Symmetry groups and Graovac−Pisanski index of some linear polymers

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Abstract. Suppose G is a graph with vertex set $V(G)$. The Graovac–Pisanski index of G is defined as $GP(G) = \frac{1}{2}|V(G)|^2\delta(G)$, where

$$\delta(G) = \frac{1}{|\Gamma||V(G)|}\sum_{u\in V(G)}\sum_{g\in\Gamma} d(u, g(u)).$$

This is a type of graph invariant that is combined distance and symmetry of molecules under consideration. The aim of this paper is to compute the symmetry groups and Graovac–Pisanski index of some linear polymers.

1. Introduction

Throughout this paper all graphs will be assumed to be simple and undirected. This means that they don't have loops, multiple and directed edges. Suppose G is such a graph with vertex set $V(G)$ and edge set $E(G)$. An edge $e \in E(G)$ will be written as $e = xy$, where $x, y \in V(G)$. A graph G is called *r-regular* if degrees of all vertices are equal to r.

The *molecular graph* of a molecule M is a simple graph in which atoms and chemical bonds are in one-to-one correspondences with vertices and edges, respectively. A *path* P_n is a sequence $x_1, x_2, \ldots, x_n$ of different vertices in which x_i and x_{i+1}, $1 \leqslant i \leqslant n-1$, are adjacent. The number of edges in a path is called its length. A *cycle graph* C_n is a graph constructed from the path P_n by adding a new edge x_1x_n. The *complete graph* K_n is an $n-$vertex graph in which all pairs of different vertices are adjacent. A graph G is *connected* if for each vertex x, y in G, there exists a path connecting them.

A *permutation* on a set X is a one-to-one function from X onto X. The set of all permutations on a set X is denoted by S_X. It is well-known that S_X is a group under composition of functions. The order of an element x in a group G is denoted by $O(x)$. An element $\theta \in S_{V(G)}$ is said to be an *automorphism* if the following condition is satisfied:

$$\forall x, y \in V(G) \;\; xy \in E(G) \Longleftrightarrow \theta(x)\theta(y) \in E(G).$$

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The set of all automorphisms of G is denoted by $Aut(G)$ which is a group under composition of functions. It is easy to see that $Aut(G)$ is a subgroup of $S_{V(G)}$. The graph G is called *vertex-transitive* if and only if for each $x, y \in V(G)$ there exists an automorphism $g \in Aut(G)$ such that $g(x) = y$. It is easy to see that vertex-transitive graphs are regular. We refer the interested readers to the famous book of Biggs [3], for more information on this topic.

Suppose G is a group containing two subgroups H and K in such a way that $H \trianglelefteq G$, $|H \cap K| = 1$ and $G = HK = \{xy \mid x \in H,\ y \in K\}$. Then we say that G is a *semi-direct product* of H by K and write $G = H : K$. For an example, we consider the set of all permutations on $X = \{1, 2, 3\}$, i.e., $S_X = \{(), (1, 2, 3), (1, 3, 2), (1, 2), (1, 3), (2, 3)\}$, where $()$ is the identity permutation. Then by choosing $H = \{(), (1, 2, 3), (1, 3, 2)\}$ and $K = \{(), (1, 2)\}$, we can see that $H \trianglelefteq S_X$, $K \leqslant S_X$, $|H \cap K| = 1$ and $S_X = HK$. Hence, S_X can be written as the semi-direct product $H : K$ of its subgroups.

Suppose G is a graph and $x, y \in V(G)$. The length of a minimum path connecting x and y is denoted by $d(x, y)$. It is easy to see that $(V(G), d)$ is a metric space with distance function $d(-, -)$. If G is connected then the *Wiener index* $W(G)$ is defined as the sum of distances between all pairs of vertices in G [18].

Graovac and Pisanski [8] in an innovating work applied the symmetry group of the graph under consideration to generalize the Wiener index and obtain a good correlation with some physico-chemical properties of molecules. To explain, we assume that G is a graph, $\Gamma \leqslant Aut(G)$ and $g \in \Gamma$. Define the *distance number* of g, $\delta(g)$, to be the average of $d(u, g(u))$ overall vertices $u \in V(G)$ and $\delta(G) = \frac{1}{|\Gamma|}\sum_{g\in G}\delta(g) = \frac{1}{|\Gamma||V(G)|}\sum_{u\in V(G)}\sum_{g\in\Gamma} d(u, g(u))$. The *Graovac–Pisanski index* (GP index for short) of G with respect to Γ, $GP_\Gamma(G)$, is defined as $GP_\Gamma(G) = \frac{|V(G)|^2}{2|\Gamma|}\sum_{g\in\Gamma}\delta(g)$. If $\Gamma = Aut(G)$ then we write $GP(G)$ as $GP_\Gamma(G)$. It is easy to see that the GP index of G can be computed by $GP(G) = \frac{1}{2}|V(G)|^2\delta(G)$. Ashrafi and Shabani [2] computed the GP index of graphs that can be represented as some graph operations and in [12], some upper and lower bounds for this graph invariant are presented. In 2016, Ghorbani and Klavžar [7] computed this topological index by cut method and Tratnik [17] generalized their method and calculated the closed formulas for the GP index of zig-zag tubulenes. In [13], the GP index of the cycle C_n with respect to all subgroups of $Aut(C_n)$ and the GP index of $(3, 6)-$ and $(5, 6)-$fullerene graphs with respect to a subgroup of their symmetry groups are computed. Finally in [15], the Graovac-Pisanski polynomial of a graph was presented by which the authors extended some well-known results from Hosoya polynomial to its symmetry-based version. In the mentioned paper, this polynomial for some classes of chemical graphs containing linear phenylene and its hexagonal squeeze, and the ortho-, meta- and para-polyphenylene chains were calculated.

Phenylenes are polycyclic conjugated molecules possessing both six- and four-membered rings [9]. Following Došlić and Litz [5], a polymer with phenylene as the basic building block is called a polyphenylene. In the mentioned paper, some exact formulas for the numbers of matchings and independent sets in three types of uniform chains are given. The authors also presented some results on polyphenylene dendrimers. In this paper, the GP index of the molecular graphs presented in [6, 9] are computed. Our calculations are done with the aid of TopoCluj [4], HyperChem [11] and GAP [16]. Our group theory notations are standard and can be taken mainly from [1, 10, 14, 16].

2. Main result

The aim of this section is to compute the symmetry groups, their orbits and GP index of the para chain of length n, $3-$uniform cactus chain, caterpilar $CAT(n_1, \ldots, n_r)$, corona product $P_n \circ P_2$, an ortho-chain of length n, ladder graph L_n and the $2-$connected linear polymer with triangular faces R_n. These graphs will be defined later. We start by computing the GP index of a para chain of length n, Figure 1.

