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Resolving an Open Problem on the Exponential Arithmetic-Geometric Index of Unicyclic Graphs

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Abstract: Recently the exponential arithmetic-geometric index (EAG) was introduced. The exponential arithmetic-geometric index (EAG) of a graph G is defined as $EAG(G) = \sum\limits_{v_iv_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}$, where d_i represents the degree of the vertex v_i in G. The characterization of extreme structures in relation to graph invariants from the class of unicyclic graphs is an important problem in discrete mathematics. Cruz, Rada and Sanchez [Extremal unicyclic graphs with respect to vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 481–503] proposed a unified method for finding extremal unicyclic graphs for exponential degree-based graph invariants. However, in the case of EAG, this method is insufficient to generate the maximal unicyclic graph. Consequently, the same article presented an open problem for the investigation of the maximal unicyclic graph with respect to this invariant. This article completely characterizes the maximal unicyclic graph in relation to EAG.

Keywords: extremal graph; exponential arithmetic-geometric index; unicyclic graph

MSC: 05C90; 05C07; 05C35

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1. Introduction

In recent years, graph theory has become a crucial tool in the field of chemistry, particularly in the study of molecular structures. A topological index is a numerical quantity that is associated with a molecular graph, used to describe specific physicochemical properties. Since Wiener introduced the first such index [43], many other indices have been developed depending on various graph parameters, including degree, distance, and eccentricity [2,3,15,26–28,30]. Among these, degree-based indices have received significant attention since the 1970s due to their strong correlation with molecular properties. One important example is the arithmetic-geometric index, introduced in [37]. Let G be a simple connected graph, whose vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(G)$. The degree of the j-th vertex v_j is denoted by d_j. The arithmetic-geometric index (AG) is defined as

$$AG(G) = \sum_{v_iv_j \in E(G)} \frac{d_i + d_j}{2\sqrt{d_id_j}}.$$

Numerous publications have extensively studied the mathematical properties of AG, specifically the extremal problems and bounds. Shegehalli et al. [38,39] calculated AG for different classes of graphs. Milovanović et al. [31] determined some upper bounds on AG for simple connected graphs. Li and Zhang [25] provided sharp bounds on AG of line graphs. Hertz et al. [23] identified the extremal chemical graphs for AG. Maximal chemical trees with respect to AG were characterized in [41]. More studies on AG can be found in references [22,36,45]. To improve the discriminative ability of topological indices, researchers introduced exponential versions of these indices in 2019 [35]. In [8,10], researchers provided a characterization of the extremal trees for the exponential Randić index. Das et al. [14] explored the extremal graphs for the exponential atom-bond connectivity index.

Jahanbani et al. [24] determined the lowest value of the exponential forgotten index for trees. Das and Mondal [16] examined sharp bounds on the exponential geometric-arithmetic index of bipartite graphs. More studies on this concept can be found in references [4–6,9,11,17]. In this paper, we focus on the exponential arithmetic-geometric index (EAG), which is defined as

$$EAG(G) = \sum_{v_i v_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}}.$$

The investigation of extremal structures within different classes of graphs is a critical area of research in discrete mathematics. In particular, the identification of extremal unicyclic graphs is a major challenge. Moon and Park [32] explored the extremal values of the geometric-arithmetic index for unicyclic graphs and identified those that attained these extreme values. Extremal unicyclic graphs for AG were characterized in [42]. Liu et al. [29] provided a complete classification of extremal unicyclic graphs for the Lanzhou index. In [18,20], researchers described the maximal unicyclic graph for exponential second Zagreb and augmented Zagreb indices. For more insights into extremal unicyclic graphs, readers can refer to [1,7,12,13,19,21,33,34]. Cruz et al.[12] introduced a unified method for the identification of extremal unicyclic graphs for exponential degree-based indices, which was successfully applied to many well-known indices. However, they discovered that this method is insufficient to generate the maximal unicyclic graph in the case of EAG. Because of this, the following open problem was posed in [12]:

Problem 1. [12] Characterize the maximal unicyclic graph with respect to EAG in terms of graph order.

