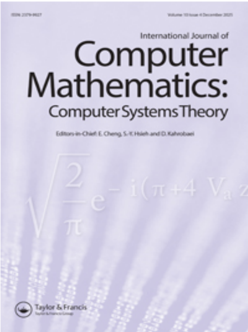

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Zagreb indices and size of a graph associated to a ring with Python syntax

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ABSTRACT
For a graph with edges and vertices, the general zeroth-order Randić index measures the sum of the degree of each vertex to the power of nonzero ω. Meanwhile, the zero divisor graph of a commutative ring R is the set of all zero divisors in R in which two vertices are adjacent if their product is zero. In this paper, the Zagreb indices of the zero divisor graph for the commutative ring $\mathbb{Z}_{p^kq}$ are found for the cases $\omega = 1, 2,$ and 3 where k is a positive integer, p and q are primes with $p < q$.

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1. Introduction

For the most part, a topological index, also called a molecular descriptor, is a numerical property that remains unchanged for a chemical graph. Many studies have been conducted on topological indices of graphs in recent years 1,6,9,10,14,15,18,24,25. In graph theory, an undirected graph $\Gamma = (V, E)$ consists of a set of vertices, V, and a set of edges, E. This research is motivated by a deep interest regarding the structural complexities of the zero divisor graph associated to commutative rings. Originating from the concept of zero divisors in rings, this graph offers a distinctive framework for analysing and understanding the algebraic properties of these mathematical structures. Its insights hold significant value across diverse applications, including network design, social networking, cryptographic frameworks and communication systems. Ali et al. [4] proposed three novel graph-theoretic encryption algorithms to enhance the quality of encryption methods, offering robust tools for securing confidential communication. Building on this foundation, Anderson and Livingston introduced and studied a zero divisor graph where

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the vertices represent nonzero zero divisors, as detailed in [5]. Axtell et al. [7] examined the presence of cut vertices in zero-divisor graphs of finite commutative rings. Pi et al. [23] described the girth and diameter of the zero divisor graph of $\mathbb{Z}_n$. The relations between the number of vertices of the zero-divisor graph, the compressed zero-divisor graph, the structure of the ring R and the eigenvalues of finite commutative rings R have been found by Mönius in [20]. Recently, Ali et al. [2] examined the zero divisor graphs for the ring of Gaussian integers modulo m, the ring of integers modulo n and some quotient polynomial rings. In [3], Ali et al. further studied some bounds for the multiset dimensions of compressed zero divisor graphs (CZDGs) associated with rings.

This paper focuses on the general zeroth-order Randić index, a degree-based topological index commonly used by chemists. In 2005, the general zeroth-order Randić index was developed by Li and Zheng [19]. The general zeroth-order Randić index is also known as the general first Zagreb index [8]. In pharmaceutical engineering, Mehak and Bhatti [22] stated that the general zeroth-order Randić index aids in testing the chemical and pharmacological characteristics of drug molecules. It provides a theoretical basis for drug manufacturing, potentially reducing the need for extensive experimental testing. Elumalai and Mansour in [12] found the expected value of the general zeroth-order Randic index for all bar graphs. Du et al. [11] obtained the minimum value of the zeroth-order general Randić index on the graphs with a given clique number and identified the associated distinctive extremal graphs. Vetrik et al. [26] presented bounds on this topological index for trees and distance k-domination number. Matejić et al. [21] discovered multiple upper and lower limits for the zeroth-order general Randić index. In this study, the general zeroth-order Randić index of the zero divisor graph for the ring $\mathbb{Z}_{p^kq}$, where k is a positive integer, p and q are primes and $p < q$, is computed. The general zeroth-order Randić index is found using the notations $R_1^0(\Gamma(\mathbb{Z}_{p^kq}))$, $R_2^0(\Gamma(\mathbb{Z}_{p^kq}))$ and $R_3^0(\Gamma(\mathbb{Z}_{p^kq}))$ to represent the cases $\omega = 1, 2$ and 3, respectively.

2. Preliminaries and known results

This section briefly introduces the concepts and definitions of ring theory, graph theory and topological index.

Definition 2.1: ([13]) Let R be a ring. A nonzero element is the zero divisor if the product of the element with another nonzero element of the ring is equal to zero.

Definition 2.2: ([5]) The zero divisor graph of R, denoted as $\Gamma(R)$, is a graph with vertices consisting of the zero divisors of R. Two distinct vertices, a and b, are adjacent if $ab = ba = 0$.

In this paper, we denote $Z(R)$ to represent the set of all zero divisors in the ring R is the set of vertices of the zero divisor graph of a ring R is denoted by $V(\Gamma(R))$.

Definition 2.3: ([19]) Let Γ be a connected graph and $\deg(a)$ be the degree of a in the graph. Then the general zeroth-order Randić index,

$$R^0_\omega = \sum_{u \in V(\Gamma)} (deg(a))^\omega,$$

where ω is an arbitrary real number.

The following three propositions are needed in our proof in the next section.

Proposition 2.1: *([16]) For any graph* Γ, $\sum_{a \in V(\Gamma)} deg(a) = 2|E(\Gamma)|$.

