

WIENER AND HARARY INDICES OF THE GENERALIZED ZERO-DIVISOR GRAPH

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ABSTRACT. Let R be a commutative ring, and let $Z^*(R)$ denote the set of all non-zero zero-divisors in R . The generalized zero-divisor graph of R , denoted by $\Gamma'(R)$, is a simple (undirected) graph with the vertex set $Z^*(R)$, and two distinct vertices x and y are adjacent in $\Gamma'(R)$ if and only if $x^n y = 0$ or $y^n x = 0$, for some positive integer n . The Wiener and Harary indices are topological indices widely used in chemistry to analyze the structures of molecules. In this paper, we determine the Wiener and Harary indices of $\Gamma'(\mathbb{Z}_n)$ for $n = pq, p^2q, p^2q^2$, where p, q are distinct primes.

Keywords: Zero-divisor graph; Wiener index; Harary index; distance matrix.

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1. INTRODUCTION

The study of topological indices has gained considerable attention in mathematical chemistry due to their ability to capture essential structural features of molecular graphs. Among these, the Wiener index and the Harary index are two classical and widely used descriptors. The Wiener index, first introduced by H. Wiener [16] in 1947, has proven particularly effective in correlating molecular structure with physicochemical properties such as boiling points, stability, and branching in alkanes. The Harary index was introduced by Plašić et al. [14] and Ivanciuc et al. [7] in 1993. Based on reciprocal distances, the Harary index emphasizes molecular compactness and has been successfully applied in

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modelling biological activity and thermodynamic behaviour. Their mathematical simplicity, combined with strong predictive power in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies, makes these indices fundamental tools for exploring structure-property relationships. Studying these indices not only deepens our understanding of graph-theoretic properties but also contributes to practical applications in drug design, materials science, and nanotechnology. This motivates a systematic investigation of the Wiener and Harary indices across various classes of graphs, aiming to uncover new patterns, bounds, and chemical interpretations.

I. Beck [4] introduced the concept of the zero-divisor graph for commutative rings. It is a graph with the vertex set R , and two distinct vertices are adjacent if their product is zero. Motivated by the work of Beck, later in 1999, Anderson and Livingston [2] modified the zero-divisor graph for commutative rings. They used the same adjacency, but the vertex set is the set of zero-divisors in R . They denoted this graph by $\Gamma(R)$. In a subsequent development, Redmond [15] introduced the zero-divisor graph for a non-commutative ring. Beaugris et al. [3] studied the weak zero-divisor graph of finite commutative rings. It is a graph with a vertex set consisting of non-zero elements of a ring R , and the vertices x and y are adjacent if and only if $(xy)^n = 0$ for some positive integer n . A $*$ -ring is a ring equipped with a function, known as an involution, which satisfies the following properties for all elements $x, y \in R$: $(x + y)^* = x^* + y^*$, $(xy)^* = y^*x^*$, and $(x^*)^* = x$. In [10], the concept of the generalized zero-divisor graph for a $*$ -ring R , denoted by $\Gamma'(R)$, was introduced. This graph is defined as a simple undirected graph whose vertex set includes all non-zero left zero-divisors of R . Two distinct vertices x and y are connected by an edge if there exists a positive integer n such that either $x^n y^* = 0$ or $y^n x^* = 0$. If R is a commutative ring, then the involution on R is the identity. The study of the algebraic structures and zero-divisor graphs is explored by many authors; see [8, 9, 11, 13]. A recent investigation into zero-divisor graphs and their associated energies is presented in [12]. In [1], Ahmadi and Jahani-Nezhad examined the energy and Wiener index of the zero-divisor graph $\Gamma(\mathbb{Z}_n)$, for the cases $n = pq, p^2q$, where p, q are primes.

In this paper, we determine the distance matrix and find the Wiener index and Harary index of $\Gamma'(\mathbb{Z}_n)$, for $n = pq, p^2q, p^2q^2$, where p, q are distinct primes.

We begin with the necessary definitions and terminology. A *graph* $G = (V, E)$ consists of a set V of vertices and a multiset E of unordered pairs of vertices, known as *edges*. The *degree of a vertex* $v \in V$, denoted by $d(v)$, is the number of vertices adjacent to v , counting multiple edges if present. In a graph $G = (V, E)$, a *path* is a sequence of distinct vertices $v_1, v_2, \dots, v_n$ such that each consecutive pair of vertices (v_i, v_{i+1}) is connected by an edge in E . A graph G is *connected* if there is a path between every pair of distinct vertices in G . A *complete graph* is a simple, undirected graph in which every pair of distinct vertices is connected by exactly one edge. The complete graph on n vertices is denoted by K_n . A graph G is called *bipartite* if its vertex set $V(G)$ can be partitioned into two disjoint sets such that no two vertices within the same set are adjacent. A *complete bipartite graph* is a bipartite graph in which every vertex in one set is adjacent to every vertex in the other set. If the two sets contain m and n vertices, respectively, the complete bipartite graph is denoted by $K_{m,n}$. The *distance* between two distinct vertices x and y in a graph G , denoted by $d(x, y)$, refers to the length of the shortest path connecting them. The *distance matrix* of graph G with n vertices $v_1, v_2, \dots, v_n$ is denoted by $D(G) = [d_{ij}]_{n \times n}$, and is the matrix such that, $d_{ij} = d(v_i, v_j)$. The *Wiener index* of a graph G , written as $W(G)$, is defined as the sum of the distances between all unordered pairs of vertices of G , i.e., $W(G) = \sum_{x, y \in V(G)} d(x, y)$. The *Harary index* of a graph G , denoted by $H(G)$, is the

sum of the reciprocals of the distances between all unordered pairs of vertices of G , i.e., $H(G) = \sum_{x,y \in V(G)} \frac{1}{d(x,y)}$. Readers can refer to [5, 6, 17] for more details on the Wiener index, graph theory, and Harary index, respectively.

