-1)^{\frac{1}{2}}(x+2)}{(x+1)^{\frac{3}{2}}} + \frac{1}{(x+1)^{\frac{1}{2}}(x+3)^{\frac{3}{2}}}. \end{aligned}$$

Let

$$A = \frac{x^2+3x-1}{x^{\frac{1}{2}}(x+2)^{\frac{3}{2}}},\ \ B = \frac{1}{(x+1)^{\frac{1}{2}}(x+3)^{\frac{3}{2}}},\ \ C = \frac{(x-1)^{\frac{1}{2}}(x+2)}{(x+1)^{\frac{3}{2}}},$$

then $g'(x) = A + B - C$. In order to prove $g'(x) > 0$, it is equivalent to prove $A + B > C$. Since $x \geq 2$, we get that $A, B, C > 0$. Then it will be enough to show that $(A + B)^2 > C^2$. It suffices to prove that $(2AB)^2 > (C^2 - A^2 - B^2)^2$. That is,

$$\frac{4(x^2+3x-1)^2}{x(x+1)(x+2)^3(x+3)^3} > \left[\frac{(x-1)(x+2)^2}{(x+1)^3} - \frac{(x^2+3x-1)^2}{x(x+2)^3} - \frac{1}{(x+1)(x+3)^3}\right]^2,$$

which can be rewritten as

$$\begin{aligned}&4x(x+2)^3(x+3)^3(x+1)^5(x^2+3x-1)^2\\ >&[x(x-1)(x+3)^3(x+2)^5 - (x+1)^3(x+3)^3(x^2+3x-1)^2 - x(x+1)^2(x+2)^3]^2.\end{aligned}$$

That is, $8x^{15} + 256x^{14} + 3560x^{13} + 28435x^{12} + 143948x^{11} + 474448x^{10} + 973836x^9 + 935916x^8 - 864916x^7 - 4418570x^6 - 7129340x^5 - 6374456x^4 - 3208660x^3 - 770428x^2 - 43308x - 729 > 0$, which is true for $x \geq 2$. The result holds.

Similar to the proof of (ii), we also obtain that (iii) holds. We complete the proof of this lemma. □

Lemma 2.3. *Let $a \in \{2, 3\}$. Let the function $h(x) = (x-2)\sqrt{1-\frac{2}{x+2}} - (x-1)\sqrt{1-\frac{2}{x+1}} + 2\sqrt{1-\frac{2}{x+3}}$ for $x \geq a$. Then $h(x) \geq h(a)$ holds with equality if and only if $x = a$.*

Proof. We first prove $\lim_{x\to+\infty} h(x) = 1$. Let the function $h_1(t) = (x-t)\sqrt{1-\frac{2}{x+t}}$ for $t \in [1, 2]$. By the Lagrange mean value theorem, we have

$$\begin{aligned}&\lim_{x\to+\infty}\left[(x-2)\sqrt{1-\frac{2}{x+2}} - (x-1)\sqrt{1-\frac{2}{x+1}}\right]\\ =&\lim_{x\to+\infty}[h_1(2) - h_1(1)]\\ =&\lim_{x\to+\infty} h_1'(\xi)\quad (1 < \xi < 2)\\ =&\lim_{x\to+\infty}\frac{-x^2+(1-2\xi)x-\xi^2+3\xi}{(x+\xi)^{\frac{3}{2}}(x+\xi-2)^{\frac{1}{2}}}\\ =&-1.\end{aligned}$$

Then we get $\lim_{x\to+\infty} h(x) = \lim_{x\to+\infty}\left[(x-2)\sqrt{1-\frac{2}{x+2}} - (x-1)\sqrt{1-\frac{2}{x+1}}\right] + \lim_{x\to+\infty} 2\sqrt{1-\frac{2}{x+3}} = -1+2 = 1$. By virtue of the MATLAB software, the equation $h'(x) = 0$ has a root $x_0 \approx 6.9609$. Similar to the proof of Lemma 2.2(ii), we can obtain that $h(x)$ is increasing in $[a, x_0)$ but decreasing in $[x_0, +\infty)$. Since $h(2) \approx 0.9718 < h(+\infty) = 1$ and $h(3) \approx 0.9934 < h(+\infty) = 1$, the result holds. □

3. Results

In this section, we will determine the maximum ABS index of graphs among $\mathcal{U}(n, d)$ for $4 \leq d \leq n-2$ and characterize the corresponding extremal graphs.