Proposition 2.2: *([17]) Let* $\mathbb{Z}_n$ *be the ring of integers modulo n, where n can be expressed as* $n = p_1^{k_1} p_2^{k_2} \cdots p_m^{k_m}$, *such that* $p_1, p_2, \ldots, p_m$ *are distinct prime numbers,* $k_1, k_2, \ldots, k_m \in \mathbb{N}$, *and* $m \in \mathbb{N}$. *Then the ring* $\mathbb{Z}_n$ *has at least a zero divisor, and the number of its zero divisors is*

$$n - n\left(1 - \frac{1}{p_1}\right)\left(1 - \frac{1}{p_2}\right)\cdots\left(1 - \frac{1}{p_m}\right) - 1.$$

3. Results and discussion

For the rest of this discussion, we concentrate on the ring $\mathbb{Z}_{p^k q}$, for positive integers k, p and q are primes with $p < q$. Some results related to the zero divisor graph of the commutative ring $\mathbb{Z}_{p^k q}$, denoted as $\Gamma(\mathbb{Z}_{p^k q})$, are discussed in this section. In the following propositions, we list the set of all zero divisors, denoted as $Z(\mathbb{Z}_{p^k q})$ and the number of zero divisors, denoted as $|Z(\mathbb{Z}_{p^k q})|$, in the commutative ring $\mathbb{Z}_{p^k q}$.

Proposition 3.1: *The set of all zero divisors,*

$$Z(\mathbb{Z}_{p^k q}) = \{p, 2p, 3p, \ldots, (p^{k-1}q - 1)p\} \cup \{q, 2q, 3q, \ldots, (p^k - 1)q\}.$$

Proof: Let a be a zero divisor of the ring $\mathbb{Z}_{p^k q}$. Then $Z(\mathbb{Z}_{p^k q})$ is given in the following:

(a) Suppose $a \in \mathbb{Z}_{p^k q}$ with $\gcd(a, p) > 1$ and A_1 is $Z(\mathbb{Z}_{p^k q})$ for a. Then $A_1 = \{p, 2p, 3p, 4p, \ldots, p(p^{k-1}q - 1)\}$ with the cardinality $(p^{k-1}q - 1)$.
(b) Suppose $a \in \mathbb{Z}_{p^k q}$ with $\gcd(a, q) > 1$ and A_2 is $Z(\mathbb{Z}_{p^k q})$ for a. Then $A_2 = \{q, 2q, 3q, 4q, \ldots, q(p^k - 1)\}$ with the cardinality $(p^k - 1)$.
(c) Suppose $a \in \mathbb{Z}_{p^k q}$ with $\gcd(a, pq) = pq$ and $A_1 \cap A_2$ is the set of all zero divisors of a. Then $A_1 \cap A_2 = \{pq, 2pq, 3pq, 4pq, \ldots, pq(p^{k-1} - 1)\}$ with the cardinality $(p^{k-1} - 1)$.

Therefore, $Z(\mathbb{Z}_{p^k q}) = A_1 \cup A_2 = \{p, 2p, 3p, \ldots, p(p^{k-1}q - 1)\} \cup \{q, 2q, 3q, \ldots, q(p^k - 1)\}$. ■

Proposition 3.2: *The number of zero divisors in the commutative ring* $\mathbb{Z}_{p^k q}$,

$$|Z(\mathbb{Z}_{p^k q})| = p^{k-1}(q - 1) + p^k - 1.$$

Proof: By using the inclusion–exclusion principle, we have

$$\begin{aligned}|Z(\mathbb{Z}_{p^kq})| &= |A_1 \cup A_2| \\ &= |A_1| + |A_2| - |A_1 \cap A_2|.\end{aligned}$$

Then, by using Proposition 3.1 with their cardinalities,

$$\begin{aligned}|Z(\mathbb{Z}_{p^kq})| &= (p^{k-1}q - 1) + (p^k - 1) - (p^{k-1} - 1) \\ &= p^{k-1}(q-1) + p^k - 1.\end{aligned}$$

■

Next the degree of a vertex in $\Gamma(\mathbb{Z}_{p^kq})$ is separated into three cases as given in Propositions 3.3, 3.4 and 3.5.

Proposition 3.3: *Let* $a \in Z(\mathbb{Z}_{p^kq})$ *with* $\gcd(a, p^kq) = p^i$ *for* $i = 1, 2, \ldots, k$. *Then* $deg(a) = p^i - 1$.

Proof: Let $a \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(a, p^kq) = p^i$, and let $b \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(b, p^kq) = p^jq$, $\gcd(b, p^kq) = p^j$ or $\gcd(b, p^kq) = q$ for $i \neq j$ where a and b are adjacent if and only if $i + j \geq k$. Since $\gcd(b, p^kq) = p^jq$, $\gcd(b, p^kq) = p^j$ or $\gcd(b, p^kq) = q$ where $j \geq k - i$, so $b \in p^{k-i}q\mathbb{Z}_{p^kq}$ and $|p^{k-i}q\mathbb{Z}_{p^kq}| = |p^{k-i}q\{0, 1, 2, 3, \ldots, p^kq - 1\}| = \frac{p^kq}{p^{k-i}q} - 1$. Thus, since $0 \notin Z(\mathbb{Z}_{p^kq})$, so $deg(a) = p^i - 1$. ■

Proposition 3.4: *Let* $a \in Z(\mathbb{Z}_{p^kq})$ *with* $\gcd(a, p^kq) = q$. *Then* $deg(a) = q - 1$.

