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Some Degree Based Topological Indices of $\mathscr{S}_i(\Re)$

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Abstract

In this paper, we introduce the concept of the closed self-inverse element graph, denoted by $\overline{\mathscr{S}_i(\Re)}$, which is obtained by relaxing the condition of vertex distinctness in the self-inverse element graph $\mathscr{S}_i(\Re)$ over a ring $\Re$. We explore in detail the adjacency matrix, its eigenvalues of $\overline{\mathscr{S}_i(\mathbb{Z}_n)}$ (i.e., the spectrum of $\overline{\mathscr{S}_i(\mathbb{Z}_n)}$), which shows interesting structural characteristics. In addition, we investigate several degree-based topological indices for $\mathscr{S}_i(\Re)$, namely; the Randić index, the general Randić index, and the atom-bond connectivity (ABC) index and many more. Furthermore, we compute the Gutman index and the Detour Gutman index for $\mathscr{S}_i(\mathbb{Z}_n)$ for the case $n = 2p^r$ and we establish a strong correlation between these indices and the Wiener index for $\mathscr{S}_i(\mathbb{Z}_n)$. This investigation provides fresh perspectives on the algebraic and topological properties of $\mathscr{S}_i(\Re)$.

Keywords: Topological indices, Adjacency matrix, Anti-circulant graph, Gutman index.

2020 Mathematics Subject Classification: 05C10, 05C50, 05C90

1. INTRODUCTION

Graph theory plays a vital role in studying the different disciplines like Computer science, Physics, Chemistry and Network Analysis etc. Due to its wide-ranging applications in different areas, researchers developed a new discipline by connecting an algebraic structure with the graph theory known as algebraic graph theory.

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It is an interdisciplinary field which utilizes algebraic tools to provide attractive proofs and insights of graph theoretic concepts. Over the last few decades, graph theory has become essential in addressing real-world problems across various disciplines.(see [24], [26], [1])

The study of topological indices, originally used to model molecular graphs in chemistry and biology but it is also valuable in the context of algebraic graphs, inspite of the fact that the two domains are obviously distinct. Algebraic graphs based on abstract algebraic structures like groups and rings can benefit from generalizing topological indices, offering deep theoretical insights, interdisciplinary applications and structural characterizations. These indices are computationally efficient and useful for analyzing large algebraic graphs. Moreover, this exploration can also lead to some new research directions and the development of topological indices change to the unique properties of algebraic graphs, enriching the broader field of graph theory. This motivate us to explore various topological indices for $\mathscr{S}_i(\Re)$.

By a graph we mean $G = (V, E)$, where $V(G)$ & $E(G)$ represent sets of all vertices & edges in G, respectively. The vertices u and v are adjacent if $E(G)$ has an edge e with endpoints u and v, i.e. $e = uv \in E(G)$, whereas e is a self loop in G if $u = v$. For a vertex $x \in G$, the sets $N(x) = \{u \in V(G)|xu \in E(G)\}$ and $N\{x\} = \{u \in V(G)|xu \in E(G)\} \cup \{x\}$ are represented open neighborhood and closed neighborhood of x, respectively. Furthermore, degree of the vertex x is $d(x) = |N(x)|$ and for any two distinct vertices u and v, $d(u, v)$ is the shortest distance, whereas $D(u, v)$ is the longest distance between u and v.

Throughout this paper, $\Re$ is a finite commutative ring with unity 1. Form [21], the set $\mathscr{S}(\Re) = \{x \in \Re|x^2 = 1\}$ is the set of all self inverse elements in $\Re$. Additionally, the self inverse element graph $\mathscr{S}_i(\Re)$ is the graph with the vertex set $V(\mathscr{S}_i(\Re)) = \Re$ and for distinct vertices u and v, $uv = e \in E(\mathscr{S}_i(\Re))$ if and only if $u + v \in \mathscr{S}(\Re)$. According to [33] Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. In [16], the first topological index was introduced by Harry Wiener for estimating the boiling point of paraffin and he named it as path number. Since then, several topological indices have been established, as they provide information of molecule structures and their properties, therefore these indices are extremely important in Molecular Chemistry. Three main classifications of topological indices are degree-based, eccentricity-based and distance-based. Our primary focus is to investigate degree-based topological indices. A brief introduction to the closed self-inverse element graph is given in the second section of this paper. In the third section, we computed the adjacency matrix and the eigenvalues for the closed self-inverse element graph, which corresponds to its spectrum. The fourth section explores several degree-based topological indices, including the geometric-arithmetic (GA), Randić, and atom-bond connectivity (ABC) indices etc. Finally, in the fifth section the Gutman and Detour Gutman indices are explored and includes a formula that relates these indices with the Wiener index for $\mathscr{S}_i(\Re)$.

2. BASIC DIFFERENCE BETWEEN $\mathscr{S}_i(\Re)$ AND $\overline{\mathscr{S}_i(\Re)}$

Throughout this paper $\Re$ is a ring and $\mathscr{S}(\Re)$ is the set of all self-inverse elements in $\Re$. The self inverse element graph of $\Re$, denoted by $\mathscr{S}_i(\Re)$ is a graph with vertex set $\Re$ and two distinct vertices x and y are adjacent in $\mathscr{S}_i(\Re)$ if and only if $x+y \in \mathscr{S}(\Re)$. If we omit the world "distinct", then this leads us to a new definition of a graph known as: "The Closed self inverse element graph $\overline{\mathscr{S}_i(\Re)}$", (i.e. this graph may have loops). Our main focus is to characterize the closed self inverse element graph and it is observed that for some cases $\overline{\mathscr{S}_i(\Re)}$ coincides with $\mathscr{S}_i(\mathbb{Z}_n)$.

Example 1. *Let $\Re = \mathbb{Z}_{12}$, and $\mathscr{S}(\Re) = \{\overline{1}, \overline{5}, \overline{7}, \overline{11}\}$, then $\overline{\mathscr{S}_i(\Re)}$ is given by Figure 1. It is observed that $\mathscr{S}(\Re)$ does not contain any element x of the form $x = y + y$, where $y \in \Re$. Therefore, $\overline{\mathscr{S}_i(\Re)}$ does not contain any loop. Hence, for this case $\overline{\mathscr{S}_i(\Re)} = \mathscr{S}_i(\Re)$.*