This paper aims to fully solve this problem by applying advanced combinatorial methods. Our goal is to develop new methods that will help us to identify the maximal unicyclic graph with respect to EAG.

2. Main Result

In this section, we address and resolve the open problem concerning the exponential arithmetic-geometric index of unicyclic graphs. To achieve this, we first establish the following essential result.

Lemma 1. *Let*

$$f(x) = \frac{x}{2\sqrt{x-1}} - \frac{x-1}{2\sqrt{3(x-4)}}, \ x \geq 5.$$

Then $f(x)$ is a strictly increasing function on $x \geq 5$.

Proof. Since

$$f(x) = \frac{x}{2\sqrt{x-1}} - \frac{x-1}{2\sqrt{3(x-4)}},$$

we have

$$f'(x) = \frac{1}{4\sqrt{x-1}}\left(\frac{x-2}{x-1}\right) - \frac{1}{4\sqrt{3}\sqrt{x-4}}\left(\frac{x-7}{x-4}\right).$$

For $x = 5$, we have $f'(x) > 0$. Otherwise, $x \geq 6$. One can easily see that

$$\frac{1}{\sqrt{x-1}} > \frac{1}{\sqrt{3}\sqrt{x-4}} \text{ and } \frac{x-2}{x-1} > \frac{x-7}{x-4},$$

and hence $f'(x) > 0$. This proves the result. □

Lemma 2. *Let*

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

Then $g(x)$ is a strictly increasing function on $x \geq 4$.

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Proof. Since $x \geq 4$, one can easily see that

$$g'(x) = \frac{1}{4\sqrt{x-1}}\left(\frac{x-2}{x-1}\right) - \frac{1}{4\sqrt{2(x+1)}}\left(\frac{x-1}{x+1}\right) > 0.$$

Therefore $g(x)$ is a strictly increasing function on $x \geq 4$. □

Lemma 3. *Let*

$$q(x) = \frac{x+3}{2\sqrt{2(x+1)}} - \frac{x+5}{4\sqrt{x+1}}.$$

Then $q(x)$ is a strictly increasing function on x.

Proof. One can easily see that

$$q'(x) = \frac{1}{4\sqrt{2}}\frac{(x-1)}{(x+1)^{3/2}} - \frac{1}{8}\frac{(x-3)}{(x+1)^{3/2}} > 0.$$

Therefore $q(x)$ is a strictly increasing function. □

Lemma 4. *For $b \leq d_j \leq d_i \leq a$,*

$$\frac{d_i + d_j}{\sqrt{d_i\,d_j}} \leq \frac{a+b}{\sqrt{a\,b}}$$

with equality if and only if $d_i = a$, $d_j = b$.

Proof. For $b \leq d_j \leq d_i \leq a$, we obtain

$$\frac{d_i}{d_j} \leq \frac{a}{b},\ \frac{d_j}{d_i} \geq \frac{b}{a}, \quad \text{and hence} \quad \left(\frac{d_i}{d_j}\right)^{1/4} - \left(\frac{d_j}{d_i}\right)^{1/4} \leq \left(\frac{a}{b}\right)^{1/4} - \left(\frac{b}{a}\right)^{1/4}.$$

Using the above result, we obtain

$$\left(\left(\frac{d_i}{d_j}\right)^{1/4} + \left(\frac{d_j}{d_i}\right)^{1/4}\right)^2 = \left(\left(\frac{d_i}{d_j}\right)^{1/4} - \left(\frac{d_j}{d_i}\right)^{1/4}\right)^2 + 4 \leq \left(\left(\frac{a}{b}\right)^{1/4} - \left(\frac{b}{a}\right)^{1/4}\right)^2 + 4,$$

$$\text{that is,}\ \sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} \leq \sqrt{\frac{a}{b}} + \sqrt{\frac{b}{a}}, \quad \text{that is,}\ \frac{d_i + d_j}{\sqrt{d_i\,d_j}} \leq \frac{a+b}{\sqrt{a\,b}}.$$

Moreover, the equality holds if and only if $d_i = a$, $d_j = b$. □

Let S'_n be a unicyclic graph of order n obtained by adding an edge to the star graph S_n (S_n is a star graph of order n).

