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Unicyclic graphs with the maximal value of Graovac-Pisanski index*

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Abstract

Let G be a graph and let Γ be its group of automorphisms. Graovac-Pisanski index of G is $\mathrm{GP}(G) = \frac{|V(G)|}{2|\Gamma|}\sum_{u\in V(G)}\sum_{\alpha\in\Gamma} d(u,\alpha(u))$, where $d(u,v)$ is the distance from u to v in G. One can observe that $\mathrm{GP}(G)=0$ if G has no nontrivial automorphisms, but it is not known which graphs attain the maximum value of Graovac-Pisanski index. In this paper we show that among unicyclic graphs on n vertices the n-cycle attains the maximum value of Graovac-Pisanski index.

Keywords: Graovac-Pisanski index, modified Wiener index, unicyclic graphs.

Math. Subj. Class.: 05C25

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1 Introduction

Wiener index, the sum of distances in a graph, is an important molecular descriptor. It was introduced by Wiener in 1949, see [18], and since then many other molecular descriptor have appeared. One of them is the Graovac-Pisanski index [8], originally known as the modified Wiener index. With this index an algebraic approach for generalizing the Wiener index was presented. Namely, as the Wiener index also the Graovac-Pisanski index is based on distances but its advantage is in considering also the symmetries of a graph, and it is known that symmetries of a molecule have an influence on its properties [14].

In his pioneering paper, Wiener showed a correlation of the Wiener index of alkanes with their boiling points [18]. It turns out that the Graovac-Pisanski index combines the symmetry and topology of molecules to obtain a good correlation with some physico-chemical properties of molecules. Recently, Črepnjak et al. showed that the Graovac-Pisanski index of some hydrocarbon molecules is correlated with their melting points [6].

This index also drew attention from theoretical point of view. Researchers are interested in the difference between the Wiener and Graovac-Pisanski index. This difference was computed in [9] for some families of polyhedral graphs. The Graovac-Pisanski index of nanostructures was studied in [1, 2, 15, 16, 17] and for some classes of fullerenes and fullerene-like molecules in [3, 11, 12]. In [13] the symmetry groups and Graovac-Pisanski index of some linear polymers were computed. Upper and lower bounds for Graovac-Pisanski index were considered in [11]. In [7] and [16] Graovac-Pisanski index was further considered from computational point of view. Exact formulae for the Graovac-Pisanski index for some graph operations are presented in [4]. Recently it was proved that for any connected bipartite graph, as well as for any connected graph on even number of vertices, the Graovac-Pisanski index is an integer number [5].

Let G be a connected graph. The *Graovac-Pisanski index* of G is defined as

$$\mathrm{GP}(G) = \frac{|V(G)|}{2|\operatorname{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \operatorname{Aut}(G)} \operatorname{dist}_G(u, \alpha(u)),$$

where $\operatorname{Aut}(G)$ is the group of automorphisms of G and $\operatorname{dist}_G(u,v)$ denotes the distance from u to v in G. However, in the paper we will use a result from [5] to compute this index. To explain the method we need some additional definitions. Let G be a graph, $u \in V(G)$ and $S \subseteq V(G)$. The *distance* of u in S, $w_S(u)$, is defined as

$$w_S(u) = \sum_{v \in S} \operatorname{dist}_G(u, v).$$

The group of automorphisms of G partitions $V(G)$ into orbits. We say that $u, v \in V(G)$ belong to the same *orbit* if there is an automorphism $\alpha \in \operatorname{Aut}(G)$ such that $\alpha(u) = v$. Let $V_1, V_2, \ldots, V_t$ be all the orbits of $\operatorname{Aut}(G)$ in G. Moreover, for every i, $1 \le i \le t$, let $v_i \in V_i$. That is, v_i's are the representatives of V_i's. It was shown in [5] that

$$\mathrm{GP}(G) = \frac{|V(G)|}{2} \sum_{i=1}^{t} w_{V_i}(v_i). \tag{1.1}$$

By (1.1), if a graph has no nontrivial automorphisms, that is if all its orbits consist of single vertices, then its Graovac-Pisanski index is 0. Hence, all graphs with no nontrivial automorphisms achieve the minimum value of Graovac-Pisanski index. More interesting is the opposite problem.

Problem 1.1. Find all graphs on n vertices with the maximum value of Graovac-Pisanski index.

This problem was solved for trees in [10]. By a long H on n vertices we denote a tree obtained from a path on $n-4$ vertices by attaching two pendent vertices to each endvertex of the path.

Theorem 1.2. *Let T be a tree on $n \geq 8$ vertices with the maximum value of Graovac-Pisanski index. Then T is either a path or a long H. Moreover,*

$$\mathrm{GP}(T) = \begin{cases} \frac{n^3-n}{8} & \text{if } n \text{ is odd,} \\ \frac{n^3}{8} & \text{if } n \text{ is even.} \end{cases}$$

For $n \leq 7$ there are also three other trees with the maximum value of Graovac-Pisanski index. However, they have the value of Graovac-Pisanski index as stated in Theorem 1.2.

In this paper we prove the following statement.

Theorem 1.3. *Let G be a unicyclic graph on n vertices with the maximum value of Graovac-Pisanski index. Then G is the n-cycle and*

$$\mathrm{GP}(C_n) = \begin{cases} \frac{n^3-n}{8} & \text{if } n \text{ is odd,} \\ \frac{n^3}{8} & \text{if } n \text{ is even.} \end{cases}$$

Observe that Graovac-Pisanski index for extremal trees and for extremal unicyclic graphs has the same value. We believe the following holds.