2. DISTANCE MATRIX

In this section, we determine the distance matrix of $\Gamma'(\mathbb{Z}_n)$, for the cases $n = pq$, p^2q , p^2q^2 for distinct primes p and q . Let R be a commutative ring; then the identity mapping is the only involution on R . The definition below gives the generalized zero-divisor graph $\Gamma'(R)$ for a commutative ring R as presented in [10].

Definition 2.1. Let R be a commutative ring. The generalized zero-divisor graph of R , denoted by $\Gamma'(R)$, is defined as a simple undirected graph whose vertex set is $Z^*(R)$, the set of non-zero zero-divisors of R . Two distinct vertices x and y are connected by an edge in $\Gamma'(R)$ if and only if there exists a positive integer n such that $x^n y = 0$ or $y^n x = 0$.

Remark 2.1. (a) For a commutative ring R , the graph $\Gamma(R)$ forms a subgraph of the generalized zero-divisor graph $\Gamma'(R)$.

(b) If x is a non-zero nilpotent element of R , then x is adjacent to every other vertex in the graph $\Gamma'(R)$ i.e., $d(x, y) = 1$ for all $y \neq x$.

Remark 2.2. Let $\phi(n)$ represent the number of positive integers less than n that are coprime to n . Then the number of non-zero zero-divisors of $\mathbb{Z}_n$ is given by $n - \phi(n) - 1$, i.e. $|Z^*(\mathbb{Z}_n)| = n - \phi(n) - 1$. Let $T_d = \{a \in \mathbb{Z}_n : (a, n) = d\}$, where (a, n) denotes the greatest common divisor of a and n . Then the cardinality of T_d is $\phi\left(\frac{n}{d}\right)$, see [18].

In the following result, we determine the distance matrix of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_n)$ for $n = pq, p^2q, p^2q^2$, where p and q are distinct primes.

Theorem 2.1. Let p, q be distinct prime numbers.

(a) The distance matrix of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{pq})$ is given by:

$$D(\Gamma'(\mathbb{Z}_{pq})) = \begin{bmatrix} 2(J - I)_{n_1 \times n_1} & J_{n_1 \times n_2} \\ J_{n_2 \times n_1} & 2(J - I)_{n_2 \times n_2} \end{bmatrix}, \quad (1)$$

where $0_{n_i \times n_j}$ is a matrix of all zeros of size $n_i \times n_j$, $J_{n_i \times n_j}$ is a matrix of all ones of size $n_i \times n_j$, and $I_{n_i \times n_i}$ is an identity matrix of size $n_i \times n_i$.

(b) The distance matrix of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{p^2q})$ is given by:

$$D(\Gamma'(\mathbb{Z}_{p^2q})) = \begin{bmatrix} 2(J - I)_{n_1 \times n_1} & J_{n_1 \times n_2} & J_{n_1 \times n_3} \\ J_{n_2 \times n_1} & 2(J - I)_{n_2 \times n_2} & J_{n_2 \times n_3} \\ J_{n_3 \times n_1} & J_{n_3 \times n_2} & (J - I)_{n_3 \times n_3} \end{bmatrix}. \quad (2)$$

(c) The distance matrix of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{p^2q^2})$ is given by:

$$D(\Gamma'(\mathbb{Z}_{p^2q^2})) = \begin{bmatrix} 2(J - I)_{n_1 \times n_1} & 2J_{n_1 \times n_2} & 2J_{n_1 \times n_3} & J_{n_1 \times n_4} & J_{n_1 \times n_5} \\ 2J_{n_2 \times n_1} & 2(J - I)_{n_2 \times n_2} & J_{n_2 \times n_3} & 2J_{n_2 \times n_4} & J_{n_2 \times n_5} \\ 2J_{n_3 \times n_1} & J_{n_3 \times n_2} & 2(J - I)_{n_3 \times n_3} & J_{n_3 \times n_4} & J_{n_3 \times n_5} \\ J_{n_4 \times n_1} & 2J_{n_4 \times n_2} & J_{n_4 \times n_3} & 2(J - I)_{n_4 \times n_4} & J_{n_4 \times n_5} \\ J_{n_5 \times n_1} & J_{n_5 \times n_2} & J_{n_5 \times n_3} & J_{n_5 \times n_4} & (J - I)_{n_5 \times n_5} \end{bmatrix}. \quad (3)$$

Proof. (a) Let $n = pq$. Then $Y_1 = \{kp : k = 1, 2, \dots, q - 1\}$, and $Y_2 = \{kq : k = 1, 2, \dots, p - 1\}$ forms a partition of $V(\Gamma'(\mathbb{Z}_{pq}))$, and $\Gamma'(\mathbb{Z}_{pq})$ is a complete bipartite graph.