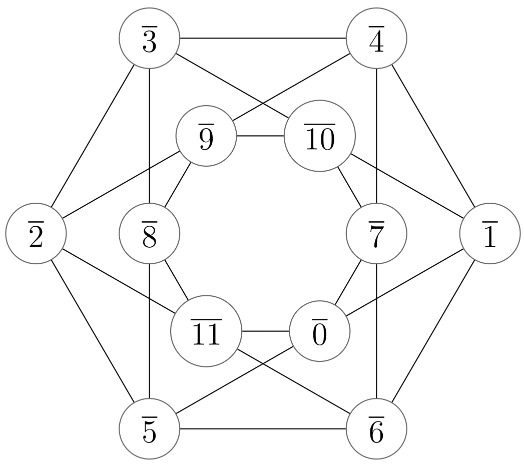

Figure 1: $\overline{\mathscr{S}_i(\mathbb{Z}_{12})}$

On the other hand, if $\Re = \mathbb{Z}_{21}$, then $\mathscr{S}(\Re) = \{\overline{1}, \overline{8}, \overline{13}, \overline{20}\}$. In this case, every element $x \in \mathscr{S}(\Re)$ can be written in the form $x = y + y$, where $y \in \Re$ i.e., $\overline{1} = \overline{11} + \overline{11}, \overline{8} = \overline{4} + \overline{4}, \overline{13} = \overline{17} + \overline{17}, \overline{20} = \overline{10} + \overline{10}$. Thus, one can clearly see in Figure 2, that there exist only four vertices namely; $\overline{11}, \overline{4}, \overline{17}, \overline{10}$ having a self loop.

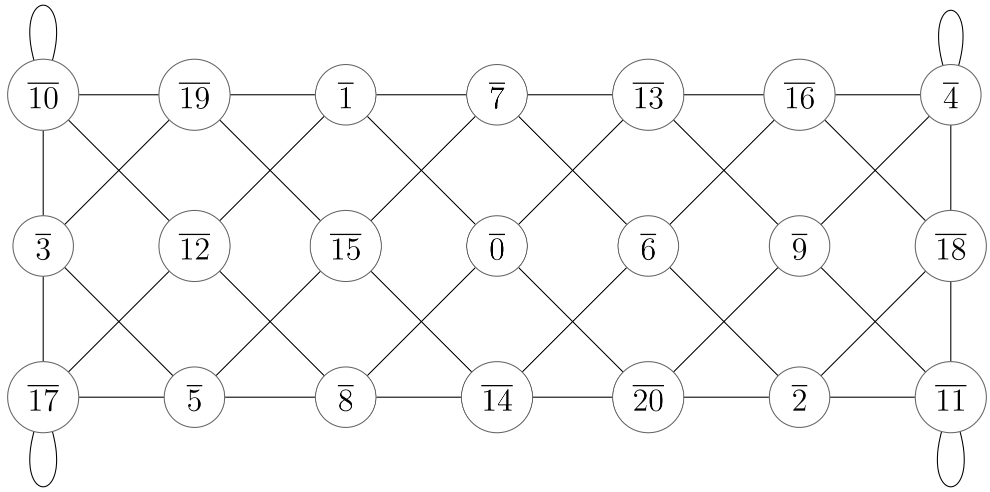

Figure 2: $\overline{\mathscr{S}_i(\mathbb{Z}_{21})}$

Now, we wish to prove one more general result in the form of a lemma about the coexistence of a closed self inverse element graph and a self inverse element graph. Before that, it is noteworthy to mention that the set $\mathscr{T}(\Re) = \{x \in \Re | x = y + y\}$(see [21]), where $y \in \Re$.

Lemma 1. *Let $\Re$ be a ring with $char(\Re) = n$. Then $\overline{\mathscr{S}_i(\Re)} = \mathscr{S}_i(\Re)$ if and only if n is an even integer.*

Proof. For a ring $\Re$, $\overline{\mathscr{S}_i(\Re)} = \mathscr{S}_i(\Re)$ if and only if for every edge $e = uv \in E(\mathscr{S}_i(\Re))$ the end vertices are always distinct. Let n be an even number, then by Lemma 2.5 in [21], $\mathscr{T}(\Re) \cap \mathscr{S}(\Re) = \phi$. Thus, by definition of $\mathscr{T}(\Re)$, there does not exist any element $y \in \mathscr{T}(\Re)$ such that $y + y = x$, for any $x \in \mathscr{T}(\Re)$. That is, there is no possibility of any self loop in $\mathscr{S}_i(\Re)$. Hence $\mathscr{S}_i(\Re) = \overline{\mathscr{S}_i(\Re)}$. On the other hand, if n is an odd number, then by Lemma 2.5 in [21], $\mathscr{T}(\Re) \cap \mathscr{S}(\Re) = \mathscr{T}(\Re)$ and this implies for every $x \in \mathscr{S}(\Re)$ there exists a unique element $y \in \mathscr{T}(\Re) \subset \Re$ such that $y + y = x$. Thus, there exist exactly $|\mathscr{S}(\Re)|$ number of self-loops in $\overline{\mathscr{S}_i(\Re)}$. □

From the above lemma, $\overline{\mathscr{S}_i(\Re)}$ has k self-loops, where $k = |\mathscr{S}(\Re)|$ is odd. This means $\overline{\mathscr{S}_i(\Re)}$ has k vertices of degree $k + 1$ and all the other $n - k$ vertices have degree k. Therefore, size of $\overline{\mathscr{S}_i(\Re)}$ is equal to $\frac{(n-k)k}{2} + \frac{k(k+1)}{2} = \frac{nk-k^2+k^2+k}{2} = \frac{(n+1)k}{2}$. This proves

Lemma 2. *If $\Re$ is a ring of order n with odd characteristic and $|\mathscr{S}(\Re)| = k$, then size of $\overline{\mathscr{S}_i(\Re)}$ is $\frac{(n+1)k}{2}$.*

Definition 1. *By [25] the category product of two graphs G_1 and G_2 is denoted by $G_1 \dot{\times} G_2$ with the vertex set $V(G_1 \dot{\times} G_2) = V(G_1) \times V(G_2)$ and two distinct vertices (x, y) and (x', y') of $G_1 \dot{\times} G_2$ are adjacent if and only if x is adjacent to x' in G_1 and y is adjacent to y' in G_2.*

Now, in our case, assume that $\Re_1$ and $\Re_2$ are two rings. Then the graph $\mathscr{S}_i(\Re_1 \times \Re_2)$ with $V(\mathscr{S}_i(\Re_1 \times \Re_2)) = \Re_1 \times \Re_2$ and two distinct vertices (u, v)& (u', v') are adjacent if and only if $(u, v) + (u', v') \in \mathscr{S}(\Re_1 \times \Re_2)$. This implies that $u + u' \in \mathscr{S}(\Re_1)$ and $v + v' \in \mathscr{S}(\Re_2)$, which means u is adjacent to u' and v is adjacent to v' in $\mathscr{S}_i(\Re_1)$ and $\mathscr{S}_i(\Re_2)$ respectively. Thus, similar to [25], it is noteworthy to mention here that

