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Research article

Computation of Hosoya and eccentricity-based topological indices of power graphs over finite groups

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Abstract: Topological indices are mathematical values based on graph models of molecular structures that characterize significant properties in terms of chemical composition, reactivity, and physicochemical properties. In this paper, we are devoted to eccentricity-based indices of power graphs over finite groups and investigate their application in the context of molecular graphs. We calculated the Zagreb eccentricity indices, eccentric connectivity index, connective eccentricity index, (adjacent) eccentric distance sum index, and the Zagreb irregularity indices. In addition, we computed the Hosoya index for the mentioned graphs, which was one of the challenging aspects of this work. These findings enhance the theoretical foundation of graph-based indices and contribute to the quantitative description of molecular graphs.

Keywords: topological indices; molecular structure; power graphs; finite groups
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1. Introduction

To determine the bioactive properties of chemical compounds, researchers have examined the topological indices and physical features in quantitative structure-property relationship (QSPR) studies. In [1], the researchers constructed a nano-QSPR model with only two substituent-based molecular descriptors to estimate the solubility of cyclopropane-functionalized fullerenes in chlorobenzene, without the need to perform expensive quantum-mechanical computations. Graph-theoretic QSPR models were also reported in [2], where the researchers used topological indices and demonstrated better results in predicting important pharmacokinetic properties of drugs using random forests, as compared to traditional models. The redefined Zagreb indices and the index of side-effect determination demonstrated the strong connection for certain essential physicochemical characterization, and these indices further optimized the QSPR modeling used for multiple sclerosis drugs [3]. The Randić index, the arithmetic-geometric index, and the atomic bond connectivity index are the most prominent topological indices in recent studies. The researchers in [4] concentrated on the derivation of the atom-bond connectivity index and its fourth version of the Cartesian products of several graphs, including the path graphs, regular graphs, and bipartite graphs. The numerical indices deliberated in this work can support the development of QSPR, which are essential in identifying bioactive compounds through physicochemical evaluations.

Eminent chemists have employed the Pólya's polynomials method [5] to compute the orbital of unsaturated hydrocarbons, a process that has drawn attention to graph theory. In this context, Hosoya developed a seminal concept known as the Hosoya polynomial [6], used for polynomial calculations of chemical graphs. Following this, the same formulations were revisited in 1996, expressed as the Wiener polynomial [7], and is often used in investigating distance-based properties. Cash [8] identified a correlation between the corresponding polynomials, enriching the understanding of these indices. Estrada et al. [9] provided a comprehensive analysis of applications of modified Wiener indices.

All graphs examined in this work are simple, having no multiple edges. Let $\mathcal{G}$ represent a finite group. The power graph $\mathcal{P}(\mathcal{G})$ is defined as a graph with vertex set $\mathcal{G}$, where two unique vertices are connected whenever one vertex is an integral power of the other. The concept of the power graph has found applications across directions, including group theory and ring theory. Perfect matchings in power graphs have been studied in [10], where the researchers demonstrated the upper and lower bounds and the maximum matching for finite nilpotent groups. The researchers in [11] focused on identifying the largest clique in power graphs and established that the number of edges is maximized when the underlying group is cyclic. The most recent survey on power graphs was published in 2021 [12]. Xiaoqi and Guo reviewed persistent topological Laplacians of simplicial, path, flag (di)graph, hyperdigraph, cellular sheaves, and N-chain complexes in a pedagogical manner [13]. Furthermore, numerous researchers have studied related algebraic concepts; see, for example, [14, 15] and the references therein. Moreover, research demonstrates the Hosoya-related properties of non-commuting and power graphs [16, 17]. In [18], Cheng et al. carried out a deeper investigation of minimal disconnecting sets, planarity, and their Laplacian energies of commuting graphs of semi-dihedral groups, while certain essential graph invariants were investigated in [19]. Moreover, the researchers in [20, 21] focused on a certain fundamental algebraic concept and the topological indices of non-commuting graphs.

Motivated by the aforementioned contributions, we focus on the power graphs of finite cyclic and non-cyclic groups. It is worth noting that computing topological indices for the power graph of any group remains a non-trivial task due to the combinatorial complexity of graph construction and variation across group structures. Nevertheless, in the growing interest, the literature reveals significant shortcomings in the enumeration of precise topological properties of power graphs. The lack of explicit and unified methodologies in the derivation of such classes of graphs is one of the major problems. This research gap is to be filled in this study, in which we will explore the analysis of eccentricity-based topological descriptors and the Hosoya characteristics of the graphs, as outlined in Table 1, offering new insights and a basis for further exploration.

The subsequent work is arranged as follows: Section 2 contains pertinent previous results and outlines the essential terminology used in this study. In Section 3, we examine several eccentricity-based topological descriptors of power graphs associated with finite cyclic and non-cyclic groups, while in Section 4, we determine the Hosoya properties for the same graphs. We conclude in Section 5, where the major findings are summarized and suggest possible directions for future research.

Table 1. List of topological indices.

Indices	Representation	Formula
First Zagreb eccentricity index [22]	$E_1(\Gamma)$	$\sum_{x\in V(\Gamma)} ec(x)^2$
Second Zagreb eccentricity index [22]	$E_2(\Gamma)$	$\sum_{x\in V(\Gamma)} ec(x)ec(y)$
Eccentric connectivity index [23]	$\xi^c(\Gamma)$	$\sum_{x\in V(\Gamma)} ec(x)d_x$
Connective eccentricity index [22]	$C^{\xi}(\Gamma)$	$\sum_{x\in V(\Gamma)} \frac{d_x}{ec(x)}$
Adjacent eccentric distance sum index [24]	$\xi^{sv}(\Gamma)$	$\sum_{x\in V(\Gamma)} \frac{ec(x)D(x)}{d_x}$
Eccentric distance sum index [23]	$\xi^d(\Gamma)$	$\sum_{x\in V(\Gamma)} ec(x)D(x)$
Zagreb related first irregularity index [25]	$IRM_1(\Gamma)$	$\sqrt{\frac{M_1(\Gamma)}{n}} - \frac{2e}{n}$
Zagreb related second irregularity index [25]	$IRM_2(\Gamma)$	$\sqrt{\frac{M_2(\Gamma)}{n}} - \frac{2e}{n}$

Note: The notation used in this table are explained in detail in Section 3.

2. Preliminaries

In this section, we introduce preliminary graph-theoretic characteristics and essential findings that support the discussions in subsequent sections.

Let Γ be a simple graph with n vertices and e edges. If v_1 and v_2 are adjacent, we write $v_1 \sim v_2$; otherwise, $v_1 \nsim v_2$. The degree (or valency) of a vertex v_1, written by d_{v_1}, corresponds to the collection of vertices connected to v_1. The degree sum is $S_v = \sum_{u\in N(v)} d_u$ of v, while $D(v) = \sum_{u\in V(\Gamma)} d(v,u)$ is the sum of all the distances from v. The distance between v_1 and v_2, denoted by $\text{dis}(v_1, v_2)$ is the length of the shortest path connecting them. The eccentricity of v_1, denoted $ec(v_1)$, is a total distance from v_1 to any other vertex in graph Γ. The diameter $\text{diam}(\Gamma)$ is the longest eccentricity amid the vertices, while the radius $\text{rad}(\Gamma)$ is the smallest such value. The join of two connected graphs Γ_1 and Γ_2, represented by $\Gamma_1 \vee \Gamma_2$, is obtained by taking their union and then adding an edge among each vertex of Γ_1 and vertices of Γ_2. A graph K_n is known as a complete graph if any two vertices of K_n are connected. A complete ℓ-partite graph is a graph if its vertex set is divided into ℓ pairwise independent sets such that each vertex in one set is connected to all vertices in the other sets. Additional notions and definitions used throughout this paper follow the conventions established in [26].

To compute the indices listed in Table 1, we utilize the edge partitions of $\mathcal{P}(\mathcal{G})$ to examine the maximum distances and reciprocal distances for each vertex. The corresponding results are summarized in Tables 2 and 3.

Table 2. Edge partitions when $\mathcal{G}$ is cyclic, for any $xy \in E(\mathcal{P}(\mathcal{G}))$.

Edge count	$(ec(x), ec(y))$ edges	(d_x, d_y) edges
$\frac{(p_2-1)(p_2-2)}{2}$	$(2, 2)$	$(n - p_1, n - p_1)$
$\frac{(p_1-1)(p_1-2)}{2}$	$(2, 2)$	$(n - p_2, n - p_2)$
$(p_2 - 1)(n - p_1 - p_2 + 2)$	$(1, 2)$	$(n - 1, n - p_1)$
$(p_1 - 1)(n - p_1 - p_2 + 2)$	$(1, 2)$	$(n - 1, n - p_2)$
$\frac{(n-p_1-p_2+2)(n-p1-p_2+1)}{2}$	$(1, 1)$	$(n - 1, n - 1)$

Table 3. Edge partitions when $\mathcal{G}$ is non-cyclic, for any $xy \in E(\mathcal{P}(\mathcal{G}))$.

