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Closed Forms for Zagreb Indices of Dihedral Orbit Graphs

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ABSTRACT

In this scientific paper, we review the Zagreb indices for the orbital graphs of the D_{2n} group by highlighting some of the geometric properties of the orbital structure created from a dihedral group. We explain that when n is an odd number, the resulting graph is a complete graph. This structural description allows us to derive explicit and precise mathematical formulas for both indices. Furthermore, we prove the existence of a mathematical relationship between the two topological indices, showing that the second Zagreb index is expressed mathematically in terms of the first Zagreb index through a multiplicative constant that depends on the order of the orbital graph. The obtained results summarize the strength of the relationship and interaction between the group structure and the indices, establishing a smooth framework for studying these indices in algebraically defined orbital graphs.

MSC..

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1. Introduction

Topological indices are fundamental and important pillars in graph theory for describing the geometric features of intersecting systems. Their use is common in modelling molecular structures in chemistry and predicting physical properties and interactions [1,2]. The first and second Zagreb indices are among the most important and prominent measures used in analysing and studying electron energy. The scope of these studies has since expanded to include the study of their mathematical properties and their relationships to the constants of other graphs [3,4,5].

Recently, there has been increased interest in studying graphs generated from algebraic systems, particularly orbital graphs under group influences. Orbits are considered vertices of the orbital graph, and the edges between them are defined by a group relationship [6]. The dihedral group is considered the ideal case study for this because the orbital graph under the influence of a group relationship (conjugation) is a complete graph when (n) is an odd number, which significantly simplifies the calculation of indices [6].

This study summarizes how to develop a precise mathematical formula for both Zagreb indices to describe the D_{2n} orbit.

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As we have arrived at and proven a mathematical formula relating the two Zagreb indices together, we show how the second Zagreb indices are described in terms of the first.

The relationship between the D_{2n} group structure and topological indices is coherent and robust. These results facilitate the analysis of topological indices in algebraic structures and provide a solid foundation for more geometrically complex forms of dihedral group effects.

2. Preliminaries

This section establishes the necessary mathematical foundation in group theory and graph theory. The primary focus of this research is the Dihedral group, denoted by D_{2n} , which represents the symmetries of a regular n -sided polygon. To explore its topological properties, we analyze its non-commuting graph G .

Definition 2.1 [10]: The dihedral group D_{2n} is the group of symmetries of a regular n -gon. It has $2n$ elements and is defined by:

$$D_{2n} = \langle r, s \mid r^n = e, s^2 = e, srs = r^{-1} \rangle$$

With n being a positive integer and $n \geq 3$.

Definition 2.2 [7]: Let G be a finite group. We define the set $\Psi \subseteq G \times G$ to consist of all ordered pairs of distinct elements in G that commute with each other and whose orders are such that the least common multiple equals two. That is,

$$\Psi = \{(x, y) \in G \times G \mid xy = yx, \quad x \neq y, \text{ lcm}(|x|, |y|) = 2\}$$

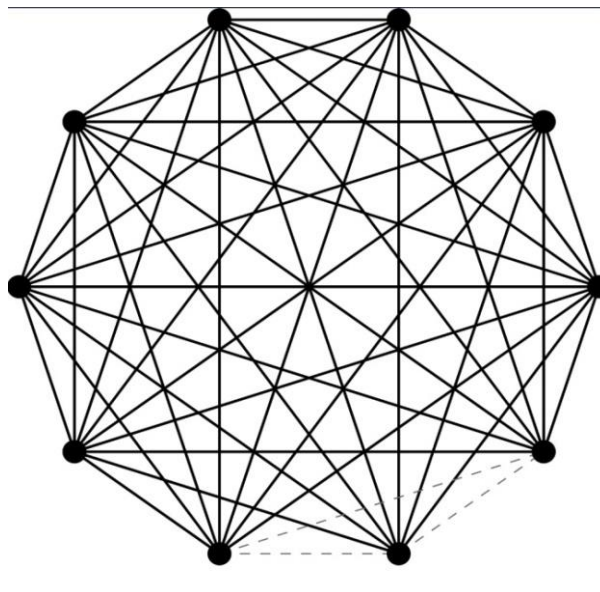
Definition 2.3 [7]: Let G be a group acting on a set X via conjugation. For an element $x \in X$, its orbit is the set of all elements obtained by conjugating x by elements of G , the orbit is written as :

$$\mathcal{O}(x) = \{gxg^{-1} : g \in G\}$$

Definition 2.4 [7]: Let G be a finite group acting on a set X by conjugation. Let $\Psi \subseteq G \times G$ be the set defined in Definition 2.2.