Theorem 1. *Let G be a unicyclic graph of order n. Then*

$$EAG(G) \leq (n-3)\,e^{\frac{n}{2\sqrt{n-1}}} + 2\,e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e \tag{1}$$

with equality if and only if $G \cong S'_n$.

Proof. Let Δ be the maximum degree in the unicyclic graph G. If $\Delta = n-1$, then $G \cong S'_n$ with

$$EAG(G) = (n-3)\,e^{\frac{n}{2\sqrt{n-1}}} + 2\,e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e$$

and hence the equality holds. For $n \leq 9$, by Sage [40], one can easily check that the result (1) holds with equality if and only if $G \cong S_n'$. Otherwise, $\Delta \leq n-2$ and $n \geq 10$. For any pendant edge $v_iv_j \in E(G)$ $(1 = d_j \leq d_i \leq n-2 < n-1)$, by Lemma 4, we obtain

$$\frac{d_i + d_j}{2\sqrt{d_id_j}} < \frac{n}{2\sqrt{n-1}}. \tag{2}$$

For any non-pendant edge $v_iv_j \in E(G)$ $(2 \leq d_j \leq d_i \leq n-2 < n-1)$, by Lemma 4, we obtain

$$\frac{d_i + d_j}{2\sqrt{d_id_j}} < \frac{n+1}{2\sqrt{2\,(n-1)}}. \tag{3}$$

For any edge $v_iv_j \in E(G)$, from (2) and (3), we obtain

$$\frac{d_i + d_j}{2\sqrt{d_id_j}} < \frac{n}{2\sqrt{n-1}} \tag{4}$$

as

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

Let k be the length of the cycle in the unicyclic graph G. Then $k \geq 3$. We consider the following two cases:

Case 1. $k = 3$. Let v_1, v_2, v_3 be the three vertices on the cycle in G. We assume that $d_1 \geq d_2 \geq d_3 \geq 2$. We consider the following cases:

Case 1.1. $d_2 = 2$. In this case $d_2 = d_3 = 2$ and hence

$$\frac{d_2 + d_3}{2\sqrt{d_2d_3}} = 1.$$

Let $E_1 = \{v_1v_2, v_2v_3, v_3v_1\}$. Using the above result with (3) and (4), we obtain

$$\begin{aligned} EAG(G) &= \sum_{v_iv_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &= e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} + \sum_{v_iv_j \in E(G)\setminus E_1} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &< 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e + (n-3)\,e^{\frac{n}{2\sqrt{n-1}}}. \end{aligned}$$

The result (1) strictly holds.

Case 1.2. $d_2 = 3$. If $d_3 = 3$, then similarly, by **Case 1.1**, we obtain

$$\begin{aligned} EAG(G) &= e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} + \sum_{v_iv_j \in E(G)\setminus E_1} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &< 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e + (n-3)\,e^{\frac{n}{2\sqrt{n-1}}}. \end{aligned}$$

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The result (1) strictly holds. Otherwise, $d_3 = 2$. Let v_4 be the vertex adjacent to the vertex v_2 other than v_1 and v_3. Since $d_2 = 3$ and $d_3 = 2$, we have

$$\frac{d_2 + d_3}{2\sqrt{d_2 d_3}} = \sqrt{\frac{25}{24}}.$$

Again since $d_2 = 3$ and $d_4 \le n-4$, by Lemma 4, we obtain

$$\frac{d_2 + d_4}{2\sqrt{d_2 d_4}} \le \frac{n-1}{2\sqrt{3\,(n-4)}}.$$

Since $n \ge 10$, by Lemma 1, we obtain

$$f(n) = \frac{n}{2\sqrt{n-1}} - \frac{n-1}{2\sqrt{3(n-4)}} \ge f(10) = \frac{5}{3} - \sqrt{\frac{9}{8}} > 0.606.$$