Let $n_1 = |Y_1| = q - 1$ and $n_2 = |Y_2| = p - 1$. If $x \in Y_1$ and $y \in Y_2$, then $d(x, y) = 1$. Hence, we get a block of all ones, i.e., $J_{n_1 \times n_2}$ corresponding to row Y_1 and column Y_2 . If $x, y \in Y_1$, then x and y are not adjacent, and $x \rightarrow z \rightarrow y$ is a path between x and y , where $z \in Y_2$, which gives $d(x, y) = 2$. Hence, a block in the distance matrix corresponding to row Y_1 and column Y_1 is given by $2(J - I)$. Similarly, we get the remaining blocks in the distance matrix. Thus, the distance matrix of $\Gamma'(\mathbb{Z}_{pq})$ with the row and column headings Y_1, Y_2 is given by:

$$D(\Gamma'(\mathbb{Z}_{pq})) = \begin{array}{c|cc} & Y_1 & Y_2 \\ \hline Y_1 & 2(J - I)_{n_1 \times n_1} & J_{n_1 \times n_2} \\ Y_2 & J_{n_2 \times n_1} & 2(J - I)_{n_2 \times n_2} \end{array},$$

where $0_{n_i \times n_j}$ is a matrix of all zeros of size $n_i \times n_j$, $J_{n_i \times n_j}$ is a matrix of all ones of size $n_i \times n_j$, and $I_{n_i \times n_i}$ is an identity matrix of size $n_i \times n_i$.

(b) Let $n = p^2q$. Partition the vertex set of $\Gamma'(\mathbb{Z}_n)$ into three classes.

Let $Y_1 = \{y \in \mathbb{Z}_n : (y, n) = p \text{ or } p^2\}$, $Y_2 = \{y \in \mathbb{Z}_n : (y, n) = q\}$, $Y_3 = \{kpq : k = 1, 2, \dots, p-1\}$. Note that the cardinality of Y_1 is $n_1 = |Y_1| = \phi\left(\frac{p^2q}{p}\right) + \phi\left(\frac{p^2q}{p^2}\right) = p(q-1)$.

Similarly $n_2 = |Y_2| = \phi\left(\frac{p^2q}{q}\right) = p(p-1)$, $n_3 = |Y_3| = p-1$ and the size of the matrix $D(\Gamma'(\mathbb{Z}_{p^2q}))$ is $p(p+q-1)-1$.

If each element of the set X is adjacent to every element of the set Y , we write $X \sim Y$. If no element of X is adjacent to any element of Y , we denote this by $X \approx Y$. The adjacency relation among the vertices of $\Gamma'(\mathbb{Z}_{p^2q})$ is depicted in Figure 1. Observe that

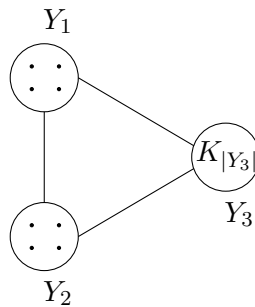


FIGURE 1. Adjacency relation among the vertices of $\Gamma'(\mathbb{Z}_{p^2q})$

$Y_1 \sim Y_2, Y_3$, $Y_2 \sim Y_3$, and $Y_3 \sim Y_3$. As every vertex of Y_1 is adjacent to every vertex in Y_2 , corresponding to the row Y_1 and the column Y_2 , we get a block of ones. Let $x, y \in Y_1$, and $z \in Y_3$, then $x \rightarrow z \rightarrow y$ is a path. That is $d(x, y) = 2$ for $x, y \in Y_1$. Hence, corresponding to the row Y_1 and the column Y_1 , we get a block of $2(J - I)$. Similarly, we get blocks of ones and $2(J - I)$ for the remaining vertices. Since $Y_2 \sim Y_3$, for $x \in Y_2$ and $y \in Y_3$, $d(x, y) = 1$. The graph $\Gamma'(\mathbb{Z}_n)$ is simple; there are no loops. Therefore, the entries on the main diagonal are 0. Hence, corresponding to the row Y_3 and the column Y_3 , we get a block of $J - I$. Thus, the distance matrix of $\Gamma'(\mathbb{Z}_{p^2q})$ with row and column headings Y_1, Y_2, Y_3 is given by

$$D(\Gamma'(\mathbb{Z}_{p^2q})) = \begin{array}{c|ccc} & Y_1 & Y_2 & Y_3 \\ \hline Y_1 & 2(J - I)_{n_1 \times n_1} & J_{n_1 \times n_2} & J_{n_1 \times n_3} \\ Y_2 & J_{n_2 \times n_1} & 2(J - I)_{n_2 \times n_2} & J_{n_2 \times n_3} \\ Y_3 & J_{n_3 \times n_1} & J_{n_3 \times n_2} & (J - I)_{n_3 \times n_3} \end{array}.$$

(c) Let $n = p^2q^2$, where p, q be distinct primes. Partition the set of non-zero zero-divisors of $\mathbb{Z}_n$ into five classes.

Let $Y_1 = \{y \in \mathbb{Z}_n : (y, n) = p\}$, $Y_2 = \{y \in \mathbb{Z}_n : (y, n) = q\}$,

$Y_3 = \{y \in \mathbb{Z}_n : (y, n) = p^2\}$, $Y_4 = \{y \in \mathbb{Z}_n : (y, n) = q^2\}$,

$Y_5 = \{k pq : k = 1, 2, \dots, pq - 1\}$.

Note that Y_5 consists of all non-zero nilpotent elements in $\mathbb{Z}_{p^2q^2}$. It is also important to observe that the sets Y_1, Y_2, Y_3, Y_4, Y_5 are pairwise disjoint. Thus,

$$P = \{Y_1, Y_2, Y_3, Y_4, Y_5\} \quad (4)$$

forms a partition of the vertex set of $\Gamma'(\mathbb{Z}_{p^2q^2})$.