Remark 1. *For two rings $\Re_1$ and $\Re_2$, $\overline{\mathscr{S}_i(\Re_1)} \dot{\times} \overline{\mathscr{S}_i(\Re_2)} \cong \mathscr{S}_i(\Re_1 \times \Re_2)$.*

3. ADJACENCY MATRIX AND ITS EIGENVALUES FOR $\overline{\mathscr{S}_i(\mathbb{Z}_n)}$

According to [10], a square matrix used to describe a finite graph is known as an adjacency matrix. Also it can be illustrated by the entries of the adjacency matrix that whether two vertices in a graph are adjacent or not. The set of eigenvalues of the adjacency matrix of graph G is called the spectrum of the graph and is denoted by $Spec(G)$. In this section, we discuss the adjacency matrix and eigenvalues of a closed self inverse element graph of $\mathbb{Z}_n$,(i.e. the spectrum of the $\overline{\mathscr{S}_i(\mathbb{Z}_n)}$).

Definition 2. *[20], Let G be a graph with n vertices, the adjacency matrix of G is a square matrix of order $n \times n$, such that*

$$a_{ij} = \begin{cases} 0, & \textit{if vertex } i \textit{ is not adjacent to vertex } j \\ 1, & \textit{if vertex } i \textit{ is adjacent to vertex } j. \end{cases}$$

Before proceeding further, it is essential to know about anti-circulant matrices. For a fixed positive integer $n \geq 2$, let $v = (a_0, a_1, ..., a_{n-2}, a_{n-1})$ be a vector in $\mathbb{C}^n$, where $\mathbb{C}$ is the set of all the complex numbers. In addition, the anti-shift operator can be defined as a function $S : \mathbb{C}^n \to \mathbb{C}^n$ such that $S(a_0, a_1, ..., a_{n-2}, a_{n-1}) = (a_1, ..., a_{n-2}, a_{n-1}, a_0)$ and thus anti-circulant matrix over $\mathbb{C}^n$ is defined as follows:

Definition 3. *[20], An anti-circulant matrix associated with vector $v = (a_0, a_1, ..., a_{n-2}, a_{n-1})$ is a square matrix, where each row vector will rotate one element to the left of the row vector that comes before it, an $n \times n$ anti-circulant matrix A is of the form*

$$A = \begin{bmatrix} a_0 & a_1 & \dots & a_{n-2} & a_{n-1} \\ a_1 & a_2 & \dots & a_{n-1} & a_0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n-2} & a_{n-1} & \dots & a_{n-4} & a_{n-3} \\ a_{n-1} & a_0 & \dots & a_{n-3} & a_{n-2} \end{bmatrix}$$

Notice that a graph is said to be an anti-circulant if its adjacency matrix is an anti-circulant matrix.

Example 2. *For $\mathbb{Z}_7$, $\mathscr{S}(\mathbb{Z}_7) = \{\overline{1}, \overline{6}\}$. Then the adjacency matrix is given by*

$$A(\overline{\mathscr{S}_i(\mathbb{Z}_7)}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

From the above example, it infers that the $\overline{\mathscr{S}_i(\mathbb{Z}_7)}$ is an anti-circulant graph and its adjacency matrix is an anti-circulant matrix associated with the vector $v = (0, 1, 0, 0, 0, 0, 1)$.

Lemma 3. *If $\Re = \mathbb{Z}_n$, then $\overline{\mathscr{S}_i(\mathbb{Z}_n)}$ is an anti-circulant graph with adjacency matrix associated to the vector $v = (a_{00}, a_{01}, a_{02}, ..., a_{0n-1})$, where*

$$a_{0j} = \begin{cases} 0, & \textit{if } j \notin \mathscr{S}(\mathbb{Z}_n) \\ 1, & \textit{if } j \in \mathscr{S}(\mathbb{Z}_n) \end{cases} \tag{1}$$

Proof. Let $\Re = \mathbb{Z}_n$. Then it is sufficient to prove that a matrix $A = [a_{ij}]$, where $i, j \in \mathbb{Z}_n$ is an anti-circulant if and only if $a_{ij} = a_{i+1,j-1}$, for all $i, j \in \mathbb{Z}_n$. Suppose A is the matrix associated to the vector $(a_{00}, a_{01}, a_{02}, ..., a_{0n-1})$, then $a_{0j} = 0$ implies $0 + j = j \notin \mathscr{S}(\mathbb{Z}_n)$ and $a_{0j} = 1$ implies $0 + j = j \in \mathscr{S}(\mathbb{Z}_n)$. Now, if $a_{ij} = 0$ implies $i + j \notin \mathscr{S}(\mathbb{Z}_n)$ and so $(i + 1) + (j - 1) \notin \mathscr{S}(\mathbb{Z}_n)$. Thus, $a_{i+1,j-1} = 0$. Similarly, $a_{ij} = 1$ implies , $a_{i+1,j-1} = 1$. Therefore, $a_{ij} = a_{i+1,j-1}$, for every $i, j \in \mathbb{Z}_n$. Hence A is an anti-circulant matrix.

□

It is observed that for any $x \in \mathbb{R}$ greatest integer function $\lfloor x \rfloor$, which rounded down real number x to the greatest integer which is less than x. This function is also known as floor function and satisfies the inequality: $x - 1 \leq \lfloor x \rfloor \leq x$, for $x \in \mathbb{R}$. Next, to calculate the eigenvalues of adjacency matrix of self inverse element graph, we are using Theorem 3.6 of [20], we mention it as

Theorem 1. *Let M be an $n \times n$ real anti-circulant matrix associated with the vector $(m_0, m_1, ..., m_{n-1})$ and $\omega = exp(\frac{2\pi\iota}{n})$, where $\in \mathbb{N}$. Let*

$$s = \lfloor \tfrac{n-1}{2} \rfloor \textit{ and } \lambda_j = \textstyle\sum_{k=0}^{n-1} m_k \omega^{jk}, j = 0, 1, ..., s.$$

If n is even, then the eigenvalues of M are

$$\lambda_0, \lambda_{\frac{n}{2}}, \pm|\lambda_j|, j = 1, 2, ..., s,$$

where $\lambda_{n/2} = \sum_{k=0}^{n-1}(-1)^k m_k$. If n is odd, then the eigenvalues of M are

$$\lambda_0, \lambda_{\frac{n}{2}}, \pm|\lambda_j|, j = 1, 2, ..., s.$$

Example 3. *Let $\Re = \mathbb{Z}_{10}$, then $\mathscr{S}(\mathbb{Z}_{10}) = \left\{\overline{1}, \overline{9}\right\}$, so the adjacency matrix is given as*

$$A(\mathscr{S}_i(\mathbb{Z}_{10})) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

by using Theorem 1 and Lemma 3, we can calculate the $Spec(\mathscr{S}_i(\mathbb{Z}_{10}))$.

