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Article

Analysis of Distance-Based Topological Polynomials Associated with Zero-Divisor Graphs

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Abstract: Chemical compounds are modeled as graphs. The atoms of molecules represent the graph vertices while chemical bonds between the atoms express the edges. The topological indices representing the molecular graph corresponds to the different chemical properties of compounds. Let a, b be are two positive integers, and $\Gamma(\mathbb{Z}_a \times \mathbb{Z}_b)$ be the zero-divisor graph of the commutative ring $\mathbb{Z}_a \times \mathbb{Z}_b$. In this article some direct questions have been answered that can be utilized latterly in different applications. This study starts with simple computations, leading to a quite complex ring theoretic problems to prove certain properties. The theory of finite commutative rings is useful due to its different applications in the fields of advanced mechanics, communication theory, cryptography, combinatorics, algorithms analysis, and engineering. In this paper we determine the distance-based topological polynomials and indices of the zero-divisor graph of the commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$ (for p, q as prime numbers) with the help of graphical structure analysis. The study outcomes help in understanding the fundamental relation between ring-theoretic and graph-theoretic properties of a zero-divisor graph $\Gamma(G)$.

Keywords: Zero divisor graph; Wiener index; Hosoya polynomial; (modified) Schulz index; (modified) Schulz polynomial

1 Introduction

Chemical graph theory is interdisciplinary research between mathematics and chemistry that deals with chemical compounds and drugs by representing them as a graph. Characteristics of chemical compounds based on topological indices would be attractive for medical and pharmaceutical researchers. This analytic research anticipates the importance of topological index-based computational methods for new drugs, medicine, and chemical compounds without performing chemical tests.

Recent improvements in nanomaterials and drugs have helped the researchers investigate the physical, biological, and chemical characteristics of new drugs and chemical compounds. To ensure the investigations' results, drug scientists perform the test of introduced chemical compounds and drugs.

Let $\mathcal{G}(V,E)$ be a simple and connected graph, while the distance between two distinct vertices $u, v \in V(\mathcal{G})$ is the number of edges in the shortest path between them, denoted as $d(u,v)$. The number of edges in the longest distance in $\mathcal{G}$ is called the diameter of the graph, denoted as $D(\mathcal{G})$. The set of all neighbors of a vertex u of $\mathcal{G}$ is called the neighborhood of u, while and the cardinality of the neighborhood of u is the degree of the vertex u, denoted as d_u.

It is interesting to establish a relation between ring-theoretic and graph-theoretic properties of the zero-divisor graph $\Gamma(\mathcal{G})$. A real-valued function $\phi: \ \mathcal{G} \to \mathbb{R}$ mapped upon the chemical structure to certain real numbers is known as a topological index. In 1947 Wiener [1], a chemist, illustrated the connection between organic compounds' Physico-chemical properties and their molecular graphs index. This index is called the Wiener index, defined as:

$$W(\mathcal{G}) = \frac{1}{2} \sum_{u \in V(\mathcal{G})} \sum_{v \in V(\mathcal{G})} d(u,v) \tag{1}$$

Besides Randic′ [2,3] introduced the Hyper-Wiener index, expressed as:

$$WW(\mathcal{G}) = \frac{1}{2} \sum_{u \in V(\mathcal{G})} \sum_{v \in V(\mathcal{G})} (d(u,v) + d(u,v)^2) \tag{2}$$

Also in 1989, Hosoya [4] introduced the Hosoya polynomial, defined as:

$$H(\mathcal{G},x) = \frac{1}{2} \sum_{u \in V(\mathcal{G})} \sum_{v \in V(\mathcal{G})} x^{d(u,v)} \tag{3}$$

For a detailed literature review on the Wiener index's applications and properties, the Hyper–Wiener index, and the Hosoya polynomial for chemical structure, see [5–9]. Schultz [10] introduced a topological index "Schultz molecular topological index" (MTI), defined as follows:

$$MTI(\mathcal{G}) = \sum_{i=1}^{n} [d(A+D)]_i \tag{4}$$

where A, D and d are the adjacency matrices, distance matrices and vector of degrees of $\mathcal{G}$ with order $n \times n$, $n \times n$ and $1 \times n$, respectively. Here the degree distance of $\mathcal{G}$ is defined as:

$$DD(\mathcal{G}) = \frac{1}{2} \sum_{\{u,v\} \subset V(\mathcal{G})} (d_u + d_v) d(u,v) \tag{5}$$