Lemma 3.1 ([3]). *The cycle C_n is the only graph possessing the minimum ABS index among all unicyclic graphs of order n for $n \geq 3$.*

Lemma 3.2. *Let U' be a graph in $\mathcal{U}(n,d)$ with the maximum ABS index for $4 \leq d \leq n-2$. Denote $P = u_0u_1u_2\ldots u_d$ and C by a diametral path and cycle of U', respectively. If $\mathcal{P}(U') \subseteq (N_{U'}(u_1) \bigcup N_{U'}(u_{d-1}))$, then $|V(P) \bigcap V(C)| \geq 2$.*

Proof. On the contrary, suppose that $|V(P) \bigcap V(C)| < 2$. Naturally, we distinguish the following two cases:

Case 1. $|V(P) \bigcap V(C)| = 0$.

Let $u_kv_1v_2\ldots v_t$ be the path connecting P and C where $2 \leq k \leq d-2$ and $t \geq 1$. Let U'' be the graph obtained from U' by applying the transformation $\Delta(u_kv_1)$. Then, according to Lemma 2.1, $U'' \in \mathcal{U}(n,d)$ and $ABS(U'') > ABS(U')$, a contradiction.

Case 2. $|V(P) \bigcap V(C)| = 1$.

We assume that $V(P) \bigcap V(C) = \{u_k\}$ and $|E(C)| = l$. Let $C = u_kw_1w_2\ldots w_{l-1}u_k$ for $l \geq 3$.

Subcase 2.1. $l \geq 4$.

Let U'' be the graph obtained from U' by applying the transformation $\Delta(u_kw_1)$. Then, according to Lemma 2.1, $U'' \in \mathcal{U}(n,d)$ and $ABS(U'') > ABS(U')$, a contradiction.

Subcase 2.2. $l = 3$.

Since $d \geq 4$, we have $d_{U'}(u_{k-1}) \geq 2$ or $d_{U'}(u_{k+1}) \geq 2$. Without loss of generality, we assume $d_{U'}(u_{k-1}) = x_2 \geq 2$. Let $d_{U'}(u_k) = x_1 \geq 4, d_{U'}(u_{k-2}) = x_3 \geq 1$. Let $U'' = U' - \{w_1w_2\} + \{w_1u_{k-1}\}$. Then,

$$\begin{aligned}ABS(U'') - ABS(U') &= (\sqrt{1-\frac{2}{x_1+x_2+1}} - \sqrt{1-\frac{2}{x_1+x_2}}) + \sqrt{1-\frac{2}{x_2+3}} - \sqrt{\frac{1}{2}} \\ &\quad + (\sqrt{1-\frac{2}{x_2+x_3+1}} - \sqrt{1-\frac{2}{x_2+x_3}}) - (\sqrt{1-\frac{2}{x_1+2}} - \sqrt{1-\frac{2}{x_1+1}}) \\ &> \sqrt{1-\frac{2}{x_2+3}} - \sqrt{\frac{1}{2}} - (\sqrt{1-\frac{2}{x_1+2}} - \sqrt{1-\frac{2}{x_1+1}}).\end{aligned}$$