Proof: Let $a \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(a, p^kq) = q$, and let $b \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(b, p^kq) = p^j$ where a and b are adjacent if and only if $j = k$. Since $\gcd(b, p^kq) = p^j$ and $j = k$, so $b \in p^k\mathbb{Z}_{p^kq}$ and $|p^k\mathbb{Z}_{p^kq}| = |p^k\{0, 1, 2, 3, \ldots, p^kq - 1\}| = \frac{p^kq}{p^k} - 1$. Thus $deg(a) = q - 1$. ■

Proposition 3.5: *Let* $a \in Z(\mathbb{Z}_{p^kq})$ *with* $\gcd(a, p^kq) = p^iq$. *Then*

$$deg(a) = \begin{cases} p^iq - 1, & \text{for } i \leq \left\lfloor \frac{k-1}{2} \right\rfloor, \\ p^iq - 2, & \text{for } i > \left\lfloor \frac{k-1}{2} \right\rfloor. \end{cases}$$

Proof: First, assume $i \leq \lfloor \frac{k-1}{2} \rfloor$. Let $a \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(a, p^kq) = p^iq$ and let $b \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(b, p^kq) = p^jq$ and $\gcd(b, p^kq) = p^j$, where a and b are adjacent if and only if $i + j \geq k$. Since $\gcd(b, p^kq) = p^jq$, $\gcd(b, p^kq) = p^j$ and $j \geq k - i$, so $b \in p^{k-i}\mathbb{Z}_{p^kq}$ and $|p^{k-i}\mathbb{Z}_{p^kq}| = |p^{k-i}\{0, 1, 2, 3, \ldots, p^kq - 1\}| = \frac{p^kq}{p^{k-i}} - 1$. Thus $deg(a) = p^iq - 1$.

Next, assume $i > \lfloor \frac{k-1}{2} \rfloor$. Let $a \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(a, p^kq) = p^iq$ and let $b \in Z(\mathbb{Z}_{p^kq})$ with $\gcd(b, p^kq) = p^jq$ and $\gcd(b, p^kq) = p^j$, where a and b are adjacent if and only if

$i+j \geq k$. Since $\gcd(b, p^k q) = p^j q$, $\gcd(b, p^k q) = p^j$ or $\gcd(b, p^k q) = q$, where $j \geq k-i$, so $b \in p^{k-i}\mathbb{Z}_{p^k q}$ and $|p^{k-i}\mathbb{Z}_{p^k q}| = |p^{k-i}\{0,1,2,3,\ldots,p^k q-1\}| = \frac{p^k q}{p^{k-i}} - 2$. Thus since $0 \notin Z(\mathbb{Z}_{p^k q})$ and $\gcd(p^i q, p^k q) = p^i q$ so $deg(a) = p^i q - 2$. ■

The number of vertices in $\Gamma(\mathbb{Z}_{p^k q})$ for a given degree is divided into three cases as shown in Propositions 3.6, 3.7 and 3.8.

Proposition 3.6: *Let $a \in V(\Gamma(\mathbb{Z}_{p^k q}))$ thus $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = p^i$. Then*

$$|V(\Gamma(\mathbb{Z}_{p^k q}))| = \begin{cases} (p^{k-i} - p^{k-(i+1)})(q-1), & \text{for } 1 \leq i \leq k-1, \\ (p^{k-i})(q-1), & \text{for } i = k. \end{cases}$$

Proof: Given $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = p^i$. Then

(i) $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i} - p^{k-(i+1)})$ for $1 \leq i \leq k-1$ and $b \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(b, q) = q$ then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = q-1$. So $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i} - p^{k-(i+1)})(q-1)$.

(ii) $|V(\Gamma(\mathbb{Z}_{p^k q}))| = p^{k-i}$ for $i = k$ and $b \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(b, q) = q$ then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = q-1$. So $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i})(q-1)$.

■

Proposition 3.7: *Let $a \in V(\Gamma(\mathbb{Z}_{p^k q}))$, thus $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = q$. Then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^k - p^{k-i})$ for $i = 1$.*

Proof: Given $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = q$. Then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^k - p^{k-i})$ for $i = 1$ and $b \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(b, q) = 1$ then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = 1$. So $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^k - p^{k-i})(1) = (p^k - p^{k-i})$. ■

Proposition 3.8: *Let $a \in V(\Gamma(\mathbb{Z}_{p^k q}))$, thus $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = p^i q$. Then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i} - p^{k-(i+1)})$ for $1 \leq i \leq k-1$.*

Proof: Given $a \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(a, p^k q) = p^i q$ then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i} - p^{k-(i+1)})$ for $1 \leq i \leq k-1$ and $b \in Z(\mathbb{Z}_{p^k q})$ where $\gcd(b, q) = 1$ then $|V(\Gamma(\mathbb{Z}_{p^k q}))| = 1$. So $|V(\Gamma(\mathbb{Z}_{p^k q}))| = (p^{k-i} - p^{k-(i+1)})$. ■

Theorem 3.1: *The number of edges for $\Gamma(\mathbb{Z}_{p^k q})$,*

$$|E(\Gamma(\mathbb{Z}_{p^k q}))| = \frac{1}{2}\left[\left((q-1)(k+1) + q(k-1) - \left(\frac{p^{k-1} - p^{\lfloor \frac{k-1}{2} \rfloor}}{p^{\lfloor \frac{3(k-1)}{2} \rfloor}(p-1)}\right)\right)(p^k - p^{k-1}) + 1 - p^{k-1}\right].$$

Proof: Using Proposition 2.1 and applying it from Propositions 3.3 to 3.8,

$$|E(\Gamma(\mathbb{Z}_{p^kq}))| = \frac{1}{2}\Bigg[(q-1)(p^k-p^{k-1}) + (q-1)\sum_{i=1}^{k-1}(p^{k-i}-p^{k-(i+1)})(p^i-1) + (q-1)\sum_{i=1+k-1}^{k} p^{k-i}(p^i-1) + \sum_{i=1}^{\left\lfloor\frac{k-1}{2}\right\rfloor}(p^{k-i}-p^{k-(i+1)})(p^iq-1) + \sum_{i=1+\left\lfloor\frac{k-1}{2}\right\rfloor}^{k-1}(p^{k-i}-p^{k-(i+1)})(p^iq-2)\Bigg].$$

