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# Computing Energy and Some Topological Indices of $\Gamma(\mathbb{Z}_n)$

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**Abstract:** For a commutative ring $R$, the total graph of $R$ which denoted by $T(\Gamma(R))$, is a graph with all elements of $R$ as vertices, and two distinct vertices $u, v \in R$ are adjacent if and only if $u + v \in Z(R)$, where $Z(R)$ denotes the set of zero-divisors of $R$. In an earlier study, we computed Wiener, hyper-Wiener, reverse Wiener, Randić, Zagreb, $ABC$ and $GA$ indices of zero-divisor graph. In this study, some computer programs are prepared to calculate the zero-divisors and adjacency matrix of the given graph which, apply these programs to compute the energy and first edge-Wiener, sum-connectivity, harmonic, augmented Zagreb and hyper-Zagreb indices.

**Keywords:** Ring, Zero-Divisor Graph, MATLAB Program, Energy, Topological Indices

## 1. Introduction

A graph $G$ consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively. The graph $G$ is *connected* if each pair of the vertices in $G$ belongs to a path. The *degree* of the vertex $u \in V(G)$, written as $d_u$, is the number of edges with $u$ as an end vertex. For two vertices $u, v \in V(G)$ we define their *distance* $d(u, v)$ as the length of any shortest path connecting $u$ and $v$ in $G$. A *regular graph* is a graph where each vertex has the same number of neighbors. A regular graph with vertices of degree $r$ is called a *$r$-regular graph* or regular graph of degree $r$. Let $R$ be a commutative ring with identity. The *total graph* of $R$ denoted by $T(\Gamma(R))$, is a graph with the vertex set $R$ such that two vertices $u$ and $v$ are adjacent if and only if $u + v \in Z(R)$. We denote the set of zero-divisors and unit elements of $R$ by $Z(R)$ and $U(R)$, respectively. This concept was firstly introduced in [1] by Anderson and Badawi. Also, the zero-divisor graph of $R$, denoted as $\Gamma(R)$. Throughout this study, let $R = \mathbb{Z}_n$ that $n = p_1 \times \cdots \times p_k$ be a positive integer, where for $i$, $1 \leq i \leq k$, $p_i$ is a distinct prime number and $p_1 < \cdots < p_k$ and suppose that $|Z(\mathbb{Z}_n)| = m$, for some positive integer $m$. Mathematical calculations are absolutely necessary to explore important concepts in chemistry. In chemical graph theory, there are many molecular descriptors (or topological indices) for a connected graph, that have very useful properties to study of chemical molecules. The use of topological indices as structural descriptors is important in proper and optimal nanostructure design. In a series of studies some topological indices are computed for nanostructures and some graphs [2-7]. This article is the continuation of the work [8], which were provided MATLAB programs, to calculate the energy and first edge-Wiener, sum-connectivity, harmonic, augmented Zagreb and hyper-Zagreb index of the given zero-divisor graph.

## 2. Methods

In this section, we recall some algebraic definitions related to the topological indices chosen for the present study. Chemical graph theory interdisciplinary science that applies graph theory to the study of molecular structures. The molecules or chemical compounds are modeled by an undirected graph named molecular graphs.

Equivalence between chemical and graph theoretical terms:

Atom≈ Vertex
Molecule ≈ Molecular graph
Covalent bond ≈ Edge
Valency of an atom ≈ Vertex degree
Skeletal structure ≈ Hydrogen-depleted graph

Topological matrix ≈ Adjacency matrix

Energy level ≈ Eigenvalue

Example 2.1 In order to make it easier for readers to understand the molecular graph, an example is given on a hydrocarbon, together with its hydrogen-depressed graph as shown in Figure 1.