Edge count	$(ec(x), ec(y))$ edges	(d_x, d_y) edges
$p_2 - 1$	$(1, 2)$	$(n - 1, p_2 - 1)$
$n - p_2$	$(1, 2)$	$(n - 1, p_1 - 1)$
$\frac{p_2(p_1-1)(p_1-2)}{2}$	$(2, 2)$	$(p_1 - 1, p_1 - 1)$
$\frac{(p_2-1)(p_2-2)}{2}$	$(2, 2)$	$(p_2 - 1, p_2 - 1)$

3. Topological properties

In this section, we explore several topological features of power graphs associated with cyclic and non-cyclic groups of order $n = p_1 p_2$. The subsequent lemma provides the key structural features of these graphs.

Lemma 1. *[27] Suppose $\mathcal{G}$ is a finite group with $|\mathcal{G}| = n = p_1 p_2$, where p_1, p_2 ($p_1 < p_2$) are different primes. Then*

- **(i)** *$\mathcal{G}$ is non-cyclic iff* $\mathcal{P}(\mathcal{G}) \cong K_1 \vee \left(\underbrace{K_{p_1-1} \cup K_{p_1-1} \cup \cdots \cup K_{p_1-1}}_{p_2} \cup K_{p_2-1} \right)$.
- **(ii)** *$\mathcal{G}$ is cyclic iff* $\mathcal{P}(\mathcal{G}) \cong K_{n-p_1-p_2+2} \vee (K_{p_1-1} \cup K_{p_2-1})$.

Consider $C(\mathcal{P}(\mathcal{G}), k)$, a collection of all those vertices of $\mathcal{P}(\mathcal{G})$ whose distance is k, that is,

$$C(\mathcal{P}(\mathcal{G}), k) = \Big\{(\ell_1, \ell_2); \ell_1, \ell_2 \in V(\mathcal{P}(\mathcal{G})) \mid \operatorname{dis}(\ell_1, \ell_2) = k\Big\}. \tag{3.1}$$

The following results from [28, Propositions 1 and 2] outlines fundamental properties of the maximum possible distance and degree in the power graphs of $\mathcal{G}$.

Proposition 1. *The total possible distances between the vertices of $\mathcal{P}(\mathcal{G})$ is described as:*

(1) If the group $\mathcal{G}$ is cyclic, then

$$\operatorname{dis}(\mathcal{P}(\mathcal{G}), i) = \begin{cases} \frac{1}{2}\left(n^2 - 3n + 2p_1 + 2p_2 - 2\right), & \textit{for } i = 1, \\ 2(p_1 - 1)(p_2 - 1), & \textit{for } i = 2. \end{cases}$$

(2) If $\mathcal{G}$ is non-cyclic, we obtain the following

$$\operatorname{dis}(\mathcal{P}(\mathcal{G}), i) = \begin{cases} \frac{p_2}{2}\left(p_1^2 - p_1 + p_2 - 1\right), & \text{for } i = 1, \\ \frac{p_2(p_1-1)(p_2-1)}{2}, & \text{for } i = 2. \end{cases}$$

Proposition 2. *The total possible degree d_x for each $x \in \mathcal{P}(\mathcal{G})$ is given by:*

(1) If $\mathcal{G}$ is cyclic, then

$$d_x = \begin{cases} n - 1, & \text{for } x \in K_{n-p_1-p_2+2}, \\ n - p_2, & \text{for } x \in K_{p_1-1}, \\ n - p_1, & \text{for } x \in K_{p_2-1}. \end{cases}$$

(2) If $\mathcal{G}$ is non-cyclic, then

$$d_x = \begin{cases} n - 1, & \text{for } x \in K_1, \\ p_1 - 1, & \text{for } x \in iK_{p_1-1}, \\ q - 1, & \text{for } x \in K_{p_2-1}. \end{cases}$$

Motivated by the above results, we determine $D(x)$, the sum of all distances from a given vertex x, in the following proposition.

Proposition 3. *For each x in $V(\mathcal{P}(\mathcal{G}))$, we have*

(1) If $\mathcal{G}$ is cyclic, then

$$D(x) = \begin{cases} n - 1, & \text{when } x \in K_{n-p_1-p_2+2}, \\ n + p_2 - 2, & \text{when } x \in K_{p_1-1}, \\ n + p_1 - 2, & \text{when } x \in K_{p_2-1}. \end{cases}$$

(2) For the case when $\mathcal{G}$ non-cyclic, we obtain

$$D(x) = \begin{cases} n - 1, & \text{when } x \in K_1, \\ 2n - p_2 - 1, & \text{when } x \in K_{p_2-1}, \\ 2n - p_1 - 1, & \text{when } x \in K_{n-p_2}. \end{cases}$$

The preceding propositions enable us to establish the following useful results.

Theorem 4. *The first and second eccentricity Zagreb indices of $\mathcal{P}(\mathcal{G})$ are described below:*

(1) If $\mathcal{G}$ is cyclic, then

$$\begin{aligned} E_1(\mathcal{P}(\mathcal{G})) =& n + 3(p_1 + p_2 - 2), \\ E_2(\mathcal{P}(\mathcal{G})) =& \frac{1}{2}(2 + n^2 + p_1 + p_2^2 + p_2 - 6n + p_2^2 + n(2p_1 + 2p_2 - 5)). \end{aligned}$$

(2) If $\mathcal{G}$ is non-cyclic, then

$$\begin{aligned} E_1(\mathcal{P}(\mathcal{G})) =& 4n - 3, \\ E_2(\mathcal{P}(\mathcal{G})) =& 2 + n + p_2(2p_1(p_1 - 3) + 2p_2 - 1). \end{aligned}$$

Proof. Consider a cyclic group $\mathcal{G}$. Then the vertex eccentricities can be examined using Table 2 along with the Propositions 1 and 2. Specifically, we have $ec(x) = 1$ and $ec(y) = 2$, where $x \in K_{n-p_1-p_2+2}$ and $y \in K_{p_1-1}$ or $y \in K_{p_2-1}$, respectively. Therefore, by applying the first eccentricity Zagreb index, we get

$$E_1(\mathcal{P}(\mathcal{G})) = (2 - p_1 + n - p_2) + 4(p_2 - 1) + 4(p_1 - 1).$$

For the second index, we use the edge partitions presented in Table 2. Then

$$\begin{aligned} E_2(\mathcal{P}(\mathcal{G})) = &\binom{2 - p_1 + n - p_2}{2} + 2(2 - p_1 + n - p_2)(p_1 - 1) + (2p_2 - 2)(2 - p_2 + n - p_1) \\ &+ 4\binom{p_2 - 1}{2} + 4\binom{p_1 - 1}{2}. \end{aligned}$$

This simplifies to

$$E_2(\mathcal{P}(\mathcal{G})) = \frac{1}{2}\left(2 + n^2 + p_1 + p_1^2 + p_2 - 6n + p_2^2 + n(2p_1 + 2p_2 - 5)\right).$$

Furthermore, the required eccentricity Zagreb indices can be determined for the non-cyclic group $\mathcal{G}$ using Table 3 along with the second parts of Propositions 1 and 2. Thus, we obtain

$$\begin{aligned} E_1(\mathcal{P}(\mathcal{G})) =& 4(p_2 - 1) + 4(n - p_2) + 1, \\ E_2(\mathcal{P}(\mathcal{G})) =& 4\binom{p_2 - 1}{2} + 4p_2\binom{p_1 - 1}{2} + n + p_2 - 2. \end{aligned}$$

After simplification, we get the desired result. □

Theorem 5. *The eccentric connectivity and connective eccentricity Zagreb indices of $\mathcal{P}(\mathcal{G})$ are as follows:*

(1) If $\mathcal{G}$ is a cyclic, then

$$\xi^c(\mathcal{P}(\mathcal{G})) = n^2 - 2 + p_1(3 - 4p_2) + 3p_2 + n(p_1 - 3 + p_2),$$

$$C^\xi(\mathcal{P}(\mathcal{G})) = \frac{1}{2}(2n^2 - 4 + p_1(3 - 2p_2) + 3p_2 - n(p_1 + p_2)).$$

(2) For the case, when $\mathcal{G}$ is non-cyclic, then

$$\xi^c(\mathcal{P}(\mathcal{G})) = 1 + n(2p_1 - 1) + 2p_2(p_2 - 1 - p_1),$$

$$C^\xi(\mathcal{P}(\mathcal{G})) = \frac{1}{2}(n - 1 + np_1 - (1 + p_1)p_2 + p_2^2).$$

Proof. If $\mathcal{G}$ is cyclic, then according to Proposition 2, we have $d_x = n - 1$ for all $x \in K_{n-p_1-p_2+2}$, $d_x = n - p_2$ for all $x \in K_{p_1-1}$, and $d_x = n - p_1$ for all $x \in K_{p_2-1}$. Additionally, the maximum eccentricity of the vertex is 2, while the remaining eccentricity values are mentioned in Table 2. Therefore,

$$\xi^c(\mathcal{P}(\mathcal{G})) = 2(n - p_2)(p_1 - 1) - (n - 1)(p_2 - 2 - n + p_1) + (2p_2 - 2)(n - p_1),$$

$$C^{\xi}(\mathcal{P}(\mathcal{G})) = (p_1 - 2 - n + p_2)(1 - n) + \frac{(p_1 - 1)(n - p_2)}{2} + \frac{(n - p_1)(p_2 - 1)}{2}.$$

