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COMPUTING WIENER INDEX OF $HAC_5C_7[p,q]$ NANOTUBES BY GAP PROGRAM

ALI IRANMANESH[1] and YASER ALIZADEH

DEPARTMENT OF MATHEMATICS, TARBIAT MODARES UNIVERSITY, P.O.BOX 14115-137, TEHRAN, IRAN.

E-mail: iranmana@modares.ac.ir

Abstract. The Wiener index of a graph $G$is defined as

$$W(G) = \frac{1}{2} \sum_{\{i,j\} \subseteq V(G)} d(i,j),$$

where $V(G)$ is the set of vertices of G and $d(i,j)$ is the distance between vertices i and j. In this paper, we give an algorithm by GAP program that can be compute the Wiener index for any graph; also we compute the Wiener index of $HAC_5C_7[p,q]$ and $HAC_5C_6C_7[p,q]$ nanotubes by this program.

Keywords: Nanotube; Wiener Index; Adjacent Vertices.

2000 Mathematics subject classification: Primary 05C12, Secondary 92E10.

1. Introduction

Let G be a connected graph. The vertex-set and edge-set of G denoted by $V(G)$ and $E(G)$ respectively. The distance between vertices i and j of G is denoted by $d(i,j)$. The Wiener index of G is denoted by $W(G)$ and is defined by

$$W(G) = \frac{1}{2} \sum_{\{i,j\} \subseteq V(G)} d(i,j) \tag{1}$$

[1]Corresponding Author

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Topological indices of nanotubes are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physicochemical properties.

The Wiener index is oldest topological indices. In 1947 chemist Harold Wiener [17] developed the most widely known topological descriptor, the Wiener index, and used in to determine physical properties of types of alkanes known as paraffins. Numerous of its chemical applications were reported and its mathematical properties are well understood. [3,4,12,14,16].

In a series of papers, the Wiener index of some nanotubes is computed [1,2,11,13,15,18 and 19], another topological indices are computed [6,7,8,9,10]. In this paper we give an algorithm for computing the Wiener index of any graph and also by this algorithm we obtain the Wiener index of $HAC_5C_7[p,q]$ and $HAC_5C_6C_7[p,q]$ nanotubes.

2. An Algorithm for the Computation of the Wiener Index

In this section, we give an algorithm that enables us to compute the Wiener index of any graph. For this purpose, the following algorithm is presented:

1) We assign to any vertex one number.
2) We determine all of adjacent vertices set of the vertex $i, i \in V(G)$ and this set denoted by $N(i)$.
3) In the start of program, we set $w = 0$, and at the end of program, the value of $\frac{1}{2}w$ will be the Wiener index of graph G.
4) The set of vertices that their distance to vertex i is equal to $t (t \geq 0)$ is denoted by $D_{i,t}$ and consider $D_{i,0} = \{i\}$. We have the following relations:

$$V = \bigcup_{i \geq 0} D_{i,t}, \quad i \in V(G) \tag{2}$$

$$W(G) = \frac{1}{2} \sum_{i \in V, t \geq 1} t \times |D_{i,t}| \tag{3}$$

According to (3), by determining these sets, we can obtain the Wiener index of the graph. The distance between vertex i and its adjacent vertices is equal to 1, therefore $D_{i,1} = N(i)$. For each $j \in D_{i,t} t \geq 1$, the distance between each vertex of set $N(j) \backslash (D_{i,t} \cup D_{i,t-1})$ and the vertex i is equal to $t+1$, thus we have $D_{i,t+1} = \bigcup_{j \in D_{i,t}} (N(j) \backslash (D_{i,t} \cup D_{i,t-1}) t \geq 1$.

According to above equation, we can obtain $D_{i,t}, t \geq 2$, for each $i \in V$. After determining each $D_{i,t}$, we add value $t \times |D_{i,t}|$ to w. Finally the Wiener index of the graph G is equal to $\frac{1}{2}w$.

Example 2.1. In [5], the Wiener index of dendrimers $T_{k,3}$, $k \geq 1$, computed and we can compute this index by above programme.

