Available online at http://scik.org
J. Math. Comput. Sci. 5 (2015), No. 1, 42-49
ISSN: 1927-5307

WIENER INDEX OF SOME NANOSTRUCTURES BY MATLAB PROGRAM

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Abstract. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. One of the most widely known topological descriptor is the Wiener index named after chemist Harold Wiener. In this paper, we propose a method for computing the Wiener index of the Cartesian product $P_m \times P_n$, $P_m \times C_n$, $C_m \times C_n$ using MATLAB. Then as our main purpose of this paper, we apply this result to compute the Wiener index of some molecular graphs related to polyomino structures and nanostructures and also characterize its property like Energy.

Keywords: Wiener Index; Matlab Program; Nanostructures.

2010 AMS Subject Classification: 82D80.

1. Introduction

A chemical graph or a molecular graph is a graph related to the structure of a chemical compound. Each vertex of this graph represented an atom of the molecule and bonds between atoms are represented by edges between the corresponding vertices. In theoretical chemistry, the physico-chemical properties of chemical compounds are often shown by the molecular graph based molecular structure descriptors, which are also referred to as topological indices. Among the various indices, which are designed to capture the different aspects of molecular structure, Wiener index is the best known one. Wiener index is the first reported distance-based topological index which was introduced by the Chemist, Harold Wiener, in 1947 [13]. It is defined as the half sum of the distances between all pairs of vertices of G.

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Received August 21, 2014

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

Where d(u,v) is the number of edges in a shortest path connecting the vertices u & v in G.

Wiener used his index, for the calculation of the boiling points of alkanes. The most important works on the geometric structures of Nano tubes, Nano tori and their topological indices were done by many authors using different software languages and different methods[1,2,3,4,5,6] In this Paper, MATLAB program is presented which is useful for computing the Wiener index of some Nano structure. Our notation is standard and mainly taken from standard books of graph theory [9].Throughout the paper, all of graphs are considered to be simple and connected. A simple graph is an undirected graph without any loops or multiple edges. Let G be a graph with the vertex set V (G) and the edge set E(G) . The distance between the vertices u and v of G is denoted by d(u,v) and defined as the number of edges in a shortest path connecting them. In this paper, we find the Wiener index of Cartesian product of Path graphs, linear polyomino chain, C_4 nanotubes and C_4 nanotori, through the adjacency matrix of a graph, which is the extension of previous paper[12].The Cartesian product G ×H of graphs G and H is a graph such that V (G ×H) = V (G) ×V (H), and any two vertices (a, b) and (u, v) are adjacent in G ×H if and only if either a = u and b is adjacent with v, or b = v and a is adjacent with u. The Wiener index of the Cartesian product graphs was studied in [7,8, 11].

2 .Wiener index of the Cartesian product of Path graphs

The following MATLAB program illustrates the adjacency matrix of the Cartesian product of path graphs., with the extension of the earlier finding [12].

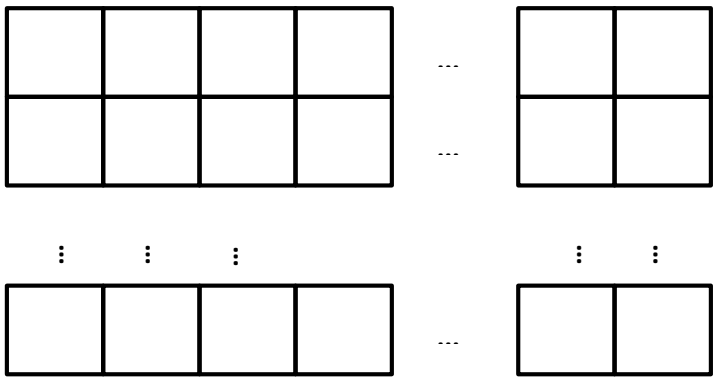

Figure 1. : $P_m \times P_n$

Cartesian product of path graph is also called as grid graph with m×n vertices.

% PROGRAMME TO CALCULATE THE ADJACENCY MATRIX OF $P_m \times P_n$

```
m= input('No. of vertices in a row m=');
n= input('No. of vertices in a column n=');
A=[];
for i=1:(m*n)-m
        A(i,i+m)=1;A(i+m,i)=1;
end
while i<=(m*n)-1
    for i=1:(m*n)-1
      A(i,i+1)=1;A(i+1,i)=1;
      if rem(i,m)==0
       A(i,i+1)=0;A(i+1,i)=0;
      end
    end
i=i+1;
end
A;
```

Corollary 2.1 Wiener index of linear polyomino chain

The graph $P_2 \times P_n$ made by n squares is called ladder graph with 2n vertices and denoted by L_n (see figure 2). Also, this graph is the molecular graph related to the polyomino structures and called the linear polyomino chain

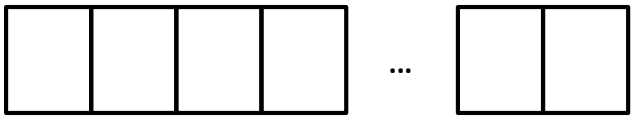

Figure 2. linear polyomino chain

3. Wiener index of C_4 nanotubes

Let G = $P_m \times C_n$, then G = TUC$_4$(m,n) is a C_4 nanotube (see figure 3) [7],[8].