Suppose G is a group and X is a set. An action of G on X is a function $\star : G \times X \longrightarrow X$ such that for all $g, h \in G$ and $x \in X$, $e \star x = x$ and $(gh) \star x = g \star (h \star x)$. The orbit of an element $x \in X$ is defined as $G \star x = \{g \star x \mid g \in G\}$. We usually write gx as $g \star x$ when there is no confusion. The size of an orbit is called its length.

Let G be a connected graph, $A \cup B \subseteq V(G)$ and $V_1, V_2, \ldots, V_r$ be the orbits of $Aut(G)$ under its natural action on $V(G)$. Define $d(A, B) = \sum_{u \in A} \sum_{v \in B} d(u, v)$. Then it can easily seen that $W(G) = \frac{1}{2} d(V, V)$. Graovac and Pisanski [8], proved that $GP(G) = |V| \sum_{i=1}^{r} \frac{W(V_i)}{|V_i|}$, where $W(V_i) = \frac{1}{2} d(V_i, V_i)$. We apply this result to compute the GP index of all polymers presented in this paper.

Theorem 2.1. *The Graovac-Pisanski index of a para chain Q_n of length n can be computed as follows:*

$$GP(Q_n) = \begin{cases} \frac{9}{4}n^3 + \frac{15}{4}n^2 + \frac{7}{4}n + \frac{1}{4} & n \text{ is odd and } n \neq 1, \\ \frac{9}{4}n^3 + \frac{15}{4}n^2 + n & n \text{ is even.} \end{cases}$$

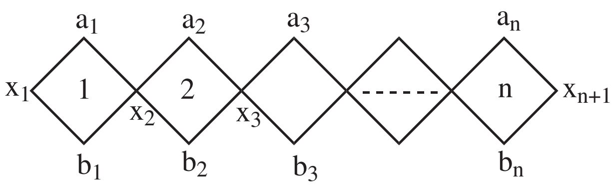

Figure 1: A para chain of length n.

Proof. The case of $n = 1$ is clear. Suppose $n > 1$ is even and consider the subset $X = \{x_1, x_2, \dots, x_{n+1}\} \subseteq V(Q_n)$, see Figure 1. It is easy to see that for each automorphism α, $\alpha(\{x_1, x_{n+1}\}) = \{x_1, x_{n+1}\}$. Hence $(\alpha(x_1) = x_1$ and $\alpha(x_{n+1}) = x_{n+1})$ or $(\alpha(x_1) = x_{n+1}$ and $\alpha(x_{n+1}) = x_1)$. If $\alpha(x_1) = x_1$ and $\alpha(x_{n+1}) = x_{n+1}$ then by definition of graph automorphism, $\alpha|_X = ()$, where $\alpha|_X$ denotes the restriction of α on the set X and $()$ is the identity permutation. If $\alpha(x_1) = x_{n+1}$ and $\alpha(x_{n+1}) = x_1$ then $\alpha|_X = (x_1\ x_{n+1})(x_2\ x_n)\dots(x_{\frac{n}{2}}\ x_{\frac{n+4}{2}})$. Define $H = \langle (a_1\ b_2), \dots, (a_n\ b_n)\rangle$. There are two permutations β_1 and β_2 induced by the unique automorphism of order two in the path graph P_{n+1} with vertex set $V(P_{n+1}) = \{1, 2, \dots, n+1\}$ and edge set $E(P_{n+1}) = \{12, 23, 34, 45, \dots, (n)(n+1)\}$. These permutations can be defined as follows:

$$\beta_1 = \begin{cases} (a_1\ a_n)(a_2\ a_{n-1})\dots(a_{\frac{n}{2}}\ a_{\frac{n+2}{2}}) & 2 \mid n. \\ (a_1\ a_n)(a_2\ a_{n-1})\dots(a_{\frac{n-1}{2}}\ a_{\frac{n+3}{2}}) & 2 \nmid n, \end{cases},$$

$$\beta_2 = \begin{cases} (b_1\ b_n)(b_2\ b_{n-1})\dots(b_{\frac{n}{2}}\ b_{\frac{n+2}{2}}) & 2 \mid n, \\ (b_1\ b_n)(b_2\ b_{n-1})\dots(b_{\frac{n-1}{2}}\ b_{\frac{n+3}{2}}) & 2 \nmid n. \end{cases}$$

It is now easy to prove $\gamma = \alpha\beta_1\beta_2$ is an automorphism of order 2 in Q_n. Define $K = \langle\gamma\rangle$. Since all generators of H has order two and they are disjoint permutations,

$$H \cong \underbrace{Z_2 \times \dots \times Z_2}_{n\ times}.$$

It is clear $|H \cap K| = 1$ and for each element $t \in X$ and each automorphism $\gamma \in H$, $\gamma(t) = t$. Thus, $H \trianglelefteq Aut(Q_n)$. If an automorphism $\gamma \in Aut(Q_n)$ fixes elementwise each element of X then $\gamma \in H$ and in other case γ can be written as the product of an element of H by $\alpha\beta_1\beta_2$. This proves that $G = H : K \cong (Z_2 \times \dots \times Z_2) : Z_2$. Therefore, the automorphism group of Q_n can be generated by automorphisms γ and $(a_i\ b_i)$, for $1 \leqslant i \leqslant n$. A similar argument shows that, when n is odd, the group $Aut(Q_n)$ can be generated by $\alpha\beta_1\beta_2$ and n permutations $(a_i\ b_i)$ for $1 \leqslant i \leqslant n$. Therefore,

$$Aut(Q_n) \cong \begin{cases} (\underbrace{Z_2 \times \dots \times Z_2}_{\text{n times}}) : Z_2 & \text{n is even,} \\ Z_2 \times \left((\underbrace{Z_2 \times \dots \times Z_2}_{\text{n-1 times}}) : Z_2 \right) & \text{n is odd and } n \neq 1. \end{cases}$$

This proves that $|Aut(Q_n)| = 2^{n+1}$, $n \neq 1$, and $Aut(Q_1) \cong D_8$. If n is even, then the orbits of $Aut(Q_n)$ on $V(Q_n)$ are $V_1 = \{x_1, x_{n+1}\}$, $V_2 = \{a_1, b_1, a_n, b_n\}$, $V_3 = \{x_2, x_n\}$, $V_4 = \{a_2, b_2, a_{n-1}, b_{n-1}\}$, $V_5 = \{x_3, x_{n-1}\}$, ..., $V_{n-1} = \{x_{n/2}, x_{n/2+2}\}$, $V_n = \{a_{n/2}, a_{n/2+1}, b_{n/2}, b_{n/2+1}\}$ and $V_{n+1} = \{x_{n/2+1}\}$. If n is odd and $n \neq 1$, then the orbits of $Aut(Q_n)$ on $V(Q_n)$ will be $U_1 = \{x_1, x_{n+1}\}$,