After the simplification of the equation using summation rules and geometric sequences, we then obtain

$$|E(\Gamma(\mathbb{Z}_{p^kq}))| = \frac{1}{2}\left[\left((q-1)(k+1)+q(k-1)-\left(\frac{p^{k-1}-p^{\left\lfloor\frac{k-1}{2}\right\rfloor}}{p^{\left\lfloor\frac{3(k-1)}{2}\right\rfloor}(p-1)}\right)\right)(p^k-p^{k-1}) + 1 - p^{k-1}\right].$$

■

Next, the main results in this research, $R^0_\omega(\Gamma(\mathbb{Z}_{p^kq}))$ for $\omega = 1, 2$ and 3 are presented in the following three theorems.

Theorem 3.2: *The general zeroth-order Randić index when* $\omega = 1$,

$$R^0_1(\Gamma(\mathbb{Z}_{p^kq})) = (p^k-p^{k-1})\left[(q-1)(k+1)+q(k-1)-\left(\frac{p^{k-1}-p^{\left\lfloor\frac{k-1}{2}\right\rfloor}}{p^{\left\lfloor\frac{3(k-1)}{2}\right\rfloor}(p-1)}\right)\right] - p^{k-1}+1.$$

Proof: Using Definition 2.3 and applying it from Propositions 3.3 to 3.8,

$$R^0_1(\Gamma(\mathbb{Z}_{p^kq})) = \sum_{a\in V(\Gamma(\mathbb{Z}_{p^kq}))}(deg(a))^1$$

$$= (p^k-p^{k-1})(q-1)^1 + (q-1)\sum_{i=1}^{k-1}(p^{k-i}-p^{k-(i+1)})(p^i-1)^1 + (q-1)\sum_{i=1+k-1}^{k} p^{k-i}(p^i-1)^1 + \sum_{i=1}^{\left\lfloor\frac{k-1}{2}\right\rfloor}(p^{k-i}-p^{k-(i+1)})(p^iq-1)^1$$

$$+ \sum_{i=1+\left\lfloor \frac{k-1}{2} \right\rfloor}^{k-1} (p^{k-i} - p^{k-(i+1)})(p^i q - 2)^1$$

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

$$- p^{k-1} + 1.$$

■

Theorem 3.3: *The general zeroth-order Randić index when $\omega = 2$*

$$R_2^0(\Gamma(\mathbb{Z}_{p^k q})) = (q-1)[(p^k - p^{k-1})(q - 2k + 1) + p^{k-1}(p^k - p + 1) - 1 + (p^k - 1)^2] + (p^k - p^{k-1}) \left[3 \left(\frac{p^{k-1} - p^{\left\lfloor \frac{k-1}{2} \right\rfloor}}{p^{\left\lfloor \frac{3(k-1)}{2} \right\rfloor}(p-1)} \right) - 2q \left(k - 1 + \left\lceil \frac{k-1}{2} \right\rceil \right) \right] + q^2(p^{2k-1} - p^k) + p^{k-1} - 1.$$

Proof: By applying the similar method as in Theorem 3.2 but with $\omega = 2$,

$$R_2^0(\Gamma(\mathbb{Z}_{p^k q})) = (p^k - p^{k-1})(q-1)^2 + (q-1) \sum_{i=1}^{k-1} (p^{k-i} - p^{k-(i+1)})(p^i - 1)^2$$

$$+ (q-1) \sum_{i=1+k-1}^{k} p^{k-i}(p^i - 1)^2 + \sum_{i=1}^{\left\lfloor \frac{k-1}{2} \right\rfloor} (p^{k-i} - p^{k-(i+1)})(p^i q - 1)^2$$

$$+ \sum_{i=1+\left\lfloor \frac{k-1}{2} \right\rfloor}^{k-1} (p^{k-i} - p^{k-(i+1)})(p^i q - 2)^2$$

$$= (q-1)[(p^k - p^{k-1})(q - 2k + 1) + p^{k-1}(p^k - p + 1) - 1 + (p^k - 1)^2] + (p^k - p^{k-1}) \left[3 \left(\frac{p^{k-1} - p^{\left\lfloor \frac{k-1}{2} \right\rfloor}}{p^{\left\lfloor \frac{3(k-1)}{2} \right\rfloor}(p-1)} \right) - 2q \left(k - 1 + \left\lceil \frac{k-1}{2} \right\rceil \right) \right] + q^2(p^{2k-1} - p^k) + p^{k-1} - 1.$$

■

Theorem 3.4: *The general zeroth-order Randić index when $\omega = 3$,*

$$R_3^0(\Gamma(\mathbb{Z}_{p^k q})) = (q-1)(p^k - p^{k-1})((q-1)^2 + 3(k-1)) + \frac{p^{3k-1} - p^{k+1}}{p+1}$$

$$- 3p^{2k-1} + 3p^{k} - p^{k-1} + 1 + (p^{k}-1)^{3}\Big] + q^{3}\left(\frac{p^{3k-1}-p^{k+1}}{p+1}\right)$$
$$- 3q^{2}(p^{2k-1}-p^{k}) - p^{k-1} + 1 - 3q^{2}\left(p^{2k-1} - p^{\left\lfloor\frac{3k-1}{2}\right\rfloor}\right)$$
$$+ (p^{k}-p^{k-1})\left[3q\left(k-1+3\left\lceil\frac{k-1}{2}\right\rceil\right) - 7\left(\frac{p^{k-1}-p^{\left\lfloor\frac{k-1}{2}\right\rfloor}}{p^{\left\lfloor\frac{3(k-1)}{2}\right\rfloor}(p-1)}\right)\right].$$