Note that the cardinality of Y_1 is $n_1 = |Y_1| = \phi\left(\frac{p^2q^2}{p}\right) = q(p-1)(q-1)$. Similarly, $n_2 = |Y_2| = \phi\left(\frac{p^2q^2}{q}\right) = p(p-1)(q-1)$, $n_3 = |Y_3| = \phi\left(\frac{p^2q^2}{p^2}\right) = q(q-1)$, $n_4 = |Y_4| = \phi\left(\frac{p^2q^2}{q^2}\right) = p(p-1)$, $n_5 = |Y_5| = pq - 1$ and the size of the matrix $D(\Gamma'(\mathbb{Z}_n))$ is $|Y_1| + |Y_2| + |Y_3| + |Y_4| + |Y_5| = pq(p+q-1) - 1$.

Observe the following:

- (1) $Y_1 \sim Y_4, Y_1 \sim Y_5, Y_1 \approx Y_1, Y_1 \approx Y_2, Y_1 \approx Y_3$.
- (2) $Y_2 \sim Y_3, Y_5, Y_2 \approx Y_1, Y_2, Y_4$.
- (3) $Y_3 \sim Y_2, Y_4, Y_5, Y_3 \approx Y_1, Y_3$.
- (4) $Y_4 \sim Y_1, Y_3, Y_5, Y_4 \approx Y_2, Y_4$.
- (5) $Y_5 \sim Y_1, Y_2, Y_3, Y_4, Y_5$.

The adjacency relation between the vertices is shown in Figure 2.

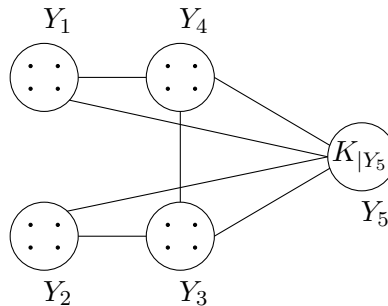


FIGURE 2. Adjacency relationship among the vertices of $\Gamma'(\mathbb{Z}_{p^2q^2})$

Using the adjacency relation shown in Figure 2 and similar to the proof of the above part (b), the distance matrix of $\Gamma'(\mathbb{Z}_{p^2q^2})$ with row and column headings Y_1, Y_2, Y_3, Y_4, Y_5 is given by

$$D(\Gamma'(\mathbb{Z}_{p^2q^2})) =$$

	Y_1	Y_2	Y_3	Y_4	Y_5
Y_1	$2(J - I)_{n_1 \times n_1}$	$2J_{n_1 \times n_2}$	$2J_{n_1 \times n_3}$	$J_{n_1 \times n_4}$	$J_{n_1 \times n_5}$
Y_2	$2J_{n_2 \times n_1}$	$2(J - I)_{n_2 \times n_2}$	$J_{n_2 \times n_3}$	$2J_{n_2 \times n_4}$	$J_{n_2 \times n_5}$
Y_3	$2J_{n_3 \times n_1}$	$J_{n_3 \times n_2}$	$2(J - I)_{n_3 \times n_3}$	$J_{n_3 \times n_4}$	$J_{n_3 \times n_5}$
Y_4	$J_{n_4 \times n_1}$	$2J_{n_4 \times n_2}$	$J_{n_4 \times n_3}$	$2(J - I)_{n_4 \times n_4}$	$J_{n_4 \times n_5}$
Y_5	$J_{n_5 \times n_1}$	$J_{n_5 \times n_2}$	$J_{n_5 \times n_3}$	$J_{n_5 \times n_4}$	$(J - I)_{n_5 \times n_5}$

□

3. WIENER AND HARARY INDICES

In this section, we compute the Wiener index and Harary index of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_n)$, for

$n = pq, p^2q, p^2q^2$, where p and q are distinct prime numbers.

Theorem 3.1. *Let p and q be distinct prime numbers. Then, the Wiener index of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{pq})$ is given by*

$$W(\Gamma'(\mathbb{Z}_{pq})) = (p-1)(p-2) + (q-1)(q-2) + (p-1)(q-1),$$

and the Harary index is

$$\frac{1}{4}(p-1)(p-2) + \frac{1}{4}(q-1)(q-2) + (p-1)(q-1).$$

Proof. According to Theorem 2.1 (a), the graph $\Gamma'(\mathbb{Z}_{pq})$ is isomorphic to the complete bipartite graph $K_{p-1, q-1}$. The Wiener index of $\Gamma'(\mathbb{Z}_{pq})$ is given by:

$$\begin{aligned} W(\Gamma'(\mathbb{Z}_{pq})) &= \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{pq}))} d(x, y) \\ &= \sum_{x \neq y \in Y_1} d(x, y) + \sum_{x \neq y \in Y_2} d(x, y) + \sum_{x \in Y_1, y \in Y_2} d(x, y) \\ &= \sum_{x \neq y \in Y_1} 2 + \sum_{x \neq y \in Y_2} 2 + \sum_{x \in Y_1, y \in Y_2} 1 \\ &= 2 \left(\frac{1}{2}(q-1)(q-2) \right) + 2 \left(\frac{1}{2}(p-1)(p-2) \right) + (p-1)(q-1) \\ &= (q-1)(q-2) + (p-1)(p-2) + (p-1)(q-1). \end{aligned}$$