From the above results, we obtain

$$\begin{aligned} e^{\frac{n}{2\sqrt{n-1}}} + e > e^{\frac{n-1}{2\sqrt{3(n-4)}}+0.606} + e > 1.83\, e^{\frac{n-1}{2\sqrt{3(n-4)}}} + e > e^{\frac{n-1}{2\sqrt{3(n-4)}}} + 0.83\, e^{\frac{\sqrt{n+2}}{2\sqrt{3}}} + e \\ \ge e^{\frac{n-1}{2\sqrt{3(n-4)}}} + 1.83\, e \\ > e^{\frac{n-1}{2\sqrt{3(n-4)}}} + e^{\sqrt{\frac{25}{24}}} \\ \ge e^{\frac{d_2+d_3}{2\sqrt{d_2 d_3}}} + e^{\frac{d_2+d_4}{2\sqrt{d_2 d_4}}}. \end{aligned}$$

Let $E_2 = E_1 \cup \{v_2 v_4\}$. By (3) and (4), we obtain

$$e^{\frac{d_1+d_2}{2\sqrt{d_1 d_2}}} < e^{\frac{n+1}{2\sqrt{2\,(n-1)}}},\ e^{\frac{d_3+d_1}{2\sqrt{d_3 d_1}}} < e^{\frac{n+1}{2\sqrt{2\,(n-1)}}},\ \text{ and }\ e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}} < e^{\frac{n}{2\sqrt{n-1}}}\ \text{ for any }\ v_i v_j \in E(G) \backslash E_2.$$

Using the above results with $|E(G)\backslash E_2| = n-4$, we obtain

$$\begin{aligned} EAG(G) &= e^{\frac{d_1+d_2}{2\sqrt{d_1 d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2 d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3 d_1}}} + e^{\frac{d_2+d_4}{2\sqrt{d_2 d_4}}} + \sum_{v_i v_j \in E(G)\backslash E_2} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}} \\ &< 2\, e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e + (n-3)\, e^{\frac{n}{2\sqrt{n-1}}}. \end{aligned}$$

The result (1) strictly holds.

Case 1.3. $d_2 \ge 4$. Let $S_1 = \{v_2 v_j \in E(G) \mid \text{ for all } v_j \in N_G(v_2)\}$, $S = S_1 \cup \{v_1 v_3\}$ and $E_3 = E(G)\backslash S$. In this case $d_1 \le n-3$, $4 \le d_2 \le \frac{n+1}{2}$, and $d_3 \ge 2$. Since $d_1 \ge d_2 \ge d_3$, by Lemma 4, we obtain

$$\frac{d_1 + d_2}{2\sqrt{d_1 d_2}} \le \frac{n+1}{4\sqrt{n-3}},\ \frac{d_2 + d_3}{2\sqrt{d_2 d_3}} \le \frac{n+5}{4\sqrt{n+1}},\ \frac{d_1 + d_3}{2\sqrt{d_1 d_3}} \le \frac{n-1}{2\sqrt{2\,(n-3)}} < \frac{n+1}{2\sqrt{2\,(n-1)}}. \tag{5}$$

Since $|E_3| = |E(G)\backslash S| = n - d_2 - 1$, by (4), we obtain

$$\sum_{v_i v_j \in E_3} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}} < (n - d_2 - 1)\, e^{\frac{n}{2\sqrt{n-1}}}. \tag{6}$$

Claim 1.
$$2\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}+e^{\frac{n+1}{4\sqrt{n-3}}}+e^{\frac{n+5}{4\sqrt{n+1}}}<2\,e^{\frac{n}{2\sqrt{n-1}}}+e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}.$$