$$\begin{aligned} \lambda_0 = \sum_{k=0}^{9} m_k \omega^{0k} &= 0.\omega^0 + 1.\omega^0 + 0.\omega^0 + 0.\omega^0 + .\omega^0 + 0.\omega^0 + .\omega^0 + 0.\omega^0 + 0.\omega^0 + 1.\omega^0 \\ &= 1 + 1 = 2. \end{aligned}$$

Similarly

$$\lambda_5 = \sum_{k=0}^{9}(-1)^k m_k = (-1)^0.0 + (-1)^1.1 + (-1)^2.0 + (-1)^3.0 + (-1)^4.0$$
$$+ (-1)^5.0 + (-1)^6.0 + (-1)^7.0 + (-1)^8.0 + (-1)^9.1$$
$$= -1 - 1 = -2.$$

Now,

$$\lambda_j = \sum_{k=0}^{n-1} m_k \omega^{jk} = \sum_{k \in \mathscr{S}(\Re)} 1.\omega^{jk} \textit{ for } 1 \leq j \leq 4.$$

Thus,

$$\begin{aligned}\lambda_1 &= \sum_{k \in \mathscr{S}(\Re)} 1.\omega^{1.k} \\ &= \omega + \omega^9 = \omega + \omega^{-1} \\ &= cos\frac{2\pi}{10} + \iota sin\frac{2\pi}{10} + cos\frac{2\pi}{10} - \iota sin\frac{2\pi}{10} = 2cos\frac{2\pi}{10},\end{aligned}$$

$$\begin{aligned}\lambda_2 &= \sum_{k \in \mathscr{S}(\Re)} 1.\omega^{2.k} \\ &= \omega^2 + \omega^{18} = \omega^2 + \omega^{-2} \\ &= cos\frac{2.2\pi}{10} + \iota sin\frac{2.2\pi}{10} + cos\frac{2.2\pi}{10} - \iota sin\frac{2.2\pi}{10} = 2cos\frac{4\pi}{10}.\end{aligned}$$

In the similar manner,

$$\lambda_3 = 2cos\frac{6\pi}{10} \textit{ and } \lambda_4 = 2cos\frac{8\pi}{10}.$$

Hence, by using Theorem 1,

$$Spec(\mathscr{S}_i(\mathbb{Z}_{10})) = \left\{\pm 2, \pm 2cos\frac{2\pi}{10}, \pm 2cos\frac{4\pi}{10}, \pm 2cos\frac{6\pi}{10}, \pm 2cos\frac{8\pi}{10}\right\}.$$

Theorem 2.

$$Spec(\overline{\mathscr{S}_i(\mathbb{Z}_n)}) = \begin{cases} \{\pm|\mathscr{S}(\mathbb{Z}_n)|, \pm|\lambda_j|\}, & \textit{if n is an even number} \\ \{|\mathscr{S}(\mathbb{Z}_n)|, \pm|\lambda_j|\}, & \textit{if n is an odd number.} \end{cases}$$

Where $j = 0, 1, 2, ..., \lfloor \frac{n-1}{2} \rfloor$ *and* $\lambda_j = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} cos\frac{2\pi jk}{n}$.

Proof. Let $\Re = \mathbb{Z}_n$. Then by Lemma 3, adjacency matrix $A(\mathscr{S}_i(\mathbb{Z}_n))$ is an anti-circulant matrix associated with the vector $v = (a_{00}, a_{01}, a_{02}, ..., a_{0n-1})$, where $a_{0,j}$ is given by equation (1). Furthermore, eigenvalues of an anti-circulant matrix can be calculated by using Theorem 1. (i.e. by using Lemma 3 and Theorem 1),

$$\lambda_0 = \sum_{k=0}^{n-1} m_k \omega^{0k} = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} 1.\omega^{0k} = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} 1 = |\mathscr{S}(\mathbb{Z}_n)|.$$

Similarly,

$$\lambda_{n/2} = \sum_{k=0}^{n-1} (-1)^k m_k = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} (-1)^k.1 = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} -1 = -|\mathscr{S}(\mathbb{Z}_n)|.$$

Now, for all $j = 1, 2, ..., [\frac{n-1}{2}]$,

$$\lambda_j = \sum_{k=0}^{n-1} m_k \omega^{jk} = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} 1\omega^{jk}.$$

Clearly, if a is the self-inverse element, so is $-a$. Therefore $\lambda_j = \omega^{aj} + ... + \omega^{-aj}$. By applying De Moivre's Theorem, we get

$$\lambda_j = cos\frac{2aj\pi}{10} + \iota sin\frac{2aj\pi}{10} + ... + cos\frac{2aj\pi}{10} - \iota sin\frac{2aj\pi}{10} = \sum_{k \in \mathscr{S}(\mathbb{Z}_n)} cos\frac{2\pi jk}{2}.$$

□

4. RESULTS ON DEGREE BASED TOPOLOGICAL INDICES OF $\mathscr{S}_i(\Re)$

This section investigates some degree-based topological indices of the graph $\mathscr{S}_i(\Re)$ derived from the M-polynomial, which have important applications in chemistry and bioinformatics. The Randić index, introduced in [22], is widely studied. The general Randić index, Atom-Bond Connectivity (ABC) index, and Geometric Arithmetic (GA) index are some of the more useful extensions of the Randić index, which are helpful in predicting molecular properties. These all degree based topological indices are very significant and play an essential role in Chemical Graph Theory; especially in Chemistry. In this section we compute all these indices by using the M-polynomial approach. Thus, the M-polynomial of a graph G is defined as,

Definition 4. *[29], Let G be a simple connected graph, then*

$$M(G;x,y)=\sum_{\delta\le i\le j\le\Delta} m_{i,j}(G)x^iy^j$$

is known as the M-polynomial of a graph G, δ is the minimum degree in G, Δ is the maximum degree in G and $m_{i,j}(G)$ is the number of edges $uv\in E$ such that $d(u)=i, d(v)=j(i,j\ge 1)$.

Degree-based topological indices are numerical values associated with a molecular graph, which represent certain structural aspects of the molecule. According [29] Degree-based topological index $I(G)$ is

$$I(G)=\sum_{i\le j} m_{i,j}(G)f(i,j), \tag{2}$$

where $f(i,j)$ is a polynomial in i,j.
The Table 1 presents some highly investigated degree based topological indices along with their formulas.
In the next theorem, we use the M-polynomial of a graph $\mathscr{S}_i(\Re)$ to provide the information about $I(\mathscr{S}_i(\Re))$ and the characterization of $I(\mathscr{S}_i(\Re))$ is on the basis of $char(\Re)$.