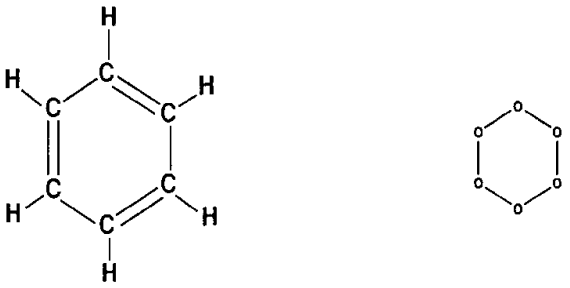

***Figure 1.*** *Structural formula and molecular graph of benzene,* $C_6H_6$.

The *adjacency matrix* of a molecular graph $G$ with $n$ vertices is an $n \times n$ matrix $A = [a_{ij}]$ defined by: $a_{ij} = 1$, if vertices $i$ and $j$ are connected by an edge and, $a_{ij} = 0$, otherwise. The *energy* of a graph $G$, often denoted $\varepsilon(G)$, is defined to be the sum of the absolute value of the eigenvalues of its adjacency matrix. Hence if $A(G)$ is the adjacency matrix of $G$, and $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A(G), then $\varepsilon(G) = \sum_{i=1}^{n} |\lambda_i|$. In chemistry the energy of a graph is extensively studied since it can be used to approximate the total $\pi$-electron energy of the molecule represented by that graph, for more details see [9, 10]. A *topological index* is a numerical parameter mathematically derived from the graph structure. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physic-chemical properties or biological activity (e.g., pharmacology).

The *Wiener index* is the oldest and one of the most studied distance-based topological indices in chemistry. It was introduced by Harold Wiener [11], equal to the sum of distances between all pairs of vertices of the graph under consideration. Other much studied distance-based topological indices are edge Wiener indices. Let $e = (x, y), f = (u, v) \in E(G)$. Set $d_1(e, f) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ and $d_0(e,f) = \begin{cases} d_1(e,f) + 1 & \text{if } e \neq f, \\ 0 & \text{if } e = f. \end{cases}$

The *first edge-Wiener index* ($W_{e_0}$) was introduced by Iranmanesh et al. [12] as follow:

$$W_{e_0} = \sum_{\{e,f\} \subseteq E(G)} d_0(e,f). \quad (1)$$

Also, vertex-degree-based topological indices discussed in this study:

Sum-connectivity (X), [13]: $X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$. (2)

*Harmonic* (*H*), [14]: $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$. (3)

Augmented Zagreb (AZI), [15]: $AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$. (4)

Hyper-Zagreb (HM), [16]: $HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$. (5)

Example 2.2 Let $G = CNC_{13}[n]$ be a defect carbon nanocone. To obtain topological indices, starting from molecular structure, viewed as a graph, and considering the number of the vertices and edges. Obviously, for $n = 1$ (see Figure 2) $|V| = 36$ and $|E| = 45$. Now, it is easy to see that $CNC_{13}[n]$ has $5n^2 + 18n + 13$ vertices and $\frac{1}{2}(15n^2 + 49n + 26)$ edges. We can see that the edge set of graph can be dividing to three partitions edges with endpoints 2 $[E_1]$, edges with endpoints $2, 3$ $[E_2]$ and edges with endpoints 3 $[E_3]$. By use an algebraic method we obtain $|E_1| = 5$, $|E_2| = 10n + 16$ and $|E_3| = \frac{1}{2}(15n^2 + 29n - 16)$.

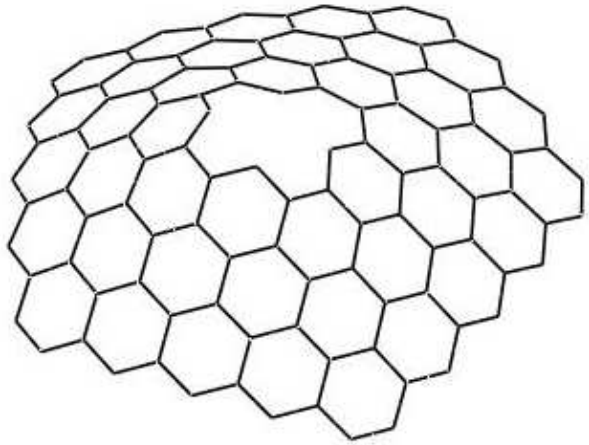

***Figure 2.*** *The graph of defect carbon nanocone,* $CNC_k[n]$ *with* $k = 13$ *and* $n = 3$.

Now, we calculate the Sum-connectivity index, Harmonic index, Augmented Zagreb index and hyper-Zagreb index for the molecular graph of Figure 2 by use an algebraic method:

a. $X(G) = \frac{1}{60}\left(75\sqrt{6}n^2 + \left(120\sqrt{5} + 145\sqrt{6}\right)n + (150 + 192\sqrt{5} - 80\sqrt{6})\right)$.

b. $H(G) = \frac{1}{30}(75n^2 + 265n + 187)$.

c. $AZI(G) = \frac{1}{128}(10935n^2 + 31381n + 9840)$.

d. $HM(G) = 270n^2 + 772n + 192$.

# 3. Results and Discussion

The goal of this section is to compute the topological indices of the zero-divisor graph $\mathbb{Z}_n$. Begin with several properties of the zero-divisor graph, which will be helpful to express of main results.