Similarly, for the non-cyclic group, we follow the same procedure along with Table 3, then we obtain

$$\xi^{c}(\mathcal{P}(\mathcal{G})) = 2(p_2 - 1)^2 - 2(p_1 - 1)(p_2 - n) + (n - 1),$$
$$C^{\xi}(\mathcal{P}(\mathcal{G})) = (n - 1) + \frac{(n - p_2)(p_1 - 1)}{2} + \frac{(p_2 - 1)^2}{2}.$$

Thus, after the simplifications

$$\xi^{c}(\mathcal{P}(\mathcal{G})) = 1 + n(2p_1 - 1) + 2p_2(p_2 - 1 - p_1),$$

$$C^{\xi}(\mathcal{P}(\mathcal{G})) = \frac{1}{2}(n - 1 + np_1 - (1 + p_1)p_2 + p_2^2).$$

Which is the required result. □

Theorem 6. *The eccentric distance sum and adjacent eccentric distance sum indices of $\mathcal{P}(\mathcal{G})$ are as:*

(1) If $\mathcal{G}$ is cyclic, we obtain

$$\xi^{d}(\mathcal{P}(\mathcal{G})) = 6 + n^2 - 5p_2 + n(-3 + p_1 + p_2) + p_1(-5 + 4p_2),$$
$$\xi^{sv}(\mathcal{P}(\mathcal{G})) = (2 - p_1 + n) - p_2 + \frac{2(p_1 - 1)(p_2 - 2 + n)}{n - p_2} + \frac{2(n - 2 + p_1)(p_2 - 1)}{n - p_1}.$$

(2) For the case when $\mathcal{G}$ is non-cyclic, we obtain

$$\xi^{d}(\mathcal{P}(\mathcal{G})) = 4n^2 - n(5 + 2p_1) + 2p_2(1 + p_1 - p_2) + 1,$$
$$\xi^{sv}(\mathcal{P}(\mathcal{G})) = \frac{1 - p_1 + 2n(2n - 3 + p_1 - 2p_2) + 4p_2}{p_1 - 1}.$$

Proof. Since the eccentric distance sum depends on the distance and eccentricity formulation, combining these expressions, we get

$$\xi^{d}(\mathcal{P}(\mathcal{G})) = (2p_2 - 2)(n + p_1 - 2) - (p_1 - n - 2 + p_2)(n - 1) + (2p_1 - 2)(n - 2 + p_2).$$

To compute the adjacent distance sum index, we apply Propositions 2 and 3, and after simplification, we obtain:

$$\xi^{sv}(\mathcal{P}(\mathcal{G})) = (2 - p_1 + n - p_2) + (p_1 - 1)\left(\frac{2(n - 2 + p_2)}{(n - p_2)}\right) + (p_2 - 1)\left(\frac{2(n - 2 + p_1)}{(n - p_1)}\right).$$

Following the same way, the corresponding indices for the non-cyclic group $\mathcal{G}$ are determine as:

$$\xi^{d}(\mathcal{P}(\mathcal{G})) = (n - 1) + (2p_2 - 2)(2n - p_2 - 1) + 2(n - p_2)(2n - p_1 - 1),$$
$$\xi^{sv}(\mathcal{P}(\mathcal{G})) = 2(2n - p_2 - 1) + (n - p_2)\left(\frac{2(p_1 + 1 - 2n)}{1 - p_1}\right) + 1.$$

After simplifications, we can get the desired results. □

We know that the first Zagreb index is represented by the degree sum of all pair of adjacent vertices, while the sum of their product is the second Zagreb index. Thus, the corresponding indices are given by

$$M_1(\Gamma) = \sum_{x_1x_2\in E(\Gamma)} [d_{x_1} + d_{x_2}] \quad \text{and} \quad M_2(\Gamma) = \sum_{x_1x_2\in E(\Gamma)} d_{x_1}d_{x_2}.$$

Furthermore, several Zagreb indices of power graphs are investigated extensively in [28]. We are now in a position to examine the first and second irregularity Zagreb indices for the power graphs of finite groups.

Theorem 7. *The first irregularity Zagreb index of $\mathcal{P}(\mathcal{G})$ of $\mathcal{G}$ is defined by*

(1) If $\mathcal{G}$ is cyclic, we obtain

$$IRM_1(\mathcal{P}(\mathcal{G})) = \sqrt{n^2 - 3 - 2n + 4p_1 + 4p_2 - 4n + \frac{(p_1 + p_2 + 2)(1 - p_1)(1 - p_2)}{n}} - \frac{2e}{n}.$$

(2) For the case when $\mathcal{G}$ is non-cyclic, we obtain

$$IRM_1(\mathcal{P}(\mathcal{G})) = \sqrt{n - 3 + p_1 + \frac{\Big((p_1 - 2)^2 p_1 + (p_2 - 2)(p_2 - 1)\Big)_2}{n}} - \frac{2e}{n},$$

where e and n are the size and order of $\mathcal{P}(\mathcal{G})$, respectively.

Proof. The first Zagreb index is represented by the summation of degrees of all pair of adjacent vertices. To compute the first irregularity Zagreb index of $\mathcal{P}(\mathcal{G})$ for a cyclic group $\mathcal{G}$, we use the edge partition provided in Table 2, along with Proposition 2, which represents the maximum degrees of each vertex of $\mathcal{P}(\mathcal{G})$. Therefore, we obtain the following:

$$\begin{aligned} IRM_1(\mathcal{P}(\mathcal{G})) =& \frac{1}{\sqrt{n}}\Bigg((2n - 2p_1)\binom{p_2 - 1}{2} + (2n - 2)\binom{n - p_1 + 2 - p_2}{2} \\ &+ (p_2 - 1)(2 - p_2 + n - p_1)\Big((n - 1) + (n - p_1)\Big) + (2n - 2p_2)\binom{p_1 - 1}{2} \\ &+ (p_1 - 1)(n - p_1 - p_2 + 2)\Big((n - 1) + (n - p_2)\Big)\Bigg)^{\frac{1}{2}} - \frac{2e}{n}, \end{aligned}$$

where e and n denote the size and order of $\mathcal{P}(\mathcal{G})$, respectively. After simplification, we get

$$IRM_1(\mathcal{P}(\mathcal{G})) = \sqrt{n^2 - 3 - 2n + 4(p_1 - n + p_2) + \frac{(p_1 + p_2 + 2)(1 - p_1)(1 - p_2)}{n}} - \frac{2e}{n}.$$

Using the same arguments when $\mathcal{G}$ is non-cyclic, then

$$IRM_1(\mathcal{P}(\mathcal{G})) = \sqrt{\frac{(p_2 + n - 2)(p_2 - 1) + (n - p_2)(n - 2 + p_1) + \binom{p_2-1}{2}(2p_2 - 2) + p_2\binom{p_1-1}{2}(2p_1 - 2)}{n}} - \frac{2e}{n}.$$

After certain essential combinatorial and addition rules, we get

$$IRM_1(\mathcal{P}(\mathcal{G})) = \sqrt{n-3+p_1+\frac{\big((p_1-2)^2p_1+(p_2-2)(p_2-1)\big)_2}{n}}-\frac{2e}{n}.$$

Which is the required result. □

Theorem 8. *The second irregularity Zagreb index of $\mathcal{P}(\mathcal{G})$ is given by*

(1) If $\mathcal{G}$ is cyclic, we get

$$IRM_2(\mathcal{P}(\mathcal{G})) = \frac{1}{\sqrt{2}}\Big(7-3n^2+n^3+2p_1^2(p_2-1)+2p_1(p_2-1)(p_2+3)-2p_2(p_2+3)$$
$$+n(6p_2-3-6p_1p_2+6p_1)+\frac{(p_1-1)(2-5p_2+p_1(2p_2-5))(p_2-1)}{n}\Big)^{\frac{1}{2}}-\frac{2e}{n}.$$

(2) For the case when G is non-cyclic, we obtain

$$IRM_2(\mathcal{P}(\mathcal{G})) = \frac{1}{\sqrt{n}}\Big(\frac{1}{2}p_2(p_1-1)^3(p_1-2)+\frac{1}{2}(p_2-1)^3(p_2-2)$$
$$+(n-1)((p_2-1)^2+(p_1-1)(n-p_2))\Big)^{\frac{1}{2}}-\frac{2e}{n}.$$

Proof. We begin the proof by considering the case when $\mathcal{G}$ is cyclic. Since the irregularity Zagreb is the degree-based index and the degrees of all vertices in $\mathcal{P}(\mathcal{G})$ are deliberated in Proposition 2 and use Table 2, we get

$$IRM_2(\mathcal{P}(\mathcal{G})) = \frac{1}{\sqrt{n}}\Big(\binom{p_1-1}{2}(n-p_2)^2+\binom{n-p_1+2-p_2}{2}(n^2-n+1)$$
$$+\binom{p_2-1}{2}(n-p_1)^2+(n-1)(n-p_1+2-p_2)(n-p_2)(p_1-1)$$
$$+(1-p_2)(p_1-n)(n-p_1+2-p_2)(n-1)\Big)^{\frac{1}{2}}-\frac{2e}{n}.$$