Theorem 3. *If $\Re$ is a ring of order n, with $char(\Re)=m$ and $|\mathscr{S}(\Re)|=k$, then $I(\mathscr{S}_i(\Re))$ is equal to the following:*

$$I(\mathscr{S}_i(\Re))=\begin{cases}\frac{nk}{2}f(k,k), \text{ when m is an even number,}\\ (k-1)kf(k,k-1)+\frac{(n+1-2k)k}{2}f(k,k), \text{ when } m \text{ is an odd number.}\end{cases}$$

Proof. Let $\Re$ be a ring with $|\Re|=n$ and $|\mathscr{S}(\Re)|=k$. If $char(\Re)$ is an even number, then by using Lemma 1 and Theorem 2.7 in [21], $\mathscr{S}_i(\Re)$ is k-regular with $\frac{nk}{2}$ number of edges. Therefore, by using equation (2),

$$I(\mathscr{S}_i(\Re))=\sum_{i\le j} m_{i,j}(\mathscr{S}_i(\Re))f(i,j)=\sum_{e\in E} f(k,k)=\frac{nk}{2}f(k,k).$$

Table 1: Degree based topological indices of a graph G

Sr. No.	Topological index	Symbol	Formula
1	Randić index [22]	$R_{-\frac{1}{2}}(G)$	$R_{-\frac{1}{2}}(G) = \sum_{e=uv\in E} \frac{1}{\sqrt{d_u d_v}}$
2	General Randić index [8]	$R_\alpha(G)$	$R_\alpha(G) = \sum_{e=uv\in E}(d_u d_v)^\alpha.$
3	Inverse Randić index [8]	$R_\alpha(G)$	$R_\alpha(G) = \sum_{e=uv\in E} \frac{1}{(d_u d_v)^\alpha}.$
4	Atom-Bond Connectivity index [12]	$ABC(G)$	$ABC(G) = \sum_{e=uv\in E} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$
5	Geometric– Arithmetic index [9]	$GA(G)$	$GA(G) = \sum_{e=uv\in E} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$
6	Harmonic index [30]	$H(G)$	$H(G) = \sum_{e=uv\in E} \frac{2}{d_u+d_v}$
7	Augmented Zagreb index [4]	$AZ(G)$	$AZ(G) = \sum_{e=uv\in E} \left\{\frac{d_u d_v}{d_u+d_v-2}\right\}^3$
8	Symmetric Division (Deg) index [11]	$SDD(G)$	$SDD(G) = \sum_{e=uv\in E} \left\{\frac{min(d_u,d_v)}{max(d_u,d_v)} + \frac{max(d_u,d_v)}{min(d_u,d_v)}\right\}$
9	Inverse Sum (Indeg) index [13]	$ISI(G)$	$ISI(G) = \sum_{e=uv\in E} \frac{d_u d_v}{d_u+d_v}$
10	Forgotten index [5]	$F(G)$	$F(G) = \sum_{e=uv\in E} {d_u}^2 + {d_v}^2$
11	Sum Connectivity index [6]	$S(G)$	$S(G) = \sum_{e=uv\in E} \frac{1}{\sqrt{d_u+d_v}}$
12	First Hyper Zagreb index [15]	$H_1(G)$	$H_1(G) = \sum_{e=uv\in E} \{d_u + d_v\}^2$
13	Second Hyper Zagreb index [32]	$H_2(G)$	$H_2(G) = \sum_{e=uv\in E} \{d_u d_v\}^2$
14	Foran index [7]	$FR(G)$	$FR(G) = \sum_{e=uv\in E} d_u\sqrt{\frac{d_u}{d_v}} + d_v\sqrt{\frac{d_v}{d_u}}$

Also, if $char(\Re)$ is odd, then by Theorem 2.8 in [4], $\mathscr{S}_i(\Re)$ is of the size $\frac{(n-1)k}{2}$, where the k number of vertices has degree $k-1$ and other $n-k$ vertices have degree k. Thus, in this theorem to calculate $I(\mathscr{S}_i(\Re))$ for the case, when $char(\Re)$ is odd, $\mathscr{S}_i(\Re)$ has precisely $k(k-1)$ number of edges with degree k and $k-1$ at their endpoints and $\frac{(n+1-2k)k}{2}$ number of edges which have both endpoints are of degree k. Therefore, for odd characteristic of $\Re$ we have

$$I(\mathscr{S}_i(\Re)) = \sum_{i\leq j} m_{i,j}(\mathscr{S}_i(\Re))f(i,j)$$
$$= \sum_{k-1\leq k} m_{k-1,k}(\mathscr{S}_i(\Re))f(k-1,k) + \sum_{k\leq k} m_{k,k}(\mathscr{S}_i(\Re))f(k,k).$$

Clearly, $m_{k-1,k}(\mathscr{S}_i(\Re)) = (k-1)k$ and $m_{k,k}(\mathscr{S}_i(\Re)) = \frac{(n+1-2k)k}{2}$, thus

$$I(\mathscr{S}_i(\Re)) = (k-1)kf(k,k-1) + \frac{(n+1-2k)k}{2}f(k,k).$$

□

On the basis of the above theorem we determine the all aforesaid topological indices in the form of a table. The Table 2 Characterize these topological indices on the basis of characteristic of ring $\Re$ (whether it is even or odd).

Next, we give some figures below in which three-dimensional graphs for the Randić index, Atom-Bond Connectivity index and Forgotten index discussed above are plotted, with respect to n (the order of the ring $\Re$) and k (the number of self-inverse elements in the ring $\Re$). These plots are generated for rings with both even and odd characteristics, which provide a comparative analysis of these topological indices on the bases of the characteristics of a ring.