Conjecture 1.4. *Let G be a graph on n vertices, $n \geq 8$, with the maximum value of Graovac-Pisanski index. Then G is either a path, or a long H, or a cycle.*

To support this conjecture we performed some computer experiments. They showed the validity of the conjecture for $n = 8$ and $n = 9$. We believe that the maximal degree of extremal graphs is small (at most 3), thus for the cases $n = 10$ and $n = 11$ we limited our computer search to maximal degrees 5 and 4, respectively, and in these cases the conjecture was confirmed as well. The graphs from the conjecture are extremal also for $n \in \{5, 6, 7\}$, however when n equals 7 there exists an additional extremal graph.

2 Proof

In this section we prove several claims which imply Theorem 1.3. Obviously, if we consider graphs of order n, we do not need to consider the multiplicative term $\frac{n}{2}$ in (1.1). Therefore we define

$$\mathrm{GPa}(G) = \sum_{i=1}^{t} w_{V_i}(v_i), \tag{2.1}$$

where $V_1, V_2, \dots, V_t$ are all the orbits of $\mathrm{Aut}(G)$ in G and $v_1, v_2, \dots, v_t$ are their representatives, respectively. Then for given n, graphs on n vertices with the maximum value of GPa are the solutions of Problem 1.1.

For a cycle on n vertices, $\mathrm{GPa}(C_n) = w_V(v)$ where v is an arbitrary vertex of C_n and $V = V(C_n)$. This implies the following statement.

Proposition 2.1. *We have*

$$\mathrm{GPa}(C_n) = \begin{cases} \frac{n^2-1}{4} & \text{if } n \text{ is odd,} \\ \frac{n^2}{4} & \text{if } n \text{ is even.} \end{cases}$$

In what follows we generalize the GPa-parameter. Let $\mathcal{Z} = \{Z_1, \dots, Z_{t_\mathcal{Z}}\}$ be a partition of $V(G)$ and let $z_i \in Z_i$, $1 \le i \le t_\mathcal{Z}$. Then

$$\mathrm{GPa}^{\mathcal{Z}}(G) = \sum_{i=1}^{t_\mathcal{Z}} w_{Z_i}(z_i).$$

In our proofs, sets Z_i will usually be unions of orbits of $\mathrm{Aut}(G)$. Nevertheless, $\mathrm{GPa}^{\mathcal{Z}}(G)$ will depend on the choice of the representatives z_i.

To prove Theorem 1.3 we start with $\mathrm{GPa}(G)$, where G is an extremal unicyclic graph on n vertices different from the n-cycle. Then in a sequence of steps we modify either the graph or the partition and in each step we obtain a larger value of $\mathrm{GPa}^{\mathcal{Z}}$. Since we terminate this process with C_n and GPa, we get the result.

Hence, let G be a unicyclic graph on n vertices with the maximum value of Graovac-Pisanski index and such that G is not the n-cycle. Then G consists of a single cycle C and trees rooted at the vertices of the cycle. In what follows, orbits of vertices of C will be important.

We start with modifying the partition by merging together some orbits of vertices which have the same distance from C. We denote by $\mathcal{X}$ the new partition of $V(G)$, while the original partition into orbits is denoted by $\mathcal{V}$. Let v be a vertex of C. If $\{v\}$ is a trivial orbit of $\mathrm{Aut}(G)$, then orbits in the v-rooted tree form sets of the partition $\mathcal{X}$. But if $\{v\}$ is not a trivial orbit of $\mathrm{Aut}(G)$, we do the following. Let O_v be the orbit of $\mathrm{Aut}(G)$ containig v and let $O_v(G)$ be the set of vertices of u-rooted trees where $u \in O_v$. We partition the vertices of $O_v(G)$ according to their distance from C. Hence, O_v alone is one set of $\mathcal{X}$, another set of $\mathcal{X}$ contains those vertices of $O_v(G)$ which are adjacent to a vertex of C, etc. We have the following statement.

Lemma 2.2. *For arbitrary choice of the representatives of sets in $\mathcal{X}$ we have*

$$\mathrm{GPa}(G) \le \mathrm{GPa}^{\mathcal{X}}(G).$$

Proof. Let X_i be a set from $\mathcal{X}$ and let x_i be an abitrary vertex of X_i. Observe that X_i is a union of several orbits of $\mathrm{Aut}(G)$. Let V_0 be an orbit of $\mathrm{Aut}(G)$ such that $V_0 \subseteq X_i$. Then $w_{V_0}(u)$ is the same for every $u \in V_0$. So let v_0 be a vertex of V_0 at the shortest distance from x_i. Then both x_i and v_0 are in the same tree rooted at a vertex of C. Assume that they are in a v-rooted tree T.