The required result can be found after applying the combinatorial rules, so we get

$$IRM_2(\mathcal{P}(\mathcal{G})) = \frac{1}{\sqrt{2}}\Big(n^3-3n^2+7+2p_1^2p_2-2p_1^2+2p_1(p_2-1)(p_2+3)-2p_2(p_2+3)$$
$$+n(6p_2-3-6p_1(p_2-1))+\frac{(1-p_2)(2-5p_2+p_1(2p_2-5))(1-p_1)}{n}\Big)^{\frac{1}{2}}-\frac{2e}{n}.$$

Using the same arguments whenever $\mathcal{G}$ is non-cyclic, then

$$IRM_2(\mathcal{P}(\mathcal{G})) = \sqrt{\frac{(p_1-1)(n-p_2)(n-1)-(p_2-1)^2(1-n)+\binom{p_2-1}{2}(p_2-1)^2+p_2\binom{p_1-1}{2}(p_1-1)^2}{n}}-\frac{2e}{n}.$$

Therefore,

$$IRM_2(\mathcal{P}(\mathcal{G})) = \frac{1}{\sqrt{n}}\Big(\frac{1}{2}(p_1p_2 - 2p_2)(p_1-1)^3 + \frac{1}{2}(p_2-1)^3(p_2-2) + (n-1)((p_2-1)^2 + (p_1-1)(n-p_2))\Big)^{\frac{1}{2}} - \frac{2e}{n}.$$

This proves the desired result. □

4. Hosoya index

In this section, we examine the well-known Hosoya index of the power graphs over certain finite groups.

A vertex incident to an edge in a matching is called matched, while those not incident to any edge in the matching are known as unmatched. The Hosoya index is a renowned topological index that counts the number of matchings in a graph. It was first introduced by Hosoya in 1971 [29]. Its applications span chemical compositions, including estimating entropy, determining boiling points, and measuring heat of vaporization. Moreover, extensive research has been devoted to computing this index for certain graph structures. The Hosoya index was explored for the power graphs of generalized quaternion and dihedral groups in [16], while the Hosoya polynomials for the same graphs were examined in [30]. However, deriving this index for the power graphs of arbitrary finite groups remains a challenging problem. Therefore, we determine the Hosoya index for the power graphs of finite cyclic and non-cyclic groups.

Theorem 9. *Let $\mathcal{G}$ be a cyclic group and $\mathcal{P}(\mathcal{G})$ its power graph. Then the Hosoya index of $\mathcal{P}(\mathcal{G})$ is given by:*

$$1 + \sum_{i=1}^{\frac{\phi(n)+1}{2}} M_1^i + \sum_{i=1}^{\frac{p_1-1}{2}} M_2^i + \sum_{i=1}^{\frac{p_2-1}{2}} M_3^i + \sum_{i=1}^{p_1-1} M_4^i + \sum_{i=1}^{p_2-1} M_5^i + M_6 + M_7 + \sum_{i=2}^{\lfloor\frac{\phi(n)+1}{2}\rfloor} M_8^i + \sum_{i=2}^{\lfloor\frac{\phi(n)+1}{2}\rfloor} M_9^i$$
$$+ \sum_{i=2}^{\frac{p_1+p_2-2}{2}} M_{10}^i + \sum_{i=3}^{\frac{n}{2}} M_{11}^i + \sum_{i=3}^{\lfloor\frac{\phi(n)+p_1}{2}\rfloor} M_{12}^i + \sum_{i=3}^{\lfloor\frac{\phi(n)+p_2}{2}\rfloor} M_{13}^i + \sum_{i=3}^{\frac{\phi(n)-p_1-p_2+3}{2}} M_{14}^i + \sum_{i=4}^{\frac{\phi(n)+p_2-s}{2}} M_{15}^i$$
$$+ \sum_{i=4}^{\frac{\phi(n)+p_1-r}{2}} M_{16}^i + \sum_{i=4}^{\frac{\phi(n)-p_2-s+2}{2}} M_{17}^i + \sum_{i=4}^{\frac{\phi(n)-p_1-r+2}{2}} M_{18}^i + \sum_{i=5}^{\frac{\phi(n)+p_1+p_2-2r-2s-1}{2}} M_{19}^i,$$

where $s \in \{1, 2, \ldots, p_1 - 2\}$, $r \in \{1, 2, \ldots, p_2 - 2\}$, and for $1 \le \ell \le 19$, M_ℓ^i is defined explicitly in the proof.

Theorem 10. *Let $\mathcal{G}$ be a non-cyclic group and $\mathcal{P}(\mathcal{G})$ its power graph. Then the Hosoya of $\mathcal{P}(\mathcal{G})$ is:* $3 + \sum_{i=1}^{\frac{p_2-1}{2}} M_2^i + \sum_{i=1}^{p_2\frac{p_1-1}{2}} M_1^i + M_3^1 + M_4^1 + \sum_{i=2}^{\frac{p_1+p_2-2}{2}} M_5^i + \sum_{i=2}^{\frac{p_1-1}{2}} M_6^i + \sum_{i=2}^{\frac{p_1-1}{2}} M_7^i + \sum_{i=2}^{\frac{p_2-1}{2}} M_8^i + \sum_{i=2}^{\frac{p_2-1}{2}} M_9^i + \sum_{i=2}^{\frac{p_1+p_2-2}{2}} M_{10}^i + \sum_{i=3}^{\frac{p_1+p_2-2}{2}} M_{11}^i + \sum_{i=3}^{\frac{p_1+p_2-2}{2}} M_{12}^i + \sum_{i=3}^{\frac{p_1+p_2-3}{2}} M_{13}^i$. *For any $1 \le \ell \le 13$, M_ℓ^i is defined explicitly in the proof.*

To prove the above results, we begin with some essential computations. The researchers in [31] examined that the complete graph K_n of order n has the largest Hosoya index among all graphs of the same order. Generally, the Hosoya index of K_n is defined by:

$$1 + \sum_{t=1}^{\lfloor \frac{n}{2} \rfloor} \frac{1}{t} \prod_{j=0}^{t-1} \binom{n-2j}{2},$$

where m_t represents the number of matchings of cardinality t, whenever $1 \le t \le \lfloor \frac{n}{2} \rfloor$. This formula enumerates all non-empty matchings in K_n, as presented in Table 4.

Table 4. Non-empty matchings in K_n, for $n \ge 2$.

K_n	m_1	m_2	m_3	m_4	$\cdots$	m_i, $(1 \le i \le n)$
K_3	$\binom{3}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2}\binom{4}{2}\binom{2}{2}$				
K_5	$\binom{5}{2}$	$\frac{1}{2}\binom{5}{2}\binom{3}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{3}\binom{6}{2}\binom{4}{2}\binom{2}{2}$			
K_7	$\binom{7}{2}$	$\frac{1}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{3}\binom{7}{2}\binom{5}{2}\binom{3}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2}\binom{8}{2}\binom{6}{2}$	$\frac{1}{3}\binom{8}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{4}\binom{8}{2}\binom{6}{2}\binom{4}{2}\binom{2}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_n	$\binom{n}{2}$	$\frac{1}{2}\binom{n}{2}\binom{n-2}{2}$	$\frac{1}{3}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}$	$\frac{1}{4}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}\binom{n-6}{2}$	$\cdots$	$\frac{1}{i}\prod_{k=0}^{i-1}\binom{n-2k}{2}$

The Hosoya polynomial of a graph Γ is defined as follows:

$$H(\Gamma, x) = \sum_{k \ge 0} \text{dis}(\Gamma, k) x^k,$$

where $\text{dis}(\Gamma, k)$ symbolizes the distance of pair of vertices (u, w) such that $\text{dis}(u, w) = k$, while $k \le \text{diam}(\Gamma)$. Similarly, the reciprocal status Hosoya polynomial of Γ was explored in [32] and is given below:

$$H_r(\Gamma, x) = \sum_{uv \in V(\Gamma)} x^{r(u)+r(v)},$$

where $r(v) = \sum_{u \in V(\Gamma), u \ne v} \frac{1}{\text{dis}(v,u)}$ is called the reciprocal transmission or the reciprocal status of v.