Theorem 3.1 [17] Let $u \in V(\Gamma(\mathbb{Z}_n))$ and $n$ be a natural number. If $n \neq 2$, then the followings hold:

a. If $n$ is prime, then $d_u = m = 1$, $(u \neq 0)$.

b. If $n$ is odd and not a prime number, then

$$d_u = \begin{cases} m-1 & u \in Z(\mathbb{Z}_n), \\ m & u \in U(\mathbb{Z}_n). \end{cases}$$

c. If $n$ is even, then $d_u = m-1$ and $\Gamma(\mathbb{Z}_n)$ is $(m-1)$-regular.

The following result is a consequence of Theorem 3.1.

Corollary 3.1 For a positive integer $n$, we have:

$$\left|E\left(\Gamma(\mathbb{Z}_n)\right)\right| = \begin{cases} \dfrac{n-1}{2} & \text{if } n \text{ is prime}, \\ \dfrac{m(n-1)}{2} & \text{if } n \text{ is odd}, \\ \dfrac{n(m-1)}{2} & \text{if } n \text{ is even}. \end{cases}$$

Note 3.1 For some values of the $\Gamma(\mathbb{Z}_n)$ is not connected. Indeed, $\Gamma(\mathbb{Z}_n)$ is not connected if and only if $n = p^k$, where $p$ is prime and $k \geq 1$. The following figures give examples of $\Gamma(\mathbb{Z}_n)$, for some values of $n$.

Example 3.1 The following figures represent some zero-divisor graphs in which Figure 3 and 4 are connected.

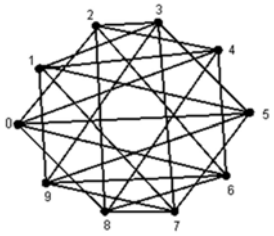


***Figure 3.*** $\Gamma(\mathbb{Z}_{10})$.

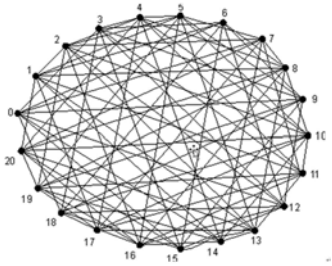

***Figure 4.*** $\Gamma(\mathbb{Z}_{21})$.

Example 3.2 The following figures represent some zero-divisor graphs in which Figure 5 and 6 are not connected.

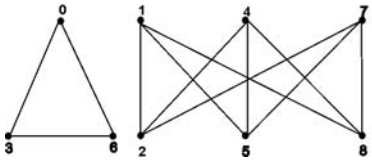


***Figure 5.*** $\Gamma(\mathbb{Z}_9)$.

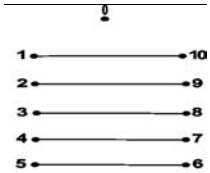


***Figure 6.*** $\Gamma(\mathbb{Z}_{10})$.

First MATLAB program is introducing a particular commutative ring $\mathbb{Z}_n$ and we will discuss the value $n$ for $\Gamma(\mathbb{Z}_n)$. Since for the calculation of topological indices the graph should be connected, therefore $n \neq p^k$, $p$ is prime and $k \geq 1$.

Program 3.1 A MATLAB program for checking different values $n$ of $\Gamma(\mathbb{Z}_n)$:

```
function [flag, Primes, Powers, N]=CHECK()
N=input('Input an integer: ');
IsPrime=isprime(1: N);
Primes=find(IsPrime);
Powers=zeros(size(Primes));
M=N;
for k=1: numel(Primes)
   while mod(M, Primes(k))==0
      Powers(k)=Powers(k)+1;
      M=M/Primes(k);
   end
end
if (sum(Powers~=0)>1)
   flag=true;
else
   flag=false;
end
```

Program 3.2 A MATLAB program compute the set zero divisors for $\Gamma(\mathbb{Z}_n)$, which is very useful in the other programs:

```
function [m]=ZeroDivisor(N, Powers, Primes)
m=[];
m(1)=0;
if((numel(Primes)>1)&&(sum(Powers~=0)>1))
   for i=1: numel(Primes)
      n=1;
      if(Powers(i)>0)
         while Primes(i)*n<N
            if(m~=Primes(i)*n)
               m=[m, Primes(i)*n];
            end
            n=n+1;
         end
      end
   end
end
m=sort(m);
end
```

Theorem 3.2 [18] Let $G$ be an arbitrary graph. Then

$$2\sqrt{|E(G)|} \leq \varepsilon(G) \leq 2|E(G)|.$$

Remark 3.1 By a well-known result on the subject of graph energy,

$$\varepsilon(G) \leq r + \sqrt{r(n-1)(n-r)},$$

for $n$-vertex $r$-regular graph $G$.

