MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **79** (2018) 451-466

ISSN 0340 - 6253

New Lower Bounds for the Geometric–Arithmetic Index

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(Received March 16, 2017)

Abstract

The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize graphs extremal with respect to them. Our main results provide lower bounds on $GA_1(G)$ involving just the minimum and the maximum degree of the graph G.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physico-chemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [13]).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches.

Probably, the best know such descriptor is the Randić connectivity index (R) [5]. Trying to improve the predictive power of the Randić index a large number of new topological descriptors resembling the original Randić index were introduced.

The first geometric-arithmetic index GA_1 was defined in [12] as

$$GA_1 = GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. Although GA_1 was introduced in 2009, there are many papers dealing with this index. For more details on this index, Randić index and their literature, the reader is referred to [6] and [7].

There exist previous works that study lower bounds on GA_1 based, for example, on the number of vertices, see [12], or the minimum and maximun degree together with the number of edges, see [1]. Our main results provide lower bounds on $GA_1(G)$ involving just the minimum and the maximum degree of the graph G (see Theorems 2.7 and 2.21, and Corollaries 2.16 and 2.17).

Throughout this work, $G = (V(G), E(G))$ denotes a (nonoriented) finite simple (without multiple edges and loops) nontrivial ($E(G) \neq \emptyset$) graph. The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize graphs extremal with respect to them.

2 GA_1 and minimum and maximum degree

If G is a graph with m edges, minimum degree δ and maximum degree Δ, then in [1] (see also [2]) we find the bounds:

$$\frac{2m\sqrt{\delta\Delta}}{\delta + \Delta} \leq GA_1(G) \leq m \,. \tag{1}$$

Remark 2.1. $GA_1(G) = \frac{2m\sqrt{\delta\Delta}}{\delta+\Delta}$ *if and only if the graph is either regular or bipartite with the two sets being respectively the set of vertices with degree* δ *and degree* Δ.

Let us recall Lemma 2.2 and Corollary 2.3 in [6].

Lemma 2.2. *Let* f *be the function* $f(t) = \frac{2t}{1+t^2}$ *on the interval* $[0, \infty)$. *Then* f *strictly increases in* $[0, 1]$, *strictly decreases in* $[1, \infty)$, $f(t) = 1$ *if and only if* $t = 1$ *and* $f(t) = f(t_0)$ *if and only if either* $t = t_0$ *or* $t = t_0^{-1}$.

Corollary 2.3. *Let* g *be the function* $g(x, y) = \frac{2\sqrt{xy}}{x+y}$ *with* $0 < a \leq x, y \leq b$. *Then* $\frac{2\sqrt{ab}}{a+b} \leq g(x, y) \leq 1$. *The equality in the lower bound is attained if and only if either* $x = a$

and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$.

Given integers $0 < \delta \le \Delta$, let us define $\mathcal{G}_{\delta,\Delta}$ as the set of graphs G with minimum degree δ, maximum degree Δ and such that:

(1) G is isomorphic to the complete graph with $\Delta + 1$ vertices $K_{\Delta+1}$, if $\delta = \Delta$,

(2) $|V(G)| = \Delta + 1$, there are Δ vertices with degree δ, if $\delta < \Delta$ and $\Delta(\delta + 1)$ is even,

(3) $|V(G)| = \Delta + 1$, there are $\Delta - 1$ vertices with degree δ and a vertex with degree $\delta + 1$, if $\delta < \Delta - 1$ and $\Delta(\delta + 1)$ is odd,

(4) $|V(G)| = \Delta + 1$, there are $\Delta - 1$ vertices with degree δ and two vertices with degree Δ, if $\delta = \Delta - 1$ and Δ is odd (and thus $\Delta(\delta + 1)$ is odd).

Remark 2.4. *Every graph $G \in \mathcal{G}_{\delta,\Delta}$ has maximum degree Δ and $|V(G)| = \Delta + 1$. Hence, every graph $G \in \mathcal{G}_{\delta,\Delta}$ is connected.*

Proposition 2.5. *For any integers $0 < \delta \le \Delta$, we have $\mathcal{G}_{\delta,\Delta} \ne \emptyset$. Let G be a graph with minimum degree δ and maximum degree Δ. Then*

$$|E(G)| \ge \frac{\Delta(\delta + 1)}{2} \quad \text{if } \Delta(\delta + 1) \text{ is even}, \qquad |E(G)| \ge \frac{\Delta(\delta + 1) + 1}{2} \quad \text{if } \Delta(\delta + 1) \text{ is odd},$$

with equality if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

Proof. There is at least one vertex $v_0 \in V(G)$ with degree Δ and Δ vertices, $v_1, \dots, v_\Delta$, adjacent to it. Since $d_{v_i} \ge \delta$, $|E(G)| \ge \frac{\Delta+\Delta\delta}{2} = \frac{\Delta(\delta+1)}{2}$. If $\Delta(\delta + 1)$ is odd, then $\frac{\Delta(\delta+1)}{2}$ is not an integer and the lower bound is at least $\frac{\Delta(\delta+1)+1}{2}$.

If the equality is attained, then $V(G) = \{v_0, v_1, \dots, v_\Delta\}$ (thus $|V(G)| = \Delta + 1$). As in Remark 2.4, we can conclude that G is connected. If $\Delta(\delta + 1)$ is even, then $d_{v_i} = \delta$ for $i = 1, \dots, \Delta$, and $G \in \mathcal{G}_{\delta,\Delta}$. If $G \in \mathcal{G}_{\delta,\Delta}$, it is clear that the equality holds. If $\Delta(\delta + 1)$ is odd, then a similar argument gives that the equality is attained if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

Finally, let us prove $\mathcal{G}_{\delta,\Delta} \ne \emptyset$. This is clear in the case (1); so, let us assume $\delta < \Delta$. Consider a graph H with $\Delta + 1$ vertices, $v_0, v_1, \dots, v_\Delta$. Assume that $d_{v_0} = \Delta$. Then, there is an edge joining v_0 with v_i for every $i > 0$.