This degree distance index was introduced in 1994 by Dobrynin et al. [11] and at the same time by Gutman [12], naming this degree distance index as "Schultz index". Klavžar et al. [13] defined the modified Schultz index of $\mathcal{G}$ as:

$$Sc^*(\mathcal{G}) = \frac{1}{2} \sum_{u \in V(\mathcal{G})} \sum_{v \in V(\mathcal{G})} (d_u \times d_v) d(u,v) \tag{6}$$

In Gutman [12], two topological polynomials of a graph $\mathcal{G}$ are defined as:

$$Sc(\mathcal{G},x)=\frac{1}{2}\sum_{u\in V(\mathcal{G})}\sum_{v\in V(\mathcal{G})}(d_u+d_v)x^{d(u,v)} \tag{7}$$

and

$$Sc^*(\mathcal{G},x)=\frac{1}{2}\sum_{u\in V(\mathcal{G})}\sum_{v\in V(\mathcal{G})}(d_u\times d_v)x^{d(u,v)} \tag{8}$$

The Schultz index $Sc(\mathcal{G})$ and modified Schultz index $Sc^*(\mathcal{G})$ for a graph $\mathcal{G}$ are defined as:

$$Sc(\mathcal{G})=\frac{\partial Sc(\mathcal{G},x)}{\partial x}|_{x=1},\quad Sc^*(\mathcal{G})=\frac{\partial Sc^*(\mathcal{G},x)}{\partial x}|_{x=1} \tag{9}$$

Immense work on Schultz polynomials and other related indices are calculated in [14–19]. Let $Z(\mathbb{R})$ be the set of zero-divisors of a commutative ring $\mathbb{R}$ having none-zero identity. Let $\Gamma(\mathbb{R})$ be the zero-divisor graph of $\mathbb{R}$ with vertices $Z(\mathbb{R})^*=Z(\mathbb{R})\backslash\{0\}$. Moreover, for distinct $a,b\in Z(\mathbb{R})^*$, the vertices a and b are adjacent if and only if $a\cdot b=0$. For further details about zero-divisor graphs, readers may refer to articles [20–27].

In this article, distance-based topological polynomials and indices of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ are broadly covered in different classes of new nanomaterial, medications, and chemical compounds with structured graphical structured analysis. To make this study useful for application-based research, some direct questions are answered to conclude the results.

2 Applications of Zero-Divisor Graphs

The interdisciplinary research in algebraic graph theory surpasses its applications, making this study quite useful in the future. The study conducted in [28,29] may serve as a fascinating survey to determine the relationship between the ring-theoretic and graph-theoretic properties of $\Gamma(\mathcal{G})$. This study starts with simple computations and leads to quite complex ring theoretic problems to prove certain properties. The main question addressed in this study is: "Is it possible that rings with the same theoretic-properties may have the same graphical construction and graphic properties or vice versa?"

In [30,31], Redmond gave all graphs up to 14 vertices as zero-divisor graphs of a commutative ring with identity. He recorded that all the rings (up to isomorphism) produced graphs and calculations located all commutative reduced rings with identity (up to isomorphism) that shows an ascent of a zero-divisor graph on n vertices for any $n\geq 1$. While studying zero-divisor graphs, a common question that comes into mind is about their uniqueness. The readers may find some applications and relation between the chemical graph theory and algebraic theory in [1,12,24].

3 Distance-Based Topological Polynomials of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$

Let $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ denotes the zero divisor graph of the commutative ring $\mathbb{Z}_{p^2}\times\mathbb{Z}_q$ is defined as: For $x\in\mathbb{Z}_{p^2}$ & $y\in\mathbb{Z}_q$, $(x,y)\notin V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))$ if and only if $x\neq p,2p,3p,\ldots,(p-1)p$ & $y\neq 0$. Let $I=\{(x,y)\notin V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)): x\neq p,2p,3p,\ldots,(p-1)p \text{ \& } y\neq 0\}$, then $|I|=(p^2-p)(q-1)$. The vertices of the set I are the non zero divisors of the commutative ring $\mathbb{Z}_{p^2}\times\mathbb{Z}_q$. Also $(0,0)\in\mathbb{Z}_{p^2}\times\mathbb{Z}_q$ is a non zero divisor. Therefore, the total number of non zero divisors are: $|I|+1=$

$(p^2-p)(q-1)+1=p^2q-p^2-pq+p+1$. There are p^2q total vertices of the commutative ring $\mathbb{Z}_{p^2}\times\mathbb{Z}_q$. Hence, there are $p^2q-(p^2q-p^2-pq+p+1)=p^2+pq-p-1$ total number of zero divisors. Hence, the order of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is $p^2+pq-p-1$ i.e., $|V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))|=p^2+pq-p-1$.