Let u be a vertex of V_0. If u is not in T then $\mathrm{dist}_G(x_i, u) = \mathrm{dist}_G(v_0, u)$ since $\mathrm{dist}_G(x_i, v) = \mathrm{dist}_G(v_0, v)$. So let u be a vertex in T. Let z be a vertex on the (unique) (v_0, u)-path at the shortest distance from v. Since v_0 is a vertex of V_0 at the shortest distance from x_i, the shortest (x_i, u)-path must contain z. Thus $\mathrm{dist}_G(v_0, u) \le \mathrm{dist}_G(x_i, u)$ and so $w_{V_0}(v_0) \le w_{V_0}(x_i)$. Consequently, $\mathrm{GPa}(G) \le \mathrm{GPa}^{\mathcal{X}}(G)$ as required. □

Now we modify the graph G, and we consider a partition $\mathcal{Y}$ of the vertex set of the modified graph inherited from the partition $\mathcal{X}$ of G. So let v be a vertex of C. If $\{v\}$ is a trivial orbit of $\mathrm{Aut}(G)$ then we do not change the v-rooted tree, and its orbits form sets of the partition $\mathcal{Y}$. Hence, in this case the sets of $\mathcal{Y}$ coincide with the sets of $\mathcal{X}$ (and also with the orbits of $\mathcal{V}$). But if $\{v\}$ is not a trivial orbit of $\mathrm{Aut}(G)$ then we change the v-rooted tree. If the v-rooted tree has p vertices in G then we replace it by a path on p vertices rooted at the endvertex, which we again denote by v. Denote by F the graph which results when all these replacements are made. Since we did not change the cycle, we denote the cycle of F again by C. Let O_v be the orbit of $\mathrm{Aut}(G)$ containing v. By our assumption $|O_v| \geq 2$. Analogously as above, let $O_v(F)$ be the set of vertices of u-rooted trees where $u \in O_v$. Partition $O_v(F)$ into p disjoint sets of $\mathcal{Y}$ according to their distance from C.

Observe that for every $Y_i \in \mathcal{Y}$ and for every two vertices $y_i^1, y_i^2 \in Y_i$ we have $w_{Y_i}(y_i^1) = w_{Y_i}(y_i^2)$. Hence when computing $\mathrm{GPa}^{\mathcal{Y}}(F)$, we can choose the representatives y_i in Y_i arbitrarily. However, orbits of F may be strictly larger than the sets Y_i. This is caused by the fact that two non-isomorphic rooted trees may have the same numbers of vertices. Our next statement follows.

Lemma 2.3. *For arbitrary choice of representatives of sets in $\mathcal{Y}$ we have*

$$\mathrm{GPa}^{\mathcal{X}}(G) \leq \mathrm{GPa}^{\mathcal{Y}}(F).$$

Proof. Let H be a graph. A ray in H is a subgraph of H which is isomorphic to a path, its first vertex has degree at least 3 in H, its last vertex has degree 1 in H and all the other vertices have degree 2 in H.

We do not prove the inequality directly. Instead, we construct a sequence of graphs $G = G^0, G^1, \dots, G^q = F$, each G^i with a partition $\mathcal{X}^i$, such that

$$\mathrm{GPa}^{\mathcal{X}^i}(G^i) \leq \mathrm{GPa}^{\mathcal{X}^{i+i}}(G^{i+1})$$

for a special choice of representatives in $\mathcal{X}^{i+1}$, where $0 \leq i \leq q-1$, $\mathcal{X}^0 = \mathcal{X}$ and $\mathcal{X}^q = \mathcal{Y}$. We remark that for every i, G^i will be a unicyclic graph with the cycle C such that if $O = \{v_1, \dots, v_t\}$ is an orbit of vertices of C in G, then all v_j-rooted trees in G^i are mutually isomorphic, $1 \leq j \leq t$. If $t = 1$ then the v_1-rooted trees in $G, G^1, \dots, F$ are mutually isomorphic and all $\mathcal{X}, \mathcal{X}^1, \dots, \mathcal{Y}$ coincide on the vertex sets of these trees. However if $t \geq 2$, then the vertex set $O_{v_1}(G^i)$ of the v_j-rooted trees, $1 \leq j \leq t$, is partitioned in $\mathcal{X}^i$ according to the distance from C, and we assume that all the representatives of these sets are in the v_1-rooted tree. This assupmtion is possible since O is an orbit in G, and although O does not need to be an orbit of G^i, the vertices of O are nicely distributed along the cycle C in G^i.

So consider i, $0 \leq i < q$. We assume that G^i is already known and we construct G^{i+1}. For this, let $O = \{v_1, \dots, v_t\}$ be an orbit of vertices of C in G, where $t \geq 2$. If the v_1-rooted tree (and so also v_j-rooted trees for $2 \leq j \leq t$) is a path rooted at the endvertex, then we are done with this orbit of G. So suppose that the v_1-rooted tree has at least two endvertices different from v_1, and consequently, at least two distinct rays starting at a common vertex. Let R_1 and R_2 be two rays starting at a vertex c such that $\mathrm{dist}_{G^i}(v_1, c)$ is maximum possible. We assume that R_1 is not shorter than R_2. If there is a representative x_j^i of X_j^i which is in R_2, then replace it by a vertex of X_j^i in R_1. Observe that this replacement does not change $\mathrm{GPa}^{\mathcal{X}^i}(G^i)$. Now delete R_2 from the v_1-rooted tree and attach it to the second vertex of R_1. Moreover, repeat the same procedure in all the other v_j-rooted trees, $2 \leq j \leq t$, and denote by G^{i+1} the resulting graph. Denote by T^i and T^{i+1} the v_1-rooted tree in G^i and G^{i+1}, respectively. If R_1 and R_2 have the same length, then this operation may create a new set in $\mathcal{X}^{i+1}$, because T^i may have smaller depth than T^{i+1}. (As is the custom, by depth we denote the largest distance from the root.) In such a case choose a representative of this new set in R_2. This is the unique case when a representative will be in R_2 in T^{i+1}.