First, suppose δ is odd. Thus, $\Delta(\delta + 1)$ is even. We have already one edge in each v_i. We are going to add edges so that $d_{v_i} = \delta$ for every $i > 0$. Let us define for every $1 \le i, j \le \Delta$, $||i - j|| = \min\{|i - j|, \Delta - |i - j|\}$ (this is, the distance between the vertices v_i and v_j in the cycle $v_1, v_2, \dots, v_\Delta, v_1$). Consider an edge v_iv_j for every pair of vertices with $||i - j|| \le \frac{\delta-1}{2}$. This is possible since $\delta - 1$ is even and $\delta - 1 < \Delta - 1$. Then, every vertex v_i with $i > 0$ satisfies that $\delta_{v_i} = \delta$ and $H \in \mathcal{G}_{\delta,\Delta}$.

Now, suppose δ and Δ are even. Thus, $\Delta(\delta+1)$ is even. Consider an edge v_iv_j for every pair of vertices with $||i-j|| \le \frac{\delta-2}{2}$ and a edge v_iv_j for every $||i-j|| = \frac{\Delta}{2}$. Notice that this is well defined since Δ is even and it is a new edge since $\frac{\Delta}{2} > \frac{\delta-2}{2}$. Then, every vertex v_i with $i>0$ satisfies that $d_{v_i} = \delta$ and $H \in \mathcal{G}_{\delta,\Delta}$.

Finally, if δ is even and Δ is odd, then $\Delta(\delta+1)$ is odd. Consider an edge v_iv_j for every pair of vertices with $||i-j|| \le \frac{\delta-2}{2}$. Now every vertex v_i with $i>0$ has degree $\delta-1$. Let us define, for every $1 \le i < j \le \Delta-1$, an edge v_iv_j if $j-i = \frac{\Delta-1}{2}$. This edge is new since $\frac{\delta-2}{2} < \frac{\Delta-1}{2}$. Now, $d_{v_i} = \delta$ for every $0 < i < \Delta$. It suffices to define an edge joining v_Δ to any non-adjacent vertex v_{i_0}, for example $i_0 = \frac{\delta}{2}+1$, and therefore, $H \in \mathcal{G}_{\delta,\Delta}$. Notice that, in this case, $d_{v_0} = \Delta$, $d_{v_{i_0}} = \delta+1$ and $d_{v_i} = \delta$ for every $i \ne 0, i_0$. ■

Proposition 2.6. *For every integers $0 < \delta \le \Delta$ and $G \in \mathcal{G}_{\delta,\Delta}$, we have*

$$GA_1(G) = \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2} \quad \text{if } \Delta(\delta+1) \text{ is even,}$$

$$\begin{aligned} GA_1(G) &= \frac{2(\Delta-1)\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2} \\ &> \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2} \quad \text{if } \Delta(\delta+1) \text{ is odd.} \end{aligned}$$

Proof. The equalities follow from the definitions of GA_1 and $\mathcal{G}_{\delta,\Delta}$. Let us see that

$$\frac{2(\Delta-1)\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2} > \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2}$$

if $\Delta(\delta+1)$ is odd. If $\delta = \Delta$, then $\Delta(\delta+1)$ is even. Thus, we can assume that $\delta < \Delta$. It suffices to check that

$$\frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} > \frac{2\sqrt{\delta\Delta}}{\delta+\Delta} \qquad \text{and} \qquad \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} - \frac{1}{2} > \delta-1.$$

The first claim follows from Lemma 2.2 and the fact that $\frac{2\sqrt{xy}}{x+y} = f(t)$ with $t = \sqrt{\frac{x}{y}}$, since $1 \le \frac{\Delta}{\delta+1} < \frac{\Delta}{\delta}$. For the second claim it suffices to check that

$$\frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} > \frac{2\delta-1}{2} \quad \Leftrightarrow \quad \sqrt{\delta(\delta+1)} > \frac{4\delta^2-1}{4\delta} \quad \Leftrightarrow$$

$$\delta(\delta+1) > \frac{16\delta^4-8\delta^2+1}{16\delta^2} \quad \Leftrightarrow \quad 16\delta^4+16\delta^3 > 16\delta^4-8\delta^2+1 \quad \Leftrightarrow \quad 16\delta^3+8\delta^2 > 1,$$

finishing the proof. ■

Theorem 2.7. *Let G be a graph with minimum degree $\delta > 0$ and maximum degree Δ. Then*

$$GA_1(G) \ge \Delta(\delta+1)\frac{\sqrt{\delta\Delta}}{\delta+\Delta}$$

with equality if and only if $\delta = 1$ *and* G *is a star graph or* $\delta = \Delta$ *and* G *is a complete graph.*

Furthermore, if $\Delta(\delta+1)$ *is odd, then*

$$GA_1(G) \geq \big(\Delta(\delta+1)+1\big)\frac{\sqrt{\delta\Delta}}{\delta+\Delta}.$$

Proof. By Proposition 2.5, $2m \geq \Delta(\delta+1)$. This inequality and the lower bound in (1) give the first inequality. If we use in this argument the second part of Proposition 2.5, then we obtain the second inequality.

If $\delta = 1$ and G is a star graph or $\delta = \Delta$ and G is a complete graph, then one can check that the equality is attained in the first inequality.

If the equality holds in the first inequality for a graph G, then Remark 2.1 gives that G is either regular or bipartite with the two sets being respectively the set of vertices with degree δ and degree Δ, and Proposition 2.5 gives that $\Delta(\delta+1)$ is even and $G \in \mathcal{G}_{\delta,\Delta}$. If $\delta = \Delta$, then G is a complete graph. If $\delta < \Delta$, then G is a bipartite graph with the two sets being the set of vertices with degree δ and degree Δ; thus, given a vertex v with degree δ, there are $\delta - 1$ edges connecting v and $\delta - 1$ vertices with degree δ; if $\delta > 1$, then this is not possible since G is a bipartite graph. Hence, $\delta = 1$ and G is a star graph. ■

Remark 2.8. *Notice that given any natural numbers* $\delta \leq \Delta$*, it is possible to define a graph* G *with minimum degree* δ*, maximum degree* Δ *and an arbitrarily large number of vertices and edges. Thus, the lower bounds we obtain for* $GA_1(G)$ *can not be compared with lower bounds that consider the number of edges as (1) or the number of vertices,* n*, as the lower bound*

$$\frac{2(n-1)^{\frac{3}{2}}}{n} \leq GA_1(G)$$

from [12].