Proof: Similarly, we obtain

$$R_3^0(\Gamma(\mathbb{Z}_{p^kq})) = \sum_{i=1}^{1}(p^{k}-p^{k-i})(q-1)^{3} + (q-1)\sum_{i=1}^{k-1}(p^{k-i}-p^{k-(i+1)})(p^{i}-1)^{3}$$
$$+ (q-1)\sum_{i=1+k-1}^{k} p^{k-i}(p^{i}-1)^{3} + \sum_{i=1}^{\left\lfloor\frac{k-1}{2}\right\rfloor}(p^{k-i}-p^{k-(i+1)})(p^{i}q-1)^{3}$$
$$+ \sum_{i=1+\left\lfloor\frac{k-1}{2}\right\rfloor}^{k-1}(p^{k-i}-p^{k-(i+1)})(p^{i}q-2)^{3}$$
$$= (q-1)(p^{k}-p^{k-1})((q-1)^{2}+3(k-1)) + \frac{p^{3k-1}-p^{k+1}}{p+1}$$
$$-3p^{2k-1} + 3p^{k} - p^{k-1} + 1 + (p^{k}-1)^{3}\Big] + q^{3}\left(\frac{p^{3k-1}-p^{k+1}}{p+1}\right)$$
$$- 3q^{2}(p^{2k-1}-p^{k}) - p^{k-1} + 1 - 3q^{2}\left(p^{2k-1} - p^{\left\lfloor\frac{3k-1}{2}\right\rfloor}\right)$$
$$+ (p^{k}-p^{k-1})\left[3q\left(k-1+3\left\lceil\frac{k-1}{2}\right\rceil\right) - 7\left(\frac{p^{k-1}-p^{\left\lfloor\frac{k-1}{2}\right\rfloor}}{p^{\left\lfloor\frac{3(k-1)}{2}\right\rfloor}(p-1)}\right)\right].$$

■

Finally, two examples of the general zeroth-order Randić index for $\Gamma(\mathbb{Z}_{p^kq})$ are shown in two cases:

(i) p is even and q is odd for some k when $\omega = 1$,
(ii) p and q are both odd for some k when $\omega = 3$.

Example 3.1: Let $p = 2$, $q = 7$ and $k = 3$, then $\Gamma(\mathbb{Z}_{56})$, is shown in Figure 1.

By Proposition 3.1, $Z(\mathbb{Z}_{56})$ is determined as follows: $Z(\mathbb{Z}_{56}) = A_1 \cup A_2 = \{2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54\} \cup \{7, 14, 21, 28, 35, 42, 49\} = \{2, 4, 6, 7, 8, 10, 12, 14, 16, 18, 20, 21, 22, 24, 26, 28, 30, 32, 34, 35, 36,$

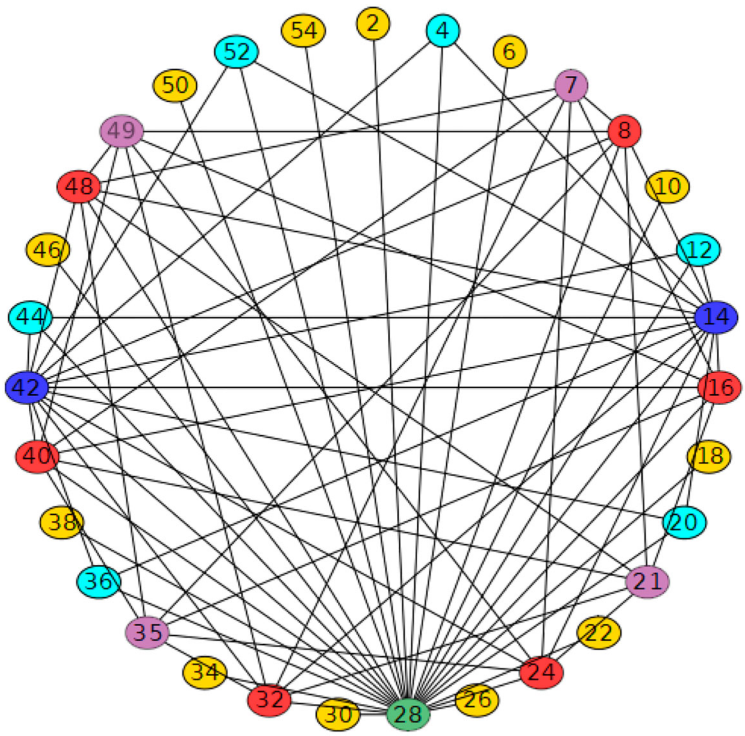

Figure 1. $\Gamma(\mathbb{Z}_{56})$ with coloured vertices.