From the above discussion and our convenience, we characterized the vertices of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ according to their degrees below as discussed in [21].

$$S_{0,1}=\{(0,y):y\in\{1,2,3,\ldots,q-1\}\},\quad |S_{0,1}|=q-1. \tag{10}$$

$$S_{1,1}=\{(x,y):x=p,2p,\ldots,(p-1)p\ and\ y\in\{1,2,\ldots,q-1\}\}, \tag{11}$$

$$|S_{1,1}|=(p-1)(q-1). \tag{12}$$

$$S_{1,0}=\{(x,0):x\in\mathbb{Z}_{p^2}\backslash\{0,p,2p,\ldots,(p-1)p\}\},\quad |S_{1,0}|=p-1. \tag{13}$$

$$S_{2,0}=\{(x,0):x=p,2p,\ldots,(p-1)p\},\quad |S_{2,0}|=p^2-p. \tag{14}$$

For $1\le i\le 2$ and $0\le j\le 1$, let $d_{i,j}$ be the degree of each vertex in $S_{i,j}$. Therefore, we get $d_{0,1}=p^2-1$, $d_{1,1}=p-1$, $d_{1,0}=pq-2$ and $d_{2,0}=q-1$.

Let $NP_t(G)$, $t\in\mathbb{Z}$, $t>0$, the number of pairs of vertices at distance t in a graph G.

Lemma 3.1: Let $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ be a zero-divisor graph, then

$$NP_1(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))=\frac{(p-1)(4pq-3p-2)}{2}.$$

Proof. The size of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is given by:

$$|S_{1,0}|(|S_{1,1}|+|S_{0,1}|)+|S_{0,1}|.|S_{2,0}|+|E(K_{|S_{1,0}|})|.$$

From Eqs. (10)–(14) and after simplification, we get

$$NP_1(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))=\frac{(p-1)(4pq-3p-2)}{2}.$$

Lemma 3.2: Let $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ be a zero-divisor graph, then

$$NP_2(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))=\frac{p(p-1)(q-1)(p^2+pq+q-6)}{2}.$$

Proof. In the following formula, the number of pairs of vertices at a distance 2 are:

$$\begin{aligned}NP_2(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))=&|S_{2,0}|_2.|S_{0,1}|+|S_{0,1}|_2.(|S_{2,0}|+|S_{1,0}|)+|S_{2,0}|.|S_{0,1}|.|S_{1,0}|+|S_{0,1}|.|S_{1,0}|.|S_{1,1}|\\&+|S_{1,1}|_2.|S_{1,0}|.\end{aligned}$$

That is,

$$\begin{aligned}NP_2(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))=&|S_{1,0}|.|S_{0,1}|\left(|S_{2,0}|+|S_{1,1}|+\frac{|S_{0,1}|-1}{2}\right)+|S_{0,1}|.|S_{2,0}|\left(\frac{|S_{2,0}|+|S_{0,1}|-2}{2}\right)\\&+|S_{1,0}|.|S_{1,1}|\left(\frac{|S_{1,1}|-1}{2}\right).\end{aligned}$$

By substituting the values of $S_{i,j}$ from Eqs. (10)–(14) and after simplification the result as follows:

$$NP_2(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = \frac{p(p-1)(q-1)(p^2+pq+q-6)}{2}.$$

Lemma 3.3: Let $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ be a zero-divisor graph, then

$$NP_3(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = p(p-1)^3(q-1)^2.$$

Proof. In the following formula, the number of pairs of vertices at a distance 3 are:

$$NP_3(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = |S_{2,0}|.|S_{1,0}|.|S_{0,1}|.|S_{1,1}|.$$

By putting the values of $S_{i,j}$ from Eqs. (10)–(14) and after simplification, the result as follows:

$$NP_3(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = p(p-1)^3(q-1)^2.$$

Now, we proved our first result in the following theorems:

Theorem 3.1: The Wiener index of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is

$$W(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = \frac{(p-1)(4pq-3p-2)}{2} + p(p-1)(q-1)(3p^2q-2p^2-5pq+4q+6p-9).$$

Proof. The diameter of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is 3. Therefore, the distance between the vertices of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is $1, 2$ and 3. The Wiener index can be obtained as follows:

$$W(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = NP_1 + 2NP_2 + 3NP_3. \tag{15}$$

By substituting the values of NP_1, NP_2 and NP_3 obtained from Lemmas 3.1–3.3, respectively into Eq. (15), we obtain the required result after simplification.

