Vol. 6, No. 2, 2024, pp. 72-82.

Molecular Topology Index of a Zero Divisor Graph on a Ring of Integers Modulo Prime Power Order

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Abstract. In chemistry, graph theory has been widely utilized to address molecular problems, with numerous applications in graph theory and ring theory within this field. One of these applications involves topological indices that represent chemical structures with numerical values. Various types of topological indices exist, including the Wiener index, the first Zagreb index, and the hyper-Wiener index. In the context of this research, the values of the Wiener index, the first Zagreb index, and the hyper-Wiener index for zero-divisor graphs on the ring of integers modulo a prime power order will be explored through a literature review and conjecture.

Keywords: first zagreb index; graph; hyper-wiener index; ring; wiener index.

1 Introduction

In chemistry, graph theory has been widely used to solve molecular problems. The structure of a molecule can be represented as a graph where the atoms are the vertices and the bonds between the atoms are the edges. There are many applications of graph theory and ring theory in chemistry. One of the applications is a topological index that represents the chemical structure with a numerical value. In addition, topological indices are useful for predicting the chemical and physical properties of molecular structures.

Research on molecular topology indices in graphs has been an interesting study in recent years. This can be seen from the many studies that have been published in various scientific journals. Research that has been studied includes the Wiener index on undirected power graphs [1], the harmonic and Gutman indices on coprime graphs on groups of integers $n = p^k$, where k is a natural number [2], the hyper-Wiener and Padmakar-Ivan indices of coprime graphs of dihedral groups [3], and topological indices of coprime graphs for dihedral groups with prime power order [4]. Apart from that, there is also research on the first Zagreb index, Wiener index, and Gutman index of power graphs in the Dihedral group [5]. Furthermore, there is also research related to topological indices on zero divisor graphs, namely the First Zagreb index [6].

Based on the presentation of research results that have been studied, this research examines the index and ex-topology of zero divisor graphs in the modulo integer ring, specifically, the Wiener index, Hyper-Wiener index, and First Zagreb on the graph.

2 Literature review

The zero divisor graph of a commutative ring *R* denoted by $\Gamma(R)$ is a graph whose vertex set is all the zero divisor elements of the commutative ring *R* and each $x, y \in R$ is connected by an edge if and only if $x \cdot y = 0$.

Lemma 1. [7] For each commutative ring R, $diam(\Gamma(R)) \leq 2$.

The Wiener index on a connected graph G, denoted by W(G), was introduced by Wiener in 1947. The Wiener index is the sum of the distances between two vertices in the graph. The Wiener index introduced by Harry Wiener is a topological index of a molecule, defined as the sum of the shortest path lengths between all pairs of vertices in a chemical graph representing non-hydrogen atoms in a molecule.

Definition 1 [8] *Given G is a connected graph. The Wiener index of G is the sum of the distances of each pair of unordered points of the graph G, written as*

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) \tag{1}$$

The following example is given to understand the definition of the Wiener index of a zero divisor graph on a modulo integer ring.

Example 1 A commutative ring \mathbb{Z}_{3^3} has zero divisor elements or $Z^*(\mathbb{Z}_{3^3}) = \{3,6,9,12,15,18,21,24\}$ with its zero divisor graph forms the following graph.

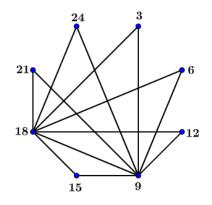


Figure 1 Coprime $\Gamma(\mathbb{Z}_{3^3})$ Graph

The following Wiener index calculation is obtained,

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Next, a definition of one of the topological indices, namely the first Zagreb index, is given as follows.

Definition 2 [9] *Given G a connected graph. The first Zagreb index of G is the sum of all* the squares of the degree of each point of G, written as

$$M_1(G) = \sum_{u \in V(G)} \deg(u)^2$$
(3)

The following example is given to understand the definition of the Zagreb index.

Example 2 A commutative ring \mathbb{Z}_{2^4} has zero divisor elements or $Z^*(\mathbb{Z}_{2^4}) =$ {2,4,6,8,10,12,14} with its zero divisor graph forms the following graph.