38, 40, 42, 44, 46, 48, 49, 50, 52, 54}. By Proposition 3.2, the number of zero divisors is the vertices of $\Gamma(\mathbb{Z}_{56})$ can be calculated as follows: $|Z(\mathbb{Z}_{56})^*| = 2^{3-1}(7-1) + 2^3 - 1 = 31$. The graph has 74 edges, as shown in Figure 1. However, by Theorem 3.1,

$$|E(\Gamma(\mathbb{Z}_{56}))| = \frac{1}{2}\left[\left((7-1)(3+1) + 7(3-1) - \left(\frac{2^{3-1} - 2^{\lfloor \frac{3-1}{2} \rfloor}}{2^{\lfloor \frac{3(3-1)}{2} \rfloor}(2-1)}\right)\right)(2^3 - 2^{3-1}) + 1 - 2^{3-1}\right] = 74.$$

Note that in Figure 1, the yellow colour represents the vertices of degree 1, cyan for vertices of degree 3, purple for degree 6, red for degree 7, blue for degree 13, and green for degree 26, which has just one vertex. By Definition 2.3, the general zeroth-order Randić index when $\omega = 1$ is calculated as follows: $R_1^0(\Gamma(\mathbb{Z}_{56})) = deg(2) + deg(4) + deg(6) + deg(7) + deg(8) + deg(10) + deg(12) + deg(14) + deg(16) + deg(18) + deg(20) + deg(21) + deg(22) + deg(24) + deg(26) + deg(28) + deg(30) + deg(32) + deg(34) + deg(35) + deg(36) + deg(38) + deg(40) + deg(42) + deg(44) + deg(46) + deg(48) + deg(49) + deg(50) + deg(52) + deg(54) = 12(1) + 6(3) + 4(6) + 6(7) + 2(13) + 1(26) = 148$.

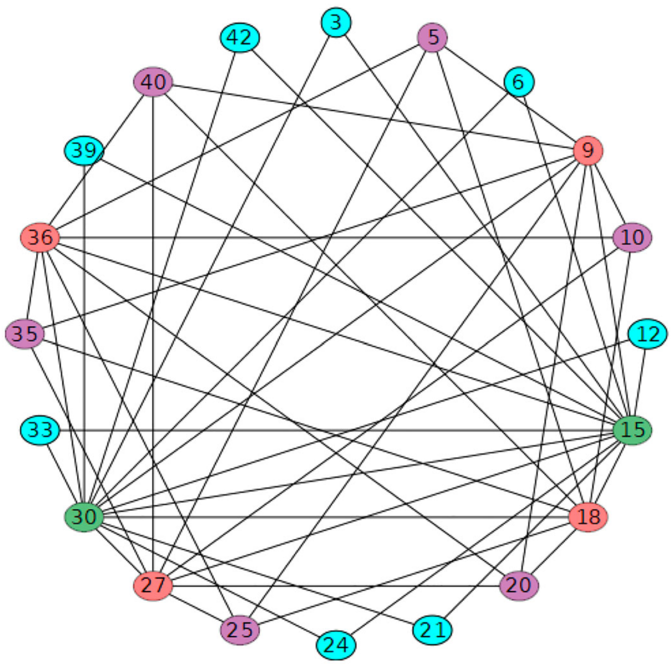

Figure 2. $\Gamma(\mathbb{Z}_{45})$ with coloured vertices.

Using Theorem 3.2 is a quick and direct way to determine the value for $R_1^0(\Gamma(\mathbb{Z}_{56}))$ when $\omega = 1$:

$$R_1^0(\Gamma(\mathbb{Z}_{56})) = (2^3 - 2^{3-1})\left((7-1)(3+1) + 7(3-1) - \left(\frac{2^{3-1} - 2^{\lfloor \frac{3-1}{2} \rfloor}}{2^{\left\lfloor \frac{3(3-1)}{2} \right\rfloor}(2-1)}\right)\right)$$
$$+1 - 2^{3-1}$$
$$= 148.$$

Example 3.2: Suppose $p = 3$, $q = 5$ and $k = 2$, then $\Gamma(\mathbb{Z}_{45})$ is illustrated in Figure 2.

By Proposition 3.1, $Z(\mathbb{Z}_{45})$ is found as follows: $Z(\mathbb{Z}_{45}) = A_1 \cup A_2 = \{3, 6, 9, 12, 15, 18, 21, 24, 27, 30, 33, 36, 39, 42\} \cup \{5, 10, 15, 20, 25, 30, 35, 40\} = \{3, 5, 6, 9, 10, 12, 15, 18, 20, 21, 24, 25, 27, 30, 33, 35, 36, 39, 40, 42\}$. According to Proposition 3.2, the number of zero divisors for $\Gamma(\mathbb{Z}_{45})$ can be determined as follows:

$$|Z(\mathbb{Z}_{45})^*| = 3^{2-1}(5-1) + 3^2 - 1 = 20.$$

Figure 2 shows that the $\Gamma(\mathbb{Z}_{45})$ has a total of 49 edges. However, by Theorem 3.1,

$$|E(\Gamma(\mathbb{Z}_{45}))| = \frac{1}{2}\left[\left((5-1)(2+1) + 5(2-1) - \left(\frac{3^{2-1} - 3^{\lfloor \frac{2-1}{2} \rfloor}}{3^{\left\lfloor \frac{3(2-1)}{2} \right\rfloor}(3-1)}\right)\right)(3^2 - 3^{2-1})\right.$$
$$\left. + 1 - 3^{2-1}\right] = 49.$$