Let $d = \mathrm{dist}_{G^i}(v_1, c)$ and let ℓ be the length of R_2. Assume that the indices of sets in $\mathcal{X}^i$ and $\mathcal{X}^{i+1}$ are chosen so that X_j^{i+1} in G^{i+1} was obtained from X_j^i in G^i and the representatives of X_j^i and X_j^{i+1} coincide whenever possible. Then $w_{X_j^i}(x_j^i)$ in G^i may differ from $w_{X_j^{i+1}}(x_j^{i+1})$ in G^{i+1} only if X_j^{i+1} contains vertices of v_k-rooted trees, $1 \leq k \leq t$, which are at distance $d+1, d+2, \dots, d+\ell+1$ from C. We distinguish three cases.

Case 1: X_j^{i+1} *contains vertices at distance* $d+1$ *from* C. Then in the v_1-rooted tree, X_j^{i+1} is smaller than X_j^i by exactly one vertex. Consequently $|X_j^i| - |X_j^{i+1}| = t$. Comparing to $\mathrm{GPa}^{\mathcal{X}^i}(G^i)$, $\mathrm{GPa}^{\mathcal{X}^{i+1}}(G^{i+1})$ is decreased by 2 due to a missing vertex in T^{i+1} and it is decreased by $(t-1)2(d+1)+c$ due to missing vertices in v_k-rooted trees $2 \leq k \leq t$. Here c represents the distances using the edges of C, that is $c = \sum_{k=2}^{t} \mathrm{dist}_G(v_1, v_k)$. Hence,

$$w_{X_j^{i+1}}(x_j^{i+1}) - w_{X_j^i}(x_j^i) = -2 - (t-1)2(d+1) - c. \tag{2.2}$$

Case 2: X_j^{i+1} *contains vertices at distance* $d+a$ *from* C, *where* $2 \leq a \leq \ell$. Then $|X_j^{i+1}| = |X_j^i|$ and comparing to $\mathrm{GPa}^{\mathcal{X}^i}(G^i)$, $\mathrm{GPa}^{\mathcal{X}^{i+1}}(G^{i+1})$, is decreased by 2 due to a shorter distance to a vertex of X_j^{i+1} in R_2. Hence,

$$w_{X_j^{i+1}}(x_j^{i+1}) - w_{X_j^i}(x_j^i) = -2. \tag{2.3}$$

Case 3: X_j^{i+1} *contains vertices at distance* $d+\ell+1$ *from* C. Then in the v_1-rooted tree, X_j^{i+1} is larger than X_j^i by exactly one vertex. Consequently $|X_j^{i+1}| - |X_j^i| = t$. Comparing to $\mathrm{GPa}^{\mathcal{X}^i}(G^i)$, $\mathrm{GPa}^{\mathcal{X}^{i+1}}(G^{i+1})$ is increased by $(t-1)2(d+\ell+1)+c$ due to new vertices in v_k-rooted trees, $2 \leq k \leq t$. Here c is the very same constant as in Case 1, that is $c = \sum_{k=2}^{t} \mathrm{dist}_G(v_1, v_k)$. In some cases, namely if X_j^i is not empty, $\mathrm{GPa}^{\mathcal{X}^i}$ is increased by at least 2 due to a new vertex in T^{i+1}, but we do not need to consider this contribution in our calculations. Hence,

$$w_{X_j^{i+1}}(x_j^{i+1}) - w_{X_j^i}(x_j^i) \geq (t-1)2(d+\ell+1) + c. \tag{2.4}$$

Since $w_{X_j^{i+1}}(x_j^{i+1}) = w_{X_j^i}(x_j^i)$ when $X_j^i \not\subseteq O_{v_i}(G^i)$, summing the expressions (2.2), (2.3) and (2.4) we get

$$\begin{aligned}\mathrm{GPa}^{\mathcal{X}^{i+1}}(G^{i+1}) - \mathrm{GPa}^{\mathcal{X}^i}(G^i) &\geq \big(-2 - (t-1)2(d+1) - c\big) - (\ell-1)2 \\ &\quad + \big((t-1)2(d+\ell+1) + c\big) \\ &= (t-2)2\ell \geq 0\end{aligned}$$

since $t \geq 2$. □

Let $Y_i \in \mathcal{Y}$. Observe that if $Y_i \cap V(C) \neq \emptyset$, then $Y_i \subseteq V(C)$. Let $\mathcal{Y}'$ be those sets of $\mathcal{Y}$ which contain vertices of $V(C)$. We define a new partition $\mathcal{Z}$ of F as follows:

$$\mathcal{Z} = \mathcal{Y} \setminus \mathcal{Y}' \cup V(C).$$

That is, we merge together all sets Y_i containing vertices of $V(C)$. All the other sets of $\mathcal{Z}$ coincide with the sets of $\mathcal{Y}$. We have the following statement.