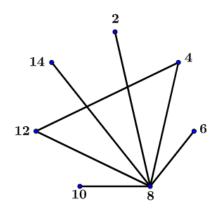


Figure 2 Coprime $\Gamma(\mathbb{Z}_{2^4})$ Graph

The following First Zagreb index calculation is obtained,

$$M_{1}(\Gamma(\mathbb{Z}_{2^{4}}) = deg(2)^{2} + deg(4)^{2} + deg(6)^{2} + deg(8)^{2} + deg(10)^{2} + deg(12)^{2} + deg(14)^{2}$$

= 1² + 2² + 1² + 6² + 1² + 2² + 1²
$$M_{1}(\Gamma(\mathbb{Z}_{2^{4}}) = 48$$
(4)

The hyper-Wiener index is a generalization of the Wiener index denoted by WW(G). The Wiener index on cyclic graphs was introduced by Randic in 1993 and extended to all connected graphs by Klein. Next, we will give a definition and example of the hyper-Wiener index.

Definition 3 [9] *Given G a connected graph. The hyper-Wiener index of G is half of the sum of the distances by the sum of the squares of the distances of each pair of unordered points from G, written as.*

$$WW(G) = \frac{1}{2} \left(\sum_{\{u,v\} \subseteq V(G)} d(u,v) + d(u,v)^2 \right)$$
(5)

Next, we give an example of the hyper-Wiener index in a commutative ring as follows.

Example 3. A commutative ring \mathbb{Z}_{2^4} has zero divisor elements or $Z^*(\mathbb{Z}_{2^4}) = \{2,4,6,8,10,12,14\}$ with its zero divisor graph forms a pattern as in Figure 2. The value of the hyper-Wiener index is obtained as follows.

$$WW(\Gamma(\mathbb{Z}_{2^4})) = 49\tag{6}$$

Next, we will give a theorem to find the Wiener index value of a simple graph that has a diameter less than or equal to two.

Theorem 1 [10] Given a graph G with diam $(G) \leq 2$, then the Wiener index of G is

$$|V(G)|(|V(G)| - 1) - |E(G)|$$
(7)

Next, we give a theorem regarding the hyper-Wiener index of the graph with the largest diameter of 2.

Theorem 2 [10] Given G a connected graph with diam $(G) \le 2$, then the hyper-Wiener index of G is

$$\frac{3}{2} |V(G)|(V(G) - 1) - 2|E(G)| \tag{8}$$

3 Results and Discussion

In this section, we explain the formula for the Wiener index, the first Zagreb index, and the hyper-Wiener index on the zero divisor graph of the modulo integer ring p^k or denoted $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k. Before determining the general formula for these indices, the basic terminology, lemmas, and properties related to zero divisor graphs on the ring are first established \mathbb{Z}_{n^k} .

3.1. Characteristics of Coprime Graphs in Zero Divisor Rings

For every commutative ring R, its zero divisor graph is connected and has a diameter of less than three. This will be used to fulfill the requirements of the lemmas and theorems that will be used to calculate the Wiener index, First Zagreb index, and Hyper-Wiener index.

Theorem 3. [11] *Given a commutative ring* R, $\Gamma(R)$ *is a connected graph with a diameter of not more than three, diam* ($\Gamma(R)$) ≤ 3 .

Based on Theorem 3, it has been proven that every ring is commutative R, then $\Gamma(R)$ is a connected graph with a diameter of not more than three, $diam(\Gamma(R)) \leq 3$. The modulo integer ring is commutative, so the diameter of the zero divisor graph is not more than three. For the case in this study, the ring \mathbb{Z}_{p^k} for a prime number p and a natural number k has a diameter of not more than two. This will be shown through the following theorem. **Theorem 4** [12] *The following statements apply:*

- 1. If a commutative ring is given \mathbb{Z}_n for n = 4 then $diam(\Gamma(\mathbb{Z}_{2^2})) = 0$.
- 2. If we are given a commutative ring \mathbb{Z}_n for $n = p^2$ with prime number $p \ge 3$ then $diam(\Gamma(\mathbb{Z}_{p^2})) = 1$.
- 3. If a commutative ring is given \mathbb{Z}_n for $n = p^k$ with p as a prime number and $k \ge 3$ is a natural number then diam $(\Gamma(\mathbb{Z}_{p^k})) = 2$.

Based on Theorem 4, it is easy to see that a commutative ring \mathbb{Z}_{p^k} for a prime number p and a natural number k has $diam(\Gamma(\mathbb{Z}_{p^k})) \leq 2$.