Theorem 11. *[30] The Hosoya polynomial of $\mathcal{P}(\mathcal{G})$ of a finite cyclic group $\mathcal{G}$ is as follows:*

$$H(\mathcal{P}(\mathcal{G}), x) = (n - p_2 - p_1 + 1)x^2 + \frac{1}{2}\left(n^2 - 3n + 2p_2 + 2p_1 - 2\right)x + n.$$

Similarly, if $\mathcal{G}$ is non-cyclic, then

$$H_r(\mathcal{P}(\mathcal{G}), x) = \frac{p_2}{2}(p_1 - 1)^2(p_2 - 1)x^2 + \frac{p_2}{2}\left(p_1^2 + p_1 - p_2 - 1\right)x + n.$$

Theorem 12. *[30] The reciprocal status Hosoya polynomials of $\mathcal{P}(\mathcal{G})$ for cyclic and non-cyclic groups $\mathcal{G}$ are, respectively, given below:*

$$\begin{aligned}H_r(\mathcal{P}(\mathcal{G}), x) &= (p_2-1)(n+2-p_2-p_1)x^{\frac{4n-p_1-3}{2}} + (n-p_2-p_1+2)(p_2-1)x^{\frac{4n-p_2-3}{2}}\\ &+ \frac{(p_1-2)(p_1-1)}{2}x^{2n-p_1-1} + \frac{(n+2-p_2-p_1)(n+1-p_2-p_1)}{2}x^{2(n-1)}\\ &+ \frac{(p_1-2)(p_1-1)}{2}x^{2n-p_2-1},\end{aligned}$$

$$\begin{aligned}H_r(\mathcal{P}(\mathcal{G}), x) &= (p_2-1)x^{\frac{3n+p_2-4}{2}} + p_2(p_1-1)x^{\frac{4n-3p_2-1}{2}} + \frac{p_2(p_1-2)(p_1-1)}{2}x^{2n-3p_2+1}\\ &+ \frac{(p_2-2)(p_2-1)}{2}x^{n+p_2-2}.\end{aligned}$$

We are now in the position to present the proofs of our theorems as mentioned above.

Proof of Theorem 9. Forming the structure of $\mathcal{P}(\mathcal{G})$ of order $n = p_1p_2$, the vertices of $K_{\phi(n)+1}$ are connected to every vertex of K_{p_1-1} and K_{p_2-1}. To determine the possible matchings between the edges of $\mathcal{P}(\mathcal{G})$, we identify the edges into the following five distinct types:
T_1: $y \sim z$, when $y,\ z \in K_{\phi(n)+1}$;
T_2: $y \sim z$, when $y,\ z \in K_{p_1-1}$;
T_3: $y \sim z$, when $y,\ z \in K_{p_2-1}$;
T_4: $y \sim z$, when $y \in K_{\phi(n)+1}$, $z \in K_{p_1-1}$;
T_5: $y \sim z$, when $y \in K_{\phi(n)+1}$, $z \in K_{p_2-1}$.

Let M_j denote the matching between the edge of $\mathcal{P}(\mathcal{G})$, where $1 \le j \le 19$. Then the total possible matchings M_j can be classified into the following categories (see Table 5):

M_1: To start a matching M_1 of order 1, we note that $K_{\phi(n)+1}$ is a complete subgraph of order $\phi(n) + 1$. Therefore, the total number of i order matchings of type M_i for $1 \le i \le \frac{\phi(n)+1}{2}$, is obtain by:

$$M_1^i = \frac{1}{i}\prod_{k=0}^{i-1}\binom{(\phi(n)+1)-2k}{2}.$$

Similarly, M_2 and M_3 types correspond to the complete subgraph $K_{p_1} - 1$ and $K_{p_2} - 1$ of order $p_1 - 1$ and $p_2 - 1$, respectively. Thus, the total possible M_i and M_j matchings of order i and j, respectively, for $1 \le i \le \frac{p_1-1}{2}$ and $1 \le i \le \frac{p_2-1}{2}$, are given as:

$$M_2^i = \frac{1}{i}\prod_{k=0}^{i-1}\binom{(p_1-1)-2k}{2} \text{ and } M_3^i = \frac{1}{i}\prod_{k=0}^{i-1}\binom{(p_2-1)-2k}{2}.$$

M_4: To determine the matching of type M_4, we first consider M_4^1, which is a matching of order 1. Since there are $p_1 - 1$ vertices in K_{p_1-1}, and each of these is connected to every vertex of $K_{\phi(n)+1}$, the total number of edges incident to K_{p_1-1} is $n - p_1 - p_2 + 2$. Therefore, $M_4^1 = (p_1-1)(n-p_1-p_2+2)$.

Now for M_4^2-type matchings of order 2, consider two edges, that is, $v_1 \sim v_2$, where $v_1 \in K_{\phi(n)+1}$ and $v_2 \in K_{p_1-1}$, and $v_3 \sim v_4$, where $v_3 \in K_{\phi(n)+1} \setminus \{v_1\}$ and $v_4 \in K_{p_1-1} \setminus \{v_2\}$, such that two edges are disjoint and each connects a vertex from $K_{\phi(n)+1}$ to K_{p_1-1}. The total possible such disjoint matchings of order 2 is $\phi(n)(n - p_1 - p_2 + 2)$. Therefore, we obtain:

$$M_4^2 = \binom{p_1 - 1}{2}\phi(n)\,(n - p_1 - p_2 + 2)\,.$$

Following the same criteria for any $2 \le i \le p_1 - 1$, we get:

$$M_4^i = \binom{p_1 - 1}{i}\phi(n)\,(n - p_1 - p_2 + 2)\,. \tag{4.1}$$

Using the similar arguments for M_5 type matchings, we have

$$M_5^i = \binom{p_2 - 1}{i}\phi(n)(n - p_1 - p_2 + 2),\ \text{for } 1 \le i \le p_2 - 1. \tag{4.2}$$

M_6: This type matching is obtained by taking the edges of T_1 as those within the complete subgraph $K_{\phi(n)+1}$, while the edges of T_2 correspond to those within K_{p_1-1}. According to Table 4, there are

$$\frac{1}{\kappa_1}\prod_{i=0}^{\kappa_1-1}\binom{\phi(n) + 1 - 2i}{2}$$

matchings of order κ_1 of $K_{\phi(n)+1}$, and the vertices of $K_{\phi(n)+1}$ are connected to the vertices of K_{p_1-1}. Thus, there must be $\kappa_2 - 1$ matchings of K_{p_1-1} together with $K_{\phi(n)+1}$.

However, when $p_1 = 3$, then there is no matching of order $\kappa_2 - 1$ in K_{p_1-1} together with $K_{\phi(n)+1}$. Hence, for $p_1 > 3$, the maximum matchings of M_6 type is expressed below:

$$M_6 = (\phi(n) + 1) + \frac{1}{\kappa_1}\prod_{i=0}^{\kappa_1-1}\binom{\phi(n) + 1 - 2i}{2}\cdot\frac{1}{\kappa_2 - 1}\prod_{j=0}^{\kappa_1-2}\binom{p_1 - 1 - 2j}{2},$$

where $1 \le \kappa_1 \le \lfloor\frac{\phi(n)+1}{2}\rfloor$, $1 \le \kappa_2 \le \frac{p_1-1}{2}$, for odd primes p_1 and p_2, such that $p_1 > 3$.

M_7: Using the same arguments as M_6 type matchings, and M_7 type matchings, given in Table 5, we obtain the following:

$$M_7 = (\phi(n) + 1) + \frac{1}{\ell_1}\prod_{i=0}^{\ell_1-1}\binom{\phi(n) + 1 - 2i}{2}\cdot\frac{1}{\ell_2 - 1}\prod_{j=0}^{\ell_2-2}\binom{p_2 - 1 - 2j}{2},$$

where $1 \le \ell_1 \le \lfloor\frac{\phi(n)+1}{2}\rfloor$, $1 \le \ell_2 \le \frac{p_2-1}{2}$, for odd primes p_1 and p_2.

M_8: There are two type of edges involved in this derivation: Edges of type T_1 and T_4. Since the order of the matchings in $K_{\phi(n)+1}$ is k, it forms an induced subgraph of type T_1. In addition, we consider the edges of type T_4, where every edge is an incident from a vertex in $K_{\phi(n)+1}$ to a vertex in K_{p_1-1}. This means that there are M_4^l type of matchings in T_4. Thus, the matchings of type M_8^i of order k for $2 \le i \le \left\lfloor\frac{\phi(n)+1}{2}\right\rfloor$ are as follows:

$$M_8^i = M_4^l\cdot\frac{1}{i - 1}\prod_{j=0}^{i-2}\binom{\phi(n) - 2j}{2},\ \text{where } M_4^l \text{ is obtained in Eq. 4.1.}$$

M_9**:** Using similar arguments as those for M_8-type, we can derive the total number of M_9-type matchings as follows: $M_9^i = M_5^l \cdot \frac{1}{i-1}\prod_{j=0}^{i-2}\binom{\phi(n)-2j}{2}$, for $2 \le i \le \left\lfloor \frac{\phi(n)+1}{2} \right\rfloor$, and M_5^l is given in Eq (4.2).

M_{10}**:** Since the edges of T_2 and T_3 types are disjoint and associated with different subgraphs, so the matchings of type M_{10} are obtained by combining a matching formed from edges of type T_2 with a matching formed from edges of type T_3. Note that in both cases, these edges belong to K_{p_1-1} and K_{p_2-1}, respectively. We denote them by F_{10}^l for $1 \le l \le \frac{p_1-1}{2}$ and H_{10}^m for $1 \le m \le \frac{p_2-1}{2}$. Therefore, for $2 \le i \le \frac{p_1+p_2-2}{2}$, we have the following:

$$\begin{aligned}
M_{10}^2 &= F_{10}^1 H_{10}^1,\\
M_{10}^3 &= F_{10}^1 H_{10}^2 + F_{10}^2 H_{10}^1,\\
M_{10}^4 &= F_{10}^1 H_{10}^3 + F_{10}^2 H_{10}^2 + F_{10}^3 H_{10}^1,\\
&\vdots\\
M_{10}^i &= \sum_{j=1}^{i-1} F_{10}^j H_{10}^{i-j},
\end{aligned}$$

where $F_{10}^j = 0$ for $j > p_1 - 1$ and $H_{10}^{i-j} = 0$ for $i - j > p_2 - 1$.