Theorem 3.3 Let $\Gamma(\mathbb{Z}_n)$ be a zero-divisor graph. Then the followings hold:

a. If $n$ is prime, then $\sqrt{2(n-1)} \leq \varepsilon(\Gamma(\mathbb{Z}_n)) \leq n-1$.

b. If $n$ is odd and not a prime number, then $\sqrt{2m(n-1)} \leq \varepsilon(\Gamma(\mathbb{Z}_n)) \leq m(n-1)$.

c. If n is even, then $\sqrt{2n(m-1)} \leq \varepsilon(\Gamma(\mathbb{Z}_n)) \leq \sqrt{(m-1)(n-1)(n-m+1)}$.

Proof. By Corollary 3.1, Theorem 3.2 and Remark 3.1, we are done.

Program 3.3 A MATLAB program for finding adjacency matrix of $\Gamma(\mathbb{Z}_n)$:

```
function A=ADJACENCYMATIRX(m, N)
A=zeros(N);
for i=1: N
   for j=i+1: N
      if sum(m==i-1)==1
         if sum(m==j-1)==1
            jam=i+j-2;
            if (sum(m==jam )==1|| jam==N || sum(m==jam-
         N)==1)
                A(i, j)=1;
            end
         else
            jam=i+j-2;
            if (sum(m==jam )==1|| jam==N || sum(m==jam-
         N)==1)
                A(i, j)=1;
            end
         end
      else
         jam=i+j-2;
         if (sum(m==jam )==1|| jam==N || sum(m==jam-
      N)==1)
            A(i, j)=1;
         end
      end
   end
end
for r=N:-1:1
   for i=N-1:-1:1
      A(r, i)=A(i, r);
   end
end
end
```

We apply Program 3.3 to compute the energy, first edge-Wiener index and vertex-degree-based topological indices of the zero-divisor graph $\mathbb{Z}_n$.

Program 3.4 A MATLAB program for computing the energy of $\Gamma(\mathbb{Z}_n)$:

```
clc;
clear;
[flag, Primes, Powers, N]=CHECK();
if(flag)
   [m]=ZeroDivisor(N, Powers, Primes);
   disp(['The number of zero divisors=',
num2str(numel(m))]);
   A=ADJACENCYMATIRX(m, N);
   e=eig(A)
   energy=sum(abs(e));
   disp(['Energy=', num2str(sum(abs(e)))]);
else
   disp('wrong input');
end
```

Using this program, we have:

***Table 1.*** *The Values of* $\varepsilon(\Gamma(\mathbb{Z}_n))$ *for* $6 \leq n \leq 40$.

| n | m | Energy of $\Gamma(\mathbb{Z}_n)$ | n | m | Energy of $\Gamma(\mathbb{Z}_n)$ |
|---|---|---|---|---|---|
| 6 | 4 | 8 | 26 | 14 | 48 |
| 10 | 6 | 16 | 28 | 16 | 64 |
| 12 | 8 | 24 | 30 | 22 | 76 |
| 14 | 8 | 24 | 33 | 13 | 72.14104977 |
| 15 | 7 | 29.47878038 | 34 | 18 | 64 |
| 18 | 12 | 40 | 35 | 11 | 81.07347241 |
| 20 | 12 | 44 | 36 | 24 | 88 |
| 21 | 9 | 43.65380658 | 38 | 20 | 72 |
| 22 | 12 | 40 | 39 | 15 | 86.4090888 |
| 24 | 16 | 56 | 40 | 24 | 100 |

Program 3.5 A MATLAB program for finding distance matrix of $\Gamma(\mathbb{Z}_n)$:

```
function D=dismat(m, N)
D=zeros(N);
m=sort(m);
for i=1: N
   for j=i+1: N
      if sum(m==i-1)==1
         if sum(m==j-1)==1
            jam=i+j-2;
            if (sum(m==jam )==1|| jam==N || sum(m==jam-
         N)==1)
                D(i, j)=1;
            else
                D(i, j)=2;
            end
         else
            jam=i+j-2;
            if (sum(m==jam )==1|| jam==N || sum(m==jam-
         N)==1)
                D(i, j)=1;
            else
                D(i, j)=2;
            end
         end
      else
         jam=i+j-2;
         if (sum(m==jam )==1|| jam==N || sum(m==jam-
      N)==1)
            D(i, j)=1;
         else
            D(i, j)=2;
         end
      end
   end
end
for r=N:-1:1
```

```
    for i=N-1:-1:1
      D(r, i)=D(i, r);
    end
  end
  end
```