To get the number of vertices in a graph, $\Gamma(\mathbb{Z}_{p^k})$, we can partition the vertices of the graph $\Gamma(\mathbb{Z}_{p^k})$ into subsets $V_1, V_2, ..., V_{k-1}$ where $V_i = \{k_i p^i : p \nmid k_i\}$ for intervals $1 \le i \le k-1$, it is easy to find that $|V_i| = (p-1) p^{n-i-1}$ for intervals $1 \le i \le k-1$ using this fact we can get Theorem 5.

Theorem 5. The number of vertices $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $p^{k-1} - 1$.

Proof. To find the number of vertices of a graph, $\Gamma(\mathbb{Z}_{p^k})$ we will describe the equation $|V_i| = (p-1) p^{n-i-1}$ for intervals $1 \le i \le k-1$ using the sigma operation to obtain the following equation.

$$\begin{aligned} \left| \mathbf{V} \big(\mathbb{Z}_{p^k} \big) \right| &= \sum_{i=1}^{(k-1)} (p-1) p^{k-i-1} \\ &= (p-1) \sum_{i=1}^{(k-1)} p^{k-i-1} \\ &= (p-1) \cdot p^{(k-1)} \cdot \sum_{i=1}^{(k-1)} p^{-i} \\ &= (p-1) \cdot p^{(k-1)} \cdot \frac{p^{-1} (1-p^{-(k-1)})}{(1-p^{-1})} \\ &= (p-1) \cdot p^{(k-1)} \cdot \frac{(1-p^{-(k-1)})}{p(1-p^{-1})} \\ &= (p-1) \cdot p^{(k-1)} \cdot \frac{(1-p^{-(k-1)})}{(p-1)} \end{aligned}$$

$$\begin{aligned} \left| \mathbf{V} \big(\mathbb{Z}_{p^k} \big) \right| &= p^{k-1} - 1 \end{aligned} \tag{9}$$

Next, we give a property that states the number of edges in a graph $\Gamma(\mathbb{Z}_{n^k})$.

Theorem 6 [13] For a positive number $n, 1 \le n \le k - 1$, the degree of the vertex v_n in the graph $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is

$$\deg(v_n) = \begin{cases} p^n - 1 & , if \ 1 \le n < \left[\frac{k}{2}\right] \\ p^n - 2 & , if \ \left[\frac{k}{2}\right] \le n \le (k - 1) \end{cases}$$
(10)

where [x] is the smallest integer greater than x.

Next, we will give a property of zero divisor graphs $\Gamma(\mathbb{Z}_{p^k})$ which states the number of edges in the graph $\Gamma(\mathbb{Z}_{p^k})$.

Theorem 7 [13] The number of sides of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $\frac{1}{2} \left[p^{k-1}(kp-k-p) - p^{k-\left\lceil \frac{k}{2} \right\rceil} + 2 \right]$.

3.2. Topology Index

Based on Consequence 1, obtained $diam(\Gamma(\mathbb{Z}_{p^k})) \leq 2$, then using Theorem 1 and Theorem 2 we can determine the general formula for the Wiener and hyper-Wiener indices of the zero divisor graph in the ring \mathbb{Z}_{p^k} for a prime number p and a natural number k.

Theorem 8 The Wiener index for $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $p^{2k-2} - 3p^{k-1} - \frac{1}{2} \left[p^{k-1}(kp-k-p) - p^{k-\frac{k}{2}} \right] + 1.$

Proof. To calculate the Wiener index value of a zero divisor graph \mathbb{Z}_{p^k} for a prime number p and a natural number k, it is enough to find the number of vertices and edges. Based on Theorem 5, the number of vertices in a graph $\Gamma(\mathbb{Z}_{p^k})$ is denoted by $|V(\Gamma(\mathbb{Z}_{p^k}))| = p^{k-1} - 1$ and the number of edges is denoted by $|E(\Gamma(\mathbb{Z}_{p^k}))|$, by using Theorem 6 we get that the number of edges of a zero divisor graph $\Gamma(\mathbb{Z}_{p^k})$ is $\frac{1}{2}[p^{k-1}(kp-k-p) - p^{k-\frac{k}{2}}] + 2]$. Next, to determine the number of Wiener indices, Theorem 1 can be used to obtain the Wiener index from the graph $\Gamma(\mathbb{Z}_{p^k})$ as follows.

$$W(\Gamma(\mathbb{Z}_{p^{k}})) = |V(\mathbb{Z}_{p^{k}})|(|V(\mathbb{Z}_{p^{k}})| - 1) - |E(\mathbb{Z}_{p^{k}})|$$