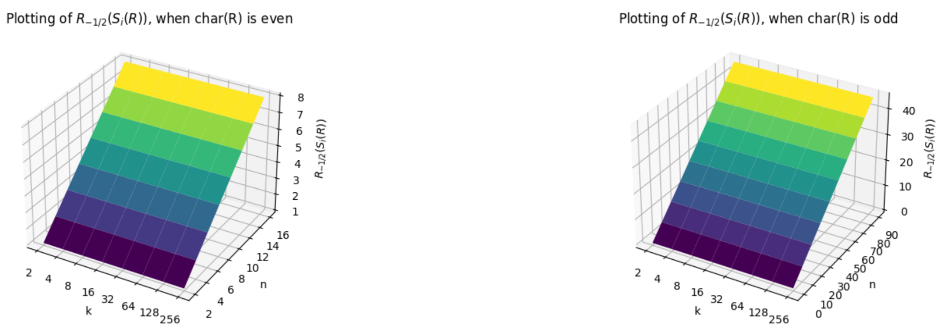

Figure 3: Three dimensional plot of the Randić index

Table 2: Degree based topological indices of a graph $\mathscr{S}_i(\Re)$, for even and odd characteristic of $\Re$

Sr. No.	Symbol	f(x,y)	$\mathrm{I}(\mathscr{S}_\mathrm{i}(\Re))$, when $\mathrm{char}(\Re)$ is even	$\mathrm{I}(\mathscr{S}_\mathrm{i}(\Re))$, when $\mathrm{char}(\Re)$ is odd
1	Randić index	$\frac{1}{\sqrt{xy}}$	$\frac{n}{2}$	$\sqrt{k(k-1)}+\frac{(n+1-2k)}{2}$
2	General Randić index	$(xy)^\alpha$	$\frac{nk^{2\alpha+1}}{2}$	$k(k-1)^{\alpha+1}+\frac{(n+1-2k)k^{2\alpha+1}}{2}$
3	Inverse Randić index	$\frac{1}{(xy)^\alpha}$	$\frac{nk^{1-2\alpha}}{2}$	$k(k-1)^{1-\alpha}+\frac{(n+1-2k)k^{1-2\alpha}}{2}$
4	Atom-Bond Connectivity index	$\sqrt{\frac{x+y-2}{xy}}$	$n\sqrt{\frac{k-1}{2}}$	$\sqrt{k(k-1)(2k-3)}+(n+1-2k)\sqrt{\frac{k-1}{2}}$
5	Geometric–Arithmetic index	$\frac{2\sqrt{xy}}{x+y}$	$\frac{nk}{2}$	$\frac{2k(k-1)^{3/2}}{2k-1}+\frac{(n+1-2k)k^2}{4}$
6	Harmonic index	$\frac{2}{x+y}$	$\frac{nk}{2}$	$\frac{2k(k-1)}{2k-1}+\frac{n+1-2k}{2}$
7	Augmented Zagreb index	$\left\{\frac{xy}{x+y-2}\right\}^3$	$\frac{nk^7}{16(k-1)^3}$	$\frac{k(k-1)^4}{(2k-3)^3}+\frac{(n+1-2k)k^7}{16(k-1)^3}$
8	Symmetric Division (Deg) index	$\left(\frac{min(x,y)}{max(x,y)}+\frac{max(x,y)}{min(x,y)}\right)$	nk	$(k-1)^2+k^2+(n+1-2k)k$
9	Inverse Sum (Indeg) index	$\frac{xy}{x+y}$	$\frac{nk^2}{4}$	$\frac{k^2(k-1)^2}{2k-1}+\frac{(n+1-2k)k^2}{4}$
10	Forgotten index	x^2+y^2	nk^3	$k^3(k-1)+k(k-1)^3+(n+1-2k)k^3$
11	Sum Connectivity index	$\frac{1}{\sqrt{x+y}}$	$\frac{n}{2}\sqrt{\frac{k}{2}}$	$\frac{k(k-1)}{\sqrt{2k-1}}+\frac{(n+1-2k)\sqrt{k}}{2^{3/2}}$
12	First Hyper Zagreb index	$\{x+y\}^2$	$2nk^3$	$k(k-1)(2k-1)^2+2(n+1-2k)k^3$
13	Second Hyper Zagreb index	$\{xy\}^2$	$\frac{nk^5}{2}$	$k(k-1)^3+\frac{(n+1-2k)k^3}{2}$
14	Foran index	$x\sqrt{\frac{x}{y}}+y\sqrt{\frac{x}{y}}$	nk^2	$k^{5/2}(k-1)^{1/2}+k^{1/2}(k-1)^{5/2}+(n+1-2k)k^2$

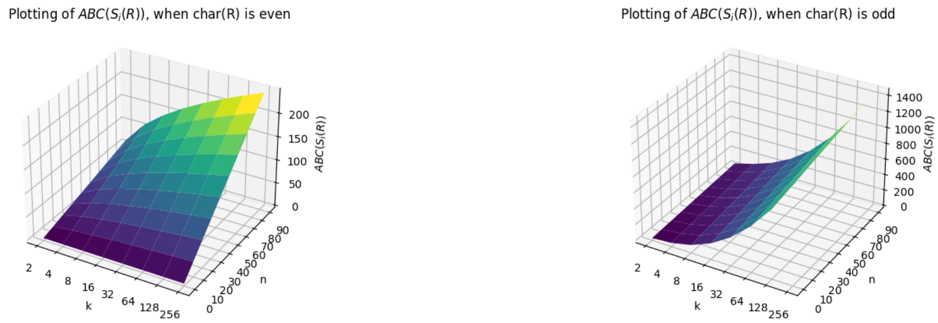

Figure 4: Three dimensional plot of the Atom-Bond Connectivity index

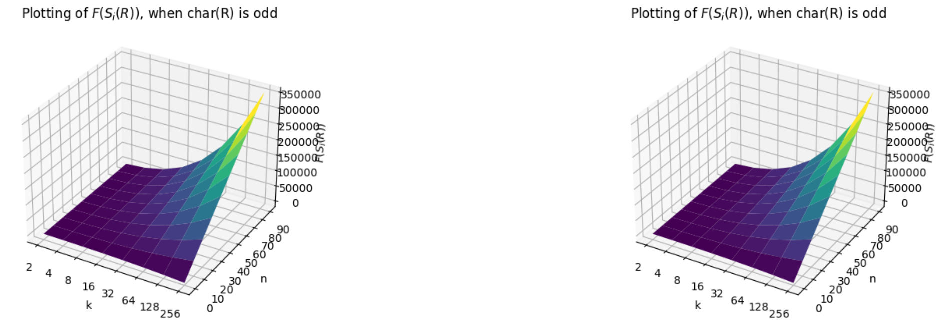

Figure 5: Three dimensional plot of the Forgotten index

We conclude this section, by providing two different graphical representations in Figure 6 and 7 for the different topological indices $I(\mathscr{S}_i(\Re))$. In particular, these graphs are made for a fixed value of k (here, k = 4), in order to show how the topological indices behave when the ring $\Re$ has either even or odd characteristic. The Figure 6 depicts the topological indices when $\Re$ has an even characteristic, while the Figure 7 illustrates the indices for the odd characteristic of $\Re$. These visualizations highlight the impact of the characteristic of a ring on the topological indices, thereby providing deeper insights into the structural properties of under varying algebraic conditions.