We say that a graph G with minimum degree δ and maximum degree Δ is *minimal* if $GA_1(G) \leq GA_1(\Gamma)$ for every graph Γ with minimum degree δ and maximum degree Δ.

Proposition 2.9. *For any integers* $0 < \delta \leq \Delta$*, let* G *be a graph with minimum degree* δ *and maximum degree* Δ *which is minimal for those* δ *and* Δ*. Then*

$$\frac{\Delta(\delta+1)}{2} \leq |E(G)| \leq \Delta\delta \quad \text{if } \Delta(\delta+1) \text{ is even,}$$
$$\frac{\Delta(\delta+1)+1}{2} \leq |E(G)| \leq \Delta\delta \quad \text{if } \Delta(\delta+1) \text{ is odd,}$$
$$\Delta + 1 \leq |V(G)| \leq \frac{\Delta(2\delta-1)}{\delta} + 1.$$

For $|E(G)|$, the lower bound is attained if and only if $G \in \mathcal{G}_{\delta,\Delta}$ and the upper bound is attained if and only if $G = K_{\delta,\Delta}$.

Proof. By Proposition 2.5, if $\Delta(\delta+1)$ is even, $\frac{\Delta(\delta+1)}{2} \le |E(G)|$ and, if $\Delta(\delta+1)$ is odd, $\frac{\Delta(\delta+1)+1}{2} \le |E(G)|$. By Corollary 2.3, for every edge uv, $\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} \le \frac{2\sqrt{d_u d_v}}{d_u+d_v}$. Therefore, by (1), if $|E(G)| > \Delta\delta$, then $GA_1(G) > \Delta\delta\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} = GA_1(K_{\delta,\Delta})$ leading to contradiction.

It is immediate to see that $\Delta + 1 \le |V(G)|$ since there is a vertex with degree Δ and Δ vertices adjacent to it. Now suppose $|V(G)| > \frac{\Delta(2\delta-1)}{\delta} + 1$. By hypothesis, there is a vertex with degree Δ and more than $\frac{\Delta(2\delta-1)}{\delta}$ vertices with degree at least δ. Thus, $|E(G)| > \delta\Delta$, leading to contradiction.

By Proposition 2.5, the lower bound for $|E(G)|$ is attained if and only if $G \in \mathcal{G}_{\delta,\Delta}$. By Corollary 2.3, the upper bound for $|E(G)|$ is attained if and only if $G = K_{\delta,\Delta}$. ■

Let us denote by $K_{\delta,\Delta}$ the complete bipartite graph with a partition K_1, K_2 with δ and Δ vertices respectively. Notice that the vertices in K_1 have degree Δ and the vertices in K_2 have degree δ. It was proved in [6] that $GA_1(K_{\delta,\Delta}) = \frac{2\delta\Delta\sqrt{\delta\Delta}}{\delta+\Delta}$.

Let $H_{\delta,\Delta}$ be any graph in $\mathcal{G}_{\delta,\Delta}$. Note that if $\delta = 1$, then $H_{1,\Delta} = K_{1,\Delta}$.

Proposition 2.10. *For any integers $1 < \delta \le \Delta$, we have*

(1) *if $\frac{\Delta}{\delta} > (2+\sqrt{3})^2$, then $GA_1(H_{\delta,\Delta}) > GA_1(K_{\delta,\Delta})$,*

(2) *if $\frac{\Delta}{\delta} < (2+\sqrt{3})^2$ and $\Delta(\delta+1)$ is even, then $GA_1(H_{\delta,\Delta}) < GA_1(K_{\delta,\Delta})$.*

Proof. By Lemma 2.2, $f(t)$ is decreasing in $[1,\infty)$ and $f\left(\sqrt{\frac{\Delta}{\delta}}\right) = \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}$.

If $\frac{\Delta}{\delta} > (2+\sqrt{3})^2$, then

$$\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} = f\left(\sqrt{\frac{\Delta}{\delta}}\right) < f(2+\sqrt{3}) = \frac{2(2+\sqrt{3})}{1+(2+\sqrt{3})^2} = \frac{1}{2}.$$

Therefore, Proposition 2.6 and $\delta > 1$ give

$$GA_1(H_{\delta,\Delta}) \ge \Delta\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2} > \Delta\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} + \Delta(\delta-1)\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} = GA_1(K_{\delta,\Delta}).$$

If $\frac{\Delta}{\delta} < (2+\sqrt{3})^2$ and $\Delta(\delta+1)$ is even, then

$$\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} = f\left(\sqrt{\frac{\Delta}{\delta}}\right) > f(2+\sqrt{3}) = \frac{2(2+\sqrt{3})}{1+(2+\sqrt{3})^2} = \frac{1}{2},$$

$$GA_1(H_{\delta,\Delta}) = \Delta\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2} < \Delta\delta\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} = GA_1(K_{\delta,\Delta}).$$

■

It may be wondered if

$$GA_1(G) \geq \min\left\{GA_1(H_{\delta,\Delta}), GA_1(K_{\delta,\Delta})\right\}. \tag{2}$$

The following example shows that the answer is negative.

Example 2.11. *Let us suppose $\delta = 4$ and $\Delta = 56$. Consider a graph G with 57 vertices, two of them, a_1, a_2 with degree 56 and the rest, $b_1, \ldots, b_{55}$ with degree 4. Let us assume the edges are as follows. There is an edge $a_i b_j$ for every i, j, an edge $a_1 a_2$ and the vertices $b_1, \ldots, b_{55}$ induce a cycle of length 55. Note that these edges produce the claimed degree in each vertex.*

Notice that G has 166 edges, one of them joins two vertices of degree 56, 110 of them join vertices with degree 56 with vertices with degree 4 and 55 of them join vertices with degree 4. Therefore, $GA_1(G) = \frac{2\cdot 110\sqrt{4\cdot 56}}{4+56} + 56 = \frac{220\sqrt{224}}{60} + 56 \approx 110.8776$.

However, $GA_1(H_{4,56}) = \frac{112\sqrt{224}}{60} + 84 \approx 111.9377$, and $GA_1(K_{4,56}) = \frac{448\sqrt{224}}{60} \approx$ 111.7508.