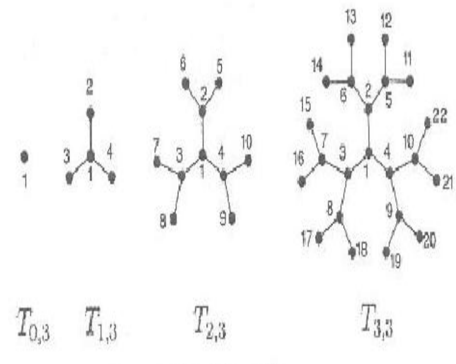

Figure1. Denderimers $T_{k,3}$

From [5], we have:
$n(T_{k,3}) = 1 + 3(2^k - 1)$
and its Wiener index is
$W(T_{k,3}) = (3k - 15)2^{2k} + 18 \times 2^k - 3$.
For computing of the Wiener index of $T_{k,3}$ by the above programme, at first we assign to any vertex one number (See Fig. 1); according to this numbering, the set of adjacent vertices to each vertex $1 \leq i \leq n$ is obtained by the following programm (part 1). In fact part 1 of the program is the presentation of the graph. We use the part 2 for compute the Wiener index of the graph.

```
k:=5;# (for example)
n:=1+3*(2 ^ k-1);
N:=[];
K1:=[2,3,4];
N[1]:=K1;
for i in K1 do
if k=1 then N[i]:=[1];
else
  N[i]:=[2*i+1,2*(i+1)];
  Add(N[i],1);fi;
od;
K2:=[..1+3*(2^(k-1)-1)];
for i in K2 do
  N[i]:=[2*i+1,2*(i+1)];
Add(n[i],Int(i-1)/2));
od;
K3:=[2+3*(2^(k-1)-1)..n];
for i in K3 do
```

```
if k=1 then N[i]:=[1];
else N[i]:=[Int(i-1)/2];fi;
od;

w:=0;
D:=[];
for i in [1..n] do
  D[i]:=[];
  u:=[i];
  D[i][1]:=N[i];
  u:=Union(u,D[i][1]);
  w:=w+Size(D[i][1]);
  s:=1;
  t:=1;
  while s <> 0 do
    D[i][t+1]:=[];
    for j in D[i][t] do
      for m in Difference (N[j],u) do
        AddSet(D[i][t+1],m);
      od;
    od;
  u:=Union(u,D[i][t+1]);
  w:=w+(t+1)*Size(D[i][t+1]);
  if D[i][t+1]=[] then s:=0;
    fi;
  t:=t+1;
    od;
  od;
w:=w/2;# (This value is equal to Wiener index of the graph)
```

In table 1, the Wiener index of $T_{k,3}$ for some k is obtained. (By the above program)

Table 1. The Wiener index of $T_{k,3}$

K	n	$W(T_{k,3})$
1	4	9
2	10	117
3	22	909
4	46	5661
5	94	31293
6	190	160893
7	382	788733
8	766	3740157
9	1534	17310717
10	3070	78661629

3. Computing the Wiener Index of $HAC_5C_7[p,q]$ Nanotube by GAP Program

A C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7. It can cover either a cylinder or a torus. In this section we compute the Wienere index of $HAC_5C_7[p,q]$ nanotube by GAP program.

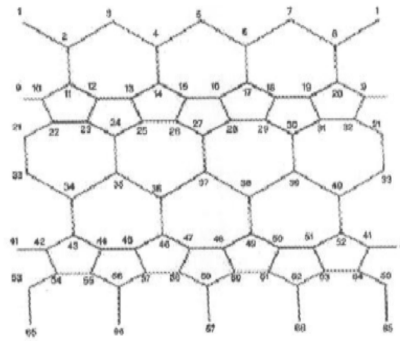

Figure2. $HAC_5C_7[4,2]$

We denote the number of heptagons in one row by p. In this nanotube, the three first rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q. In each period there are $8p$ vertices and p vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to $8pq + p$.

We partition the vertices of this graph to following sets:

- K_1: The vertices of first row whose number is $2p$.
- K_2: The vertices of the first row in each period except the first one whose number is $2p(q-1)$.
- K_3: The vertices of the second rows in each period whose number is $3pq$.
- K_4: The vertices of the third row in each period whose number is $3pq$.
- K_5: The last vertices of the graph whose number is p.

Figure 3 shows the rows of m-th period.
We write a program to obtain the adjacent vertices set to each vertex in the sets K_i, $i = 1 \ldots 5$. We can obtain the adjacent vertices set to each vertex by the join of these programs. In this program, the value of x is the assign number of vertex i in that period.

The following program computes the Wiener index of $HAC_5C_7[p,q]$ nanotube for arbitrary p and q.

```
p:=3; q:=7;# (for example)
n:=8*p*q+p;
N:=[];
K1:=1..2*p];V1:=[2..2*p-1];
```