$U_2 = \{a_1, b_1, a_n, b_n\}$, $U_3 = \{x_2, x_n\}$, $U_4 = \{a_2, b_2, a_{n-1}, b_{n-1}\}$, …, $U_{n-1} = \{a_{(n-1)/2}, b_{(n-1)/2}, a_{(n+3)/2}, b_{(n+3)/2}\}$, $U_n = \{x_{(n+1)/2}, x_{(n+3)/2}\}$ and $U_{n+1} = \{a_{(n+1)/2}, b_{(n+1)/2}\}$. To compute the Graovac-Pisanski index of this graph, we consider the following cases:

1. n is even. In this case, $Aut(Q_n)$ has exactly $n+1$ orbits under its natural action on $V(Q_n)$. Since $|V_{n+1}| = 1$, $W(V_{n+1}) = 0$. On the other hand, we have exactly $\frac{n}{2}$ orbits of size 2 and $\frac{n}{2}$ orbits of size 4. Now a simple calculation shows that $W(V_1) = 2n$, $W(V_2) = 8n-4$, …, $W(V_{n-3}) = 8$, $W(V_{n-2}) = 28$, $W(V_{n-1}) = 4$ and $W(V_n) = 4$. Therefore,

$$\begin{aligned} GP(Q_n) &= |V| \sum_{i=1}^{n+1} \frac{W(V_i)}{|V_i|} \\ &= (3n+1)\left(\frac{4+8+\cdots+2n}{2} + \frac{12+28+\cdots+8n-4}{4}\right) \\ &= \frac{9}{4}n^3 + \frac{15}{4}n^2 + n. \end{aligned}$$

2. n is odd and $n \neq 1$. In this case, again $Aut(Q_n)$ has exactly $n+1$ orbits under its natural action on $V(Q_n)$. On the other hand, by above calculations $\frac{n+3}{2}$ orbits have length 2 and other orbits have length 4. For orbits of length 2, we have $W(U_{n+1}) = 2$, $W(U_n) = 2$, $W(U_{n-2}) = 6$, …, $W(U_1) = 2n$, and for orbits of length 4, $W(U_{n-1}) = 20$, $W(U_{n-3}) = 36$, …, $W(U_2) = 8n-4$. Therefore,

$$\begin{aligned} GP(Q_n) &= |V| \sum_{i=1}^{n+1} \frac{W(V_i)}{|V_i|} \\ &= (3n+1)\left(\frac{2}{2} + \frac{2+6+\ldots+2n}{2} + \frac{20+36+\ldots+8n-4}{4}\right) \\ &= \frac{9}{4}n^3 + \frac{15}{4}n^2 + \frac{7}{4}n + \frac{1}{4}. \end{aligned}$$

This completes the proof. □

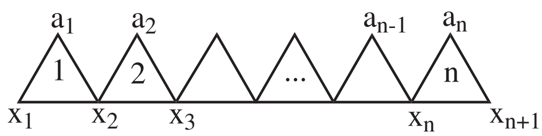

Figure 2: A 3-uniform cactus chain T_n.

Theorem 2.2. *The Graovac-Pisanski index of a 3-uniform cactus chain T_n, Figure 2, can be computed as follows:*

$$GP(T_n) = \begin{cases} \frac{1}{2}n^3 + \frac{5}{4}n^2 + n + \frac{1}{4} & n \text{ is odd and } n \neq 1, \\ \frac{1}{2}n^3 + \frac{5}{4}n^2 + \frac{3}{2}n + \frac{1}{2} & n \text{ is even.} \end{cases}$$

Proof. If n is odd and $n \neq 1$, then the automorphism group of T_n can be generated by $(x_1\ a_n)(a_1\ x_{n+1})\ (x_2\ x_n)(x_3\ x_{n-1})\cdots(x_{\frac{n+1}{2}}\ x_{\frac{n+3}{2}})(a_2\ a_{n-1})\cdots(a_{\frac{n-1}{2}}\ a_{\frac{n+3}{2}})$, $(x_1\ a_1)$ and $(a_n\ x_{n+1})$. Moreover, if n is even, then $Aut(T_n)$ is generated by $\alpha = (x_1\ a_n)(a_1\ x_{n+1})(x_2\ x_n)\cdots(x_{\frac{n}{2}}\ x_{\frac{n}{2}+2})(a_2\ a_{n-1})\cdots(a_{\frac{n}{2}}\ a_{\frac{n}{2}+1})$ and $\beta = (x_1\ a_1)$. Since $\alpha\beta \neq \beta\alpha$ and $\alpha\beta$ has order 4, $Aut(T_n) \cong D_8$. Note that two non-commuting elements δ and τ of order two generate a dihedral group of order $2O(\delta\tau)$. Therefore,

$$Aut(T_n) \cong \begin{cases} S_3 & n = 1 \\ D_8 & n \neq 1 \end{cases}.$$

To compute the GP index of T_n, we first calculate the orbits of $Aut(T_n)$ under its natural action on $V(T_n)$. If n is even, then $Aut(T_n)$ has exactly n orbits containing one orbit of length 1, one orbit of length 4 and $n-2$ orbits of length 2. These are $V_1 = \{x_{\frac{n}{2}+1}\}$, $V_2 = \{a_1, x_1, a_n, x_{n+1}\}$, $V_i = \{x_i, x_{n-i+2}\}$ and $V_i' = \{a_i, a_{n-i+1}\}$, $2 \leqslant i \leqslant \frac{n}{2}$. Our calculations show that $W(V_1) = 0$, $W(V_2) = 4n+2$ and $W(V_i) = W(V_i') = n - 2i + 2$, $2 \leqslant i \leqslant \frac{n}{2}$. Therefore,

$$\begin{aligned} GP(T_n) &= |V| \sum_{i=1}^{n} \frac{W(V_i)}{|V_i|} \\ &= (2n+1)\left(\frac{4n+2}{4} + \frac{1}{2} \times 2 \times (2 + 4 + \cdots + (n-2))\right) \\ &= \frac{1}{2}n^3 + \frac{5}{4}n^2 + \frac{3}{2}n + \frac{1}{2}. \end{aligned}$$