Also, by Proposition 2.5, any graph with minimum degree 4 and maximum degree 56 has at least 140 edges (while G has 166). By Theorem 2.7 we have that any graph G' with minimum degree 4 and maximum degree 56 satisfies that $GA_1(G') \geq 56 \cdot 5\frac{\sqrt{224}}{60} \approx 69.8443$. Notice that his lower bound is relatively far from the results obtained from G, $H_{4,56}$ and $K_{4,56}$.

However, (2) holds if we have either $\delta = 1$ or $\delta = \Delta$ (see Theorem 2.7). Furthermore, (2) also holds if δ and Δ are close enough, as the following results show.

Theorem 2.12. *Let G be a graph with minimum degree $\delta > 0$ and maximum degree $\Delta \geq 2$. If*

$$\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} \geq \frac{\Delta(\delta-1)}{\Delta(\delta-1)+2}, \tag{3}$$

then

$$GA_1(G) \geq \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2}. \tag{4}$$

Furthermore, if $\Delta(\delta+1)$ is odd,

$$\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} \geq \frac{\Delta(\delta-1)}{\Delta(\delta-1)+2} \quad and \quad \frac{3\sqrt{\delta\Delta}}{\delta+\Delta} + \delta - \frac{1}{2} \geq \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1}, \tag{5}$$

then

$$GA_1(G) \geq \frac{2(\Delta-1)\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2}. \tag{6}$$

If Δ and δ verify (3), then the equality in (4) is attained if and only if $\Delta(\delta+1)$ is even and $G \in \mathcal{G}_{\delta,\Delta}$. If Δ and δ verify (5) and $\Delta(\delta+1)$ is odd, then the equality in (6) is attained if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

Proof. Suppose $G \notin \mathcal{G}_{\delta,\Delta}$. Then, by Proposition 2.5, G has at least $\frac{\Delta(\delta+1)}{2}+1$ edges. By (1), this implies that

$$GA_1(G) \geq \Big(\frac{\Delta(\delta+1)}{2}+1\Big)\frac{2\sqrt{\delta\Delta}}{\delta+\Delta}. \tag{7}$$

Let us denote $\varepsilon = \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}$. Then, it suffices to check that

$$\Big(\frac{\Delta(\delta+1)}{2}+1\Big)\varepsilon \geq \Delta\varepsilon + \frac{\Delta(\delta-1)}{2}.$$

Thus, it is readily seen that

$$\Big(\frac{\Delta(\delta+1)}{2}+1\Big)\varepsilon \geq \Delta\varepsilon + \frac{\Delta(\delta-1)}{2} \quad \Leftrightarrow \quad \varepsilon\Big(\frac{\Delta(\delta+1)}{2}+1-\Delta\Big) \geq \frac{\Delta(\delta-1)}{2} \quad \Leftrightarrow$$

$$\varepsilon\Big(\frac{\Delta(\delta-1)+2}{2}\Big) \geq \frac{\Delta(\delta-1)}{2} \quad \Leftrightarrow \quad \varepsilon \geq \frac{\Delta(\delta-1)}{\Delta(\delta-1)+2}.$$

If $\Delta(\delta+1)$ is odd and $G \notin \mathcal{G}_{\delta,\Delta}$, then by Proposition 2.5, G has at least $\frac{\Delta(\delta+1)+1}{2}+1$ edges. By (1), this implies that

$$GA_1(G) \geq \Big(\frac{\Delta(\delta+1)+1}{2}+1\Big)\frac{2\sqrt{\delta\Delta}}{\delta+\Delta}. \tag{8}$$

Then, it suffices to check that

$$\Big(\frac{\Delta(\delta+1)+1}{2}+1\Big)\varepsilon \geq (\Delta-1)\varepsilon + \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2}.$$

Since $\varepsilon \geq \frac{\Delta(\delta-1)}{\Delta(\delta-1)+2}$, the argument from the even case implies that

$$\Big(\frac{\Delta(\delta+1)}{2}+1\Big)\varepsilon \geq \Delta\varepsilon + \frac{\Delta(\delta-1)}{2} = (\Delta-1)\varepsilon + \varepsilon + \frac{\Delta(\delta-1)}{2}$$

and it suffices to check that

$$\frac{3\varepsilon}{2} + \frac{\Delta(\delta-1)}{2} \geq \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2}.$$

Since, by hypothesis

$$\frac{3}{2}\varepsilon + \delta - \frac{1}{2} \geq \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1},$$

then the result follows immediately.

Proposition 2.6 gives that the equality in (4) is attained if $\Delta(\delta+1)$ is even and $G \in \mathcal{G}_{\delta,\Delta}$, and that the equality in (6) is attained if $\Delta(\delta+1)$ is odd and $G \in \mathcal{G}_{\delta,\Delta}$.

Assume that Δ and δ verify (3). Proposition 2.6 gives that if the equality is attained in (4) for some G, then $\Delta(\delta+1)$ is even. Assume that the equality is attained in (4) for some $G \notin \mathcal{G}_{\delta,\Delta}$. Thus, the equality is attained in (7). Remark 2.1 and (1) give that $|E(G)| = \frac{\Delta(\delta+1)}{2} + 1$ and G is either regular or bipartite with the two sets being respectively the set of vertices with degree δ and degree Δ. If G is regular, then $\delta = \Delta$ and $\frac{\Delta(\Delta+1)}{2} + 1 = |E(G)| = \frac{n\Delta}{2}$, where $n = |V(G)|$. So, $2 = \Delta(n-1-\Delta)$ and, since $\Delta \geq 2$, we conclude $\Delta = 2$ and $n-1-\Delta = 1$; hence, G is a 2-regular graph with $n = 4$ vertices, i.e., $G \cong C_4$. Assume now that G is bipartite with the two sets being respectively the set of vertices with degree δ and degree Δ (thus, $\Delta > \delta$). Then there exists a vertex $v_0 \in V(G)$ of degree Δ with neighbors $v_1, \dots, v_\Delta \in V(G)$ of degree δ; since G is a bipartite graph,

$$\frac{\Delta(\delta+1)}{2} + 1 = |E(G)| \geq \Delta\delta, \qquad \Delta + 2 \geq \Delta\delta \,.$$

If $\delta \geq 2$, then $\Delta + 2 \geq 2\Delta$, $2 \geq \Delta$ and we conclude $\Delta = \delta = 2$, a contradiction. If $\delta = 1$, then G is isomorphic to the union of r graphs $K_{1,\Delta}$, since G is bipartite, and we have

$$\Delta + 1 = \frac{\Delta(\delta+1)}{2} + 1 = |E(G)| = r\Delta, \qquad 1 = (r-1)\Delta \,.$$

Hence, $\Delta = 1$, a contradiction. We conclude that if the equality is attained in (4) for some $G \notin \mathcal{G}_{\delta,\Delta}$, then $(\Delta, \delta) = (2,2)$ and $G \cong C_4$, but we have $GA_1(C_4) = 4 > 3 = \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2}$, a contradiction. Therefore, if $G \notin \mathcal{G}_{\delta,\Delta}$, then the inequality (4) is strict.