5. GUTMAN INDEX AND DETOUR GUTMAN INDEX

In [17], Gutman introduced the modified Schultz index which he referred to as the Gutman index. It is evident to note here that in case of acyclic structures (acyclic structures are those graphs which does not contain any cycle), the structural characteristics of a molecular structure given by the Gutman index is in concordance

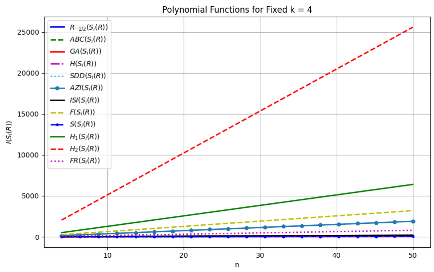

Figure 6: $\mathbf{I}(\mathscr{S}_{\mathbf{i}}(\Re))$ for even characteristic

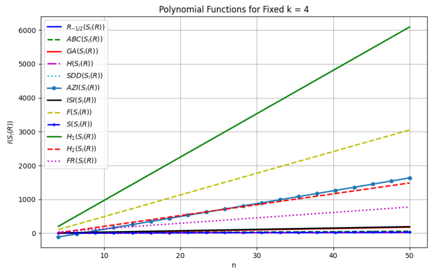

Figure 7: $\mathbf{I}(\mathscr{S}_{\mathbf{i}}(\Re))$ for odd characteristic

with the the structural characteristics of a molecular structure given by the Wiener index. The Gutman index of a graph G, denoted by Gut(G) is calculated as the sum over all pairs of vertices u and v in G, with half the product of their vertex degrees and the distance between them. In acyclic connected graph $d(x, y) = D(x, y)$, but for the graphs which contain cycles, we have $d(x, y) \neq D(x, y)$. Furthermore, in [31] a new index of a graph G fame as Detour Gutman index is examined and this index is the Gutman index with respect to detour distance [14]. In this section, we compute the Gutman and Detour Gutman indices for the graph $\mathscr{S}_i(\mathbb{Z}_n)$, when $n = 2p^r$, where p is an odd prime number. We begin with the following definitions:

Definition 5. *[31], The Gutman index for the graph G is given by the formula*

$$Gut(G) = \sum_{\{u,v\} \subset V(G)} d_u d_v d(u, v).$$

Definition 6. *[31], The Detour Gutman index for a graph G is symbolized by $DGut(G)$ and is defined as*

$$DGut(G) = \sum_{\{u,v\} \subset V(G)} d_u d_v D(u, v).$$

Theorem 4. *If $n = 2p^r$, then $Gut(\mathscr{S}_i(\mathbb{Z}_n)) = \frac{n^3}{2}$ and $DGut(\mathscr{S}_i(\mathbb{Z}_n)) = \frac{3n^3}{2}$*

Proof. Let $n = 2p^r$. Then by Lemma 1 and Theorem 4.2 in [21], $\mathscr{S}_i(\mathbb{Z}_n) \cong C_n$ i.e., $\mathscr{S}_i(\mathbb{Z}_n)$ is a cycle graph with n vertices, which means every vertex has degree 2. Let $\mathscr{S}_i(\mathbb{Z}_n)$ is a cyclic graph of the form $u_1 \leftrightarrow u_2 \leftrightarrow u_3 \leftrightarrow ... \leftrightarrow u_{n-1} \leftrightarrow u_n \leftrightarrow u_1$, where $u_i \in V$, for $1 \leq i \leq n$ and the symbol $\leftrightarrow$ represents the adjacency of two vertices. Clearly, $\mathscr{S}_i(\mathbb{Z}_n)$ has ${}^nC_2$ number of distinct pairs of vertices. Out of these ${}^nC_2$ number of pairs, the n pairs namely; $\{u_1, u_2\}, \{u_2, u_3\}, ..., \{u_{n-1}, u_n\}, \{u_n, u_1\}$ are the pairs in which vertices are at unit distance from each other and the n pairs namely; $\{u_1, u_3\}, \{u_2, u_4\}, ..., \{u_{n-1}, u_1\}, \{u_n, u_2\}$, are those having vertices at distance 2. Continuing in this fashion, there are $\frac{n}{2}$ pairs namely; $\left\{u_1, u_{\frac{n}{2}}\right\}, \left\{u_2, u_{\frac{n}{2}+1}\right\}, ..., \left\{u_{n-1}, u_{\frac{n}{2}-1}\right\}, \{u_n, u_2\}$ in which vertices are at distance $\frac{n}{2}$ from each other. Thus, by the definition of Gutman index, we have

$$
\begin{aligned}
Gut(\mathscr{S}_i(\mathbb{Z}_n)) &= \sum_{\{u,v\}\subset V(G)} d_u d_v d(u,v) \\
&= \{2.2.1 + 2.2.1 + ... + 2.2.1\}\ (n \text{ times }) \\
&+ \{2.2.2 + 2.2.2 + ... + 2.2.2\}\ (n \text{ times }) + ... \\
&+ \left\{2.2.(\frac{n}{2} - 1) + 2.2.(\frac{n}{2} - 1) + ... + 2.2.(\frac{n}{2} - 1)\right\}\ (n \text{ times }) \\
&+ \left\{2.2.\frac{n}{2} + 2.2.\frac{n}{2} + ... + 2.2.\frac{n}{2}\right\}\ (\frac{n}{2} \text{ times }) \\
&= 4\left\{1n + 2n... + (\frac{n}{2} - 1)n + \frac{n}{2}\frac{n}{2}\right\} \\
&= 4\left\{(1 + 2 + ... + (\frac{n}{2} - 1))n + \frac{n^2}{4}\right\} \\
&= 4\left\{(\frac{n}{2} - 1)(\frac{n}{2})\frac{n}{2} + \frac{n^2}{4}\right\} \\
&= 4(\frac{n^3}{8}) = \frac{n^3}{2}.
\end{aligned}
$$

On the other hand, the Detour Gutman index will be calculated by using the longest distance between the pairs of vertices. Thus, the Detour Gutman index for $\mathscr{S}_i(\mathbb{Z}_n)$ i.e., for the cycle graph can be calculated similarly as Gutman index except distances. Therefore, for all pairs of vertices, where the distance between vertices is 1, the longest distance will become $n - 1$. Similarly, for those pairs in which vertices are at distance