It is easy to check that the function $\sqrt{1-\frac{2}{x+3}}$ is strictly increasing in $[3, +\infty)$. According to Lemma 2.2(i), $f(x) = \sqrt{1-\frac{2}{x+1}} - \sqrt{1-\frac{2}{x}}$ is monotonously decreasing in $[3, +\infty)$. Since $x_2 \geq 2$ and $x_1 \geq 4$, then $ABS(U'') - ABS(U') > \sqrt{1-\frac{2}{5}} - \sqrt{\frac{1}{2}} - f(x_1+1) \geq \sqrt{\frac{3}{5}} - \sqrt{\frac{1}{2}} - f(5) = 2\sqrt{\frac{3}{5}} - \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} > 0$, a contradiction. The proof of this lemma is completed. □

Let U_n^d be the graph obtained from a path $u_0u_1u_2\ldots u_d$ with a new vertex w by adding the edges wu_1 and wu_3 and then attaching $n-d-2$ pendent vertices to u_1, as depicted in Figure 2. We get that

$$ABS(U_n^d) = (n-d-1)\sqrt{1-\frac{2}{n-d+2}} + 2\sqrt{1-\frac{2}{n-d+3}} + M_1, \tag{3.1}$$

where $M_1 = 2\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}}$ if $d = 4$; $M_1 = 3\sqrt{\frac{3}{5}} + (d-5)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}$ if $d \geq 5$.

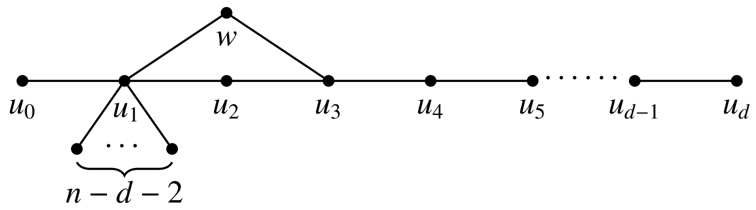

Figure 2. U_n^d for $4 \le d \le n-2$.

For $4 \le d \le n-2$, we investigate the ABS index of graphs among $\mathcal{U}(n,d)$ beginning with $d = n-2$.

Theorem 3.1. *Let U' be a graph in $\mathcal{U}(d+2,d)$ with the maximum ABS index for $d \ge 4$. Then $U' \cong U_{d+2}^d$, where U_{d+2}^d is depicted in Figure 2 for $n = d+2$.*

Proof. We denote a diametral path of U' by $P = u_0u_1u_2\dots u_d$ and the cycle by C. Since $|V(U')| = d+2$, there is exactly one vertex w and $\{w\} = V(U')\backslash V(P)$. Then, $C = u_ku_{k+1}wu_k$ for $0 \le k \le d-1$, or $C = u_ku_{k+1}u_{k+2}wu_k$ for $0 \le k \le d-2$.

Claim 1. $\{u_0, u_d\} \bigcap V(C) = \emptyset$.

On the contrary, suppose $u_d \in V(C)$. Thus, $C = u_{d-1}u_dwu_{d-1}$ or $C = u_{d-2}u_{d-1}u_dwu_{d-2}$.

Case 1. $C = u_{d-1}u_dwu_{d-1}$.

Let $U'' = U' - \{u_dw\} + \{u_{d-2}w\}$. Then, $ABS(U'') - ABS(U') = \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}} > 0$, a contradiction.

Case 2. $C = u_{d-2}u_{d-1}u_dwu_{d-2}$.

Let $U'' = U' - \{u_dw\} + \{u_{d-1}w\}$. Then, $ABS(U'') - ABS(U') = \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}} > 0$, a contradiction.

From Cases 1 and 2, we obtain $u_d \notin V(C)$. Similarly, we get $u_0 \notin V(C)$. Claim 1 holds.

Claim 2. $|E(C)| = 4$.