Assume that Δ and δ verify (5) and that the equality is attained in (6) for some $G \notin \mathcal{G}_{\delta,\Delta}$. Thus, the equality is attained in (8). Remark 2.1 and (1) give that $|E(G)| = \frac{\Delta(\delta+1)+1}{2} + 1$ and G is either regular or bipartite with the two sets being respectively the set of vertices with degree δ and degree Δ. If G is regular, then $\delta = \Delta$ and $\Delta(\Delta+1)$ is even, leading to contradiction with the number of edges. Assume now that G is bipartite with the two sets being respectively the set of vertices with degree δ and degree Δ (thus, $\Delta > \delta$). Then there exists a vertex $v_0 \in V(G)$ of degree Δ with neighbors $v_1, \dots, v_\Delta \in V(G)$ of degree δ; since G is a bipartite graph,

$$\frac{\Delta(\delta+1)+1}{2} + 1 = |E(G)| \geq \Delta\delta, \qquad \Delta + 3 \geq \Delta\delta \,.$$

Since $\Delta(\delta+1)$ is odd, we have $\delta \geq 2$. Thus, $\Delta + 3 \geq 2\Delta$, $3 \geq \Delta > \delta \geq 2$ and we conclude $\Delta = 3$, $\delta = 2$ and $|E(G)| = 6$. Hence, G has two vertices with degree 3 and three vertices with degree 2 and it is isomorphic either to the cycle graph C_5 with an additional edge or to the complete bipartite graph $K_{2,3}$. One can check that for these graphs the equality in (6) is strict, a contradiction. We conclude that the equality is not attained in (6) if $G \notin \mathcal{G}_{\delta,\Delta}$. ∎

Remark 2.13. *Notice that in Theorem 2.12, since* $\frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} \le 1$ *for every* $\delta < \Delta$*, to assure the second condition in the case where* $\Delta(\delta+1)$ *is odd, this is,*

$$\frac{3\sqrt{\delta\Delta}}{\delta+\Delta} + \delta - \frac{1}{2} \ge \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1},$$

it suffices to check that

$$\frac{3\sqrt{\delta\Delta}}{\delta+\Delta} + \delta - \frac{3}{2} \ge \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1},$$

or equivalently,

$$\delta\left(1 - \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}\right) \ge \frac{3}{2}\left(1 - \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\right).$$

A nontrivial connected graph with maximum degree at most four is a *molecular graph* representing hydrocarbons [10]. Theorem 2.12 allows to obtain sharp inequalities for molecular graphs.

Corollary 2.14. *Let* G *be a molecular graph with minimum degree* $\delta > 0$ *and maximum degree* Δ*. If* $(\delta, \Delta) \neq (2,3)$*, then*

$$GA_1(G) \ge \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2},$$

with equality if and only if $G \in \mathcal{G}_{\delta,\Delta}$*. If* $(\delta, \Delta) = (2,3)$*, then*

$$GA_1(G) \ge \frac{2(\Delta-1)\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{2\sqrt{(\delta+1)\Delta}}{\delta+1+\Delta} + \frac{2\delta\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2} = \frac{8\sqrt{6}}{5} + 1,$$

with equality if and only if $G \in \mathcal{G}_{2,3}$*.*

Proof. Since G is a molecular graph, $\Delta(\delta+1)$ is even if and only if $(\delta, \Delta) \neq (2,3)$. One can check that, in this case, (δ, Δ) satisfies (3) in Theorem 2.12. Thus, Theorem 2.12 gives the first part of the corollary. It is easy to check that $(\delta, \Delta) = (2,3)$ satisfies (5) in Theorem 2.12. Hence, Theorem 2.12 gives the second part of the corollary. ■

Corollary 2.15. *Let* G *be a graph with minimum degree* $\delta > 0$ *and maximum degree* $\Delta = \delta + h \ge 2$*. If* $(16-h^2)\Delta^3 + (2h^3+2h^2-32h-16)\Delta^2 + (-h^4-2h^3+15h^2+16h+16)\Delta - 16h \ge 0$*, then*

$$GA_1(G) \ge \frac{2\Delta\sqrt{\Delta(\Delta-h)}}{2\Delta-h} + \frac{\Delta(\Delta-h-1)}{2}.$$

Proof. By Theorem 2.12 and $\delta = \Delta - h$, it suffices to check that

$$\frac{2\sqrt{\Delta(\Delta-h)}}{2\Delta-h} \ge \frac{\Delta(\Delta-(h+1))}{\Delta(\Delta-(h+1))+2}.$$

Thus,

$$\frac{2\sqrt{\Delta(\Delta-h)}}{2\Delta-h} \geq \frac{\Delta(\Delta-(h+1))}{\Delta(\Delta-(h+1))+2} \Leftrightarrow 2\sqrt{\Delta(\Delta-h)} \geq \frac{\Delta(\Delta-(h+1))(2\Delta-h)}{\Delta(\Delta-(h+1))+2} \Leftrightarrow$$

$$4(\Delta-h) \geq \frac{\Delta(\Delta-(h+1))^2(2\Delta-h)^2}{\Delta^2(\Delta-(h+1))^2+4\Delta(\Delta-(h+1))+4} \Leftrightarrow$$

$$4(\Delta-h)\Delta^2(\Delta-(h+1))^2+16\Delta(\Delta-h)(\Delta-(h+1))+16(\Delta-h)$$

$$\geq \Delta(\Delta-(h+1))^2(2\Delta-h)^2 \Leftrightarrow$$

$$\Delta(\Delta-(h+1))^2[4\Delta(\Delta-h)-(2\Delta-h)^2]+16(\Delta-h)[\Delta(\Delta-(h+1))+1] \geq 0 \Leftrightarrow$$

$$-h^2\Delta(\Delta-(h+1))^2+16(\Delta-h)[\Delta^2-h\Delta-\Delta+1] \geq 0 \Leftrightarrow$$

$$(16-h^2)\Delta^3+(2h^3+2h^2-32h-16)\Delta^2+(-h^4-2h^3+15h^2+16h+16)\Delta-16h \geq 0.$$