Furthermore, the Harary index is given by:

$$\begin{aligned} W(\Gamma'(\mathbb{Z}_{pq})) &= \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{pq}))} \frac{1}{d(x, y)} \\ &= \sum_{x \neq y \in Y_1} \frac{1}{d(x, y)} + \sum_{x \neq y \in Y_2} \frac{1}{d(x, y)} + \sum_{x \in Y_1, y \in Y_2} \frac{1}{d(x, y)} \\ &= \sum_{x \neq y \in Y_1} \frac{1}{2} + \sum_{x \neq y \in Y_2} \frac{1}{2} + \sum_{x \in Y_1, y \in Y_2} 1 \\ &= \frac{1}{2} \left(\frac{1}{2}(q-1)(q-2) \right) + \frac{1}{2} \left(\frac{1}{2}(p-1)(p-2) \right) + (p-1)(q-1) \\ &= \frac{1}{4}(q-1)(q-2) + \frac{1}{4}(p-1)(p-2) + (p-1)(q-1). \end{aligned}$$

□

Theorem 3.2. *Let p and q be distinct prime numbers. Then the Wiener index of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{p^2q})$ is given by*

$$W(\Gamma'(\mathbb{Z}_{p^2q})) = p \left(\frac{p}{3}(2p^2 - 5p - 2) + pq(p + q - 2) - 1 \right),$$

and the Harary index is

$$H(\Gamma'(\mathbb{Z}_{p^2q})) = \frac{1}{4} (p^2((p+q)^2 - 2(p+q+5)) - 5pq + 4p + 9).$$

Proof. Let the sets Y_1, Y_2, Y_3 be as given in the proof of Theorem 2.1 (b) and $n_1 = |Y_1| = p(q-1)$, $n_2 = |Y_2| = p(p-1)$, $n_3 = |Y_3| = p-1$. Let $y_i, y_j \in V(G)$, then $y_i, y_j \in Y_1 \cup Y_2 \cup Y_3$. Consider the following cases.

Case (i): Let $y_i, y_j \in Y_1$. Then $d(y_i, y_j) = 2$, since $y_i \sim z \sim y_j$ is a path, where $z \in Y_3$. Since $|Y_1| = n_1$. Therefore

$$\sum_{y_i \neq y_j \in Y_1} d(y_i, y_j) = \frac{1}{2} \sum_{i=1}^{n_1} \sum_{j=1, j \neq i}^{n_1} d(y_i, y_j) = \frac{1}{2} \sum_{i=1}^{n_1} \sum_{j=1, j \neq i}^{n_1} 2 = n_1(n_1 - 1). \quad (5)$$

Furthermore,

$$\sum_{y_i \neq y_j \in Y_1} \frac{1}{d(y_i, y_j)} = \frac{1}{2} \sum_{i=1}^{n_1} \sum_{j=1, j \neq i}^{n_1} \frac{1}{d(y_i, y_j)} = \frac{1}{2} \sum_{i=1}^{n_1} \sum_{j=1, j \neq i}^{n_1} \frac{1}{2} = \frac{n_1(n_1 - 1)}{4}. \quad (6)$$

Case (ii): Let $y_i, y_j \in Y_2$. Since no element in Y_2 is adjacent to any other element within Y_2 , the induced subgraph on Y_2 contains no edges and $y_i \sim z \sim y_j$ is a path for $z \in Y_3$. Therefore $d(y_i, y_j) = 2$. Hence similar to Case (i) we get

$$\sum_{y_i \neq y_j \in Y_2} d(y_i, y_j) = n_2(n_2 - 1). \quad (7)$$

$$\sum_{y_i \neq y_j \in Y_2} \frac{1}{d(y_i, y_j)} = \frac{n_2(n_2 - 1)}{4}. \quad (8)$$

Case (iii): Let $y_i, y_j \in Y_3$. Since each element of Y_3 is adjacent to every other element of Y_3 , $d(y_i, y_j) = 1$. Therefore

$$\sum_{y_i \neq y_j \in Y_3} d(y_i, y_j) = \frac{1}{2} \sum_{i=1}^{n_3} \sum_{j=1, j \neq i}^{n_3} d(y_i, y_j) = \frac{1}{2} \sum_{i=1}^{n_3} \sum_{j=1, j \neq i}^{n_3} 1 = \frac{n_3(n_3 - 1)}{2}. \quad (9)$$

As $d(y_i, y_j) = 1$, we get

$$\sum_{y_i \neq y_j \in Y_3} \frac{1}{d(y_i, y_j)} = \sum_{y_i \neq y_j \in Y_3} d(y_i, y_j) = \frac{n_3(n_3 - 1)}{2}. \quad (10)$$

Case (iv): Label the elements of Y_1 as $x_1, x_2, \dots, x_{n_1}$ and Y_2 as $y_1, y_2, \dots, y_{n_2}$. Let $x_i \in Y_1$ and $y_j \in Y_2$, then the distance between x_i and y_j in the graph is $d(x_i, y_j) = 1$. Therefore

$$\sum_{x_i \in Y_1, y_j \in Y_2} d(x_i, y_j) = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} d(x_i, y_j) = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} 1 = n_1 n_2 \quad (11)$$

As $d(x_i, y_j) = 1$, we get

$$\sum_{x_i \in Y_1, y_j \in Y_2} \frac{1}{d(x_i, y_j)} = \sum_{x_i \in Y_1, y_j \in Y_2} d(x_i, y_j) = n_1 n_2 \quad (12)$$