In the following theorems, we determined the Hosoya polynomial of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$.

Theorem 3.2: The Hosoya polynomial of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is

$$H(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) = \frac{(p-1)(4pq-3p-2)}{2}x + \frac{p(p-1)(q-1)(p^2+pq+q-6)}{2}x^2 + p(p-1)^3(q-1)^2x^3.$$

Proof. Since,

$$H(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) = (NP_1)x + (NP_2)x^2 + (NP_3)x^3. \tag{16}$$

From Lemmas 3.1–3.3, we obtain

$$H(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) = \frac{(p-1)(4pq-3p-2)}{2}x + \frac{p(p-1)(q-1)(p^2+pq+q-6)}{2}x^2 + p(p-1)^3(q-1)^2x^3.$$

Theorem 3.3: The Hyper-Wiener index of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is:

$$WW(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = (p-1)(12p^3q^2-21p^3q+9p^3-21p^2q^2+45p^2q-24p^2-41pq+15pq^2+27p-2).$$

Proof. We know that

$$\begin{aligned} WW(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) &= \frac{1}{2}\sum_{u\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}\ \sum_{v\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}(d(u,v)+d(u,v)^2) \\ &= W(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))+\frac{1}{2}\sum_{u\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}\ \sum_{v\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))} d(u,v)^2 \\ &= W(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))+(1)^2NP_1+(2)^2NP_2+(3)^2NP_3. \end{aligned}$$

From Theorem 3.1 and Lemma 3.1–3.3

$$\begin{aligned} WW(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) &= \frac{(p-1)(4pq-3p-2)}{2}+p(p-1)(q-1)(3p^2q-2p^2-5pq+4q+6p-9) \\ &\quad +1^2\frac{(p-1)(4pq-3p-2)}{2}+2^2\frac{p(p-1)(q-1)(p^2+pq+q-6)}{2} \\ &\quad +3^2p(p-1)^3(q-1)^2. \end{aligned}$$

After simplification, we obtain

$$WW(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = (p-1)(12p^3q^2-21p^3q+9p^3-21p^2q^2+45p^2q-24p^2-41pq+15pq^2+27p-2).$$

Theorem 3.4: The Schultz polynomial for $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is given by:

$$\begin{aligned} Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) &= (p^4q-p^4+p^3q^2+p^3q-p^3-11p^2q+6p^2-pq^2+9pq-4)x+(5p^4q^2-10p^4q \\ &\quad +5p^4-8p^3q^2+9p^3q-p^3+2p^2q^2+12p^2q-14p^2-pq^2-9pq+10p+2q^2-2q) \\ &\quad \times x^2+p(p-1)^3(q-1)^2(p+q-2)x^3. \end{aligned}$$

Proof. By inserting the coefficient of (d_u+d_v) in the Hosoya polynomial, we obtain the Schultz polynomial of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$, yielding

$$\begin{aligned} Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) &= \frac{1}{2}\sum_{u\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}\ \sum_{v\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}(d_u+d_v)x^{d(u,v)} \\ &= |S_{0,1}|.|S_{2,0}|.(d_{0,1}+d_{2,0})x+|S_{1,0}|.|S_{0,1}|.(d_{1,0}+d_{0,1})x+|S_{1,1}|.|S_{1,0}|.(d_{1,1}+d_{1,0})x \\ &\quad +|S_{1,0}|_2.2(d_{1,0})x+|S_{2,0}|_2.|S_{0,1}|.2(d_{2,0})x^2+|S_{2,0}|.|S_{1,0}|.|S_{1,1}|.(d_{2,0}+d_{1,0})x^2 \\ &\quad +|S_{0,1}|.|S_{1,0}|.|S_{1,1}|.(d_{1,1}+d_{0,1})x^2+|S_{0,1}|_2.(|S_{2,0}|+|S_{1,0}|).2(d_{0,1})x^2 \\ &\quad +|S_{1,1}|_2.|S_{1,0}|.2(d_{1,1})x^2+|S_{0,1}|.|S_{1,0}|.|S_{1,1}|.|S_{2,0}|.(d_{1,1}+d_{2,0})x^3. \end{aligned}$$