We now assume that n is odd. Then we have one orbit of length 1, one orbit of length 4 and $n-2$ orbits of length 2. These are $U_1 = \{a_{\frac{n+1}{2}}\}$, $U_2 = \{a_1, x_1, a_n, x_{n+1}\}$, $U_3 = \{x_{\frac{n+1}{2}}, x_{\frac{n+3}{2}}\}$, $U_4 = \{x_2, x_n\}$, $U_5 = \{a_2, a_{n-1}\}$, $U_6 = \{x_3, x_{n-1}\}$, $U_7 = \{a_3, a_{n-2}\}$, $\ldots$, $U_{n-1} = \{a_{\frac{n-1}{2}}, a_{\frac{n+3}{2}}\}$ and $U_n = \{x_{\frac{n-1}{2}}, x_{\frac{n+5}{2}}\}$. By our calculations, $W(U_1) = 0$, $W(U_2) = 4n+2$, $W(U_3) = 1$, $W(U_4) = W(U_5) = n-2$, $W(U_6) = W(U_7) = n-4$, $\ldots$, $W(U_{n-1}) = W(U_n) = 3$. Therefore,

$$\begin{aligned} GP(T_n) &= |V| \sum_{i=1}^{n} \frac{W(V_i)}{|V_i|} \\ &= (2n+1)\left(\frac{4n+2}{4} + \frac{1}{2} + \frac{1}{2} \times 2 \times (3 + 5 + \cdots + (n-2))\right) \\ &= \frac{1}{2}n^3 + \frac{5}{4}n^2 + n + \frac{1}{4}, \end{aligned}$$

which completes our proof. □

The *caterpilar* $CAT(n_1, \ldots, n_r)$ is a tree with vertex set

$$\underbrace{\{v_1, \ldots, v_r\}}_{A} \cup \underbrace{\{v_{11}, \ldots, v_{1n_1}\}}_{A_1} \cup \ldots \cup \underbrace{\{v_{r1}, \ldots, v_{rn_r}\}}_{A_r}$$

in which A is the vertex set for a path v_1, v_2, ..., v_r and A_i, $1 \leqslant i \leqslant r$, is a set of pendant vertices that all of them are adjacent with v_i, see Figure 3.

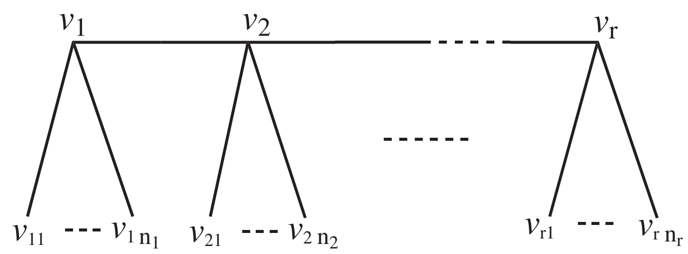

Figure 3: The caterpilar $CAT(n_1, \ldots, n_r)$.

Theorem 2.3. *The Graovac-Pisanski index of* $CAT(n_1, \ldots, n_r)$ *can be computed as follows:*

(1) *If for some i and j with $i + j = r + 1$, we have $n_i \neq n_j$ then*

$$GP(CAT(n_1, \ldots, n_r)) = \left(\sum_{i=1}^{r} n_i\right)^2 - r^2.$$

(2) *If $n_1 = n_2 = \cdots = n_r = n$, then*

$$GP(CAT(n, \ldots, n)) = \begin{cases} f(n,r) & r \text{ is even}, \\ g(n,r) & r \text{ is odd}, \end{cases}$$

where $f(n,r) = \left(\frac{1}{8}r^3 + r^2\right)n^2 + \left(\frac{1}{2}r^2 + \frac{1}{4}r^3\right)n - \frac{1}{2}r^2 + \frac{1}{8}r^3$ *and*

$$g(n,r) = \left(\frac{1}{8}r^3 + r^2 - \frac{1}{8}r\right)n^2 + \left(-\frac{3}{4}r + \frac{1}{2}r^2 + \frac{1}{4}r^3\right)n - \frac{5}{8}r - \frac{1}{2}r^2 + \frac{1}{8}r^3.$$

Proof. Set $\mathcal{L} = CAT(n_1, \ldots, n_r)$ and P is the induced subgraph of A. It is easy to see that $S_{A_i} \leqslant Aut(\mathcal{L})$, $1 \leqslant i \leqslant r$. Since $A_i \cap A_j = \emptyset$, $1 \leqslant i \neq j \leqslant r$, one can easily seen that $S_{A_1}S_{A_2}\ldots S_{A_r} \cong S_{A_1} \times S_{A_2} \times \cdots \times S_{A_r}$ and so $Aut(\mathcal{L})$ has a subgroup H isomorphic to $S_{A_1} \times S_{A_2} \times \cdots \times S_{A_r}$. Our main proof will consider two separate cases as follows:

1. Suppose for some i and j with $i+j=r+1$, we have $n_i \neq n_j$. From Figure 3, one can easily seen that $H = Aut(\mathcal{L})$ and H has exactly $2r$ orbits under its natural action on $V(\mathcal{L})$. These orbits are $\{v_1\}$, $\{v_2\}$, ..., $\{v_r\}$ and A_1, ..., A_r. Since $W(A_i) = {n_i}^2 - n_i$, $|A_i| = n_i$ and $|V| = r + \sum_{i=1}^{r} n_i$,

$$\begin{aligned} GP(\mathcal{L}) &= |V| \sum_{i=1}^{2r} \frac{W(V_i)}{|V_i|} \\ &= \left(r + \sum_{i=1}^{r} n_i \right) \left(\sum_{i=1}^{r} \frac{{n_i}^2 - n_i}{n_i} \right) \\ &= \left(\sum_{i=1}^{r} n_i \right)^2 - r^2. \end{aligned}$$

2. $n_1 = n_2 = \cdots = n_r = n$. Choose f to be the automorphism of order 2 in $Aut(P)$ and extend f to an automorphism $\overline{f}$ of $\mathcal{L}$ by defining $f(x) = x$, for each $x \in \bigcup_{i=1}^{r} A_i$. If r is even then $Aut(\mathcal{L}) = H \cup \overline{f} H$ and so $Aut(\mathcal{L}) \cong (S_{A_1} \times S_{A_2} \times \cdots \times S_{A_r}) : Z_2$. Furthermore, $Aut(\mathcal{L})$ can be generated by $(v_{i1}\ v_{i2})$, $(v_{i1}\ v_{i3})$, ..., $(v_{i1}\ v_{in_i})$ and $\prod (v_i\ v_j)(v_{i1}\ v_{j1})(v_{i2}\ v_{j2})(v_{i3}\ v_{j3}) \cdots (v_{in_i}\ v_{jn_i})$, where $1 \leqslant i \leqslant \frac{n}{2}$, $\frac{n}{2}+1 \leqslant j \leqslant n$ and $i+j=r+1$. Therefore, $Aut(\mathcal{L})$ has exactly r orbits such that $\frac{r}{2}$ of them have length 2 and others have length $2n$. These are $V_i = \{v_i, v_j\}$ and $V_i' = \{v_{i1}, v_{i2}, v_{i3}, \ldots, v_{in}, v_{j1}, v_{j2}, v_{j3}, \ldots, v_{jn}\}$, where $1 \leqslant i \leqslant \frac{r}{2}$, $\frac{r}{2}+1 \leqslant j \leqslant r$ and $i+j=r+1$. Our calculations show that, $W(V_i) \in \{1, 3, 5, 7, \ldots, r-1\}$ and $W(V_i') \in \{5n^2 - 2n, 5n^2 - 2n + 2n^2, \ldots, (r+3)n^2 - 2n\}$, where $1 \leqslant i \leqslant \frac{r}{2}$. Therefore,