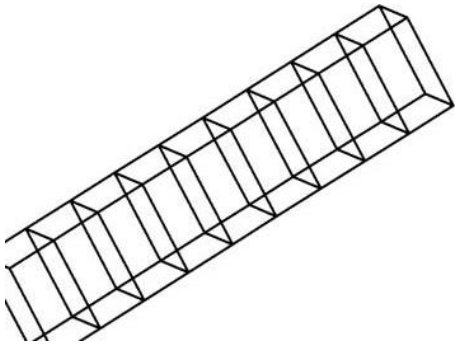

Figure 3. C_4 nanotube

% PROGRAMME TO CALCULATE THE ADJACENCY MATRIX OF C_4 NANOTUBE

```
p= input('No. of vertices in a row p=');
q= input('No. of vertices in a column q=');
A=[];
for i=1:(p*q)-p
        A(i,i+p)=1;A(i+p,i)=1;
end
while i<=(p*q)-1
    for i=1:(p*q)-1
      A(i,i+1)=1;A(i+1,i)=1;
      if rem(i,p)==0
       A(i,i+1)=0;A(i+1,i)=0;
      end
    end
i=i+1;
end
for i=1:p:(p*q)-p+1
        A(i,i+p-1)=1;A(i+p-1,i)=1;
end
A;
```

4. Wiener index of C_4 nanotorous

Let G = $C_m \times C_n$, then G = TUC$_4$(m.n) is a C_4 nanotorus (see figure 4) [7,8].

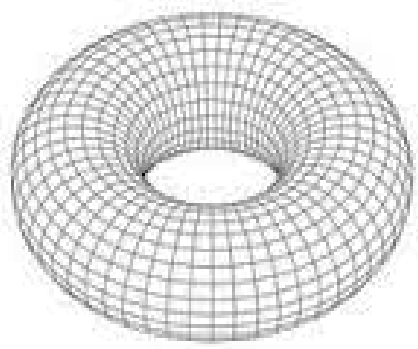

Figure 4. C_4 nanotorous

% PROGRAMME TO CALCULATE THE ADJACENCY MATRIX OF C_4 NANOTORUS

```
p= input('No. of vertices in a row p=');
q= input('No. of vertices in a column q=');
A=[];
for i=1:(p*q)-p
        A(i,i+p)=1;A(i+p,i)=1;
end
while i<=(p*q)-1
    for i=1:(p*q)-1
      A(i,i+1)=1;A(i+1,i)=1;
      if rem(i,p)==0
       A(i,i+1)=0;A(i+1,i)=0;
      end
    end
i=i+1;
end
for i=1:p:(p*q)-p+1
        A(i,i+p-1)=1;A(i+p-1,i)=1;
end
for i=1:p
        A(i,i+(q*p)-p)=1;A(i+(q*p)-p,i)=1;
end
A;
```

5. Illustration

Table 1: Wiener Index of grid graphs

$W(P_m \times P_n)$		N								
		2	3	4	5	6	7	8	9	10
m	2	8	25	56	105	176	273	400	561	760
	3		72	154	280	459	700	1012	1404	1885
	4			320	570	920	1386	1984	2730	3640
	5				1000	1595	2380	3380	4650	6125
	6					2520	3731	5264	7155	9440
	7						5488	7700	10416	13685
	8							10752	14484	18960
	9								19440	25365
	10									33000

Table 2: Wiener Index of C_4 NANO TORI

$W(C_m \times C_n)$		Q							
		3	4	5	6	7	8	9	10
p	3	54	120	210	351	525	768	1053	1425
	4		256	440	720	1064	1536	2088	2800
	5			750	1215	1785	2560	3465	4625
	6				1944	2835	4032	5427	7200
	7					4116	5824	7812	10325
	8						8192	10944	14400
	9							14580	19125
	10								25000

Table 3: Wiener Index of C_4 NANO TOROUS

$W(P_m \times C_n)$		q							
		3	4	5	6	7	8	9	10
p	2	25	56	105	176	273	400	561	760
	3	63	138	255	423	651	948	1323	1785
	4	136	288	520	848	1288	1856	2568	3440
	5	235	490	875	1415	2135	3060	4215	5625
	6	387	792	1395	2232	3339	4752	6507	8640
	7	574	1162	2030	3227	4802	6804	9282	12285
	8	832	1664	2880	4544	6720	9472	12864	16960
	9	1134	2250	3870	6075	8946	12564	17010	22365
	10	1525	3000	5125	8000	11725	16400	22125	29000

6. Conclusions

According to [12] and using the above MATLAB program, we can compute this index quickly. We tested the algorithm to calculate the Wiener index of some nano structures and classified its characterization like Energy [10]. Linear polyomino chain is non-hypo, non -hyper energetic for p=2, $q \geq 3$, C_4 Nanotori is non- hypo, non- hyper energetic for $p \geq 2$, $q \geq 3$,C_4 Nanotorus is non-hypo, non-hyper energetic for $p > 3, q \geq 4$.

Conflict of Interests

The author declares that there is no conflict of interests.

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