= $(p^{k-1} - 1)(p^{k-1} - 2) - \frac{1}{2}[p^{k-1}(kp - k - p) - p^{k-\frac{k}{2}} + 2]$

$$= p^{(2k-2)} - 3p^{k-1} + 2 - \frac{1}{2} \left[p^{k-1}(kp - k - p) - p^{k-\left[\frac{k}{2}\right]} \right] - 1$$
$$W\left(\Gamma(\mathbb{Z}_{p^k})\right) = p^{(2k-2)} - 3p^{k-1} - \frac{1}{2} \left[p^{k-1}(kp - k - p) - p^{k-\left[\frac{k}{2}\right]} \right] + 1 \qquad (11)$$

The value of the first Zagreb index of the graph $\Gamma(\mathbb{Z}_{p^k})$ is given below.

Theorem 9 The First Zagreb Index of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $p^k(p^{k-1}-1) - 2(k-1)\left(\left\lfloor\frac{k}{2}\right\rfloor - 1\right) p^{k-1} - 4(p-1)\left(k - \left\lfloor\frac{k}{2}\right\rfloor\right) p^{k-1} + 3p^{k-\left\lfloor\frac{k}{2}\right\rfloor} + p^{k-1} - 4$

Proof. To calculate the value of the first Zagreb index of a zero divisor graph \mathbb{Z}_{p^k} for a prime number p and a natural number k, it is enough to find the number of vertices and the degree of each vertex. By using Consequence 2 and Theorem 5 we can see the number of vertices and the degree of each vertex. From the definition of the first Zagreb index, an equation can be created as follows.

$$\begin{split} M_1\left(\Gamma(\mathbb{Z}_{p^k})\right) &= \sum_{v \in V\left(\Gamma(\mathbb{Z}_{p^k})\right)} (\deg(v))^2 \\ &= \sum_{i=1}^{\binom{k}{2}-1} (p-1) \ p^{k-i-1} \ \left(p^i-1\right)^2 + \sum_{i=\binom{k}{2}}^{(k-1)} (p-1) \\ &= (p-1) \left[\sum_{i=1}^{\binom{k}{2}-1} \ p^{k-i-1} \ \left(p^i-1\right)^2 + \\ &\qquad \sum_{i=\binom{k}{2}}^{(k-1)} \ p^{k-i-1} \ \left(p^i-2\right)^2\right] \\ &= (p-1) \left[\sum_{i=1}^{\binom{k}{2}-1} \ p^{k-i-1} \ \left((p^{2i}-2p^i+1)\right) + \\ &\qquad \sum_{i=\binom{k}{2}}^{(k-1)} \ p^{k-i-1} \ \left(p^{2i}-4p^i+4\right)\right] \\ &= \left[\sum_{i=1}^{\binom{k-1}{2}-1} \ \left(p^{k+i-1}-2p^{k-1}+p^{k+i-1}\right) + \\ &\qquad \sum_{i=\binom{k}{2}}^{(k-1)} \ \left(p^{k+i-1}-4p^{k-1}+4p^{k+i-1}\right)\right] (p-1) \end{split}$$

$$= (p-1) \left[\sum_{i=1}^{(k-1)} p^{k+i-1} - 2 \sum_{i=1}^{\binom{k}{2}-1} p^{k-1} + \sum_{i=1}^{\binom{k}{2}-1} p^{k-1} - 4 \sum_{i=\binom{k}{2}}^{(k-1)} p^{(k-1)} + 4 \sum_{i=\binom{k}{2}}^{(k-1)} p^{k-i-1} \right]$$

$$= (p-1) \left[\left(\frac{p^{k}(p^{k-1}-1)}{(p-1)} \right) - 2 \left(\left[\frac{k}{2} \right] - 1 \right) p^{k-1} - 4 \left(k - \left[\frac{k}{2} \right] \right) p^{k-1} + \left(\frac{\binom{3p^{k-\binom{k}{2}}+p^{k-1}-4}{(p-1)}}{(p-1)} \right) \right]$$

$$M_{1} \left(\Gamma(\mathbb{Z}_{p^{k}}) \right) = p^{k}(p^{k-1}-1) - 2(p-1) \left(\left[\frac{k}{2} \right] - 1 \right) p^{k-1} - 4(p-1) \left(\left[\frac{k}{2} \right] \right) p^{k-1} + 3p^{k-\binom{k}{2}} + p^{k-1} - 4 \right]$$
(12)

The hyper-Wiener index values of the graph $\Gamma(\mathbb{Z}_{n^k})$ are given below.