On the contrary, suppose $C = u_ku_{k+1}wu_k$ where $1 \le k \le d-2$ by Claim 1. As $d \ge 4$, we have $max\{d_{U'}(u_{k-1}), d_{U'}(u_{k+2})\} = 2$. Without loss of generality, we assume that $d_{U'}(u_{k-1}) = 2$ for $2 \le k \le d-2$. Let $d_{U'}(u_{k-2}) = x$, where $x \in \{1,2\}$. Let $U'' = U' - \{wu_k\} + \{wu_{k-1}\}$. Then, $ABS(U'') - ABS(U') = \sqrt{1-\frac{2}{x+3}} - \sqrt{1-\frac{2}{x+2}} - (\sqrt{1-\frac{2}{6}} - \sqrt{1-\frac{2}{5}}) = f(x+2) - f(5)$. According to Lemma 2.2(i) and $x+2 \le 4 < 5$, we have $f(x+2) - f(5) > 0$. Hence, $ABS(U'') > ABS(U')$, a contradiction. Claim 2 holds.

By Claims 1 and 2, we obtain that $C = u_ku_{k+1}u_{k+2}wu_k$ for $1 \le k \le d-3$. For $k = 1$ or $k = d-3$, $U' \cong U_{d+2}^d$. For $2 \le k \le d-4$, $ABS(U') - ABS(U_{d+2}^d) = 2\sqrt{\frac{1}{2}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} > 0$. Thus, $U' \cong U_{d+2}^d$. □

In what follows, we investigate the ABS index of graphs among $\mathcal{U}(n,d)$ for $4 \le d \le n-3$. It would be necessary to introduce the following definition.

Definition 3.1. *Let $G \in \mathcal{U}(n,d)$ and $v \in \mathcal{P}(G)$ for $2 \le d \le n-3$. The vertex v is called a removable pendent vertex if $G - v \in \mathcal{U}(n-1,d)$.*

Lemma 3.3. *Let U' be a graph in $\mathcal{U}(n,d)$ with the maximum ABS index for $4 \le d \le n-3$. Then U' contains at least one removable pendent vertex.*

Proof. On the contrary, we suppose that U' contains no removable pendent vertex. Denote a diametral path of U' by $P = u_0u_1u_2\dots u_d$ and the cycle of U' by C. Recall that $\mathcal{P}(U')$ is the set of all pendent vertices of U'. We known that $\mathcal{P}(U') \ne \emptyset$ by Lemma 3.1. Then, $G - v \in \mathcal{U}(n-1,d-1)$ for any

$v \in \mathcal{P}(U')$. If there exists in U' a pendent vertex $v \notin \{u_0, u_d\}$, then $U' - v \in \mathcal{U}(n-1, d)$. Thus, $\mathcal{P}(U') \subseteq \{u_0, u_d\}$. Without loss of generality, we assume u_0 is a pendent vertex of U'. Also, we obtain $|V(P) \bigcap V(C)| \geq 2$ by Lemma 3.2. Denote C by $u_k u_{k+1} \ldots u_{k+t} w_s w_{s-1} \ldots w_1 u_k$, where $1 \leq k < k+t \leq d$, $t \geq 1$, and $w_1, w_2, \ldots, w_s \in V(C) \backslash V(P)$. Since $d \leq n-3$, we get that $s \geq 2$ and $t \leq s+1$.

Case 1. $t < s+1$.

Let U'' be the graph obtained from U' by applying the transformation $\Delta(u_k w_1)$. Then, according to Lemma 2.1, $U'' \in \mathcal{U}(n, d)$ and $ABS(U'') > ABS(U')$, a contradiction.

Case 2. $t = s+1$.

Let $d_{U'}(u_{k-1}) = x$ for $x \geq 1$. Let $U'' = U' - \{u_k w_1, w_1 w_2\} + \{u_{k+1} w_1, u_{k+1} w_2\}$, then $U'' \in \mathcal{U}(n, d)$. According to Lemma 2.2(i) and $x \geq 1$, we have

$$\begin{aligned} ABS(U'') - ABS(U') &= 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - (\sqrt{1 - \frac{2}{x+3}} - \sqrt{1 - \frac{2}{x+2}}) \\ &= 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - f(x+2) \\ &\geq 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - f(3) \\ &= 3\sqrt{\frac{2}{3}} - \sqrt{\frac{3}{5}} - 3\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}} > 0, \end{aligned}$$

a contradiction. The proof of this lemma is completed. □

Lemma 3.4. *Let U' be a graph in $\mathcal{U}(n, d)$ with the maximum ABS index for $4 \leq d \leq n-3$. If v is a removable pendent vertex of U' and w is the vertex adjacent to v, then $|N_{U'}(w) \backslash \mathcal{P}(U')| \geq 2$.*