$$\begin{aligned} GP(\mathcal{L}) &= |V| \sum_{i=1}^{r} \frac{W(V_i)}{|V_i|} \\ &= (n+1)r \left[\frac{1+3+\cdots+r-1}{2} + \frac{5n^2 - 2n + \cdots + (r+3)n^2 - 2n}{2n} \right] \\ &= \left(\frac{1}{8} r^3 + r^2 \right) n^2 + \left(\frac{1}{2} r^2 + \frac{1}{4} r^3 \right) n - \frac{1}{2} r^2 + \frac{1}{8} r^3. \end{aligned}$$

If r is odd then $S_{A_{\frac{r+1}{2}}}$ will be a characteristic subgroup and

$$\begin{aligned} Aut(\mathcal{L}) &\cong \left[\left(S_{A_1} \times S_{A_2} \times \cdots \times S_{A_{\frac{r-1}{2}}} \times S_{A_{\frac{r+3}{2}}} \times \cdots \times S_{A_r} \right) : Z_2 \right] \times S_{A_{\frac{r+1}{2}}} \\ &\cong \left[\underbrace{(S_n \times S_n \times \cdots \times S_n \times S_n \times \cdots \times S_n)}_{\text{r-1 times}} : Z_2 \right] \times S_n. \end{aligned}$$

Moreover, $Aut(\mathcal{L})$ can be generated by $(v_{i1}\ v_{i2})$, ..., $(v_{i1}\ v_{in_i})$ and $\prod (v_i\ v_j)$ $(v_{i1}\ v_{j1}) \cdots (v_{in_i}\ v_{jn_i})$, where $1 \leqslant i \leqslant \frac{n-1}{2}$, $\frac{n+3}{2} \leqslant j \leqslant n$ and $i+j=r+1$. On the other hand, $Aut(\mathcal{L})$ has exactly $r+1$ orbits, one orbit of length 1, one orbit of length n, $\frac{r-1}{2}$ orbits of length 2, and $\frac{r-1}{2}$ orbits of length $2n$. These are $U_1 = \{v_{\frac{r+1}{2}}\}$, $U_2 = \{v_{\frac{r+1}{2}1}, v_{\frac{r+1}{2}2}, \cdots, v_{\frac{r+1}{2}n}\}$, $U_i = \{v_i, v_j\}$ and $U_i' = \{v_{i1}, v_{i2}, \ldots, v_{in}, v_{j1}, v_{j2}, \ldots, v_{jn}\}$, where $1 \leqslant i \leqslant \frac{r-1}{2}$, $\frac{r+3}{2} \leqslant j \leqslant r$ and $i + j = r + 1$. By our calculations, $W(U_1) = 0$, $W(U_2) = n(n-1)$, $W(U_i) \in \{2, 4, \ldots, r-1\}$ and $W(U_i') \in \{6n^2-2n, 8n^2-2n, \ldots, (r+3)n^2-2n\}$. Therefore,

$$\begin{aligned}
GP(\mathcal{L}) &= |V| \sum_{i=1}^{r+1} \frac{W(V_i)}{|V_i|} \\
&= (n+1)r \left[\frac{n(n-1)}{n} + \frac{2+4+\cdots+r-1}{2} \right. \\
&\qquad \left. + \frac{6n^2-2n+\cdots+(r+3)n^2-2n}{2n} \right] \\
&= \left(\frac{1}{8}r^3 + r^2 - \frac{1}{8}r\right) n^2 + \left(-\frac{3}{4}r + \frac{1}{2}r^2 + \frac{1}{4}r^3\right) n - \frac{5}{8}r - \frac{1}{2}r^2 + \frac{1}{8}r^3.
\end{aligned}$$

This completes our argument. □

Note that our previous theorem covers the case when for some i, j with $i+j = r+1$, n_i is not equal to n_j and another case when all n_i are the same. It is easy to see that $Aut(\mathcal{L}) = H$ or $H : Z_2$. For example, we do not cover the case that $CAT(2,3,4,3,2)$. Our method shows that $Aut(CAT(2,3,4,3,2)) \cong (Z_2 \times S_3 \times S_4 \times S_3 \times Z_2) : Z_2$ and a simple GAP program shows that in this case $GP(\mathcal{L}) = 399$.

Suppose G and H are two graphs. The *corona product* $G \circ H$ is a graph constructed from G and $|V(G)|$ copies of H by connecting the i^{th} vertex of G to each vertex of the i^{th} copy of H, $1 \leqslant i \leqslant |V(G)|$.

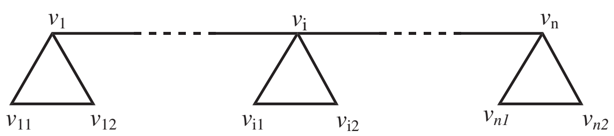

Figure 4: The corona product $P_n \circ P_2$.

Theorem 2.4. *The Graovac-Pisanski index of $P_n \circ P_2$, Figure 4, can be computed by the following formula:*

$$GP(P_n \circ P_2) = \begin{cases} \frac{9}{8}n^3 + \frac{15}{4}n^2 & n \text{ is even}, \\ \frac{9}{8}n^3 + \frac{15}{4}n^2 - \frac{27}{8}n & n \text{ is odd}, \\ 3 & n = 1. \end{cases}$$

Proof. Depending on whether n is an even or odd number, our proof will consider two cases.