Theorem 10. The hyper-Wiener index of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is

$$\frac{3}{2}\left(p^{2k-2} - 3p^{k-1}\right) - p^{k-1}(kp - k - p) + p^{k - \left[\frac{k}{2}\right]} + 1$$
(13)

Proof. To find the number of hyper-Wiener indices in a commutative ring \mathbb{Z}_{p^k} , simply find the number of vertices and edges in the graph $\Gamma(\mathbb{Z}_{p^k})$. In Theorem 3 we give a property guaranteeing that every commutative ring of a zero divisor graph is a connected graph with a diameter of not more than three ($diam(\Gamma(R)) \leq 3$). Then it continues with Theorem 4 which guarantees that every commutative ring \mathbb{Z}_n with $n = p^k$ for a prime number p and a natural number k, has $diam(\Gamma(\mathbb{Z}_{p^k})) \leq 2$. Hence, the main condition in Theorem 2 is fulfilled, namely that the graph G is connected and has $diam(G) \leq 2$. Using Theorem 2 we can determine the number of hyper-Wiener indices of a commutative ring simply by finding the number of vertices of the graph that $\Gamma(\mathbb{Z}_{p^k})$ are in Consequence 2 denoted by $|V(\Gamma(\mathbb{Z}_{p^k}))| = p^{k-1} - 1$. Meanwhile, the number of edges of the graph $\Gamma(\mathbb{Z}_{p^k})$ is in Theorem 6, namely $|E(\Gamma(\mathbb{Z}_{p^k}))| = \frac{1}{2}[p^{k-1}(kp - k - p) - p^{k-[\frac{k}{2}]} + 2]$. Then by substituting the number of vertices and edges of the graph $\Gamma(\mathbb{Z}_{p^k})$ is Theorem 2, we get the number of hyper-Wiener indices of the graph $\Gamma(\mathbb{Z}_{p^k})$ as follows.

$$WW(\mathbb{Z}_{p^{k}}) = \frac{3}{2} |V(\mathbb{Z}_{p^{k}})| (|V(\mathbb{Z}_{p^{k}})| - 1) - 2|E(\mathbb{Z}_{p^{k}})|$$

$$= \frac{3}{2} (p^{k-1} - 1)(p^{k-1} - 2) - 2 \cdot \frac{1}{2} \left[p^{k-1} \left(kp - k - p \right) - p^{k-\left[\frac{k}{2}\right]} + 2 \right]$$

$$= \frac{3}{2} (p^{2k-2} - 3p^{k-1} + 2) - \left[p^{k-1} \left(kp - k - p \right) - p^{k-\left[\frac{k}{2}\right]} + 2 \right]$$

$$= \frac{3}{2} (p^{2k-2} - 3p^{k-1}) + 3 - p^{k-1} (kp - k - p) + p^{k-\left[\frac{k}{2}\right]} - 2$$

$$WW(\mathbb{Z}_{p^{k}}) = \frac{3}{2} (p^{2k-2} - 3p^{k-1}) - p^{k-1} (kp - k - p) + p^{k-\left[\frac{k}{2}\right]} + 1 \quad (14)$$

4 Conclusion

In this research, the formulas for the Wiener index, the first Zagreb index, and the hyper-Wiener index on the zero divisor graph of the modulo integer ring \mathbb{Z}_{p^k} for a prime number p and a natural number k are obtained as follows:

- 1. The Wiener index of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $p^{2k-2} 3p^{k-1} \frac{1}{2} \left[p^{k-1}(kp k p) p^{k \left\lfloor \frac{k}{2} \right\rfloor} \right] + 1.$
- 2. The first Zagreb index of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $p^k(p^{k-1}-1) 2(k-1)\left(\left\lfloor\frac{k}{2}\right\rfloor 1\right) p^{k-1} 4(p-1)\left(k \left\lfloor\frac{k}{2}\right\rfloor\right) p^{k-1} + 3p^{k-\left\lfloor\frac{k}{2}\right\rfloor} + p^{k-1} 4.$
- 3. The hyper-Wiener index of $\Gamma(\mathbb{Z}_{p^k})$ for a prime number p and a natural number k is $\frac{3}{2}(p^{2k-2}-3p^{k-1})-p^{k-1}(kp-k-p)+p^{k-\left\lfloor\frac{k}{2}\right\rfloor}+1$.

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