From Eqs. (10), (11) and their degrees, we obtain

$$\begin{aligned} Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) =& p(p-1)(q-1)(p^2+q-2)x+(p^2+pq-3)(p-1)(q-1)x+(pq+p-3)(p-1)^2 \\ &\times(q-1)x+(pq-2)(p-1)(p-2)x+p(p-1)(q-1)^2(p^2-p-1)x^2+p(p-1)^2 \\ &\times(q-1)(pq+q-3)x^2+(p^2+p-2)(p-1)^2(q-1)^2x^2+(p-1)^2(q-1)(p+1)^2 \\ &\times(q-2)x^2+(p-1)^3(q-1)(pq-p-q)x^2+p(p-1)^3(q-1)^2(p+q-2)x^3. \end{aligned}$$

After simplification, we obtain

$$\begin{aligned} Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) =& (p^4q-p^4+p^3q^2+p^3q-p^3-11p^2q+6p^2-pq^2+9pq-4)x+(5p^4q^2-10p^4q \\ &+5p^4-8p^3q^2+9p^3q-p^3+2p^2q^2+12p^2q-14p^2-pq^2-9pq+10p+2q^2-2q) \\ &\times x^2+p(p-1)^3(q-1)^2(p+q-2)x^3. \end{aligned}$$

Theorem 3.5: The modified Schultz polynomial for $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is equal to

$$\begin{aligned} Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) =& (p-1)^2(q-1)(3p^2q-p^2+pq-5p)x+\frac{(p-1)(p-2)(pq-2)^2}{2}x \\ &+\frac{p(p-1)(q-1)}{2}(p^4q-2p^4+4p^3q-5p^3+3p^2q^2-14p^2q+12p^2-3pq^2+4pq \\ &+4p-q^2+7q-10)x^2+p(p-1)^4(q-1)^3x^3. \end{aligned}$$

Proof. By inserting the coefficient of $(d_u\times d_v)$ in the Hosoya polynomial, we obtain the modified Schultz polynomial of $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$. We have the following:

$$\begin{aligned} Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) =& \frac{1}{2}\sum_{u\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}\ \sum_{v\in V(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))}(d_u\times d_v)x^{d(u,v)} \\ =& |S_{0,1}|.|S_{2,0}|.(d_{0,1}\times d_{2,0})x+|S_{1,0}|.|S_{0,1}|.(d_{1,0}\times d_{0,1})x+|S_{1,1}|.|S_{1,0}|.(d_{1,1}\times d_{1,0})x \\ &+|S_{1,0}|_2.(d_{1,0})^2x+|S_{2,0}|_2.|S_{0,1}|.(d_{2,0})^2x^2+|S_{2,0}|.|S_{1,0}|.|S_{1,1}|.(d_{2,0}\times d_{1,0})x^2 \\ &+|S_{0,1}|.|S_{1,0}|.|S_{1,1}|.(d_{1,1}\times d_{0,1})x^2+|S_{0,1}|_2.(|S_{2,0}|+|S_{1,0}|).(d_{0,1})^2x^2 \\ &+|S_{1,1}|_2.|S_{1,0}|.(d_{1,1})^2x^2+|S_{0,1}|.|S_{1,0}|.|S_{1,1}|.|S_{2,0}|.(d_{1,1}\times d_{2,0})x^3. \end{aligned}$$

From Eqs. (10), (11) and their degrees, we obtain

$$\begin{aligned} Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) =& p(p-1)^2(q-1)^2(p+1)x+(p-1)^2(q-1)(p+1)(pq-2)x \\ &+\frac{(p-1)(p-2)(pq-2)^2}{2}x+(p-1)^3(q-1)(pq-2)x \\ &+\frac{p(p-1)(q-1)^3(p^2-p-1)}{2}x^2+p(p-1)^2(q-1)^2(pq-2)x^2+(p-1)^4 \end{aligned}$$

$$\times (q-1)^2(p+1)x^2 + \frac{(p-1)^3(q-1)(p+1)^3(q-2)}{2}x^2$$
$$+ \frac{(p-1)^4(q-1)(pq-p-q)}{2}x^2 + p(p-1)^4(q-1)^3x^3.$$