Proof of Claim 1. For $10\leq n\leq 11$, by Mathematica [44], one can easily check that the result holds. Otherwise, $n\geq 12$. By Lemma 2, the function $g(x)=\frac{x}{2\sqrt{x-1}}-\frac{x+3}{2\sqrt{2\,(x+1)}}$ is increasing on $x\geq 12$, and hence
$$g(x)\geq g(12)=\frac{6}{\sqrt{11}}-\frac{15}{2\sqrt{26}}>0.338.$$
Since $n\geq 12$, from the above, we have
$$\frac{n}{2\sqrt{n-1}}-\frac{n+3}{2\sqrt{2\,(n+1)}}>0.338>\ln 1.4,$$
$$\text{that is,}\ \ e^{\frac{n}{2\sqrt{n-1}}-\frac{n+3}{2\sqrt{2\,(n+1)}}}>1.4,\ \ \text{that is,}\ \ e^{\frac{n}{2\sqrt{n-1}}}>1.4\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}. \tag{7}$$
By Lemma 3, the function $q(x)=\frac{x+3}{2\sqrt{2\,(x+1)}}-\frac{x+5}{4\sqrt{x+1}}$ is increasing on $x\geq 12$, and hence
$$q(x)\geq q(12)=\frac{15}{2\sqrt{26}}-\frac{17}{4\sqrt{13}}>0.29.$$
Since $n\geq 12$, from the above, we have
$$\frac{n+3}{2\sqrt{2\,(n+1)}}-\frac{n+5}{4\sqrt{n+1}}>0.29>\ln\left(\frac{5}{4}\right),$$
$$\text{that is,}\ \ e^{\frac{n+3}{2\sqrt{2\,(n+1)}}-\frac{n+5}{4\sqrt{n+1}}}>\frac{5}{4},\ \ \text{that is,}\ \ 0.8\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}>e^{\frac{n+5}{4\sqrt{n+1}}}. \tag{8}$$
Since $n>5$, one can easily see that
$$\frac{n+1}{4\sqrt{n-3}}<\frac{n+1}{2\sqrt{2\,(n-1)}},\ \ \text{that is,}\ \ e^{\frac{n+1}{4\sqrt{n-3}}}<e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}.$$
Using the above result with (7) and (8), we obtain
$$\begin{aligned}2\,e^{\frac{n}{2\sqrt{n-1}}}+e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}&>2.8\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}+e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}\\&>2\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}+e^{\frac{n+5}{4\sqrt{n+1}}}+e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}\\&>2\,e^{\frac{n+3}{2\sqrt{2\,(n+1)}}}+e^{\frac{n+5}{4\sqrt{n+1}}}+e^{\frac{n+1}{4\sqrt{n-3}}}.\end{aligned}$$

This completes the proof of **Claim 1**.

For $v_j\in N_G(v_2)\backslash\{v_1,v_3\}$, we have $4\leq d_2\leq\frac{n+1}{2}$, $1\leq d_j\leq\frac{n-3}{2}$, and by Lemma 4, we obtain
$$\frac{d_2+d_j}{2\sqrt{d_2d_j}}\leq\frac{n+3}{2\sqrt{2\,(n+1)}}.$$

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Using the above result with (5), we obtain

$$\sum_{v_j:v_j\in N_G(v_2)} e^{\frac{d_2+d_j}{2\sqrt{d_2d_j}}} = e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + \sum_{v_j:v_j\in N_G(v_2)\setminus\{v_1,v_3\}} e^{\frac{d_2+d_j}{2\sqrt{d_2d_j}}}$$
$$\leq e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + (d_2-2)\, e^{\frac{n+3}{2\sqrt{2(n+1)}}}$$
$$\leq e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + (d_2-4)\, e^{\frac{n}{2\sqrt{n-1}}} \tag{9}$$

as

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

Using (5), (6), (9) and **Claim 1**, we obtain

$$EAG(G) = \sum_{v_iv_j\in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}$$
$$= e^{\frac{d_1+d_3}{2\sqrt{d_1d_3}}} + \sum_{v_j:v_j\in N_G(v_2)} e^{\frac{d_2+d_j}{2\sqrt{d_2d_j}}} + \sum_{v_iv_j\in E_3} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}$$
$$< e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + (d_2-4)\, e^{\frac{n}{2\sqrt{n-1}}} + (n-d_2-1)\, e^{\frac{n}{2\sqrt{n-1}}}$$
$$< (n-3)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-2)}}}$$
$$< (n-3)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e.$$

The result (1) strictly holds.