Lemma 2.4. *For arbitrary choice of representatives of sets in $\mathcal{Z}$ we have*

$$\mathrm{GPa}^{\mathcal{Y}}(F) \le \mathrm{GPa}^{\mathcal{Z}}(F).$$

Proof. Observe that there are three types of sets in $\mathcal{Z}$. First, if $v_1 \in V(C)$ is a trivial orbit in G, then orbits of vertices of the v_1-rooted tree are sets of $\mathcal{Z}$. Second, if $\{v_1, \dots, v_t\} \subseteq V(C)$ is a non-trivial orbit in G, that is if $t \ge 2$, then the v_i-rooted trees are paths with endvertices v_i, and sets of vertices of $O_{v_1}(F)$ in $\mathcal{Z}$ contain vertices of these t rooted trees which are at the same distance from C. Finally, $\mathcal{Z}$ contains $V(C)$. If Z_i is a set of $\mathcal{Z}$ of the first type or of the second type and $u, v \in Z_i$, then $w_{Z_i}(u) = w_{Z_i}(v)$. Hence, to prove the statement it suffices to show that

$$\sum_{Y_i \in \mathcal{Y}'} w_{Y_i}(y_i) \le w_{V(C)}(z) = \sum_{Y_i \in \mathcal{Y}'} w_{Y_i}(z)$$

where z is an arbitrary vertex of $V(C)$ and $\mathcal{Y}'$ is defined before Lemma 2.4. (Recall that y_i is a representative of Y_i in $\mathcal{Y}$.)

Thus, let $z \in V(C)$ and let $Y_i \in \mathcal{Y}'$. In what follows we show that $w_{Y_i}(y_i) \le w_{Y_i}(z)$. We distinguish four cases.

Case 1: $|Y_i| = 1$. Since $w_{Y_i}(y_i) = 0 \le \mathrm{dist}_F(z, y_i) = w_{Y_i}(z)$, we have $w_{Y_i}(y_i) \le w_{Y_i}(z)$.

Case 2: $|Y_i| = 2$. let $Y_i = \{y_i, y\}$. Then by triangle inequality

$$w_{Y_i}(y_i) = \mathrm{dist}_F(y_i, y) \le \mathrm{dist}_F(z, y_i) + \mathrm{dist}_F(z, y) = w_{Y_i}(z).$$

Hence, in the sequel we assume that $|Y_i| \ge 3$. Since Y_i is an orbit of vertices of C in G, there is a nontrivial rotational automorphism α in $\mathrm{Aut}(G)$ such that $\{\alpha^k(y_i) \mid k \in \mathbb{N}\} \subseteq Y_i$. Let r be the biggest order of a rotational automorphism of this type and let α be the corresponding automorphism. Observe that $r \ge 2$. Since $w_{Y_i}(u) = w_{Y_i}(v)$ for $u, v \in Y_i$, we assume that y_i is chosen so that $\mathrm{dist}_F(z, y_i)$ is smallest possible.

Case 3: *r is even.* Let $Y_i' = \{\alpha^k(y_i) \mid 0 \le k < r\}$. We rename vertices of Y_i' as $\{y^0, y^1, \dots, y^{r-1}\}$ so that $\mathrm{dist}_F(y_i, y^k) \le \mathrm{dist}_F(y_i, y^{k+1})$ whenever $0 \le k < r-1$. Observe that $y^0 = y_i$, the vertices $y^{2\ell-1}$ and $y^{2\ell}$ have the same distance from y_i if $1 \le \ell < r/2$ and y^{r-1} is the unique vertex of Y_i' with the largest distance from y_i. Since y_i is the vertex of Y_i with the smallest distance from z, we have

$$\mathrm{dist}_F(y^{2\ell-1}, y_i) + \mathrm{dist}_F(y_i, y^{2\ell}) = \mathrm{dist}_F(y^{2\ell-1}, z) + \mathrm{dist}_F(z, y^{2\ell})$$

for $1 \le \ell < r/2$ and also

$$\mathrm{dist}_F(y_i, y^{r-1}) = \mathrm{dist}_F(y_i, z) + \mathrm{dist}_F(z, y^{r-1}) = \tfrac{1}{2}|V(C)|.$$

Hence, $w_{Y_i'}(y_i) = w_{Y_i'}(z)$. If $Y_i = Y_i'$, we are done. Therefore, in the sequel assume that there is also a reflexion β such that $\beta(Y_i') \subseteq Y_i$ and $\beta(Y_i') \cap Y_i' = \emptyset$. Then $Y_i = Y_i' \cup \beta(Y_i')$ and $|Y_i| = 2r$. Observe that all the vertices of $\beta(Y_i')$ are obtained from arbitrary one of them using α. Thus, let y_i^β be a vertex of $\beta(Y_i')$ with the smallest distance from y_i. Then using the same arguments as above we get

$$w_{\beta(Y_i')}(y_i^\beta) = w_{\beta(Y_i')}(y_i).$$

Since $w_{\beta(Y_i')}(y_i^\beta) = w_{Y_i'}(y_i)$, we get

$$w_{Y_i}(y_i) = 2w_{Y_i'}(y_i).$$

Analogously, if $y_i^{\beta z}$ is a vertex of $\beta(Y_i')$ at the smallest distance from z, we get

$$w_{\beta(Y_i')}(y_i^{\beta z}) = w_{\beta(Y_i')}(z).$$

Since $w_{\beta(Y_i')}(y_i^{\beta z}) = w_{Y_i'}(y_i)$, we obtain $w_{Y_i}(y_i) = w_{Y_i}(z)$.