Proof. It is known that $|N_{U'}(w) \backslash \mathcal{P}(U')| \geq 1$. We will prove $|N_{U'}(w) \backslash \mathcal{P}(U')| \geq 2$ by contradiction, which implies that $|N_{U'}(w) \backslash \mathcal{P}(U')| = 1$. Let $P = u_0 u_1 \ldots u_d$ be a diametral path of U' and C be the cycle of U'. Let $\mathcal{P}^*(U')$ be the set of all removable pendent vertices of U'. By Lemma 3.3, we have $\mathcal{P}^*(U') \neq \emptyset$.

Claim 1. $\mathcal{P}^*(U') \subseteq (N_{U'}(u_1) \bigcup (N_{U'}(u_{d-1}))$.

On the contrary, suppose there exists a vertex $v_0 \in \mathcal{P}^*(U')$, but $v_0 \notin N_{U'}(u_1) \bigcup N_{U'}(u_{d-1})$. Since $|N_{U'}(w) \backslash \mathcal{P}(U')| = 1$, we have $v_0 \notin V(P) \bigcup V(C)$. Let v_1 be the vertex adjacent to v_0. Let w_1 be a non-pendent vertex adjacent to v_1. Let U'' be the graph obtained from U' by applying the transformation $\Delta(w_1 v_1)$. Then, according to Lemma 2.1, $U'' \in \mathcal{U}(n, d)$ and $ABS(U'') > ABS(U')$, a contradiction. The proof of Claim 1 is completed.

Since $\emptyset \neq \mathcal{P}^*(U') \subseteq (N_{U'}(u_1) \bigcup (N_{U'}(u_{d-1}))$, we can assume there exists a removable vertex adjacent to u_1. Then, $|N_{U'}(u_1) \backslash \mathcal{P}(U')| = 1$ and $u_0, u_1 \notin V(C)$. Let $d_{U'}(u_1) = x \geq 3$.

According to Lemma 3.2 and Claim 1, we get that $|V(P) \bigcap V(C)| \geq 2$. Then we can assume that $C = u_k u_{k+1} \ldots u_{k+t} w_s w_{s-1} \ldots w_1 u_k$, where $2 \leq k < k+t \leq d$, $t \geq 1$ and $w_1, w_2, \ldots, w_s \in V(C) \backslash V(P)$.

Claim 2. $|V(C) \backslash V(P)| = 1$.

On the contrary, suppose that $|V(C) \backslash V(P)| \geq 2$. Let $w_1, w_2 \in V(C) \backslash V(P)$. Note that $t \leq s+1$.

Case 1. $t < s+1$.

Let U'' be the graph obtained from U' by applying the transformation $\Delta(u_k w_1)$. Then, according to Lemma 2.1, $U'' \in \mathcal{U}(n, d)$ and $ABS(U'') > ABS(U')$, a contradiction.

Case 2. $t = s+1$.

Let $U'' = U' - \{u_k w_1, w_1 w_2\} + \{u_{k+1} w_1, u_{k+1} w_2\}$. Let $d_{U'}(u_{k-1}) = x_1 \geq 2$. Then we have

$$\begin{aligned} ABS(U'') - ABS(U') &= 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - \left(\sqrt{1 - \frac{2}{x_1 + 3}} - \sqrt{1 - \frac{2}{x_1 + 2}}\right) \\ &= 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - f(x_1 + 2) \quad \text{(by Lemma 2.2(i))} \\ &\geq 3\sqrt{\frac{2}{3}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} - f(4) \quad \text{(by Lemma 2.2(i) and } x_1 \geq 2) \\ &= 3\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}} - 2\sqrt{\frac{3}{5}} > 0, \end{aligned}$$

a contradiction. From Cases 1 and 2, Claim 2 holds.