After simplification, we obtain

$$Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x) = (p-1)^2(q-1)(3p^2q-p^2+pq-5p)x + \frac{(p-1)(p-2)(pq-2)^2}{2}x$$
$$+ \frac{p(p-1)(q-1)}{2}(p^4q-2p^4+4p^3q-5p^3+3p^2q^2-14p^2q+12p^2-3pq^2+4pq$$
$$+4p-q^2+7q-10)x^2 + p(p-1)^4(q-1)^3x^3.$$

Theorem 3.6: The Schultz index for $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is equal to

$$Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = (10p^4q^2-19p^4q+9p^4-15p^3q^2+19p^3q-3p^3+4p^2q^2+13p^2q-22p^2-3pq^2-9pq$$
$$+20p+4q^2-4q-4)+3p(p-1)^3(q-1)^2(p+q-2).$$

Proof. By the definition of the Schultz index $Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))$, we have the following:

$$Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = \frac{\partial Sc(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x)}{\partial x}|_{x=1}$$
$$= \frac{\partial}{\partial x}((p^4q-p^4+p^3q^2+p^3q-p^3-11p^2q+6p^2-pq^2+9pq$$
$$-4)x+(5p^4q^2-10p^4q+5p^4-8p^3q^2+9p^3q-p^3+2p^2q^2+12p^2q-14p^2-pq^2$$
$$-9pq+10p+2q^2-2q)x^2+p(p-1)^3(q-1)^2(p+q-2)x^3)|_{x=1}.$$
$$= (10p^4q^2-19p^4q+9p^4-15p^3q^2+19p^3q-3p^3+4p^2q^2+13p^2q-22p^2-3pq^2-9pq$$
$$+20p+4q^2-4q-4)+3p(p-1)^3(q-1)^2(p+q-2).$$

This completes the proof.

Theorem 3.7: The modified Schultz index for $\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)$ is equal to

$$Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = (p-1)(q-1)(p^5q-2p^5+4p^4q-5p^4+3p^3q^2-11p^3q+11p^3-3p^2q^2+2p^2q-pq^2$$
$$+6pq-5p)+3p(p-1)^4(q-1)^3+\frac{(p-1)(p-2)(pq-2)^2}{2}.$$

Proof. By the definition of the modified Schultz index $Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q))$, we have the following:

$$Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q)) = \frac{\partial Sc^*(\Gamma(\mathbb{Z}_{p^2}\times\mathbb{Z}_q),x)}{\partial x}|_{x=1}$$
$$= \frac{\partial}{\partial x}((p-1)^2(q-1)(3p^2q-p^2+pq-5p)x + \frac{(p-1)(p-2)(pq-2)^2}{2}x$$

$$
\begin{aligned}
&+\frac{p(p-1)(q-1)}{2}(p^4q-2p^4+4p^3q-5p^3+3p^2q^2-14p^2q+12p^2-3pq^2+4pq\\
&+4p-q^2+7q-10)x^2+p(p-1)^4(q-1)^3x^3)|_{x=1}\\
=&(p-1)(q-1)(p^5q-2p^5\\
&+4p^4q-5p^4+3p^3q^2-11p^3q+11p^3-3p^2q^2+2p^2q-pq^2+6pq-5p)\\
&+3p(p-1)^4(q-1)^3+\frac{(p-1)(p-2)(pq-2)^2}{2}.
\end{aligned}
$$

This completes the proof.

Open Problem 3.8: Let a, b be any positive integers, then determine the distance-based topological polynomials and indices for the zero divisor graph $\Gamma(\mathbb{Z}_a \times \mathbb{Z}_b)$ of the commutative ring $\mathbb{Z}_a \times \mathbb{Z}_b$.

4 Conclusion

In this article, we analyzed the graph structure to determine the distance-based topological polynomials and indices for the zero divisor graph $\Gamma(\mathbb{Z}_{p^2} \times \mathbb{Z}_q)$ of the commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$. The results support the open problem and broadly display different classes of new medications, nanomaterials and chemical structures. These outcomes are also useful to clarify the fundamental topologies of graphs. This article also presents some interesting results that interplay a relation between zero-divisors and chemical graph theory.

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