M_{11}**:** This type of matching is obtained by considering T_1, T_2, and T_3 types of edges, which correspond to $K_{\phi(n)+1}$, K_{p_1-1}, and K_{p_2-1}, respectively. Since all subgraphs are disjoint, the matchings of order i for $3 \le i \le \frac{n}{2}$ can be expressed as A_{11}^l, B_{11}^m, and C_{11}^t, where $1 \le l \le \frac{\phi(n)+1}{2}$, $1 \le m \le \frac{p_1-1}{2}$, and $1 \le t \le \frac{p_2-1}{2}$. Therefore,

$$\begin{aligned}
M_{11}^3 &= A_{11}^1 B_{11}^1 C_{11}^1,\\
M_{11}^4 &= A_{11}^1 B_{11}^1 C_{11}^2 + A_{11}^1 B_{11}^2 C_{11}^1 + A_{11}^2 B_{11}^1 C_{11}^1,\\
&\vdots\\
M_{11}^i &= \sum_{j=2}^{i} A_{11}^{j-1} B_{11}^{i-j} C_{11}^{i-j-1},
\end{aligned}$$

where $A_{11}^j = 0$ for $j > \phi(n) + 1$, $B_{11}^{i-j} = 0$ for $i - j > p_1 - 1$, and $C_{11}^{i-j-1} = 0$ for $i - j - 1 > p_2 - 1$.

M_{12}**:** Let M_{12}^i represent the i order matchings, for $i = 1, 2$. In this case, $M_{12}^i = 0$. Observe that the edges of types T_1 and T_2 are disjoint, while the edges of T_2 are connected with those of T_4, forming a bridge among the disjoint subgraphs. There are $\phi(n) + 1$ edges connecting every vertex of T_2 to those in T_4. Now, let A_{12}^l and B_{12}^m denote the matchings of T_1 and T_2, respectively, for $1 \le l \le \left\lfloor \frac{\phi(n)+1}{2} \right\rfloor$ and $1 \le m \le \left\lfloor \frac{p_1-1}{2} \right\rfloor$. Thus, the possible matchings of type M_{12}^i of order i for $3 \le i \le \left\lfloor \frac{\phi(n)+p_1}{2} \right\rfloor$ is given by:

$$M_{12}^i = (p_1 - 1)(\phi(n) + 1) \sum_{j=1}^{i} A_{12}^j B_{12}^{i-j},$$

where $A_{12}^j = 0,$ for $j > \phi(n) + 1$ and $B_{12}^{i-j} = 0,$ for $i - j > p_1 - 1$.

M_{13}**:** Using the similar argument as those for M_{12} type, we can determine the i order matchings of M_{13} type for $3 \leq i \leq \left\lfloor \frac{\phi(n)+p_2}{2} \right\rfloor$. Thus,

$$M_{13}^{i} = (p_2 - 1)(\phi(n) + 1) \sum_{j=1}^{i} C_{13}^{j} D_{13}^{i-j},$$

where $C_{13}^{j} = 0$ for $j > \phi(n) + 1$ and $D_{13}^{i-j} = 0$ for $i - j > p_1 - 1$ denote the matchings of T_1 and T_3, respectively.

M_{14}**:** M_{14} matchings are formed by combining the edges of T_1, T_4, and T_5. Let M_{14}^{i} denote the i order matchings for $i = 1, 2$. In this case, we have $M_{14}^{i} = 0$. Furthermore, every vertex of $K_{\phi(n)+1}$ is edge incident to each vertex of K_{p_1-1} and K_{p_2-1}. Therefore, there are $i = \phi(n) - p_1 - p_2 + 3$ matchings between uv edges such that $u, v \in K_{\phi(n)+1}$ and $u, v \notin K_{p_1-1}$, $u, v \notin K_{p_2-1}$. Then, the matchings of the subgraph $K_{\phi(n)-p_1-p_2+3}$ of order i for $3 \leq i \leq \frac{\phi(n)-p_1-p_2+3}{2}$ are given as

$$\frac{1}{i} \prod_{j=0}^{i-1} \binom{\phi(n) - p_1 - p_2 - 2j + 3}{2}.$$

Hence, the total number of matchings of M_{14} is:

$$M_{14}^{i} = (\phi(n) + 1)(p_1 - 1)(p_2 - 1) \cdot \frac{1}{i} \prod_{j=0}^{i-1} \binom{\phi(n) - p_1 - p_2 - 2j + 3}{2}.$$

M_{15}**:** It is based on the matching classification in Table 5. Let M_{15}^{i} denote the total possible i order matchings for $i \in \{1, 2, 3\}$. In this case, we have $M_{15}^{i} = 0$. Matchings of type M_{15} consist of edges considered from T_1, T_2, T_3, and T_4 types. Note that the edges of T_3 correspond to the edges of K_{p_2-1}. Let A_{15}^{l} denote the T_3 type matchings of order l, whenever $1 \leq l \leq \frac{p_2-1}{2}$. In addition, every vertex of $K_{\phi(n)+1}$ is adjacent to K_{p_1-1} in T_4. Thus, there are $p_1 - 1$ order matchings of T_4 and it is denoted by s, where $s \in \{1, 2, \ldots, p_1 - 2\}$. From the remaining vertices of $K_{\phi(n)+2-p_1}$ and K_{p_1-s-1}, we define B_{25}^{m} as the matchings of $K_{\phi(n)+2-p_1}$ for $1 \leq m \leq \frac{\phi(n)+2-p_1}{2}$ and K_{p_1-s-1} depending on s, which determine the order of T_4 type matchings. Therefore, the possible matchings of M_{15}^{i} for $4 \leq i \leq \frac{\phi(n)+p_2-s}{2}$ are as follows:

$$M_{15}^{i} = \left[\sum_{s=1}^{p_1-1} s X_{15}^{s} \right] \left[\sum_{j=1}^{i-3} B_{15}^{j} A_{15}^{i-j} \right],$$

where $X_{15}^{s} = \frac{1}{k-s} \prod_{j=0}^{k-s} \binom{p_1-s-2j-1}{2}$, $B_{15}^{j} = 0$, for $j > \frac{p_2-1}{2}$, and $A_{15}^{i-j} = 0$, for $i - j > \left(\frac{\phi(n)-p_1+2}{2} \right)$.

M_{16}**:** Every matching of this type of order is i for $4 \leq i \leq \frac{\phi(n)+p_1-r}{2}$, where $r \in \{1, 2, \ldots, p_2 - 2\}$ can be obtain using similar arguments as in M_{15}. Thus, we get:

$$M_{16}^{i} = \left[\sum_{r=1}^{p_2-1} r Y_{16}^{r} \right] \left[\sum_{j=1}^{i-3} T_{16}^{j} U_{16}^{i-j} \right],$$

where

$$T_{16} = \frac{1}{l}\prod_{k=0}^{l-1}\binom{p_1-1-2k}{2}, \quad U_{16} = \frac{1}{m}\prod_{k=0}^{m-1}\binom{\phi(n)-p_1+2-2k}{2}, \quad T_{16}^{j} = 0 \quad \text{for } j > \frac{p_1-1}{2},$$

$$U_{16}^{i-j} = 0 \quad \text{for } i-j > \left(\frac{\phi(n)-p_2+2}{2}\right), \quad Y_{16}^{r} = \frac{1}{k-r}\prod_{j=0}^{k-r}\binom{p_2-r-2j-1}{2}.$$

M_{17}: Every matching of type M_{17}^{i} of order i can be generated by considering the edges of types T_1, T_2, T_4, and T_5. The edges of T_1 form the complete subgraph $K_{\phi(n)+1}$, and the vertices of $K_{\phi(n)+1}$ are incident to every vertex of K_{p_1-1} and K_{p_2-1}, and suppose

$$A_{17}^{l} = \frac{1}{l}\prod_{t=0}^{l-1}\binom{\phi(n)-p_1-p_2+3-2t}{2}, \text{ for } 1 \le l \le \frac{\phi(n)-p_1-p_2+3}{2},$$

represent the matchings in $K_{\phi(n)-p_1-p_2+3}$ obtained after removing common matchings with K_{p_1-1}. Furthermore, let $s \in \{1, 2, \ldots, p_1-1\}$ denote the number of matchings between xy edges such that $x \in K_{\phi(n)+1}$, $y \in K_{p_2-1}$ and

$$B_{17}^{m} = \frac{1}{m}\prod_{t=0}^{m-1}\binom{p_1-s-1-2t}{2}, \text{ where } 1 \le m \le \frac{p_1-1-s}{2}$$

is the matchings set of K_{p_1-1-s}. Therefore, the matchings of type M_{17}^{i} of order i, where $4 \le i \le \frac{\phi(n)-p_2-s+2}{2}$, are given as:

$$M_{17}^{i} = s(\phi(n)+1)[(p_1-1)(p_2-1)]\sum_{j=1}^{i-3} A_{17}^{j}B_{17}^{i-j}, \quad \text{where } 1 \le s \le p_1-1, \text{ and}$$

$$A_{17}^{j} = 0, \quad \text{for } j > \frac{\phi(n)-p_1-p_2+3}{2}, \quad B_{17}^{i-j} = 0, \quad \text{for } i-j > \frac{p_1-1-s}{2}.$$