Similarly, $\sum_{x \in Y_1, y \in Y_3} d(x, y) = \sum_{x \in Y_1, y \in Y_3} \frac{1}{d(x, y)} = n_1 n_3$ and

$$\sum_{x \in Y_2, y \in Y_3} d(x, y) = \sum_{x \in Y_2, y \in Y_3} \frac{1}{d(x, y)} = n_2 n_3. \text{ Therefore}$$

$$\begin{aligned} \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{p^2q}))} d(x, y) &= \sum_{x \neq y \in Y_i, i=1,2,3} d(x, y) + \sum_{x \in Y_i, y \in Y_j, i \neq j} d(x, y) \\ &= n_1(n_1 - 1) + n_2(n_2 - 1) + \frac{n_3(n_3 - 1)}{2} + n_1 n_2 + n_1 n_3 + n_2 n_3 \\ &= n_1^2 - n_1 + n_2^2 - n_2 + \frac{n_3^2}{2} - \frac{n_3}{2} + n_1 n_2 + n_1 n_3 + n_2 n_3 \\ &= p^2(q - 1)^2 - p(q - 1) + p^2(p - 1)^2 - p(p - 1) + \frac{(p - 1)^2}{2} \\ &\quad - \frac{p - 1}{2} + p(q - 1)p(p - 1) + p(q - 1)(p - 1) + p(p - 1)(p - 1) \\ &= p \left(\frac{p}{3}(2p^2 - 5p - 2) + pq(p + q - 2) - 1 \right). \end{aligned}$$

Hence the Wiener index of $\Gamma'(\mathbb{Z}_{p^2q})$ is

$$W(\Gamma'(\mathbb{Z}_{p^2q})) = p \left(\frac{p}{3}(2p^2 - 5p - 2) + pq(p + q - 2) - 1 \right).$$

$$\begin{aligned} \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{p^2q}))} \frac{1}{d(x, y)} &= \sum_{x \neq y \in Y_i, i=1,2,3} \frac{1}{d(x, y)} + \sum_{x \in Y_i, y \in Y_j, i \neq j} \frac{1}{d(x, y)} \\ &= \frac{n_1(n_1 - 1)}{4} + \frac{n_2(n_2 - 1)}{4} + \frac{n_3(n_3 - 1)}{2} + n_1 n_2 + n_1 n_3 + n_2 n_3 \\ &= \frac{1}{4} (n_1^2 - n_1 + n_2^2 - n_2 + 2n_3^2 - 2n_3 + 4n_1 n_2 + 4n_1 n_3 + 4n_2 n_3) \\ &= \frac{1}{4} (p^2(q - 1)^2 - p(q - 1) + p^2(p - 1)^2 - p(p - 1) + 2(p - 1) \\ &\quad - 2(p - 1) + 4p(q - 1)p(p - 1) + 4p(q - 1)(p - 1) + 4p(p - 1)(p - 1)) \\ &= \frac{1}{4} (p^2((p + q)^2 - 2(p + q + 5)) - 5pq + 4p + 9). \end{aligned}$$

Thus, the Harary index of $\Gamma'(\mathbb{Z}_{p^2q})$ is

$$H(\Gamma'(\mathbb{Z}_{p^2q})) = \frac{1}{4} (p^2((p + q)^2 - 2(p + q + 5)) - 5pq + 4p + 9).$$

□

Theorem 3.3. Let p and q be distinct prime numbers. Then the Wiener index of the generalized zero-divisor graph $\Gamma'(\mathbb{Z}_{p^2q^2})$ is given by

$$\begin{aligned} W(\Gamma'(\mathbb{Z}_{p^2q^2})) &= q^4(p^2 - 2p + 2) + q^3(2p^3 - 4p^2 + 5p - 4) \\ &\quad + q^2(p^4 - 4p^3 + 6p^2 - 6p + 2) + q \left(p^3 - 4p^2 + \frac{5}{2}p \right) + \frac{3}{2}, \end{aligned}$$

and the Harary index is given by (23).

Proof. Let the sets $Y_1, Y_2, \dots, Y_5$ be as given in the proof of Theorem 2.1 (c), and let $n_1 = |Y_1| = q(p - 1)(q - 1)$, $n_2 = |Y_2| = p(p - 1)(q - 1)$, $n_3 = |Y_3| = q(q - 1)$, $n_4 = |Y_4| =$

$p(p-1)$, $n_5 = |Y_5| = pq - 1$ (see Theorem 2.1 (c)). As in the above part (b), consider the following cases.

Case (i): Let $x, y \in Y_i$, $i \in \{1, 2, 3, 4\}$. Since no element of Y_i is adjacent to any other element within Y_i and the path $x \sim z \sim y$ exists for any $z \in Y_5$, it follows that $d(x, y) = 2$. Similar to the proof of the above part (b), we have $\sum_{x \neq y \in Y_i} d(x, y) = n_i(n_i - 1)$,

and $\sum_{x \neq y \in Y_i} \frac{1}{d(x, y)} = \frac{n_i(n_i - 1)}{4}$ for $i = 1, 2, 3, 4$.

Case (ii): Let $x \neq y \in Y_5$. Since each element of Y_5 is adjacent to every other element in Y_5 , the distance between any two elements $x, y \in Y_5$ is $d(x, y) = 1$. Then, similar to Case (iii) of the above part (b), we have $\sum_{x \neq y \in Y_5} d(x, y) = \sum_{x \neq y \in Y_5} \frac{1}{d(x, y)} = \frac{n_5(n_5 - 1)}{2}$.