Note that in Figure 2, the vertex colours are as follows: cyan colour represents vertices of degree 2, purple for vertices of degree 4, red for degree 8 and green for degree 13. By Definition 2.3, the calculation for $R_3^0(\Gamma(\mathbb{Z}_{45}))$ when $\omega = 3$ consists of the following steps: $R_3^0(\Gamma(\mathbb{Z}_{45})) = deg(3)^3 + deg(5)^3 + deg(6)^3 + deg(9)^3 + deg(10)^3 + deg(12)^3 + deg(15)^3 + deg(18)^3 + deg(20)^3 + deg(21)^3 + deg(24)^3 + deg(25)^3 + deg(27)^3 + deg(30)^3 + deg(33)^3 + deg(35)^3 + deg(36)^3 + deg(39)^3 + deg(40)^3 + deg(42)^3 = 8(2)^3 + 6(4)^3 + 4(8)^3 + 2(13)^3 = 6890$. Using Theorem 3.4, $R_3^0(\Gamma(\mathbb{Z}_{45})) = (5-1)[(3^2 - 3^{2-1})((5-1)^2 + 3(2-1)) + \frac{3^{3(2)-1} - 3^{2+1}}{3+1} - 3(3^{2(2)-1}) + 3(3^2) - 3^{2-1} + 1 + (3^2-1)^3] + 5^3(\frac{3^{3(2)-1} - 3^{2+1}}{3+1}) - 3(5^2)(3^{2(2)-1} - 3^2) - 3^{2-1} + 1 - 3(5^2)(3^{2(2)-1} - 3^{\lfloor \frac{3(2)-1}{2} \rfloor}) + (3^2 - 3^{2-1})[3(5)(2 - 1 + 3\lceil \frac{2-1}{2} \rceil) - 7(\frac{3^{2-1} - 3^{\lfloor \frac{2-1}{2} \rfloor}}{3^{\lfloor \frac{3(2-1)}{2} \rfloor}(3-1)})] = 6890$.

The answers from the example above show that the results are identical when applying the definition and the general formula.

4. Python syntax for computing the general zeroth-order Randić index of $\Gamma(\mathbb{Z}_{p^k q})$

In this section, the Python syntax to compute the general zeroth-order Randic index of $\Gamma(\mathbb{Z}_{p^k q})$ is presented. First, we used Python syntax to construct a zero divisor graph of commutative ring integers modulo n as follows.

```
import networkx as nx
import matplotlib.pyplot as plt
import math

# Definition of the zero divisor graph for Gamma_Z_(p^k)q
def zero_divisor_graph(p, q, k):
    n = (p ** k) * q
    zero_divisors = []

    for x in range(1, n):
        for y in range(1, n):
            if (x * y) % n == 0 and x != y:
                zero_divisors.append((x, y))

    G = nx.Graph()
    G.add_nodes_from(range(1, n))

    for zero_divisor in zero_divisors:
        G.add_edge(zero_divisor[0], zero_divisor[1])

        # Removing unconnected nodes or vertices
    largest_cc = max(nx.connected_components(G), key=len)
    unconnected_nodes = set(G.nodes) - largest_cc
    G.remove_nodes_from(unconnected_nodes)

    return G
```

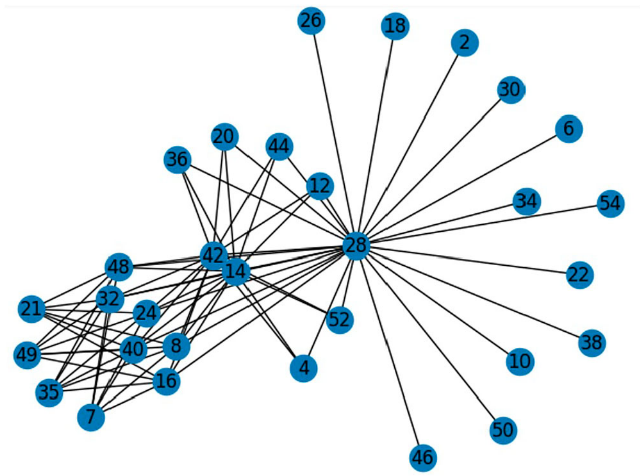

Figure 3. Output Python of $\Gamma(\mathbb{Z}_{56})$.

This paper focuses on $n = p^k q$, where p and q are primes and $q > p$. The following code is the function to check whether the number is a prime.

```
#Function to Check Prime Number
def isNotPrime(z):
  factor=0
  for i in range (1,z+1):
    if z%i==0:
      factor +=1
  if factor==2:
      return False
  else :
      return True
```

Next, we need to input the values of p, q and k. The zero divisor graph of $\mathbb{Z}_{p^k q}$ will be processed if the inputs are correct.

```
p=0
q=0
while p>=q or isNotPrime(p) or isNotPrime(q):
  p=int(input("p:"))
  k=int(input("k:"))
  q=int(input("q:"))
  if p>=q or isNotPrime(p) or isNotPrime(q):
    print("p must be smaller than q where p and q prime number, please
    ↪ input again")
Gamma_Z_pkq=zero_divisor_graph(p, q, k)
```

Figure 3 shows the Python output of $\Gamma(\mathbb{Z}_{56})$ for $p = 2, q = 7$ and $k = 3$ in Example 3.1. Figure 4 shows the Python output of $\Gamma(\mathbb{Z}_{45})$ for $p = 3, q = 5$ and $k = 2$ in Example 3.2.