M_{18}: Similarly, the matchings of type M_{18}^{i} of order i for $4 \le i \le \frac{\phi(n)-p_1-r+2}{2}$, with $r \in \{1, 2, \ldots, p_2-1\}$ can be obtained as follows:

$$U_{18}^{l} = \frac{1}{l}\prod_{j=0}^{l-1}\binom{\phi(n)-p_1-p_2-2j+3}{2}, \quad \text{for } 1 \le l \le \frac{\phi(n)-p_1-p_2+3}{2},$$

$$T_{18}^{m} = \frac{1}{m-r}\prod_{t=o}^{m-r-1}\binom{p_2-r-1-2t}{2}, \quad \text{for } 1 \le m \le \frac{p_2-r-1}{2}.$$

Therefore,

$$M_{18}^{i} = r\,(\phi(n)+1)\,[(p_1-1)(p_2-1)]\sum_{j=1}^{i-3} U_{18}^{j}T_{18}^{i-j},$$

where $U_{18}^{j} = 0$ for $j > \frac{\phi(n)-p_1-p_2+3}{2}$ and $T_{18}^{i-j} = 0$ for $i-j > \frac{p_2-r-1}{2}$, $\quad r \in \{1, 2, \ldots, p_2-1\}$.

M_{19}**:** Since the edges of T_1, T_2, and T_3 correspond to the complete subgraphs $K_{\phi(n)+1}$, K_{p_1-1}, and K_{p_2-1}, respectively, and since the edges of type T_4 and T_5 share common vertices, we have $M^t_{19} = 0$ for $1 \le t \le 4$. Next, let s denote the number of edges in a matching of type T_4, where $1 \le s \le p_1 - 1$, and let r denote the total possible edges in a T_5 matchings, where $1 \le r \le p_2 - 1$. After removing s number of edges from $K_{\phi(n+1)}$ and K_{p_1-1} and r edges from $K_{\phi(n+1)}$ and K_{p_2-1}, we obtain the remaining matchings of the subgraphs $K_{\phi(n)-s-r+1}$, K_{p_1-s-1}, and K_{p_2-r-1}:

$$\frac{1}{k}\prod_{j=0}^{k-1}\binom{\phi(n)-r-s-2j+1}{2}, \quad \frac{1}{l}\prod_{t=0}^{l-1}\binom{p_1-s-2t-1}{2}, \quad \text{and} \quad \frac{1}{m}\prod_{u=0}^{m-1}\binom{p_2-r-2u-1}{2}.$$

Combining all these terms with the T_4 and T_5 type edges, the total possible matchings of M^i_{19} of order i for $5 \le i \le \frac{\phi(n)+p_1+p_2-2r-2s-1}{2}$ are obtained as follows:

$$\begin{aligned} M_{19} = r + s + \frac{1}{k}\prod_{j=0}^{k-1}\binom{\phi(n)-s-r-2j+1}{2} + \frac{1}{l}\prod_{t=0}^{l-1}\binom{p_1-s-2t-1}{2} \\ + \frac{1}{m}\prod_{u=0}^{m-1}\binom{p_2-r-2u-1}{2}, \quad \text{where } 1 \le s \le p_1-1, \quad 1 \le r \le p_2-1, \\ 1 \le k \le \frac{\phi(n)-r-s+1}{2}, \quad 1 \le l \le \frac{p_1-s-1}{2}, \quad \text{and } 1 \le m \le \frac{p_2-r-1}{2}. \end{aligned}$$

Table 5. Classification of all possible types of matchings in $\mathcal{P}(\mathcal{G})$.

Types	Descriptions
M_1	Matching between T_1
M_2	Matching between T_2
M_3	Matching between T_3
M_4	Matching between T_4
M_5	Matching between T_5
M_6	Matching between T_1 and T_2
M_7	Matching between T_1 and T_3
M_8	Matching between T_1 and T_4
M_9	Matching between T_1 and T_5
M_{10}	Matching between T_2 and T_3
M_{11}	Matching between T_1, T_2 and T_3
M_{12}	Matching between T_1, T_2 and T_4
M_{13}	Matching between T_1, T_3 and T_5
M_{14}	Matching between T_1, T_4 and T_5
M_{15}	Matching between T_1, T_2, T_3 and T_4
M_{16}	Matching between T_1, T_2, T_3, and T_5
M_{17}	Matching between T_1, T_2, T_4 and T_5
M_{18}	Matching between T_1, T_3, T_4 and T_5
M_{19}	Matching between T_1, T_2, T_3, T_4 and T_5

Hence, by combining the cases mentioned in Table 5 and counting the arguments, we get the required result.

We are now ready to determine the Hosoya index of the power graphs associated with finite non-cyclic groups.

Proof of Theorem 10. To establish this result, we apply the second part of Lemma 1 with Table 3. Based on this partition, $\mathcal{P}(\mathcal{G})$ contains the following possible types of edges:
T_1: $a \sim b$ for $a, b \in K_{p_1-1}$;
T_2: $a \sim b$ for $a, b \in K_{p_2-1}$;
T_3: $a \sim b$ for $a = e,\ b \in K_{p_1-1}$;
T_4: $a \sim b$ for $a = e,\ b \in K_{p_2-1}$.

According to the edge types discussed above, the following M_ℓ matchings for $1 \leq \ell \leq 13$ can occur between the edges of $\mathcal{P}(\mathcal{G})$:

M_1: One can see that the induced subgraph of T_1 is complete, i.e, K_{p_1-1}, and the total matchings of order l in K_{p_1-1}, for $1 \leq l \leq \frac{p_1-1}{2}$ is $M_1 = \frac{1}{l}\prod_{j=0}^{l-1}\binom{p_1-1-2j}{2}$. Since there are p_2 copies of K_{p_1-1}, the total number of matchings of type M_1^i, for $1 \leq i \leq \frac{p_2(p_1-1)}{2}$ is given by

$$M_1^i = \frac{p_2}{i}\prod_{j=0}^{i-1}\binom{p_1-1-2j}{2}.$$

M_2: Using the same arguments as in the case of M_1, the total i order matchings of M_2, for $1 \leq i \leq \frac{p_2-1}{2}$ is $M_2^i = \frac{1}{i}\prod_{j=0}\binom{p_2-2j-1}{2}$.

M_3: It is evident from the structure of graph $\mathcal{P}(\mathcal{G})$ that the identity element of $\mathcal{G}$ is connected to every vertex. We conclude that for any edge of T_3, identity e is shared across all p_2 copies of K_{p_1-1}. Hence, $M_3^1 = 1$.

Similar reasoning applies to M_4 and M_{10}, leading to the conclusion that $M_4^1 = 1$ and $M_{10}^1 = 1$, respectively.

M_5: It is clear from the classifications of edge types that T_1 and T_2 given in Table 6 are disjoint. Therefore, a matching of type M_5 is obtained by combining matchings formed from T_1 type edges with those from T_2 type edges. Since every edge of T_1 is also an edge of K_{p_1-1}, this results in the l order matchings of A_5^l for $1 \leq l \leq \frac{p_2-1}{2}$. Similarly, the edges of T_2 corresponds to those in K_{p_2-1}, yielding B_5^l matchings of order m, where $1 \leq m \leq \frac{p_2-1}{2}$. The expressions of these matchings are

$$A_5^l = \frac{1}{l}\prod_{J=0}^{l-1}\binom{p_1-1-2J}{2}, \quad B_5^m = \frac{1}{m}\prod_{s=0}^{m-1}\binom{p_2-2s-1}{2}.$$

Furthermore, there are p_2 copies of K_{p_1-1}, each connected only to the identity element. Thus, the total number of matchings of M_5^i of order i for $2 \leq i \leq \frac{p_1+p_2-1}{2}$, is given by:

$$M_5^1 = 0, \quad M_5^2 = p_2 A_5^1 B_5^1, \quad M_5^3 = p_2\left(A_5^1 B_5^1 + A_5^2 B_5^1\right),$$
$$M_5^4 = p_2\left(A_5^1 B_5^1 + A_5^2 B_5^2 + A_5^3 B_5^1\right)$$

$$\vdots$$

$$M_5^i = \sum_{t=1}^{i-1} A_5^t B_5^{i-t}, \text{ where } A_5^t = 0 \text{ for } t > \frac{p_1-1}{2}, \quad B_5^{i-t} = 0 \text{ for } i-t > \frac{p_2-1}{2}.$$