1. n is even. In this case, the generators of $Aut(P_n \circ P_2)$ are $(v_{k1}\ v_{k2})$, $1 \leqslant k \leqslant n$, and $\prod(v_i\ v_j)(v_{i1}\ v_{j1})(v_{i2}\ v_{j2})$, $1 \leqslant i \leqslant \frac{n}{2}$, $\frac{n}{2}+1 \leqslant j \leqslant n$ and $i+j=n+1$. Our calculations show that the orbits of this action are $V_i = \{v_i, v_j\}$ and $V_i' = \{v_{i1}, v_{i2}, v_{j1}, v_{j2}\}$. Furthermore, $W(V_1) = n-1$, $W(V_2) = n-3$, ..., $W(V_{\frac{n}{2}}) = 1$, $W(V_1') = 4n+6$, $W(V_2') = 4n-2$, ..., $W(V_{\frac{n}{2}}') = 14$. Therefore,

$$\begin{aligned} GP(P_n \circ P_2) &= |V| \sum_{i=1}^{n} \frac{W(V_i)}{|V_i|} \\ &= 3n \left[\frac{1+3+\cdots+n-1}{2} + \frac{14+22+30+\cdots+4n+6}{4} \right] \\ &= \frac{9}{8}n^3 + \frac{15}{4}n^2. \end{aligned}$$

2. n is odd. The generators of $Aut(P_n \circ P_2)$ are $(v_{k1}\ v_{k2})$, $1 \leqslant k \leqslant n$ and $\prod(v_i\ v_j)(v_{i1}\ v_{j1})(v_{i2}\ v_{j2})$, $1 \leqslant i \leqslant \frac{n-1}{2}$, $\frac{n+3}{2} \leqslant j \leqslant n$ and $i+j=n+1$. This group has exactly $n+1$ orbits under its natural action. These orbits are $U = \{v_{\frac{n+1}{2}}\}$, $U' = \{v_{\frac{n+1}{2}1}, v_{\frac{n+1}{2}2}\}$, $\frac{n+1}{2}$ orbits $U_i = \{v_i, v_j\}$ of size 2 and $\frac{n-1}{2}$ orbits $U_i' = \{v_{i1}, v_{i2}, v_{j1}, v_{j2}\}$ of size 4. Moreover, $W(U) = 0$, $W(U') = 1$, $W(U_1) = n-1$, $W(U_2) = n-3$, ..., $W(U_{\frac{n-1}{2}}) = 2$, $W(U_1') = 4n+6$, $W(U_2') = 4n-2$, ..., $W(U'_{\frac{n-1}{2}}) = 18$. Therefore,

$$\begin{aligned} GP(P_n \circ P_2) &= |V| \sum_{i=1}^{n+1} \frac{W(V_i)}{|V_i|} \\ &= 3n \left[0 + \frac{1}{2} + \frac{2+4+\cdots+n-1}{2} + \frac{18+26+\cdots+4n+6}{4} \right] \\ &= \frac{9}{8}n^3 + \frac{15}{4}n^2 - \frac{27}{8}n. \end{aligned}$$

This completes the proof. □

Theorem 2.5. *The Graovac-Pisanski index of an ortho-chain O_n, Figures $5-7$, of length n is computed as follows:*

$$GP(O_n) = \begin{cases} \frac{9}{8}n^3 + \frac{33}{8}n^2 + \frac{17}{4}n + 1 & n \text{ is even,} \\ \frac{9}{8}n^3 + \frac{33}{8}n^2 + \frac{19}{8}n + \frac{3}{8} & n \text{ is odd.} \end{cases}$$

Proof. There are two possible cases, depending on whether n is even or odd.

1. n is even. It can be proved that the automorphism group $Aut(O_n)$ is generated by the permutations $(1\ a_2)$, $(n+1\ b_{n-1})$ and $(a_1\ b_n)(1\ b_{n-1})(a_2\ n+1)(2\ n)(b_1\ a_n)(a_3\ b_{n-2})(3\ n-1)\ (b_2\ a_{n-1})(a_4\ b_{n-3})\cdots(\frac{n}{2}\ \frac{n}{2}+2)(b_{\frac{n}{2}-1}\ a_{\frac{n}{2}+2})$

$(a_{\frac{n}{2}+1}\ b_{\frac{n}{2}})$. Moreover, the group has exactly $\frac{3n}{2}$ orbits. These orbits are $U_1 = \{\frac{n}{2}+1\}$, $U_2 = \{a_{\frac{n}{2}+1}, b_{\frac{n}{2}}\}$, $U_3 = \{\frac{n}{2}, \frac{n}{2}+2\}$, $U_4 = \{a_{\frac{n}{2}}, b_{\frac{n}{2}+1}\}$, $U_5 = \{\frac{n}{2}-1, \frac{n}{2}+3\}$, $U_6 = \{b_{\frac{n}{2}-1}, a_{\frac{n}{2}+2}\}$, $U_7 = \{a_{\frac{n}{2}-1}, b_{\frac{n}{2}+2}\}$, $U_8 = \{\frac{n}{2}-2, \frac{n}{2}+4\}$, $U_9 = \{b_{\frac{n}{2}-2}, a_{\frac{n}{2}+3}\}$, …, $U_{\frac{3n-10}{2}} = \{a_3, b_{n-2}\}$, $U_{\frac{3n-8}{2}} = \{2, n\}$, $U_{\frac{3n-6}{2}} = \{b_2, a_{n-1}\}$, $U_{\frac{3n-4}{2}} = \{b_1, a_n\}$, $U_{\frac{3n-2}{2}} = \{a_1, b_n\}$ and $U_{\frac{3n}{2}} = \{1, a_2, b_{n-1}, n+1\}$. On the other hand, $W(U_1) = 0$, $W(U_2) = W(U_3) = 2$, $W(U_4) = W(U_5) = W(U_6) = 4$, $W(U_7) = W(U_8) = W(U_9) = 6$, $W(U_{\frac{3n-10}{2}}) = W(U_{\frac{3n-8}{2}}) = W(U_{\frac{3n-6}{2}}) = n-2$, $W(U_{\frac{3n-4}{2}}) = n$, $W(U_{\frac{3n-2}{2}}) = n+2$ and $W(U_{\frac{3n}{2}}) = 4n+4$.

Therefore,

$$
\begin{aligned}
GP(O_n) &= |V|\sum_{i=1}^{\frac{3n}{2}} \frac{W(V_i)}{|V_i|} \\
&= (3n+1)\left[\frac{0}{1} + \frac{2+2}{2} + \frac{4+4+4}{2} + \frac{6+6+6}{2}\right. \\
&+ \left.\cdots + \frac{n-2+n-2+n-2}{2} + \frac{n}{2} + \frac{n+2}{2} + \frac{4n+4}{4}\right] \\
&= (3n+1)\left[0 + 2 + \frac{3}{2}\left(\underbrace{4+6+\cdots+n-2}_{\frac{n-4}{2}}\right) + \frac{n}{2} + \frac{n+2}{2} + n + 1\right] \\
&= \frac{9}{8}n^3 + \frac{33}{8}n^2 + \frac{17}{4}n + 1.
\end{aligned}
$$

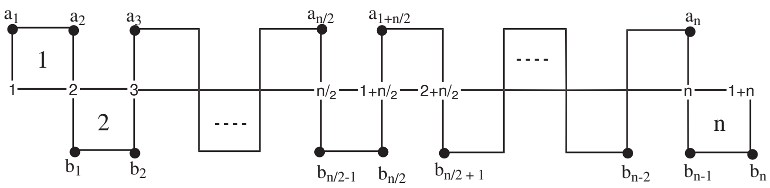

Figure 5: An ortho-chain of length n, n is even.