■

Let us denote

$$P(h,\Delta) = (16-h^2)\Delta^3+(2h^3+2h^2-32h-16)\Delta^2+(-h^4-2h^3+15h^2+16h+16)\Delta-16h.$$

Therefore, we obtain the following polynomials with the following real solutions (rounded off to one decimal):

If $h=0$, $P(0,\Delta)=16\Delta^3-16\Delta^2+16\Delta$, real root: 0.

If $h=1$, $P(1,\Delta)=15\Delta^3-44\Delta^2+44\Delta-16$, real root: 1.3.

If $h=2$, $P(2,\Delta)=12\Delta^3-56\Delta^2+76\Delta-32$, real root: 2.7.

If $h=3$, $P(3,\Delta)=7\Delta^3-40\Delta^2+64\Delta-48$, real root: 3.8.

If $h=4$, $P(4,\Delta)=16\Delta^2-64\Delta-64$, real roots: -0.8 and 4.8.

If $h=5$, $P(5,\Delta)=-9\Delta^3+124\Delta^2-404\Delta-80$, real roots: -0.2, 5.9 and 8.1.

If $h=6$, $P(6,\Delta)=-20\Delta^3+296\Delta^2-1076\Delta-96$, real roots: -0.1, 6.9 and 8.

If $h=7$, $P(7,\Delta)=-33\Delta^3+544\Delta^2-2224\Delta-112$, real roots: -0.1, 7.9 and 8.6.

This, together with Theorem 2.7 and Corollary 2.15, yields the following:

Corollary 2.16. *Let G be a graph with minimum degree $\delta>0$ and maximum degree $\Delta=\delta+h\geq 2$. If we have*

(1) $h=0$ *or* $h=1$, *for every* $\Delta\geq 2$,

(2) $h=2$, *for every* $\Delta\geq 3$,

(3) $h=3$, *for every* $\Delta\geq 4$,

(4) $h=4$, *for every* $\Delta\geq 5$,

(5) $h=5$, *for every* $\Delta\in\{6,7,8\}$,

(6) $h=6$, *for every* $\Delta\in\{7,8\}$,

(7) $h\geq 7$ *and* $\Delta=h+1$,

then

$$GA_1(G) \ge \frac{2\Delta\sqrt{\Delta(\Delta-h)}}{2\Delta-h} + \frac{\Delta(\Delta-h-1)}{2}.$$

Corollary 2.17. *Let G be a graph with maximum degree $\Delta \ge 2$ and minimum degree $\delta = \Delta - 1$. Then*

$$GA_1(G) \ge \frac{2\Delta\sqrt{\Delta(\Delta-1)}}{2\Delta-1} + \frac{\Delta(\Delta-2)}{2}, \quad \text{if } \Delta \text{ is even,}$$
$$GA_1(G) \ge \frac{4(\Delta-1)\sqrt{\Delta(\Delta-1)}}{2\Delta-1} + \frac{(\Delta-2)^2-1}{2} + 1, \quad \text{if } \Delta \text{ is odd,}$$

with equalities if and only if $G \in \mathcal{G}_{\Delta-1,\Delta}$.

Proof. As we saw above, $P(1,\Delta) = 15\Delta^3 - 44\Delta^2 + 44\Delta - 16 \ge 0$ for every $\Delta \ge 2$. Furthermore, since this inequality is strict for every $\Delta \ge 2$, the bound is only attained if $G \in \mathcal{G}_{\Delta-1,\Delta}$.

If Δ is odd (and therefore, $\Delta \ge 3$), then by Theorem 2.12, and Remark 2.13, the second result follows trivially from the fact that $\delta \ge 2 > \frac{3}{2}$. Also, since the inequality is strict, the bound is only attained if $G \in \mathcal{G}_{\Delta-1,\Delta}$ ■

Corollary 2.16 has also the following consequence.

Corollary 2.18. *Let G be a graph with minimum degree $\delta > 0$ and maximum degree $2 \le \Delta \le 8$. Then*

$$GA_1(G) \ge \frac{2\Delta\sqrt{\delta\Delta}}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2}.$$

Lemma 2.19. *If $28 \le a \le \Delta$, then*

$$\frac{2\sqrt{a\Delta}}{\Delta+a} > 2\frac{2\sqrt{2\Delta}}{\Delta+2}. \tag{9}$$

Proof.

$$\frac{2\sqrt{a\Delta}}{\Delta+a} > 2\frac{2\sqrt{2\Delta}}{\Delta+2} \quad\Leftrightarrow\quad \frac{\sqrt{a}}{\Delta+a} > \frac{2\sqrt{2}}{\Delta+2} \quad\Leftrightarrow$$
$$a(\Delta+2)^2 > 8(\Delta+a)^2 \quad\Leftrightarrow\quad (a-8)\Delta^2 - 12a\Delta - 8a^2 + 4a > 0.$$

Since $28 \le a \le \Delta$, then $(a-8)\Delta^2 - 12a\Delta - 8a^2 + 4a \ge (a-28)\Delta^2 + 4a > 0$ and (9) holds. ■

Lemma 2.20. *If $2 \le b \le 27$ and $\Delta \ge 30$, then*

$$(b-1)\frac{2\sqrt{2b}}{b+2} > b\frac{2\sqrt{2\Delta}}{\Delta+2}\ . \tag{10}$$

Proof. We have

$$(b-1)\frac{2\sqrt{2b}}{b+2} > b\frac{2\sqrt{2\Delta}}{\Delta+2} \quad \Leftrightarrow \quad \frac{b-1}{(b+2)\sqrt{b}} > \frac{\sqrt{\Delta}}{\Delta+2}\,.$$

Let us define

$$A(b) = \frac{b-1}{(b+2)\sqrt{b}}, \qquad B(\Delta) = \frac{\sqrt{\Delta}}{\Delta+2}\,.$$

One can check that $\min_{2\le b\le 27} A(b) = A(27)$ and $\max_{\Delta\ge 30} B(\Delta) = B(30)$. Since $A(27) = \frac{26}{29\sqrt{27}} > \frac{\sqrt{30}}{32} = B(30)$, we conclude that (10) holds. ■

Theorem 2.21. *Let G be a graph with minimum degree 2 and maximum degree $\Delta \ge 28$. Then,*

$$GA_1(G) \ge 2\Delta\frac{2\sqrt{2\Delta}}{\Delta+2}\,,$$

and the equality is attained if and only if $G = K_{2,\Delta}$.