The **orbit graph** Γ_G is defined as follows:

- The vertex set $V(\Gamma_G)$ consists of the distinct **orbits** of the action of G on Ψ , i.e., $V(\Gamma_G) = \{\mathcal{O}(x, y) : (x, y) \in \Psi\}$.
- Two distinct vertices $\mathcal{O}_1$ and $\mathcal{O}_2$ are said to be adjacent if and only if there exist representatives $(x_1, y_1) \in \mathcal{O}_1$ and $(x_2, y_2) \in \mathcal{O}_2$ such that they satisfy a specified structural relation.

Figure 1. The orbit graph K_n of D_{2n}

Definition 2.5 [8]: The degree of vertex $v \in V(G)$, denoted by $\deg(v)$, is the number of edges adjacent to v . The structural properties of a graph, particularly its connectivity, are primarily characterized by the vertex degree. This degree is defined as the total count of edges incident to a specific vertex within the graph's architecture. These degree-based metrics serve as the foundation for calculating various topological descriptors.

Zagreb's first and second indices are considered fundamental concepts in mathematical chemistry. In 2012, Mezreggar and Ashrafi generalized some topological indices to graphs [4], with particular attention to the D_{2n} group. The following sections provide the formal definitions and analytical evaluations for the first and second Zagreb indices as applied to the graphs of finite groups.

Definition 2.6 [9]: The first Zagreb index for a connected graph Γ_G is determined by sum of the squares of the degrees of all vertices in the set Γ_G :

$$M_1(\Gamma_G) = \sum_{v \in V(\Gamma_G)} (\deg(v))^2$$

Definition 2.7 [9]: The second Zagreb index is calculated based on the edges of the graph, representing the sum of the products of the degrees of all pairs of adjacent vertices :

$$M_2(\Gamma_G) = \sum_{u,v \in E(\Gamma_G)} \deg(u) \deg(v)$$

Lemma 1. For a complete graph K_n , every pair of distinct vertices is connected by an edge. Consequently, each vertex is adjacent to all other $n - 1$ vertices, and the total number of edges in the graph is $\frac{n(n-1)}{2}$.

3. Results And Discussions

In this section, we present analytical calculations for the first and second Zagreb indices, specifically for the graphs associated with dihedral groups (D_{2n}). The study focuses on evaluating these two indices and determining the relationship between them to provide a deeper understanding of the topological behavior of D_{2n} within the framework of graph theory.

Proposition 3.1: Let $G = D_{2n}$, where n is an odd integer. Then the orbit graph Γ_G is a complete graph.

Proof. First, we explicitly determine the vertex set. The vertices correspond to the orbits of the conjugation action of G on Ψ .

For odd n , all reflections in D_{2n} form a single conjugacy class, while rotations form separate classes depending on their order.

Thus, the action partitions Ψ into a finite number of distinct orbits.

Next, consider any two distinct vertices $\mathcal{O}_1 \neq \mathcal{O}_2$. By the structure of D_{2n} and the conjugation action, representatives of these orbits can be related through conjugation by suitable elements of G , ensuring adjacency under the adopted definition.

Hence, every pair of distinct vertices is adjacent, and therefore $\Gamma_G \cong K_m$, i.e., it is a complete graph. ■

Proposition 3.2: The number of vertices of Γ_G is equal to m , such that $m = \frac{n+1}{2}$, $n \in \mathbb{N}$.

Proof. The vertices of Γ_G correspond to the distinct orbits of the action of D_{2n} on Ψ . Under this action, the elements of Ψ are partitioned into pairs due to the symmetry of reflections, with exactly one orbit remaining fixed.

Hence, the total number of orbits is

$$m = \frac{n+1}{2}, n \in \mathbb{N}.$$

Therefore, the number of vertices of Γ_G is $(m = \frac{n+1}{2}, n \in \mathbb{N})$. ■

Remark : Since Γ_G is isomorphic to the K_m it follows from Lemma 1. That every vertex has degree $(m - 1)$ and the total number of edges is $\frac{m(m-1)}{2}$. These properties are essential for computing the Zagreb indices in closed form.

Theorem 3.1: Let Γ_G the orbit graph of D_{2n} acting on a set Ψ . If $\Gamma_G \cong K_m$, then the first and second zagreb indices are given by :

- $M_1(\Gamma_G) = m(m - 1)^2$
- $M_2(\Gamma_G) = \frac{m(m-1)^3}{2}$

Proof : Let K_m be a complete graph on m vertices. By definition, every vertex in K_m is adjacent to all other $(m - 1)$ vertices. Hence, for each vertex $(v \in V(K_m))$, we have $\deg(v) = m - 1$.