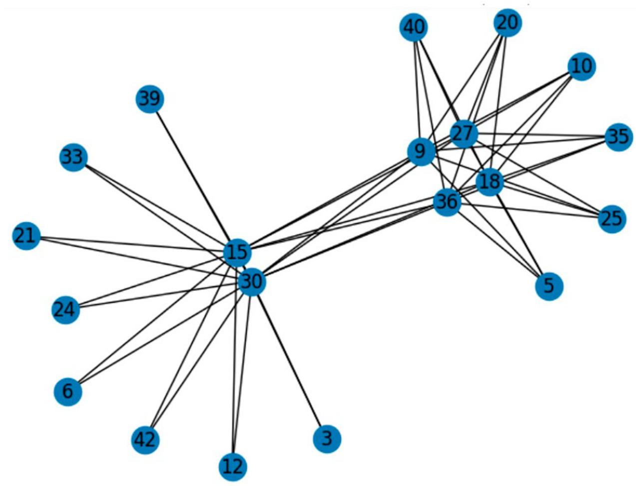

Figure 4. Output Python of $\Gamma(\mathbb{Z}_{45})$.

The following are the Python syntax for the cases $\omega = 1, 2$ and 3.

```
# General Zeroth-Order Randić Index when omega = 1
def GZORIomega1(p,q,k):
 return (((q - 1) * (k + 1) + q * (k - 1) - ((p**(k - 1) - p**(math.floor((k - 1) / 2))) / (p**(math.floor(3 * (k - 1) / 2)) * (p - 1)))) * (p**k - p**(k - 1)) + 1 - p**(k - 1))

# General Zeroth-Order Randić Index when omega = 2
def GZORIomega2(p,q,k):
  term1b = (q - 1) * ((p**k - p**(k - 1)) * (q - 2*k + 1) + p**(k - 1) * (p**k - p + 1) - 1 + (p**k - 1)**2)
  term2b = (p**k - p**(k - 1)) * (3*((p**(k - 1) - p**math.floor((k - 1)/2)) / (p**math.floor(3*(k - 1)/2) * (p - 1))) - 2*q*(k - 1 + math.ceil((k - 1)/2)))
  term3b = q**2 * (p**(2*k - 1) - p**k) + p**(k - 1) - 1
  return term1b + term2b + term3b

# General Zeroth-Order Randić Index when omega = 3
def GZORIomega3(p,q,k):
  term1c = (q - 1) * ((p**k - p**(k - 1)) * ((q - 1)**2 + 3*(k - 1)) + (p**(3*k - 1) - p**(k + 1)) / (p + 1) - 3*p**(2*k - 1) + 3*p**k - p**(k - 1) + 1 + (p**k - 1)**3)
  term2c = q**3 * ((p**(3*k - 1) - p**(k + 1)) / (p + 1)) - 3*q**2 * (p**(2*k - 1) - p**k) - p**(k - 1) + 1 - 3*q**2 * (p**(2*k - 1) - p**math.floor((3*k - 1)/2))
  term3c = (p**k - p**(k - 1)) * (3*q*(k - 1 + 3*math.ceil((k - 1)/2)) - 7*((p**(k - 1) - p**math.floor((k - 1)/2)) / (p**math.floor(3*(k - 1)/2)*(p - 1))))
  return term1c + term2c+ term3c
```

The following is the general zeroth-order Randic index for any value of t.

```
def General_Zeroth_Order_Randic_Index_omega(t):
    sum2 = 0
    for i in Gamma_Z_pkq.nodes():
        sum2 += Gamma_Z_pkq.degree(i)**t
    return sum2
```

Next the Python code used to compute the general zeroth-order Randic index using both theorem and definition is shown below. The output depends on the values of p, k and q.

```
print("General Zeroth-Order Randić Index for omega=1 => By Theorem 3.2: ", GZORIomega1(p,q,k) , "  => By Definition 2.3:", General_Zeroth_Order_Randic_Index_omega(1))
print("General Zeroth-Order Randić Index for omega=2 => By Theorem 3.3: ", GZORIomega2(p,q,k) , "  => By Definition 2.3:", General_Zeroth_Order_Randic_Index_omega(2))
print("General Zeroth-Order Randić Index for omega=3 => By Theorem 3.4: ", GZORIomega3(p,q,k) , "  => By Definition 2.3:", General_Zeroth_Order_Randic_Index_omega(3))
```

The following gives the output of this code.

```
p:3
k:2
q:5
General Zeroth-Order Randić Index for omega=1 => By Theorem 3.2:  98.0  => By Definition 2.3: 98
General Zeroth-Order Randić Index for omega=2 => By Theorem 3.3:  722.0   => By Definition 2.3: 722
General Zeroth-Order Randić Index for omega=3 => By Theorem 3.4:  6890.0   => By Definition 2.3: 6890
```

```
p:2
k:3
q:7
General Zeroth-Order Randić Index for omega=1 => By Theorem 3.2:  148.0   => By Definition 2.3: 148
General Zeroth-Order Randić Index for omega=2 => By Theorem 3.3:  1518.0   => By Definition 2.3: 1518
General Zeroth-Order Randić Index for omega=3 => By Theorem 3.4:  25066.0   => By Definition 2.3: 25066
```

This output shows that the results by theorems obtained and by definition are the same.

5. Conclusion

In this paper, the set of all zero divisors, the number of zero divisors, the degree of a vertex, the number of vertices and edges of the zero divisor graph for the commutative ring $\mathbb{Z}_{p^k q}$ are determined. Furthermore, the Zagreb indices of the zero divisor graph for the cases $\omega = 1, 2$ and 3 have been computed and the general formulas have been obtained. The computations are accelerated by the general formulas of these topological indices, particularly for larger values of p, k and q. Python is one of the easiest programming languages to learn because it has a compact and straightforward syntax. In this research, Python is utilized to facilitate the calculation of the Zagreb indices.

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Disclosure statement

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