2. n is odd. The generators of $Aut(O_n)$ are $(1\ 1{+}n)(2\ n)\cdots(\frac{1+n}{2}\ \frac{3+n}{2})\ (a_1\ a_{1+n})$ $(a_2\ a_n)\ \cdots\ (a_{\frac{1+n}{2}}\ a_{\frac{3+n}{2}})\,(b_1\ b_{n-1})\,(b_2\ b_{n-2})\cdots(b_{\frac{n-1}{2}}\ b_{\frac{n+1}{2}})$, $(1\ a_2)$ and $(1{+}n\ a_n)$. Furthermore, the number of orbits of this group under its natural action is $\frac{3n-1}{2}$ and the orbits are $V_1 = \{a_{\frac{n+1}{2}}, a_{\frac{n+3}{2}}\}$, $V_2 = \{\frac{n+1}{2}, \frac{n+3}{2}\}$, $V_3 = \{b_{\frac{n-1}{2}}, b_{\frac{n+1}{2}}\}$, $V_4 = \{\frac{n-1}{2}, \frac{n+5}{2}\}$, $V_5 = \{a_{\frac{n-1}{2}}, a_{\frac{n+5}{2}}\}$, $V_6 = \{\frac{n-3}{2}, \frac{n+7}{2}\}$, $V_7 = \{b_{\frac{n-3}{2}}, b_{\frac{n+3}{2}}\}$, $V_8 = \{a_{\frac{n-3}{2}}, a_{\frac{n+7}{2}}\}$, $V_9 = \{\frac{n-5}{2}, \frac{n+9}{2}\}$, $V_{10} = \{b_{\frac{n-5}{2}}, b_{\frac{n+5}{2}}\}$, …, $V_{\frac{3n-11}{2}} = \{a_3, a_{n-1}\}$, $V_{\frac{3n-9}{2}} = \{2, n\}$, $V_{\frac{3n-7}{2}} = \{b_2, b_{n-2}\}$, $V_{\frac{3n-5}{2}} = \{b_1, b_{n-1}\}$, $V_{\frac{3n-3}{2}} = \{a_1, a_{n+1}\}$ and $V_{\frac{3n-1}{2}} = \{1, a_2, 1+n, a_n\}$.

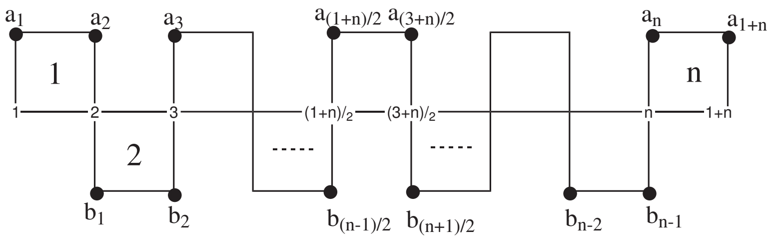

Figure 6: An ortho-chain of length n, $n \overset{4}{\equiv} 1$.

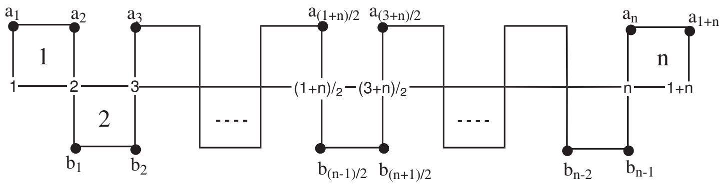

Figure 7: An ortho-chain of length n, $n \overset{4}{\equiv} 3$.

To compute the Graovac-Pisanski index of this graph, $n \neq 3$, we note that $W(V_5) = W(V_6) = W(V_7) = 5$, $W(V_8) = W(V_9) = W(V_{10}) = 7$, $W(V_{\frac{3n-11}{2}}) = W(V_{\frac{3n-9}{2}}) = W(V_{\frac{3n-7}{2}}) = n-2$, $W(V_{\frac{3n-5}{2}}) = n$, $W(V_{\frac{3n-3}{2}}) = n+2$, $W(V_{\frac{3n-1}{2}}) = 4n+4$. Finally, if $n \overset{4}{\equiv} 1$ then $W(V_1) = W(V_2) = 1$, $W(V_3) = W(V_4) = 3$, and if $n \overset{4}{\equiv} 3$ then $W(V_2) = W(V_3) = 1$ and $W(V_1) = W(V_4) = 3$.
Therefore,

$$
\begin{aligned}
GP(O_n) &= |V| \sum_{i=1}^{\frac{3n-1}{2}} \frac{W(V_i)}{|V_i|} \\
&= (3n+1) \left[\frac{1+1}{2} + \frac{3+3}{2} + \frac{5+5+5}{2} + \frac{7+7+7}{2} \right. \\
&+ \left. \cdots + \frac{n-2+n-2+n-2}{2} + \frac{n}{2} + \frac{n+2}{2} + \frac{4n+4}{4} \right] \\
&= (3n+1) \left[1 + 3 + \frac{3}{2}(5+7+\cdots+n-2) + \frac{n}{2} + \frac{n+2}{2} + n + 1 \right] \\
&= \frac{9}{8}n^3 + \frac{33}{8}n^2 + \frac{19}{8}n + \frac{3}{8}.
\end{aligned}
$$

This completes the proof of our theorem. □

In the next theorem the Graovac-Pisanski index of ladder graph L_n, Figures 8 − 9, which is also known as the linear polyomino is computed [6].

Theorem 2.6. *The Graovac-Pisanski index of the ladder graph L_n can be computed as follows:*

$$GP(L_n) = \begin{cases} \frac{n^3}{2} + \frac{5n^2}{2} + 3n + 1 & n \text{ is even,} \\ \frac{n^3}{2} + \frac{5n^2}{2} + \frac{7n}{2} + \frac{3}{2} & n \text{ is odd.} \end{cases}$$

Proof. We first note that $Aut(L_1) \cong D_8$ and $Aut(L_n) \cong Z_2 \times Z_2$, for $n \neq 1$. If n is even, then $Aut(L_n)$ can be generated by $\prod_{k=1}^{n+1}(a_k\ b_k)$ and $\prod_{i=1}^{n-1}(a_i\ a_{i+1})(b_i\ b_{i+1})$, i is odd. If n is odd, then the permutations $\prod_{t=1}^{n+1}(a_t\ b_t)$ and $\prod_{j=1}^{n}(a_j\ a_{j+1})$ $(b_j\ b_{j+1})$ will generate the group $Aut(L_n)$, where j is odd positive integer.