Case 4: *r is odd.* Let $Y_i' = \{\alpha^k(y_i) \mid 0 \leq k < r\}$. Then proceeding analogously as in Case 3 one gets

$$w_{Y_i'}(z) = w_{Y_i'}(y_i) + \mathrm{dist}_F(y_i, z),$$

and so $w_{Y_i}(y_i) \leq w_{Y_i}(z)$ if $Y_i = Y_i'$. Hence, assume that there is a reflexion β such that $\beta(Y_i') \subseteq Y_i$ and $\beta(Y_i') \cap Y_i' = \emptyset$. Again, $Y_i = Y_i' \cup \beta(Y_i')$ and $|Y_i| = 2r$, and all the vertices of $\beta(Y_i')$ are obtained from arbitrary one of them using α. Thus, let y_i^β be a vertex of $\beta(Y_i')$ with the shortest distance from y_i. Then analogously as in Case 3 one gets

$$w_{Y_i'}(y_i) = w_{\beta(Y_i')}(y_i^\beta) = w_{\beta(Y_i')}(y_i) - \mathrm{dist}_F(y_i^\beta, y_i)$$

and so

$$w_{Y_i}(y_i) = 2w_{Y_i'}(y_i) + \mathrm{dist}_F(y_i^\beta, y_i).$$

Also, let $y_i^{\beta z}$ be a vertex of $\beta(Y_i')$ with the shortest distance from z. Then analogously as above we get

$$w_{Y_i'}(y_i) = w_{\beta(Y_i')}(y_i^{\beta z}) = w_{\beta(Y_i')}(z) - \mathrm{dist}_F(y_i^{\beta z}, z)$$

and so

$$w_{Y_i}(z) = 2w_{Y_i'}(y_i) + \mathrm{dist}_F(y_i^{\beta z}, z) + \mathrm{dist}_F(y_i, z).$$

Since

$$\mathrm{dist}_F(y_i^\beta, y_i) \leq \mathrm{dist}_F(y_i^{\beta z}, y_i) \leq \mathrm{dist}_F(y_i^{\beta z}, z) + \mathrm{dist}_F(y_i, z),$$

we get $w_{Y_i}(y_i) \leq w_{Y_i}(z)$. □

Finally, we are in a position to prove the last lemma which implies Theorem 1.3. Observe that there is a strict inequality in Lemma 2.5.

Lemma 2.5. *We have*

$$\mathrm{GPa}^{\mathcal{Z}}(F) < \mathrm{GPa}(C_n).$$

Proof. Analogously as in Lemma 2.3, we prove the statement by a sequence of steps. Let $O^1, \ldots, O^q$ be all orbits of vertices of C in G, such that for every $v \in O^i$ the v-rooted tree is nontrivial (i.e., it has more than one vertex). Observe that if the v-rooted tree is nontrivial in G, then the v-rooted tree in F is also nontrivial. Assume that $|O^1| \geq |O^2| \geq \cdots \geq |O^q|$.

We consecutively create unicyclic graphs $F = F^0, F^1, \dots, F^q = C_n$ with partitions $\mathcal{Z} = \mathcal{Z}^0, \mathcal{Z}^1, \dots, \mathcal{Z}^q$, respectively, and for every i, $0 \le i < q$, we show that $\mathrm{GPa}^{\mathcal{Z}^i}(F^i) < \mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$. The graph F^{i+1} is obtained from F^i by moving the vertices of v-rooted trees, where $v \in O^{i+1}$, into the unique cycle C^i of F^i. Now we describe the process in detail.

Choose i, $0 \le i < q$. For $v \in O^{i+1}$, let $p+1$ be the number of vertices of v-rooted tree in F^i (or in G, since the numbers of vertices of v-rooted trees in G and F are the same). By our assumption $p \ge 1$. Orient the cycle C^i of F^i and for every vertex $u \in V(C^i)$ let u^f be the vertex following u on C^i. Let $v \in O^{i+1}$. Delete the p non-root vertices of the v-rooted tree from F^i and subdivide the edge vv^f exactly p times. Repeat this procedure for all vertices of O^{i+1} and denote by F^{i+1} the resulting unicyclic graph. The partition $\mathcal{Z}^{i+1}$ is exactly the same as $\mathcal{Z}^i$, the only exception is that instead of the set $V(C^i)$ and various sets partitioning $O_v(F^i)$ for $v \in O^{i+1}$ we have just the set $V(C^{i+1})$ in $\mathcal{Z}^{i+1}$. We assume that if a set of $\mathcal{Z}^i$ is identical with a set of $\mathcal{Z}^{i+1}$, then they have the same representatives.

Let $Z' \in \mathcal{Z}^i$ and $Z^* \in \mathcal{Z}^{i+1}$ such that $Z' = Z^*$. Then Z' is a collection of vertices of $O_u(F^i)$, i.e., of u-rooted trees for $u \in O^j$, where $j > i+1$. Since the distances between these vertices cannot be shorter in F^{i+1} than in F^i (they can be only larger due to the extension of C^i to C^{i+1}), we have $w_{Z'}(z') \le w_{Z^*}(z^*)$ where z' is a representative of Z' in F^i and z^* is a representative of Z^* in F^{i+1}. Hence, it suffices to check the contribution of $V(C^{i+1})$ in $\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$ and in $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ the contribution of $V(C^i)$ and of the sets of non-root vertices of v-rooted trees for $v \in O^{i+1}$. Let $t = |O^{i+1}|$. Analogously as in the proof of Lemma 2.4 we distinguish four cases. In these cases, we set $c = |V(C^i)|$. Moreover, by δ_a we denote the parity of a. That is $\delta_a = 1$ if a is odd and $\delta_a = 0$ if a is even.