Program 3.6 A MATLAB program for finding minimum of a vector of numbers:

```
  function [k]=mini(V)
  [m, n]=size(V);
  k=V(1);
  for i=2: n
    if V(i)<k
      k=V(i);
    end
  end
  end
```

Program 3.7 The program compute the first edge-Wiener index of $\Gamma(\mathbb{Z}_n)$. This program includes several sub programs:

```
  clc;
  clear;
  [flag, Primes, Powers, N]=CHECK();
  c=1;
  for i=1: numel(Primes)
    if Powers(i)~=0
      primes2(c)=Primes(i);
      c=c+1;
    end
  end
  if(flag)
    [m]=ZeroDivisor(N, Powers, Primes);
    A=ADJACENCYMATIRX(m, N);
    D=dismat(m, N);
    k=0; We=0; We0=0;
    for i=1: size(A, 1)
      for j=1: size(A, 1)
        if i < j & A(i, j)==1
          k=k+1;
          x(k)=i;
          y(k)=j;
        end
      end
    end
    for i=1: k
      for j=1: k
        if i~=j
          F=[D(x(i), x(j)), D(x(i), y(j)), D(y(i), x(j)),
        D(y(i), y(j))];
          We(i, j)=mini(F)+1;
        else
          We(i, j)=0;
        end
      end
    end
    for i=1: k
      for j=1: k
        We0=We0+(We(i, j)/2);
      end
    end
    disp(['first edge-Wiener index=', num2str(We0)]);
  else
    disp('wrong input');
  end
```

Lemma 3.1 Let G be an arbitrary graph. Then G is r-regular if and only if one of the followings holds:

a. $X(G) = \frac{1}{\sqrt{2r}}|E(G)|$.

b. $H(G) = \frac{1}{r}\,|E(G)|$.

c. $\mathrm{AZI(G)} = \left(\frac{r^2}{2(r-1)}\right)^3 |E(G)|$.

d. $HM(G) = 4r^2\,|E(G)|$.

Proof. The proof is clear.

In order to provide a unified approach to the results discussed in next theorem, we express the following notation.

Note 3.2 *Let $uv$ be an arbitrary edge. Three cases may occur:*

(i) $u, v \in Z(\mathbb{Z}_n)$.

Since the degree of a vertex $v \in Z(\mathbb{Z}_n)$ is $m-1$, then the number of $d_u \times d_v$ is $A = \sum_{i=1}^{k}\binom{\frac{n}{p_i}}{2}$.

(ii) $u \in Z(\mathbb{Z}_n) - \{0\}$ and $v \in U(\mathbb{Z}_n)$.

Since the degree of a vertex $v \in Z(\mathbb{Z}_n)$ is $m-1$, the number of unit vertices adjacent to a vertex $v \in Z(\mathbb{Z}_n)$ is $m - \frac{n}{p_i}$. So, the coefficient of $m \times (m-1)$ is $B = \sum_{i=1}^{k}(m - \frac{n}{p_i})\left(\frac{n}{p_i} - 1\right)$.

(iii) $u, v \in U(\mathbb{Z}_n)$.

Similar to the previous cases, we have $C = \frac{m(n-1)}{2} - \left[\sum_{i=1}^{k}\binom{\frac{n}{p_i}}{2} + \sum_{i=1}^{k}(m - \frac{n}{p_i})\left(\frac{n}{p_i} - 1\right)\right]$.

Now, we calculate the sum-connectivity index, harmonic index, augmented Zagreb index and hyper-Zagreb index of $\Gamma(\mathbb{Z}_n)$ by use an algebraic method.