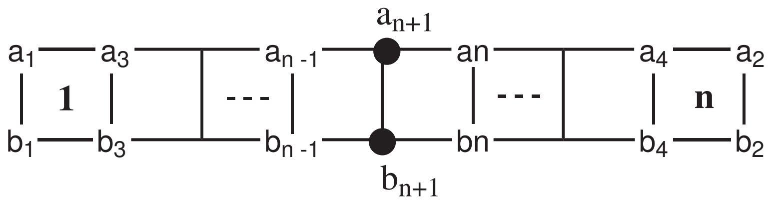

Figure 8: The graph L_n, when n is even.

If n is even, then this group has $\frac{n}{2} + 1$ orbits, and the orbits are $V_1 = \{a_{n+1}, b_{n+1}\}$ of length 2 and other orbits which have length 4 are $V_2 = \{a_1, b_1, a_2, b_2\}$, $V_3 = \{a_3, b_3, a_4, b_4\}, \ldots, V_{\frac{n}{2}+1} = \{a_{n-1}, b_{n-1}, a_n, b_n\}$. On the other hand, $W(V_1) = 1$, $W(V_{\frac{n}{2}+1}) = 12$, $W(V_{\frac{n}{2}}) = 20$, $W(V_{\frac{n}{2}-1}) = 28, \ldots, W(V_2) = 4n + 4$. Therefore,

$$\begin{aligned} GP(L_n) &= |V| \sum_{i=1}^{\frac{n}{2}+1} \frac{W(V_i)}{|V_i|} \\ &= (2n+2)\left(\frac{1}{2} + \frac{12 + 20 + 28 + \cdots + 4n + 4}{4}\right) \\ &= \frac{n^3}{2} + \frac{5n^2}{2} + 3n + 1. \end{aligned}$$

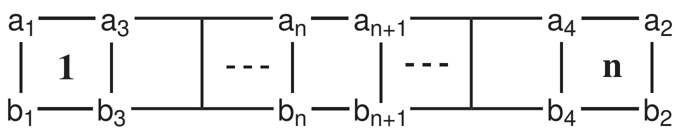

Figure 9: The graph L_n, when n is odd.

If n is odd, then this group has $\frac{n+1}{2}$ orbits of length 4, and the orbits are $V_1 = \{a_1, b_1, a_2, b_2\}$, $V_2 = \{a_3, b_3, a_4, b_4\}, \ldots, V_{\frac{n+1}{2}} = \{a_n, b_n, a_{n+1}, b_{n+1}\}$. Furthermore,

$W(V_{\frac{n+1}{2}}) = 8$, $W(V_{\frac{n-1}{2}}) = 16$, $W(V_{\frac{n-3}{2}}) = 24$, ..., $W(V_1) = 4n + 4$. Therefore,

$$\begin{aligned} GP(L_n) &= |V| \sum_{i=1}^{\frac{n+1}{2}} \frac{W(V_i)}{|V_i|} \\ &= (2n+2)\left(\frac{8 + 16 + 24 + \cdots + 4n + 4}{4}\right) \\ &= \frac{n^3}{2} + \frac{5n^2}{2} + \frac{7n}{2} + \frac{3}{2}, \end{aligned}$$

which completes our argument. □

We end this paper by computing the Graovac-Pisanski index of a 2-connected linear polymer with triangular faces R_n.

Theorem 2.7. *The Graovac-Pisanski index of a* $2-$*connected linear polymer with triangular faces* R_n*, Figure* 10*, is computed as*

$$GP(R_n) = \begin{cases} \frac{n^3}{16} + \frac{n^2}{2} + \frac{5n}{4} + 1 & n \text{ is even}, \\ \frac{n^3}{16} + \frac{3n^2}{8} + \frac{11n}{16} + \frac{3}{8} & n \text{ is odd}. \end{cases}$$

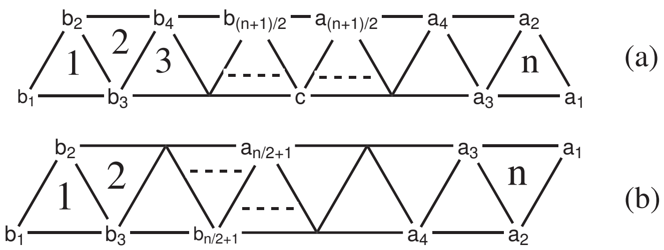

Figure 10: (a) R_n, n is odd; (b) R_n, n is even.

Proof. It is clear that $Aut(R_1) \cong S_3$, $Aut(R_2) \cong Z_2 \times Z_2$ and $Aut(R_n) \cong Z_2$, when $n \geq 3$. To compute the Graovac-Pisanski index, we first assume that n is even. Then $V_i = \{a_i, b_i\}$, $1 \leqslant i \leqslant \frac{n}{2} + 1$, $W(V_1) = \frac{n}{2} + 1$, $W(V_2) = \frac{n}{2}$, ..., $W(V_{\frac{n}{2}}) = 2$ and $W(V_{\frac{n}{2}+1}) = 1$. Therefore,

$$\begin{aligned} GP(R_n) &= |V| \sum_{i=1}^{\frac{n}{2}+1} \frac{W(V_i)}{|V_i|} \\ &= (n+2)\left(\frac{1 + 2 + 3 + \cdots + \frac{n}{2} + 1}{2}\right) \\ &= \frac{n^3}{16} + \frac{n^2}{2} + \frac{5n}{4} + 1. \end{aligned}$$

If n is odd then $V_j = \{a_j, b_j\}$, $1 \leqslant j \leqslant \frac{n+1}{2}$, $V_{\frac{n+3}{2}} = \{c\}$, $W(V_1) = \frac{n+1}{2}$, $W(V_2) = \frac{n-1}{2}$, $\ldots$, $W(V_{\frac{n-1}{2}}) = 2$, $W(V_{\frac{n+1}{2}}) = 1$ and $W(V_{\frac{n+3}{2}}) = 0$. Therefore,

$$\begin{aligned} GP(R_n) &= |V| \sum_{j=1}^{\frac{n+3}{2}} \frac{W(V_j)}{|V_j|} \\ &= (n+2)\left(\frac{0}{1} + \frac{1+2+3+\cdots+\frac{n+1}{2}}{2}\right) \\ &= \frac{n^3}{16} + \frac{3n^2}{8} + \frac{11n}{16} + \frac{3}{8}. \end{aligned}$$

□

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