Proof. Let x_0 be a vertex such that $d_{x_0} = \Delta$. Let $C_1, \dots, C_k$ be the connected components of $G\backslash\{x_0\}$ and $R_i = V(C_i) \cap N(x_0)$ for every $1 \le i \le k$ where $N(x_0)$ denotes the set of vertices in G adjacent to x_0. Let $r_i := |R_i|$ and notice that $\sum_{i=1}^{k} r_i = \Delta$. Denote by Γ_i the subgraph of G induced by $V(C_i) \cup \{x_0\}$ (thus, $\cup_{i=1}^{k}\Gamma_i = G$).

If C_i has at least r_i edges, then $\sum_{uv\in E(C_i)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \ge r_i\frac{2\sqrt{2\Delta}}{\Delta+2}$. Since $|E(\Gamma_i)| = |E(C_i)|+r_i$, we have that

$$\sum_{uv\in E(\Gamma_i)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \ge 2r_i\frac{2\sqrt{2\Delta}}{\Delta+2}\,.$$

If C_i has less than r_i edges then, since R_i has r_i vertices and $R_i \subseteq C_i$ with C_i connected, it follows that $R_i = V(C_i)$ and C_i is a tree with exactly $r_i - 1$ edges.

Suppose there is a vertex $v \in R_i$, such that $d_v \ge 28$. Recall that v is adjacent to x_0 with $d_{x_0} = \Delta$. Thus, by Lemma 2.19, $\frac{2\sqrt{d_v\Delta}}{\Delta+d_v} > 2\frac{2\sqrt{2\Delta}}{\Delta+2}$. Since apart from the edge x_0v, there are r_i-1 edges joining x_0 and the vertices in $R_i\backslash\{v\}$ and r_i-1 edges in C_i, it follows that

$$\sum_{uv\in E(\Gamma_i)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} > 2r_i\frac{2\sqrt{2\Delta}}{\Delta+2}\,.$$

Otherwise, if v_i is the vertex in R_i with maximum degree and $d_{v_i} \le 27$, then $\frac{2\sqrt{d_u d_{v_i}}}{d_u+d_{v_i}} \ge \frac{2\sqrt{2d_{v_i}}}{d_{v_i}+2}$ for every vertex $u \in N(v_i) \setminus \{x_0\}$. Therefore, by Lemma 2.20, if $A(d_{v_i}) > B(\Delta)$

$$\sum_{u\in N(v_i)\backslash\{x_0\}} \frac{2\sqrt{d_u d_{v_i}}}{d_u+d_{v_i}} \ge (d_{v_i}-1)\frac{2\sqrt{2d_{v_i}}}{d_{v_i}+2} > d_{v_i}\frac{2\sqrt{2\Delta}}{\Delta+2}.$$

Since apart from these edges there are $r_i - d_{v_i}$ edges in C_i and r_i edges joining x_0 and the vertices in R_i, it follows that

$$\sum_{uv\in E(\Gamma_i)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} > 2r_i \frac{2\sqrt{2\Delta}}{\Delta + 2}.$$

Notice that $A(d_{v_i}) > B(\Delta)$ for every $\Delta \geq 30$, if $\Delta = 29$ and $d_{v_i} \leq 26$ and if $\Delta = 28$ and $d_{v_i} \leq 25$. Therefore, if every component C_i either satisfies one of these cases, or has r_i edges, or has a vertex with degree at least 28, then

$$GA_1(G) = \sum_{i=1}^{k} \sum_{uv\in E(\Gamma_i)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} > \sum_{i=1}^{k} 2r_i \frac{2\sqrt{2\Delta}}{\Delta + 2} = 2\Delta \frac{2\sqrt{2\Delta}}{\Delta + 2} = GA_1(K_{2,\Delta}).$$

Therefore, to finish the proof it suffices to check the following cases:

Case 1. Suppose $\Delta = 29$ and there is a vertex v_i adjacent to x_0 such that $d_{v_i} = 27$, $v_i \in C_1$ and C_1 has $r_1 - 1$ edges. Then, there are exactly two vertices adjacent to x_0 which are not adjacent to v_i. Let us assume, relabeling if necessary, that these are x_{28} and x_{29}, and $v_i = x_1$. Therefore, G has one edge joining x_0 to x_1 where $d_{x_0} = 29$ and $d_{x_1} = 27$, 28 edges joining x_0 to a vertex x_i with $d_{x_i} \geq 2$ and 26 edges joining x_1 to x_j for $2 \leq j \leq 27$ with $d_{x_j} \leq 27$. If G has 58 edges, then trivially $GA_1(G) \geq GA_1(K_{2,29})$. If $|E(G)| \leq 57$, then there are at most two edges left. Since $d_{x_{28}} \geq 2$ and $d_{x_{29}} \geq 2$ either there is an edge $x_{28}x_{29}$ or there are two edges joining x_{28} and x_{29} to the same or two different vertices in $\{x_2, \dots, x_{27}\}$ or there is an edge $x_{28}x_{29}$ and some extra edge joining two vertices in $\{x_2, \dots, x_{29}\}$. Thus, either there is an edge joining two vertices with degree 2 or two edges joining a vertex with degree 2 or 3 to a vertex with degree 3 or 4. Since $2\frac{2\sqrt{2\cdot 3}}{2+3} > 2\frac{2\sqrt{2\cdot 4}}{2+4} > 1$, it follows that

$$GA_1(G) \geq \frac{2\sqrt{29\cdot 27}}{56} + 28\frac{2\sqrt{29\cdot 2}}{31} + 26\frac{2\sqrt{27\cdot 2}}{29} + 1$$

and it suffices to check that $1.999 \approx \frac{2\sqrt{29\cdot 27}}{56} + 1 > 4\frac{2\sqrt{29\cdot 2}}{31} \approx 1.965$.