Case 2. $k \geq 4$. Let $v_1, v_2, \ldots, v_k$ be the vertices on the cycle $C_k\,(k \geq 4)$. We can assume that $d_1 = \max\{d_i : v_i \in V(C_k)\}$. Then $d_1 \leq n-k+2 \leq n-2$ and $d_i \geq 2\,(2 \leq i \leq k)$. Then by Lemma 4, for $v_1v_2 \in E(C_k)$ and $v_1v_k \in E(C_k)$, we obtain

$$\frac{d_1+d_2}{2\sqrt{d_1\,d_2}} \leq \frac{n}{2\sqrt{2\,(n-2)}} \quad\text{and}\quad \frac{d_1+d_k}{2\sqrt{d_1\,d_k}} \leq \frac{n}{2\sqrt{2\,(n-2)}}. \tag{10}$$

Since $v_2v_3 \in E(C_k)$ and $v_3v_4 \in E(C_k)$ with $2 \leq d_2, d_3, d_4 \leq \frac{n-k+4}{2} \leq \frac{n}{2}$, by Lemma 4, we obtain

$$\frac{d_2+d_3}{2\sqrt{d_2\,d_3}} \leq \frac{n+4}{4\sqrt{n}} \quad\text{and}\quad \frac{d_3+d_4}{2\sqrt{d_3\,d_4}} \leq \frac{n+4}{4\sqrt{n}}. \tag{11}$$

Claim 2.

$$2\, e^{\frac{n+4}{4\sqrt{n}}} < e^{\frac{n}{2\sqrt{n-1}}} + e.$$

Proof of Claim 2. For $10 \leq n \leq 12$, by Mathematica [44], one can easily check that the result holds. Otherwise, $n \geq 13$. Let us consider a function

$$h(x) = \frac{x}{\sqrt{x-1}} - \frac{x+4}{2\sqrt{x}}, \quad x \geq 13.$$

Then we have

$$h'(x) = \frac{1}{4x^{3/2}\,(x-1)^{3/2}}\left[2\,x^{3/2}\,(x-2) - (x-4)\,(x-1)^{3/2}\right] > 0.$$

Thus $h(x)$ is an increasing function on $x \geq 13$ and hence

$$h(x) \geq h(13) = \frac{13}{\sqrt{12}} - \frac{17}{2\sqrt{13}} > 1.395 > 2\ln 2.$$

From the above, we obtain

$$\frac{n}{\sqrt{n-1}} - \frac{n+4}{2\sqrt{n}} > 2\ln 2,$$

that is,

$$e^{\frac{n}{2\sqrt{n-1}} - \frac{n+4}{4\sqrt{n}}} > 2,$$

that is,

$$2\,e^{\frac{n+4}{4\sqrt{n}}} < e^{\frac{n}{2\sqrt{n-1}}} < e^{\frac{n}{2\sqrt{n-1}}} + e.$$

This completes the proof of **Claim 2**.

Let p be the number of pendant vertices in G. Since G has cycle length at least 4, we have $p \leq n-4$. Since $\frac{n+1}{\sqrt{2\,(n-1)}} < \frac{n}{\sqrt{n-1}}$, using (3), we obtain

$$\sum_{\substack{v_iv_j \in E(G)\setminus\{v_2v_3, v_3v_4\},\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} < (n-p-2)\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} \leq 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + (n-p-4)\,e^{\frac{n}{2\sqrt{n-1}}}. \tag{12}$$

Using the above result with (2), (11) and **Claim 2**, we obtain

$$\begin{aligned}
EAG(G) &= \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j = 1}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} + \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}\\
&< p\,e^{\frac{n}{2\sqrt{n-1}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_4}{2\sqrt{d_3d_4}}} + \sum_{\substack{v_iv_j \in E(G)\setminus\{v_2v_3, v_3v_4\},\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}\\
&< p\,e^{\frac{n}{2\sqrt{n-1}}} + 2\,e^{\frac{n+4}{4\sqrt{n}}} + (n-p-4)\,e^{\frac{n}{2\sqrt{n-1}}} + 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}\\
&< (n-3)\,e^{\frac{n}{2\sqrt{n-1}}} + 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e.
\end{aligned}$$

The result (1) strictly holds. This completes the proof of the theorem. □

3. Concluding Remarks

An open problem that was stated in [12] has been resolved in this paper. It has been determined that the maximal unicyclic graph with respect to EAG can be described in terms of graph order n.

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