Claim 3. $d_{U'}(u_d) = 1$.

On the contrary, suppose that $d_{U'}(u_d) = 2$. By Claim 2, we can assume $V(C) \backslash V(P) = \{w_1\}$. Then we have $C = u_{d-1} u_d w_1 u_{d-1}$ or $C = u_{d-2} u_{d-1} u_d w_1 u_{d-2}$.

Case 1. $C = u_{d-1} u_d w_1 u_{d-1}$.

Let $U'' = U' - \{u_d w_1\} + \{u_{d-2} w_1\}$. Since $d \geq 4$, we can assume that $d_{U'}(u_{d-3}) = x \geq 2$. Then

$$ABS(U'') - ABS(U') = \sqrt{1 - \frac{2}{x+3}} - \sqrt{1 - \frac{2}{x+2}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{5}} > 0,$$

a contradiction.

Case 2. $C = u_{d-2} u_{d-1} u_d w_1 u_{d-2}$.

Let $U'' = U' - \{u_d w_1\} + \{u_{d-1} w_1\}$. Then $ABS(U'') - ABS(U') = \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}} > 0$, a contradiction.

From Cases 1 and 2, the proof of Claim 3 is completed.

Claim 4. $E(C) = 4$.

On the contrary, according to Claim 2, suppose that $|E(C)| = 3$. By Claims 1 and 3, we can assume that $C = u_k u_{k+1} w_1 u_k$ where $2 \leq k \leq d - 2$ and $w_1 \in V(C) \backslash V(P)$. Let $d_{U'}(u_1) = x \geq 3$.

Case 1. $k = 2$.

Let $U'' = U' - \{w_1 u_2\} + \{w_1 u_1\}$. According to Lemma 2.2(ii) and $x \geq 3$, we have

$$\begin{aligned} ABS(U'') - ABS(U') &= (x-1)\sqrt{1 - \frac{2}{x+2}} - (x-1)\sqrt{1 - \frac{2}{x+1}} + \sqrt{1 - \frac{2}{x+3}} - \sqrt{\frac{2}{3}} \\ &= g(x) - \sqrt{\frac{2}{3}} \\ &\geq g(3) - \sqrt{\frac{2}{3}} = 2\sqrt{\frac{3}{5}} - 2\sqrt{\frac{1}{2}} > 0, \end{aligned}$$

a contradiction.

Case 2. $3 \leq k \leq d - 3$.

Let $U'' = U' - \{w_1 u_k, w_1 u_{k+1}\} + \{w_1 u_1, w_1 u_3\}$. Let $u_{k+2} = y \geq 1$. According to Lemmas 2.2(i) and 2.3, we have

$$ABS(U'') - ABS(U') = (x-2)\sqrt{1 - \frac{2}{x+2}} - (x-1)\sqrt{1 - \frac{2}{x+1}} + 2\sqrt{1 - \frac{2}{x+3}}$$

$$
\begin{aligned}
&-(\sqrt{1-\frac{2}{y+3}}-\sqrt{1-\frac{2}{y+2}})-\sqrt{\frac{2}{3}}\\
&=h(x)-f(y+2)-\sqrt{\frac{2}{3}}\\
&\geq h(3)-f(3)-\sqrt{\frac{2}{3}}\quad(\text{by } x\geq 3 \text{ and } y\geq 1)\\
&=\sqrt{\frac{3}{5}}+\sqrt{\frac{2}{3}}+\sqrt{\frac{1}{3}}-3\sqrt{\frac{1}{2}}>0,
\end{aligned}
$$

a contradiction. From Cases 1 and 2, the proof of Claim 4 is completed.

From above four Claims, we have $C = u_k u_{k+1} u_{k+2} w_1 u_k$ for $2 \leq k \leq d-3$, $d_{U'}(u_1) = x \geq 3$, $d_{U'}(u_d) = 1$. Let $u_{k+3} = y \geq 1$. Finally, we will complete the proof of this lemma in the following two cases:

Case 1. $k = 2$.