2, the longest distance between them is $n-2$. Thus, we have

$$\begin{aligned}
DGut(\mathscr{S}_i(\mathbb{Z}_n)) &= \sum_{\{u,v\}\subset V(G)} d_u d_v D(u,v) \\
&= \{2.2.(n-1) + 2.2.(n-1) + ... + 2.2.(n-1)\} \ (n \text{ times }) \\
&+ \{2.2.(n-2) + 2.2.(n-2) + ... + 2.2.(n-2)\} \ (n \text{ times }) + ... \\
&+ \left\{2.2.(\frac{n}{2}+1) + 2.2.(\frac{n}{2}+1) + ... + 2.2.(\frac{n}{2}+1)\right\} (n \text{ times }) \\
&+ \left\{2.2.\frac{n}{2} + 2.2.\frac{n}{2} + ... + 2.2.\frac{n}{2}\right\} (\frac{n}{2} \text{ times }) \\
&= 4\left\{(n-1)n + (n-2)n ... + (\frac{n}{2}+1)n + \frac{n}{2}\frac{n}{2}\right\} \\
&= 4\left\{((n-1) + (n-2) + ... + (\frac{n}{2}+1))n + \frac{n^2}{4}\right\} \\
&= 4\left\{n(\frac{n(n-1)}{2} - \frac{1}{2}(\frac{n}{2}+1)\frac{n}{2}) + \frac{n^2}{4}\right\} \\
&= 4\left\{n(\frac{n^2}{2}\frac{n}{2} - \frac{n^2}{8} - \frac{n}{4}) + \frac{n^2}{4}\right\} \\
&= 4\left\{\frac{n^3}{2} - \frac{n^2}{2} - \frac{n^3}{8} - \frac{n^2}{4} + \frac{n^2}{4}\right\} \\
&= 2\left(\frac{3n^3}{4} - n^2\right).
\end{aligned}$$

□

Theorem 5. *If n is an even number, then $Gut(\mathscr{S}_i(\mathbb{Z}_n)) = k^2 W(\mathscr{S}_i(\mathbb{Z}_n))$ and $DGut(\mathscr{S}_i(\mathbb{Z}_n)) = 2|E|(n-1) - k^2 W(\mathscr{S}_i(\mathbb{Z}_n))$, where $k = |\mathscr{S}_i(\mathbb{Z}_n)|$ and $W(\mathscr{S}_i(\mathbb{Z}_n))$ is the Wiener index of graph $\mathscr{S}_i(\mathbb{Z}_n)$.*

Proof. Let n be an even number, then by [21] $\mathscr{S}_i(\mathbb{Z}_n)$ is a $k-$regular graph with $k = |\mathscr{S}(\mathbb{Z}_n)|$. By [16], the Wiener index is

$$W(\mathscr{S}_i(\mathbb{Z}_n)) = \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d(u,v).$$

Now, by definition of Gutman index, we have

$$Gut(\mathscr{S}_i(\mathbb{Z}_n)) = \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d_u d_v d(u,v),$$

but $d_u = k$, for all $u \in V(\mathscr{S}_i(\mathbb{Z}_n))$. Thus,

$$Gut(\mathscr{S}_i(\mathbb{Z}_n)) = \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d_u d_v d(u,v) = k^2 \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d(u,v) = k^2 W(\mathscr{S}_i(\mathbb{Z}_n))$$

To prove further, we claim that $D(u,v) = n - d(u,v)$. Let $u, v \in \mathscr{S}_i(\mathbb{Z}_n)$ such that $d(u,v) = l$. As n is an even number, then $\mathscr{S}_i(\mathbb{Z}_n)$ has a Hamiltonian cycle of the form

$$u \leftrightarrow x_1 \leftrightarrow x_2 \leftrightarrow \ldots \leftrightarrow x_{l-1} \leftrightarrow v \leftrightarrow x_{l+1} \leftrightarrow \ldots \leftrightarrow x_{n-1} \leftrightarrow u.$$

Therefore, for longest distance between u and v there exists an alternative sequence of vertices and edges,

$$v \leftrightarrow x_{l+1} \leftrightarrow x_{l+2} \ldots \leftrightarrow x_{n-1} \leftrightarrow u.$$

Thus, $D(v,u) = n - l$ which implies $D(u,v) = n - d(u,v)$. So, by Detour Gutman index

$$\begin{aligned} DGut(\mathscr{S}_i(\mathbb{Z}_n)) &= \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d_u d_v D(u,v) \\ &= \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d_u d_v \left(n - d(u,v)\right) \\ &= k^2 \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} (n - d(u,v)) \\ &= k^2 \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} n - k^2 \sum_{\{u,v\}\subset V(\mathscr{S}_i(\mathbb{Z}_n))} d(u,v) \end{aligned}$$

The number of ways to select 2 elements out of n elements, without considering the order, is given by $\binom{n}{2} = \frac{n(n-1)}{2}$. Hence,

$$DGut(\mathscr{S}_i(\mathbb{Z}_n)) = k^2 \frac{n(n-1)}{2} n - k^2 W(\mathscr{S}_i(\mathbb{Z}_n))$$

□

By the implications of the preceding theorem, along with Theorems 1.6 and 1.7 in [28], we can rigorously derive the following corollaries.

Corollary 1. *For $\mathscr{S}_i(\mathbb{Z}_{2^r})$, the Gutman index is of the form*

$$Gut(\mathscr{S}_i(\mathbb{Z}_{2^r})) = \begin{cases} 1 & \textit{if } r = 1 \\ 32 & \textit{if } r = 2 \\ 640 & \textit{if } r = 3 \\ 16n + n^3 & \textit{if } r \geq 4. \end{cases}$$

Furthermore, Detour Gutman index is

$$DGut(\mathscr{S}_i(\mathbb{Z}_{2^r})) = \begin{cases} 1 & \textit{if } r = 1 \\ 64 & \textit{if } r = 2 \\ 2944 & \textit{if } r = 3 \\ 7n^3 - 8n^2 - 16n & \textit{if } r \geq 4. \end{cases}$$

Corollary 2. *If p is an odd prime and s is a natural number, then the Gutman index of $\mathscr{S}_i(\mathbb{Z}_n)$ is of the form*

$$Gut(\mathscr{S}_i(\mathbb{Z}_n)) = \begin{cases} \frac{2}{3}n^3 - 2n^2 + \frac{7}{3}n - 1 & \textit{if } n = p^s \\ \frac{n^3}{2} & \textit{if } n = 2p^s \\ n^3 + 16n & \textit{if } n = 4p^s \\ 2n^3 + 192n & \textit{if } n = 8p^s. \end{cases}$$

and Detour Gutman index is

$$DGut(\mathscr{S}_i(\mathbb{Z}_n)) = \begin{cases} \frac{2}{3}n^3 - 2n^2 + \frac{7}{3}n - 1 & \textit{if } n = p^s \\ \frac{3n^3}{2} - 2n^2 & \textit{if } n = 2p^s \\ 7n^3 - 8n^2 - 16n & \textit{if } n = 4p^s \\ 30n^3 - 224n & \textit{if } n = 8p^s. \end{cases}$$

Conflict of Interest

The authors declare no conflict of interest.

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