Case (iii): Suppose that $x \in Y_i, y \in Y_j, i \neq j$. If $Y_i \sim Y_j$, then $d(x, y) = 1$. If $Y_i \approx Y_j$, then $d(x, y) = 2$, since $Y_i \sim Y_5 \sim Y_j$ is a path. Let $x \in Y_1, y \in Y_2$. Then $d(x, y) = 2$. Therefore

$$\sum_{x \in Y_1, y \in Y_2} d(x, y) = \sum_{x \in Y_1} \sum_{y \in Y_2} 2 = \sum_{x \in Y_1} 2n_2 = 2n_1n_2,$$

$$\sum_{x \in Y_1, y \in Y_2} \frac{1}{d(x, y)} = \sum_{x \in Y_1} \sum_{y \in Y_2} \frac{1}{2} = \sum_{x \in Y_1} \frac{1}{2}n_2 = \frac{n_1n_2}{2}.$$

Similarly, if $x \in Y_1, y \in Y_3$, then $d(x, y) = 2$.

Therefore $\sum_{x \in Y_1, y \in Y_3} d(x, y) = 2n_1n_3$, and $\sum_{x \in Y_1, y \in Y_3} \frac{1}{d(x, y)} = \frac{n_1n_3}{2}$.

Case (iv): Let $x \in Y_1, y \in Y_4$. Then $d(x, y) = 1$. Therefore

$$\sum_{x \in Y_1, y \in Y_4} d(x, y) = \sum_{x \in Y_1, y \in Y_4} \frac{1}{d(x, y)} = \sum_{x \in Y_1} \sum_{y \in Y_4} 1 = \sum_{x \in Y_1} n_4 = n_1n_4.$$

And, $\sum_{x \in Y_1, y \in Y_5} d(x, y) = \sum_{x \in Y_1, y \in Y_5} \frac{1}{d(x, y)} = n_1n_5$.

Similarly, we consider the remaining cases. Note that if $Y_i \approx Y_j$, then $d(x, y) = 2$ and we have $\sum_{x \in Y_i, y \in Y_j, i \neq j} d(x, y) = 2n_in_j$ and $\sum_{x \in Y_i, y \in Y_j, i \neq j} \frac{1}{d(x, y)} = \frac{n_in_j}{2}$. If $Y_i \sim Y_j$, then

$d(x, y) = 1$ and we have $\sum_{x \in Y_i, y \in Y_j, i \neq j} d(x, y) = \sum_{x \in Y_i, y \in Y_j, i \neq j} \frac{1}{d(x, y)} = n_in_j$. We now proceed

to compute the total sum of the distances between all pairs of vertices in the graph. Let $x \in Y_1$ and $y \in Y_i, i \in \{1, 2, \dots, 5\}$. Then

$$\begin{aligned} \sum_{i=1}^5 \sum_{x \in Y_1, x \neq y \in Y_i} d(x, y) &= n_1(n_1 - 1) + 2n_1n_2 + 2n_1n_3 + n_1n_4 + n_1n_5 \\ &= n_1(n_1 - 1 + 2n_2 + 2n_3 + n_4 + n_5). \end{aligned} \quad (13)$$

Similarly, if $x \in Y_2$ and $y \in Y_i, i \in \{2, 3, 4, 5\}$, then

$$\begin{aligned} \sum_{i=2}^5 \sum_{x \in Y_2, x \neq y \in Y_i} d(x, y) &= n_2(n_2 - 1) + n_2n_3 + 2n_2n_4 + n_2n_5 \\ &= n_2(n_2 - 1 + n_3 + 2n_4 + n_5). \end{aligned} \quad (14)$$

If $x \in Y_3$ and $y \in Y_i, i \in \{3, 4, 5\}$, then

$$\begin{aligned} \sum_{i=3}^5 \sum_{x \in Y_3, x \neq y \in Y_i} d(x, y) &= n_3(n_3 - 1) + n_3n_4 + n_3n_5 \\ &= n_3(n_3 - 1 + n_4 + n_5). \end{aligned} \quad (15)$$

If $x \in Y_4$ and $y \in Y_i, i \in \{4, 5\}$, then

$$\begin{aligned} \sum_{i=4}^5 \sum_{x \in Y_4, x \neq y \in Y_i} d(x, y) &= n_4(n_4 - 1) + n_4n_5 \\ &= n_4(n_4 - 1 + n_5). \end{aligned} \quad (16)$$

If $x \in Y_5$ and $y \in Y_5$, then

$$\sum_{x \neq y \in Y_5} d(x, y) = \frac{n_5(n_5 - 1)}{2}. \quad (17)$$

Adding equations (13) to (17) gives the Wiener index of $\Gamma'(\mathbb{Z}_{p^2q^2})$. Hence

$$\begin{aligned} W(\Gamma'(\mathbb{Z}_{p^2q^2})) &= \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{p^2q^2}))} d(x, y) \\ &= n_1(n_1 - 1 + 2n_2 + 2n_3 + n_4 + n_5) + n_2(n_2 - 1 + n_3 + 2n_4 + n_5) \\ &\quad + n_3(n_3 - 1 + n_4 + n_5) + n_4(n_4 - 1 + n_5) + \frac{n_5(n_5 - 1)}{2} \\ &= n_1^2 + n_2^2 + n_3^2 + n_4^2 + \frac{n_5^2}{2} - (n_1 + n_2 + n_3 + n_4 + n_5) + \frac{n_5}{2} \\ &\quad + n_1(2n_2 + 2n_3 + n_4 + n_5) + n_2(n_3 + 2n_4 + n_5) + n_3(n_4 + n_5) + n_4n_5 \\ &= q^2(p-1)^2(q-1)^2 + p^2(p-1)^2(q-1)^2 + q^2(q-1)^2 + p^2(p-1)^2 \\ &\quad + (pq-1)^2 - pq(p+q-1) + 1/2 + (1/2)pq \\ &\quad + q(p-1)(q-1)(2p(p-1)(q-1) + p(p-1) + pq-1) \\ &\quad + p(p-1)(q-1)(q(q-1) + 2p(p-1) + pq-1) \\ &\quad + q(q-1)(p(p-1) + pq-1) + p(p-1)(pq-1) \\ &= -p(p-1) + 2q^4 - 4q^3 + 3/2 - 3p^2q - 6pq^2 + p^2q^4 - 4p^2q^3 - 2pq^4 \\ &\quad + 5p^2q^2 + 5pq^3 + p^4q^2 - 4p^3q^2 + (9/2)pq + p^2 + 2q^2 - p + 2p^3q^3 \\ &\quad + p(p-1)pq + (pq)^2 - 2(pq) \\ &= q^4(p^2 - 2p + 2) + q^3(2p^3 - 4p^2 + 5p - 4) + q^2(p^4 - 4p^3 + 6p^2 - 6p + 2) \\ &\quad + q\left(p^3 - 4p^2 + \frac{5}{2}p\right) + \frac{3}{2}. \end{aligned}$$