Case 1: $t = 1$. By Proposition 2.1, $V(C^i)$ contributes $\frac{1}{4}(c^2 - \delta_c)$ to $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ and $V(C^{i+1})$ contributes $\frac{1}{4}((c+p)^2 - \delta_{c+p})$ to $\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$. Let $O^{i+1} = \{v_1\}$. Denote by T the v_1-rooted tree in F^i. Since T is a tree on $p+1$ vertices, the orbits of T contribute to $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ at most $\frac{1}{4}((p+1)^2 - \delta_{p+1})$ by Theorem 1.2. So

$$\begin{aligned}4\big(\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i)\big) &\ge (c+p)^2 - \delta_{c+p} - c^2 + \delta_c - (p+1)^2 + \delta_{p+1}\\ &\ge (c+p)^2 - c^2 - (p+1)^2 - 1\\ &= 2p(c-1) - 2 > 0\end{aligned}$$

since $c \ge 3$ and $p \ge 1$.

Case 2: $t = 2$. In this case the v-rooted trees are paths whenever $v \in O^{i+1}$. Since the contribution to $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ of j-th vertices of these paths (i.e., of vertices at distance j from the roots) is at most $j + c/2 + j$, the total contribution of non-root vertices of v-rooted trees, $v \in O^{i+1}$, is at most $2\binom{p+1}{2} + \frac{1}{2}cp$. Since the contribution of $V(C^i)$ is $\frac{1}{4}(c^2 - \delta_c)$ and the contribution of $V(C^{i+1})$ is $\frac{1}{4}((c+2p)^2 - \delta_{c+2p})$, where $\delta_{c+2p} = \delta_c$, we get

$$\begin{aligned}4\big(\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i)\big) &\ge (c+2p)^2 - \delta_c - c^2 + \delta_c - 8\tbinom{p+1}{2} - 2cp\\ &\ge (c+2p)^2 - c^2 - 4p^2 - 4p - 2cp\\ &= 2p(c-2) > 0\end{aligned}$$

since $c \ge 3$ and $p \ge 1$.

In the remaining cases we may assume that there is a nontrivial rotational automorphism α of F^i such that when $v \in O^{i+1}$ then also $\alpha(v) \in O^{i+1}$. Let r be the biggest order of such a rotational automorphism α, and moreover, let α be such that the distance s between v and $\alpha(v)$ is the smallest possible. Then $c = r \cdot s$.

Case 3: *r is even.* Then $r \geq 2$. Let $v_0 \in O^{i+1}$. Denote $O' = \{\alpha^k(v_0) \mid 0 \leq k < r\}$. First assume that $|O^{i+1}| = 2r$. Hence there is also a reflexion β such that $\beta(O') \subseteq O^{i+1}$ and $\beta(O') \cap O' = \emptyset$. Let $v_1 \in O^{i+1}$ such that the distance t between v_0 and v_1 is the smallest possible. Then $t \leq s/2$ and $v_1 \in \beta(O')$. Observe that now $t \geq 1$ and $s \geq 2$. Since $c = rs$ is even, the contribution of $V(C^i)$ to $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ is $\frac{1}{4}r^2s^2$. The contribution of $V(C^{i+1})$ to $\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$ is $\frac{1}{4}r^2(s+2p)^2$. Now we calculate the contribution of non-root vertices of v-rooted trees when $v \in O^{i+1}$. These trees are paths and the contribution of j-th vertices is

$$\begin{aligned}
&2(s+2j) + 2(2s+2j) + \cdots + 2\big((\tfrac{r}{2}-1)s+2j\big) + (\tfrac{r}{2}s+2j)\\
&\quad + (t+2j) + (s+t+2j) + \cdots + \big((\tfrac{r}{2}-1)s+t+2j\big) + (s-t+2j)\\
&\quad + (2s-t+2j) + \cdots + \big((\tfrac{r}{2}-1)s-t+2j\big) + (\tfrac{r}{2}s-t+2j)\\
&\qquad = 4(s+2j) + 4(2s+2j) + \cdots + 4\big((\tfrac{r}{2}-1)s+2j\big) + 2(\tfrac{r}{2}s+2j) + 2j\\
&\qquad = \tfrac{1}{2}r^2s + 2j(2r-1).
\end{aligned}$$

So the contribution of non-root vertices of v-rooted trees, $v \in O^{i+1}$, is

$$\sum_{j=1}^{p}\Big(\tfrac{1}{2}r^2s + 2j(2r-1)\Big) = \tfrac{1}{2}r^2sp + (p^2+p)(2r-1).$$

Hence

$$\begin{aligned}
\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i) &\geq \tfrac{1}{4}r^2s^2 + r^2sp + r^2p^2 - \tfrac{1}{4}r^2s^2\\
&\qquad - \tfrac{1}{2}r^2sp - 2rp^2 - 2rp + p^2 + p\\
&= p^2(r-1)^2 + p\big(r(\tfrac{1}{2}rs-2)+1\big) > 0
\end{aligned}$$

since $r \geq 2$, $s \geq 2$ and $p \geq 1$.