Therefore, the first Zagreb index is given by

$$M_1(K_m) = \sum_{v \in V(K_m)} (\deg(v))^2 = m(m - 1)^2,$$

since there are (m) vertices, each having degree $(m - 1)$.

Next, we compute the second Zagreb index. The number of edges in (K_m) is

$$|E(K_m)| = \frac{m(m-1)}{2}.$$

For every edge $(uv \in E(K_m))$, both endpoints have degree $(m - 1)$, and hence $\deg(u) \deg(v) = (m - 1)^2$

Thus, we obtain

$$M_2(K_m) = \sum_{v \in V(K_m)} \deg(u) \deg(v) = \frac{m(m - 1)^3}{2}, \blacksquare$$

4. Relation Between The Zagreb Indices

The relationship between the two Zagreb indices established in this research holds for all regular graphs. The novelty of this study lies in proving that the orbit graph of a dihedral group, when n is odd, under the action on the set Ψ , forms a complete graph. This result allows the reduction of the computation of the first and second Zagreb

indices to closed-form expressions, providing a strong connection between the algebraic structure of the group and the invariant properties of the graph.

Theorem 4.1: For the orbit graph $\Gamma_G \cong K_m$, the first and second Zagreb indices satisfy the following linear relationship :

$$M_2(\Gamma_G) = \frac{m-1}{2} M_1(\Gamma_G)$$

Proof: By Theorem (1-2)

Then

$$\begin{aligned} RHS &= \frac{m-1}{2} M_1(\Gamma_G) \\ &= \frac{m-1}{2} [m(m-1)^2] \\ RHS &= \frac{m(m-1)^3}{2} \end{aligned}$$

Hence

$$RHS = M_2(\Gamma_G) \quad \blacksquare$$

Example 4.1: Consider the orbit graph of D_{18} , where ($n = 9$).

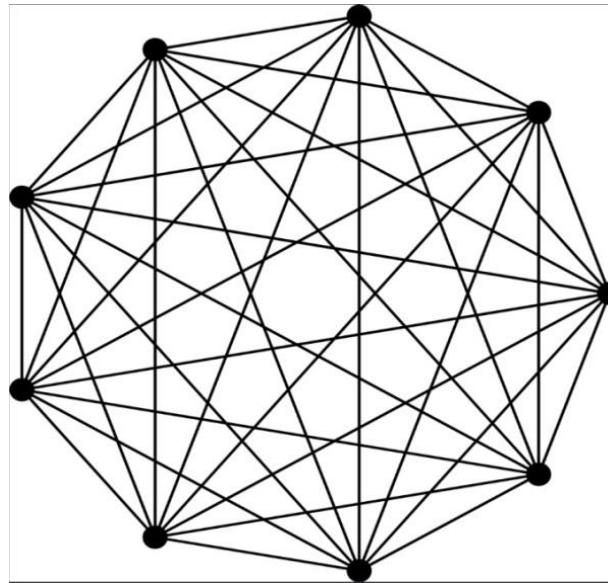


Figure 2. The orbit graph K_9 of D_{18}

Since n is odd, it follows from **Proposition 3.1** that the orbit graph is complete. Suppose that the resulting orbit graph has $m = 9$ vertices. (see Figure 2).

$$\text{Then, } \Gamma_G \cong K_m$$

Therefore,

$$|V| = 9 \quad \text{and} \quad |E| = \frac{n(n-1)}{2} = 36$$

Since, $(\Gamma_G \cong K_9)$ has

$$\deg(v) = (9 - 1) = 8$$

Now, we compute the Zagreb indices.

First and second Zagreb index

$$M_1(\Gamma_G) = m(m-1)^2 = 576$$

$$M_2(\Gamma_G) = \frac{m(m-1)^3}{2} = 2304$$

The relationship between the two indicators

$$M_2(\Gamma_G) = \frac{m-1}{2} M_1(\Gamma_G) = \frac{8}{2} \times 576 = 2304$$

5. Conclusion

Topological indices are typically studied within the framework of connected graphs; therefore, in this work, attention was restricted to the case in which the orbit graph of the dihedral group is connected. For D_{2n} with odd n , this graph was shown to be complete, which allows for a simplified treatment of degree-based indices.

Relying on this structural property, the first and second Zagreb indices of the orbit graph were computed in explicit closed forms by utilizing the well-known properties of complete graphs. In addition, a direct relationship between these two indices was obtained, revealing that one can be expressed in terms of the other through a simple functional dependence.

The results of this study help simplify the study of the Zagreb indices for D_{2n} orbitals to basic calculations simply by

describing the structure of the graph. This provides a straightforward explanation of how some algebraic features of

the groups affect the numerical constants associated with the graph.

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