Next, we calculate the Harary index of $\Gamma'(\mathbb{Z}_{p^2q^2})$.

First, we determine the reciprocals of the distances between all pairs of vertices in the graph. Let $x \in Y_1$ and $y \in Y_i, i \in \{1, 2, \dots, 5\}$. Then

$$\begin{aligned} \sum_{i=1}^5 \sum_{x \in Y_1, x \neq y \in Y_i} \frac{1}{d(x, y)} &= \frac{n_1(n_1 - 1)}{4} + \frac{n_1 n_2}{2} + \frac{n_1 n_3}{2} + n_1 n_4 + n_1 n_5 \\ &= \frac{n_1}{4}(n_1 - 1 + 2n_2 + 2n_3 + 4n_4 + 4n_5). \end{aligned} \quad (18)$$

Similarly, if $x \in Y_2$ and $y \in Y_i, i \in \{2, 3, 4, 5\}$, then

$$\begin{aligned} \sum_{i=2}^5 \sum_{x \in Y_2, x \neq y \in Y_i} \frac{1}{d(x, y)} &= \frac{n_2(n_2 - 1)}{4} + n_2 n_3 + \frac{n_2 n_4}{2} + n_2 n_5 \\ &= \frac{n_2}{4}(n_2 - 1 + 4n_3 + 2n_4 + 4n_5). \end{aligned} \quad (19)$$

If $x \in Y_3$ and $y \in Y_i, i \in \{3, 4, 5\}$, then

$$\begin{aligned} \sum_{i=3}^5 \sum_{x \in Y_3, x \neq y \in Y_i} \frac{1}{d(x, y)} &= \frac{n_3(n_3 - 1)}{4} + n_3 n_4 + n_3 n_5 \\ &= \frac{n_3}{4}(n_3 - 1 + 4n_4 + 4n_5). \end{aligned} \quad (20)$$

If $x \in Y_4$ and $y \in Y_i, i \in \{4, 5\}$, then

$$\begin{aligned} \sum_{i=4}^5 \sum_{x \in Y_4, x \neq y \in Y_i} \frac{1}{d(x, y)} &= \frac{n_4(n_4 - 1)}{4} + n_4 n_5 \\ &= \frac{n_4}{4}(n_4 - 1 + 4n_5). \end{aligned} \quad (21)$$

If $x \in Y_5$ and $y \in Y_5$, then

$$\sum_{x \in Y_5, x \neq y \in Y_5} \frac{1}{d(x, y)} = \frac{n_5(n_5 - 1)}{2}. \quad (22)$$

The Harary index of $\Gamma'(\mathbb{Z}_{p^2 q^2})$ is obtained by summing the expressions given in equations (18) through (22). Thus,

$$\begin{aligned} H(\Gamma'(\mathbb{Z}_{p^2 q^2})) &= \sum_{x \neq y \in V(\Gamma'(\mathbb{Z}_{p^2 q^2}))} \frac{1}{d(x, y)} \\ &= \frac{n_1}{4}(n_1 - 1 + 2n_2 + 2n_3 + 4n_4 + 4n_5) + \frac{n_2}{4}(n_2 - 1 + 4n_3 + 2n_4 + 4n_5) \\ &\quad + \frac{n_3}{4}(n_3 - 1 + 4n_4 + 4n_5) + \frac{n_4}{4}(n_4 - 1 + 4n_5) + \frac{n_5(n_5 - 1)}{2} \\ &= \frac{1}{4}[(n_1^2 + n_2^2 + n_3^2 + n_4^2 + 2n_5^2) - (n_1 + n_2 + n_3 + n_4 + 2n_5) + \\ &\quad n_1(2n_2 + 2n_3 + 4n_4 + 4n_5) + n_2(4n_3 + 2n_4 + 4n_5) + n_3(4n_4 + 4n_5) + \\ &\quad 4n_4 n_5], \end{aligned} \quad (23)$$

where $n_i = |Y_i|$ as given in Theorem 2.1 (c). □

4. CONCLUSIONS

The Wiener and Harary indices are significant topological indices in chemical graph theory and network analysis. They quantify structural features of molecules and network topologies and are extensively applied in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. The Wiener index is particularly useful in drug design, molecular stability assessment, and the prediction of physicochemical properties. Meanwhile, the Harary index evaluates the efficiency of information spread and interaction potential within a network. In this paper, we investigated the Wiener and Harary indices of $\Gamma'(\mathbb{Z}_n)$ for specific values of n . Future research will aim to extend this analysis to a broader range of values and develop algorithmic methods for efficiently computing these indices, along with exploring their applications across various domains.

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