Let $U'' = U' - \{w_1u_2, w_1u_4\} + \{w_1u_1, w_1u_3\}$. According to Lemma 2.2(i) and (ii), we have

$$
\begin{aligned}
ABS(U'')-ABS(U') &= (x-1)(\sqrt{1-\frac{2}{x+2}}-\sqrt{1-\frac{2}{x+1}})+\sqrt{1-\frac{2}{x+3}}\\
&\quad-(\sqrt{1-\frac{2}{y+3}}-\sqrt{1-\frac{2}{y+2}})-\sqrt{\frac{3}{5}}\\
&=g(x)-f(y+2)-\sqrt{\frac{3}{5}}\\
&\geq g(3)-f(3)-\sqrt{\frac{3}{5}}\quad(\text{by } x\geq 3 \text{ and } y\geq 1)\\
&=\sqrt{\frac{3}{5}}+\sqrt{\frac{2}{3}}+\sqrt{\frac{1}{3}}-3\sqrt{\frac{1}{2}}>0,
\end{aligned}
$$

a contradiction.

Case 2. $3 \leq k \leq d-3$.

Let $U'' = U' - \{w_1u_k, w_1u_{k+2}\} + \{w_1u_1, w_1u_3\}$. According to Lemmas 2.2 (i) and 2.3, we have

$$
\begin{aligned}
ABS(U'')-ABS(U') &= (x-2)\sqrt{1-\frac{2}{x+2}}-(x-1)\sqrt{1-\frac{2}{x+1}}+2\sqrt{1-\frac{2}{x+3}}\\
&\quad-(\sqrt{1-\frac{2}{y+3}}-\sqrt{1-\frac{2}{y+2}})+\sqrt{\frac{1}{2}}-2\sqrt{\frac{3}{5}}\\
&=h(x)-f(y+2)+\sqrt{\frac{1}{2}}-2\sqrt{\frac{3}{5}}\\
&\geq h(3)-f(3)+\sqrt{\frac{1}{2}}-2\sqrt{\frac{3}{5}}\quad(\text{by } x\geq 3 \text{ and } y\geq 1)\\
&=2\sqrt{\frac{2}{3}}+\sqrt{\frac{1}{3}}-2\sqrt{\frac{1}{2}}-\sqrt{\frac{3}{5}}>0,
\end{aligned}
$$

a contradiction. □

Theorem 3.2. *Let U' be a graph in $\mathcal{U}(n,d)$ with the maximum ABS index for $4 \le d \le n-2$. Then $U' \cong U_n^d$, where U_n^d is depicted in Figure 2.*

Proof. We will prove the theorem holds by induction on n. The theorem holds for $n = d+2$ by Theorem 3.1. Now we assume the theorem holds for $n-1$ where $n \ge d+3$. According to Lemma 3.3, the graph U' contains a removable pendent vertex, say v, that is $U'-v \in \mathcal{U}(n-1,d)$. Let w be the vertex adjacent to v. By Lemma 3.4, we have $|N_{U'}(w)\backslash\mathcal{P}(U')| \ge 2$. Let $N_{U'}(w) = \{v, v_1, v_2, \ldots, v_{t-1}\}$ for $3 \le t \le n-d+1$ and $d_{U'}(v_i) = x_i$ for $1 \le i \le t-1$. We can assume $v_1, v_2 \in N_{U'}(w)\backslash\mathcal{P}(U')$, that is, $x_1 \ge 2, x_2 \ge 2$. By virtue of inductive hypothesis and Eq (3.1), we have