Theorem 3.4 *It holds that:*

*a.*

$$X\big(\Gamma(\mathbb{Z}_n)\big) = \begin{cases} \frac{n\sqrt{2m-2}}{4} & \text{if } n \text{ is even and } n \neq 2^{\alpha_1}, \\ \frac{A}{\sqrt{2m-2}} + \frac{B}{\sqrt{2m-1}} + \frac{C}{\sqrt{2m}} & \text{if } n \text{ is odd and } n \neq {p_1}^{\alpha_1}. \end{cases}$$

*b.*

$$H\big(\Gamma(\mathbb{Z}_n)\big) = \begin{cases} \frac{n}{2} & \text{if } n \text{ is even and } n \neq 2^{\alpha_1}, \\ \frac{A}{m-1} + \frac{2B}{2m-1} + \frac{C}{m} & \text{if } n \text{ is odd and } n \neq {p_1}^{\alpha_1}. \end{cases}$$

*c.*

$$AZI\big(\Gamma(\mathbb{Z}_n)\big) =$$

$$\begin{cases} \frac{n(m-1)^7}{16(m-2)^3} & \text{if } n \text{ is even and } n \neq 2^{\alpha_1}, \\ A\left(\frac{(m-1)^6}{(2m-4)^3}\right) + B\left(\frac{m^2-m}{2m-3}\right)^3 + C\left(\frac{m^2}{2m-2}\right)^3 & \text{if } n \text{ is odd and } n \neq p_1^{\alpha_1}. \end{cases}$$

*d.*

$$HM(\Gamma(\mathbb{Z}_n)) = \begin{cases} 2n(m-1)^3 & \text{if } n \text{ is even and } n \neq 2^{\alpha_1}, \\ A(2m-2)^2 + B(2m-1)^2 + C(2m)^2 & \text{if } n \text{ is odd and } n \neq {p_1}^{\alpha_1}. \end{cases}$$

Proof. The formulas follow immediately from apply the precedent definitions, Lemma 3.1 and Note 3.2.

Program 3.8 A MATLAB program for finding degree of a vertex:

```
function [z]=degv(A, m)
z=0;
for a=A(m,:)
   z=z+a;
end
end
```

Program 3.9 We offer a MATLAB program for calculating vertex-degree-based topological indices of $\Gamma(\mathbb{Z}_n)$:

```
clc;
clear;
[flag, Primes, Powers, N]=CHECK();
c=1;
for i=1: numel(Primes)
   if Powers(i)~=0
      primes2(c)=Primes(i);
      c=c+1;
   end
end
if(flag)
   [m]=ZeroDivisor(N, Powers, Primes);
   A=ADJACENCYMATIRX(m, N);
   k=0; X=0; H=0; AZI=0; HM=0;
   for i=1: size(A, 1)
      for j=1: size(A, 1)
         if i < j & A(i, j)==1
            k=k+1;
            x(k)=i;
            y(k)=j;
         end
      end
   end
   for i=1: k
      X=X+(1/sqrt((degv(A, x(i))+degv(A, y(i)))));
      H=H+(2/(degv(A, x(i))+degv(A, y(i))));
      AZI=AZI+((degv(A, x(i))*degv(A, y(i)))/(degv(A,
   x(i))+degv(A, y(i))-2))^3;
      HM=HM+((degv(A, x(i))+degv(A, y(i)))^2);
   end
   disp(['Sum-connectivity index=', num2str(X)]);
   disp(['Harmonic index=', num2str(H)]);
   disp(['Augmented Zagreb index=', num2str(AZI)]);
   disp(['Hyper-Zagreb index=', num2str(HM)]);
else
   disp('wrong input');
end
```

To investigate the efficiency of Program 3.7 and Program 3.9, we consider two graphs which depicted in Figure 3 and 4.

Example 3.3 The values of $W_{e_0}(\Gamma(\mathbb{Z}_n)), X(\Gamma(\mathbb{Z}_n)), H(\Gamma(\mathbb{Z}_n)), AZI(\Gamma(\mathbb{Z}_n))$ and $HM(\Gamma(\mathbb{Z}_n))$ for $n = 10, 21$ are as follows:

***Table 2.*** *Some values of the topological indices of $\Gamma(\mathbb{Z}_n)$.*

| $n$ | $W_{e_0}(\Gamma(\mathbb{Z}_n))$ | $X(\Gamma(\mathbb{Z}_n))$ | $H(\Gamma(\mathbb{Z}_n))$ | $AZI(\Gamma(\mathbb{Z}_n))$ | $HM(\Gamma(\mathbb{Z}_n))$ |
|---|---|---|---|---|---|
| **10** | 530 | 7.9057 | 5 | 762.9395 | 2500 |
| **21** | 7947 | 21.7203 | 10.4902 | 10396.3589 | 26688 |

# 4. Conclusion

In fact, we made a connection between commutative ring theory, graph theory and topological indices. The main purpose of this study is to extend some results given in [8]. We have mentioned here some MATLAB programs, to calculate the adjacency matrix of the given graphs. Then we compute the energy and some topological indices by these programs.

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