In the case when $|O^{i+1}| = r$, the contribution of $V(C^{i+1})$ is $\frac{1}{4}r^2(s+p)^2$ and the contribution of j-th vertices in v-rooted trees, $v \in O^{i+1}$, is

$$2(s+2j) + 2(2s+2j) + \cdots + 2\big((\tfrac{r}{2}-1)s+2j\big) + (\tfrac{r}{2}s+2j) = \tfrac{1}{4}r^2s + 2j(r-1).$$

So the contribution of non-root vertices of v-rooted trees, $v \in O^{i+1}$, is

$$\sum_{j=1}^{p}\Big(\tfrac{1}{4}r^2s + 2j(r-1)\Big) = \tfrac{1}{4}r^2sp + (p^2+p)(r-1).$$

Hence

$$\begin{aligned}
\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i) &\geq \tfrac{1}{4}r^2s^2 + \tfrac{1}{2}r^2sp + \tfrac{1}{4}r^2p^2 - \tfrac{1}{4}r^2s^2\\
&\qquad - \tfrac{1}{4}r^2sp - rp^2 - rp + p^2 + p\\
&= p^2(\tfrac{r}{2}-1)^2 + p\big(r(\tfrac{1}{4}rs-1)+1\big) > 0
\end{aligned}$$

since in this case $r \geq 4$, $s \geq 1$ and $p \geq 1$.

Case 4: *r is odd.* Then $r \geq 3$. Let $v_0 \in O^{i+1}$ and $O' = \{\alpha^k(v_0) \mid 0 \leq k < r\}$. First assume that $|O^{i+1}| = 2r$. Hence there is also a reflexion β such that $\beta(O') \subseteq O^{i+1}$ and $\beta(O') \cap O' = \emptyset$. Let $v_1 \in O^{i+1}$ such that the distance t between v_0 and v_1 is the smallest possible. Then $t \leq s/2$ and $v_1 \in \beta(O')$. The contribution of $V(C^i)$ to $\mathrm{GPa}^{\mathcal{Z}^i}(F^i)$ is $\frac{1}{4}(r^2s^2 - \delta_{rs})$. The contribution of $V(C^{i+1})$ to $\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$ is $\frac{1}{4}\big(r^2(s+2p)^2 - \delta_{r(s+2p)}\big)$. Now we calculate the contribution of non-root vertices of v-rooted trees when $v \in O^{i+1}$. These trees are paths and the contribution of j-th vertices is

$$\begin{aligned}
&2(s+2j) + 2(2s+2j) + \cdots + 2(\tfrac{r-1}{2}s+2j) \\
&\quad + (t+2j) + (s+t+2j) + \cdots + (\tfrac{r-1}{2}s+t+2j) \\
&\quad + (s-t+2j) + (2s-t+2j) + \cdots + (\tfrac{r-1}{2}s-t+2j) \\
&\qquad = 4(s+2j) + 4(2s+2j) + \cdots + 4(\tfrac{r-1}{2}s+2j) + (t+2j) \\
&\qquad = \tfrac{1}{2}(r^2-1)s + 2j(2r-1) + t.
\end{aligned}$$

So the contribution of non-root vertices of v-rooted trees, $v \in O^{i+1}$, is

$$\begin{aligned}
\sum_{j=1}^{p}\Big(\tfrac{1}{2}(r^2-1)s + 2j(2r-1) + t\Big) &= \tfrac{1}{2}(r^2-1)sp + (p^2+p)(2r-1) + pt \\
&\leq \tfrac{1}{2}r^2sp + (p^2+p)(2r-1)
\end{aligned}$$

since $-\frac{1}{2}sp + pt \leq 0$. Hence

$$\begin{aligned}
\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i) &\geq \tfrac{1}{4}r^2s^2 + r^2sp + r^2p^2 - \tfrac{1}{4}\delta_{rs} - \tfrac{1}{4}r^2s^2 + \tfrac{1}{4}\delta_{rs} \\
&\quad - \tfrac{1}{2}r^2sp - 2rp^2 - 2rp + p^2 + p \\
&= p^2(r-1)^2 + p\big(r(\tfrac{1}{2}rs-2)+1\big) > 0
\end{aligned}$$

since $r \geq 3$, $s \geq 2$ and $p \geq 1$.

In the case when $|O^{i+1}| = r$, the contribution of $V(C^{i+1})$ to $\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1})$ is $\frac{1}{4}\big(r^2(s+p)^2 - \delta_{r(s+p)}\big)$ and the contribution of j-th vertices in v-rooted trees, $v \in O^{i+1}$, is

$$2(s+2j) + 2(2s+2j) + \cdots + 2(\tfrac{r-1}{2}s+2j) = \tfrac{1}{4}(r^2-1)s + 2j(r-1).$$

So the contribution of non-root vertices of v-rooted trees, $v \in O^{i+1}$, is

$$\sum_{j=1}^{p}\Big(\tfrac{1}{4}(r^2-1)s + 2j(r-1)\Big) = \tfrac{1}{4}(r^2-1)sp + (p^2+p)(r-1).$$

Hence

$$\begin{aligned}
\mathrm{GPa}^{\mathcal{Z}^{i+1}}(F^{i+1}) - \mathrm{GPa}^{\mathcal{Z}^i}(F^i) &\geq \tfrac{1}{4}r^2s^2 + \tfrac{1}{2}r^2sp + \tfrac{1}{4}r^2p^2 - \tfrac{1}{4} - \tfrac{1}{4}r^2s^2 \\
&\quad - \tfrac{1}{4}(r^2-1)sp - rp^2 - rp + p^2 + p \\
&= p^2(\tfrac{r}{2}-1)^2 + p\big(r(\tfrac{1}{4}rs-1) + \tfrac{1}{4}s + 1\big) - \tfrac{1}{4} > 0
\end{aligned}$$

since in this case $r \geq 3$, $s \geq 1$ and $p \geq 1$. (Observe that the second bracket is at least $\frac{2}{4}$ if $r = 3$ and $s = 1$.) □

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