$$\begin{aligned}
ABS(U') &= ABS(U'-v) + \sqrt{1-\frac{2}{t+1}} + \sum_{i=1}^{t-1}\left(\sqrt{1-\frac{2}{t+x_i}} - \sqrt{1-\frac{2}{t+x_i-1}}\right)\\
&\le ABS(U_{n-1}^d) + \sqrt{1-\frac{2}{t+1}} + \sum_{i=1}^{t-1}\left(\sqrt{1-\frac{2}{t+x_i}} - \sqrt{1-\frac{2}{t+x_i-1}}\right)\\
&= (n-d-2)\sqrt{1-\frac{2}{n-d+1}} + 2\sqrt{1-\frac{2}{n-d+2}} + M_1\\
&\quad + \sqrt{1-\frac{2}{t+1}} + \sum_{i=1}^{t-1}\left(\sqrt{1-\frac{2}{t+x_i}} - \sqrt{1-\frac{2}{t+x_i-1}}\right).
\end{aligned}$$

According to Lemma 2.2(i), we get that $\sqrt{1-\frac{2}{t+x_i}} - \sqrt{1-\frac{2}{t+x_i-1}}$ is decreasing with respect to x_i for $i = 1, 2, \ldots, t-1$, where $x_1, x_2 \ge 2$, and $x_3, \ldots, x_{t-1} \ge 1$. Hence,

$$\begin{aligned}
ABS(U') &\le (n-d-2)\sqrt{1-\frac{2}{n-d+1}} + 2\sqrt{1-\frac{2}{n-d+2}} + M_1 + \sqrt{1-\frac{2}{t+1}}\\
&\quad + 2\left(\sqrt{1-\frac{2}{t+2}} - \sqrt{1-\frac{2}{t+1}}\right) + (t-3)\left(\sqrt{1-\frac{2}{t+1}} - \sqrt{1-\frac{2}{t}}\right)\\
&= (n-d-2)\sqrt{1-\frac{2}{n-d+1}} + 2\sqrt{1-\frac{2}{n-d+2}} + M_1\\
&\quad + 2\sqrt{1-\frac{2}{t+2}} + (t-4)\sqrt{1-\frac{2}{t+1}} - (t-3)\sqrt{1-\frac{2}{t}}.
\end{aligned}$$

According to Lemma 2.2(iii), we have that $\varphi(t) = 2\sqrt{1-\frac{2}{t+2}} + (t-4)\sqrt{1-\frac{2}{t+1}} - (t-3)\sqrt{1-\frac{2}{t}}$ is increasing with respect to t. Since $3 \le t \le n-d+1$, then

$$\begin{aligned}
ABS(U') &\le (n-d-2)\sqrt{1-\frac{2}{n-d+1}} + 2\sqrt{1-\frac{2}{n-d+2}} + M_1\\
&\quad + 2\sqrt{1-\frac{2}{n-d+3}} + (n-d-3)\sqrt{1-\frac{2}{n-d+2}} - (n-d-2)\sqrt{1-\frac{2}{n-d+1}}\\
&= (n-d-1)\sqrt{1-\frac{2}{n-d+2}} + 2\sqrt{1-\frac{2}{n-d+3}} + M_1
\end{aligned}$$

$= ABS(U_n^d)$.

Thus, $ABS(U') \leq ABS(U_n^d)$ holds with equality if and only if $ABS(U'-v) \cong ABS(U_{n-1}^d)$, $x_1 = x_2 = 2$, $x_3 = \cdots = x_{t-1} = 1$, and $t = n - d + 1$, that is, $U' \cong U_n^d$. The proof of this theorem is completed. □

4. Conclusions

In this paper, we have determined the sharp upper bound on the ABS index of unicyclic graphs among $\mathcal{U}(n,d)$ and characterized the corresponding extremal graphs. In the future, we will study the sharp lower bound on the ABS index of unicyclic graphs among $\mathcal{U}(n,d)$. Meanwhile, we are also interested in investigating the extremal ABS indices of unicyclic graphs with other parameters given, such as degree sequence, independence number, and domination number, etc.

Author contributions

Zhen Wang: Writing-original draft, Writing-review & editing and Methodology; Kai Zhou: Formal analysis and Software. All authors have read and agreed to the published version of the manuscript.

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 no conflict of interest in this article.

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