M_6: This type of matching is obtained by considering one edge of type T_3 and at least one edge of T_1 type. Note that every edge of T_1 is also an edge of K_{p_1-1}, so any matching involving edges of T_1 is also a matching of K_{p_1-1}. Furthermore, every edge of T_3 shares a common vertex (the identity), which is connected to all vertices in every p_2 copies of K_{p_1-1}. Therefore, a matching of type M_6 of order i is obtained by combining one edge from T_3 with a matching of order $i-1$ in K_{p_1-1}. Hence,

$$M_6^i = 1 + \frac{1}{i-1}\prod_{j=0}^{i-2}\binom{p_1-2j-1}{2} + \frac{p_2-1}{i}\prod_{j=0}^{i-1}\binom{p_1-2j-1}{2}, \text{ where } 2 \le i \le \frac{p_1-1}{2}.$$

M_7: Using the similar argument as for the M_6 type matchings, we can compute the number of matchings to types M_7 and M_9, respectively:

$$M_7^i = 1 + \frac{p_2}{i}\prod_{j=0}^{i-1}\binom{p_1-2j-1}{2}, \text{ where } 2 \le i \le \frac{p_1-1}{2}.$$

$$M_9^i = 1 + \frac{1}{i-1}\prod_{s=0}^{i-2}\binom{p_2-2s-1}{2}, \text{ where } 2 \le i \le \frac{p_2-1}{2}.$$

M_8: In this type, a matching of M_8 is obtained by selecting one edge from T_3 and at least one edge from the T_2 type. Therefore, the M_8^i matching of order i, for $2 \le i \le \frac{p_2-1}{2}$ is:

$$M_8^i = 1 + \frac{1}{i}\prod_{s=0}^{i-1}\binom{p_2-1-2s}{2}.$$

M_{11}: To determine the matchings of type M_{11}, one can see the possible partitions in Table 6 by considering the combinations involving edges from T_1, T_2, and T_3. At least one edge of T_3 shares a common vertex with T_1, while T_2 and T_3 remain disjoint. This leads to the following cases:

Case I: If we consider only one induced subgraph K_{p_1-1}, with the edge set of type T_1 denoted by A_{11}^l of order l, the edge set of type T_2 by B_{11}^m of order m, and the edge set of type T_3 by C_{11}^1 of order 1, then the total matchings of type M_{11}^i of order i, whenever $3 \le i \le \frac{p_1+p_2-2}{2}$, is given below:

$$M_{11}^i = \sum_{j=21}^{i-1} C_{11}^1 A_{11}^j B_{11}^{i-j}, \quad A_{11}^j = 0, \text{ for } j > \frac{p_1-1}{2}, \quad B_{11}^{i-j} = 0, \text{ for } i-j > \frac{p_2-1}{2},$$

where $A_{11}^l = \frac{1}{l-1}\prod_{j=0}^{l-2}\binom{p_1-1-2j}{2}$, $B_{11}^m = \frac{1}{11}\prod_{s=0}^{m-1}\binom{p_2-1-2s}{2}$.

Case II: Suppose we consider all the subgraphs K_{p_1-1} induced by the edges of type T_2, and let A^l_{11}, B^m_{11}, and C^1_{11} represent the total possible matchings of order l, m, and 1, respectively, corresponding to T_1, T_2, and T_3 type edges, respectively. Then, a matching of type M^i_{11} of order i is obtained by taking an l-order matching among T_1 type edges and m-order matching among T_2 type of edges, for $1 \le l \le \frac{p_1-2}{2}$ and $1 \le m \le \frac{p_2-2}{2}$, respectively. Thus,

$$A^l_{11} = \frac{1}{l-1}\prod_{t=0}^{l-2}\binom{p_1-1-2j}{2}, B^m_{11} = \frac{1}{m}\prod_{t=0}^{m-1}\binom{p_2-1-2t}{2}, \text{ and } C^1_{11} = 1.$$

Therefore, for $3 \le i \le \frac{p_1+p_2-2}{2}$, we have

$$\begin{aligned}
M^3_{11} &= C^1_{11}A^1_{11}B^1_{11}\\
M^4_{11} &= C^1_{11}A^1_{11}B^2_{11} + C^1_{11}A^2_{11}B^1_{11}\\
&\vdots\\
M^i_{11} &= \sum_{j=1}^{i-2} C^1_{11}A^j_{11}B^{i-j-1}_{11}, \text{ where } A^j_{11} = 0 \text{ for } j > \frac{p_1-1}{2} B^{i-j-1}_{11} = 0 \text{ for } i-j-1 > \frac{p_2-1}{2}.
\end{aligned}$$

M_{12}**:** To prove the matchings of this type, we use the same argument as of M_{11}, and the number of M_{12} type matchings can be obtained as follows:

$$\begin{aligned}
M^i_{12} &= \sum_{j=1}^{i-2} C^1_{12}D^j_{12}E^{i-j-1}_{12}, \quad \text{where } C^1_{12} = 1, \ T_4 \text{ type edge},\\
D^l_{12} &= \frac{p_2}{l}\prod_{t=0}^{l-1}\binom{p_1-2t-1}{2}, \quad 1 \le l \le \frac{p_1-1}{2},\\
E^m_{12} &= \frac{1}{m}\prod_{s=0}^{m-2}\binom{p_2-2s-1}{2}, \quad 1 \le m \le \frac{p_2-2}{2}, \quad \text{and } D^j_{12} = 0, \quad \text{for } j > \frac{p_1-1}{2},\\
E^{i-j-1}_{12} &= 0, \quad \text{for } i-j-1 > \frac{p_2-1}{2}.
\end{aligned}$$

M_{13}**:** Finally, to determine the matching of type M_{13}, we consider adding one edge from either T_3 or T_4, as they share a common vertex. Without loss of generality, we consider T_4, where X^1_{13} represents a matching consisting of a single edge from T_4, i.e., of order 1. Additionally, let $Y^l_{13} = \frac{p_2}{l}\prod_{t=0}^{l-1}\binom{p_1-1-2t}{2}$ for $1 \le l \le \frac{p_2-1}{2}$ represent the matchings by contributing p_2 copies of K_{p_1-1}, and $Z^m_{13} = \frac{1}{m}\prod_{s=0}^{m-1}\binom{p_2-1-2s}{2}$ for $1 \le m \le \frac{p_2-2}{2}$ represent the number of matchings of K_{p_2-1}. Therefore, the total possible matching of M^i_{13} of order i, where $3 \le i \le \frac{p_1+p_2-3}{2}$, is given by:

$$\begin{aligned}
M^3_{13} &= X^1_{13}Y^1_{13}Z^1_{13},\\
M^4_{13} &= X^1_{13}Y^1_{13}Z^2_{13} + X^1_{13}Y^2_{13}Z^2_{13},\\
M^5_{13} &= X^1_{13}Y^1_{13}Z^3_{13} + X^1_{13}Y^2_{13}Z^2_{13} + X^1_{13}Y^3_{13}Z^2_{13},\\
&\vdots
\end{aligned}$$

$$M_{13}^{i} = \sum_{j=1}^{i-2} X_{13}^{1} Y_{13}^{j} Z_{13}^{i-j-1} \quad \text{for } Y_{13}^{j} = 0, j > \frac{p_1 - 1}{2}, \quad Z_{13}^{i-j-1} = 0, \text{for } i - j - 1 > \frac{p_2 - 1}{2}.$$

Table 6. Total possible matchings.

Types	Descriptions
M_1	Matching between T_1
M_2	Matching between T_2
M_3	Matching between T_3
M_4	Matching between T_4
M_5	Matching between T_1 and T_2
M_6	Matching between T_1 and T_3
M_7	Matching between T_1 and T_4
M_8	Matching between T_2 and T_3
M_9	Matching between T_2 and T_4
M_{10}	Matching between T_3 and T_4
M_{11}	Matching between T_1, T_2 and T_3
M_{12}	Matching between T_1, T_2 and T_4
M_{13}	Matching between T_1, T_2, T_3 and T_4

By combining the cases mentioned in Table 6 and counting the arguments, we get the required result.

5. Conclusions

In this study, we intended to determine the geomorphic characteristics of power graphs of finite groups. We examined certain eccentricity-based topological indices, including Zagreb eccentricity indices, the eccentric connectivity index, connective eccentricity index, eccentric distance sum index, and Zagreb irregularity indices of the power graphs of certain finite cyclic and non-cyclic groups. Furthermore, we determined the Hosoya index of the aforementioned graphs, which was one of the challenging tasks of this work.

Our findings contribute to the broader understanding of the specific algebraic graphs. Nevertheless, finding the topological indices, specifically the Hosoya index of any algebraic graph, including the power graph, Cayley graph, and conjugacy graph of any group, remains an open and challenging problem. From a chemical perspective, such algebraic characteristics are essential for developing chemical and molecular compositions. The numerical indices deliberated in this work can support the development of QSPR studies which are essential in identifying bioactive compounds through physicochemical evaluations.

Author contributions

Kalim Ullah: Conceptualization, Data curation, Investigation, Writing–original draft; Fawad Ali: Supervision, Methodology, Validation, Resources, Investigation, Writing–review and editing; Shi

Xia: Formal analysis, visualization, Resources, and editing; Muhammad Shoaib Arif: Methodology, Validation, Formal analysis; Kamleldin Abodayeah: Validation, Formal analysis and editing. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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