Case 2. Suppose $\Delta = 28$ and there is a vertex v_i adjacent to x_0 such that $d_{v_i} = 26$, $v_i \in C_1$ and C_1 has $r_1 - 1$ edges. Then, there are exactly two vertices adjacent to x_0 which are not adjacent to v_i. Let us assume, relabeling if necessary, that these are x_{27} and x_{28}, and $v_i = x_1$. Therefore, G has one edge joining x_0 to x_1 where $d_{x_0} = 28$ and $d_{x_1} = 26$, 27 edges joining x_0 to a vertex x_i with $d_{x_i} \geq 2$ and 25 edges joining x_1 to x_j for $2 \leq j \leq 26$ with $d_{x_j} \leq 26$. If G has 56 edges, then trivially $GA_1(G) \geq GA_1(K_{2,28})$. If $|E(G)| \leq 55$, then there are at most two edges left. Since $d_{x_{27}} \geq 2$ and $d_{x_{28}} \geq 2$ either there is an edge $x_{27}x_{28}$ or there are two edges joining x_{27} and x_{28} to the same or two different vertices in $\{x_2, \ldots, x_{26}\}$ or there is an edge $x_{27}x_{28}$ and some extra edge joining two vertices in $\{x_2, \ldots, x_{28}\}$. Thus, either there is an edge joining two vertices with degree 2 or two edges joining a vertex with degree 2 or 3 to a vertex with degree 3 or 4. Since $2\frac{2\sqrt{2\cdot 3}}{2+3} > 2\frac{2\sqrt{2\cdot 4}}{2+4} > 1$, it follows that

$$GA_1(G) > \frac{2\sqrt{28\cdot 26}}{54} + 27\frac{2\sqrt{28\cdot 2}}{30} + 25\frac{2\sqrt{26\cdot 2}}{28} + 1$$

and it suffices to check that $1.999 \approx \frac{2\sqrt{28\cdot 26}}{54} + 1 > 4\frac{2\sqrt{28\cdot 2}}{30} \approx 1.996$.

Case 3. Suppose $\Delta = 28$ and there is a vertex v_i adjacent to x_0 such that $d_{v_i} = 27$, $v_i \in C_1$ and C_1 has $r_1 - 1$ edges. Then, there is exactly one vertex adjacent to x_0 which is not adjacent to v_i. Let us assume, that it is x_{28}, and $v_i = x_1$. Therefore, G has one edge joining x_0 to x_1 where $d_{x_0} = 28$ and $d_{x_1} = 27$, 27 edges joining x_0 to a vertex x_i with $d_{x_i} \geq 2$ and 26 edges joining x_1 to x_j for $2 \leq j \leq 27$ with $d_{x_j} \leq 27$. If G has 56 edges, then trivially $GA_1(G) \geq GA_1(K_{2,28})$. If $|E(G)| \leq 55$, then there is at most 1 edge left. Since $d_{x_{28}} \geq 2$ there is an edge joining x_{28} to a vertex in $\{x_2, \ldots, x_{27}\}$. Thus, there is an edge joining a vertex with degree 2 to a vertex with degree 3. Hence, it follows that

$$GA_1(G) \geq \frac{2\sqrt{28\cdot 27}}{55} + 27\frac{2\sqrt{28\cdot 2}}{30} + 26\frac{2\sqrt{27\cdot 2}}{29} + \frac{2\sqrt{2\cdot 3}}{5}$$

and it suffices to check that $1.98 \approx \frac{2\sqrt{28\cdot 27}}{55} + \frac{2\sqrt{2\cdot 3}}{5} > 3\frac{2\sqrt{28\cdot 2}}{30} \approx 1.50$.

Since the inequalities in Lemmas 2.19 and 2.20 are strict, it follows from the proof that if $GA_1(G) = 2\Delta\frac{2\sqrt{2\Delta}}{\Delta+2}$, then C_i has exactly r_i edges for every $1 \leq i \leq k$. Therefore, G has 2Δ edges and Proposition 2.9 gives $G = K_{2,\Delta}$. ■

Given any odd integer $\Delta \geq 3$, let us define H_Δ as the graph with minimum degree 2, maximum degree Δ, $|V(H_\Delta)| = \Delta + 1$, and such that there are 2 vertices, x_0, x_1 with degree Δ which are adjacent and $\Delta - 1$ vertices with degree 2: $x_2, \ldots, x_\Delta$. Note that

$$GA_1(H_\Delta) = 2(\Delta - 1)\frac{2\sqrt{2\Delta}}{2+\Delta} + 1\ . \tag{11}$$

The next result shows that the conclusion of Theorem 2.21 does not hold for $\Delta < 28$.

Proposition 2.22. *For any integer* $2 \leq \Delta \leq 27$, *if* $G \in \mathcal{G}_{2,\Delta}$, *then*

$$GA_1(G) < GA_1(K_{2,\Delta}), \quad \text{if } \Delta \text{ is even,}$$
$$GA_1(H_\Delta) < GA_1(K_{2,\Delta}), \quad \text{if } \Delta \text{ is odd.}$$

Proof. If Δ is even, then $\Delta(\delta+1)$ is even and, by Proposition 2.10, $GA_1(G) < GA_1(K_{2,\Delta})$.

If Δ is odd, then by (11), $GA_1(H_\Delta) = 2(\Delta-1)\frac{2\sqrt{2\Delta}}{2+\Delta}+1$ and, since for every $2 \leq \Delta \leq 27$ we have $1 < 2\frac{2\sqrt{2\Delta}}{2+\Delta}$, we conclude $GA_1(H_\Delta) < GA_1(K_{2,\Delta})$. ■

Acknowledgement: This work was partially supported by the grants from Ministerio de Economía y Competititvidad, Agencia Estatal de Investigación (AEI) and Fondo Europeo de Desarrollo Regional (FEDER) (MTM 2015-63612P, MTM 2016-78227-C2-1-P and MTM 2015-69323-REDT), Spain, and from CONACYT (FOMIX-CONACyT-UAGro 249818), México.

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