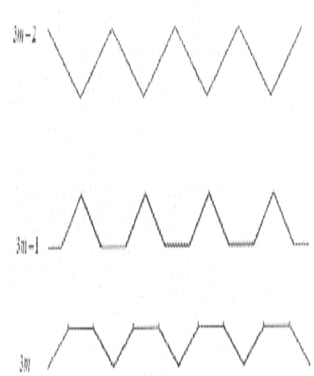

Figure3.

```
N[1]:=[2,2*p];
N[2*p]:=[2*p-1,5*p,1];
for i in V1 do
if i mod 2=0 then N[i]:=[i-1,i+1,3/2*i+2*p];
  else N[i]:=[i-1,i+1]; fi;
od; k:=[2*p+1..8*p*q];
k2:=Filtered(k,i-> i mod (8*p)in[1..2*p]);;
for i in k2 do
  x:=i mod (8*p);
  if x mod 2=1 then N[1]:=[i-1,i+1,(x-2)*(3/2)+1+i-x-3*p];
    else N[i]:=[i-1,i+1,x*(3/2)+2*p+i-x];fi;
  if x=1 then N[i]:=[i+1,i-1+2*p,i-3*p];fi;
  if x=2*p then N[i]:=[i-1,i+3*p,i-2*p+1];fi;
od;
k3:=Filtered(k,i-> 1 mod(8*p)in[2*p+1..5*p]);;
for i in k3 do
  x:=i mod (8*p);
  if(x-(2*p)) mod 3=1 then N[i]:=[i-1,i+1,i+3*p-1];
    elif (x-(2*p)) mod 3=2 then N[i]:=[i-1,i+1,i+3*p];
    elif(x-(2*p)) mod 3=0 then N[i]:=[i-1,i+1,(2/3)*(x-2*p)+i-x];fi;
  if x=2*p+1 then N[i]:=[i-1+3*p,i-1+6*p,i+1];fi;
  if x=5*p then N[i]:=[i-3*p,i-3*p+1,i-1];fi;
od;
k4:=Filtered(k,i-> i mod (8*p) in Union ([5*p+1..8*p-1],[0]));;
for i in k4 do
  x:=i mod (8*p);
  if (x-(5*p)) mod 3=1 then N[i]:[i-1,i+1,(x-(5*p)-1)*(2/3)+1+(i-x)+8*p];
```

```
  elif(x-(5*p)) mod 3=2 then N[i]:=[i-1,i+1,i-3*p];
    elif (x-5*p)) mod 3=0 then N[i]:=[i-1,i+1,i-3*p+1];fi;
  if x=5*p+1 then N[i]:=[i+3*p-1,i+1,i+3*p];fi;
  if x=0 then N[i]:=[i-1,i-3*p+1,i-6*p+1];fi;
od;
K5:=[8*p*q+1..8*p*q+p];
for i in K5 do
  x:=i-8*p*q;
  y:=8*p*(q-1)+5*p+3*x-2;
  N[i]:=[y];
  N[y][3]:=i;
od;
w:=0;
D:=[];
for i in [1..n] do
  D[i]=[];
  u:=[i];
  D[i][1]:=N[i];
  u:=Union(u,D[i][1]);
  w:=w+Size(D[i][1]); s:=1;
t:=1;
while s <> 0 do
  D[i][t+1]:=[];
  for j in D[i][t] do
    for m in Difference (N[j],u) do
      AddSet(D[i][t+1],m);
    od;
  od;
  u:=Union(u,D[i][t+1]);
  w:=w+(t+1)*Size(D[i][t+1]);
  if D[i][t+1]=[] then s:=0;
    fi;
  t:=t+1;
  od;
od;
w:=w/2;# (This value is equal to Wiener index of the graph)
```

Table 2. The Wiener index of nanotube $HAC_5C_7[p,q]$

p	q	n	w
3	1	27	1167
4	2	68	12236
4	3	100	35052
5	3	125	57915
6	4	198	187068
7	4	231	265391
7	7	399	1220219
3	6	147	134787
4	6	196	243276
4	7	228	379756
5	7	285	601855
6	8	390	1290348
7	8	455	1781535
7	9	511	2495731
8	8	520	2362824
9	9	657	4235085

4. Computing the Wiener Index of $HAC_5C_6C_7[p,q]$ Nanotube by GAP Program

A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6 and C_7. It can cover either a cylinder or a torus. In this section we compute the Wiener index of $HAC_5C_6C_7[p,q]$ nanotube similar to the precious section.

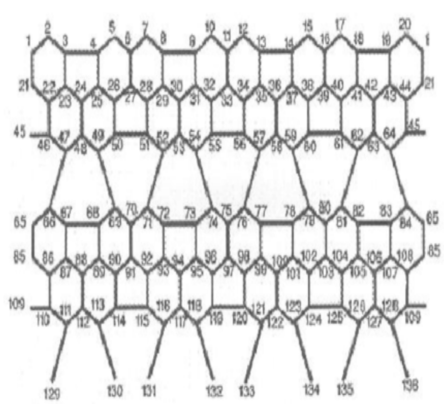

Figure4. Nanotube $HAC_5C_6C_7[4,2]$

We denote the number of pentagons in the first row by p. In this nanotube the three first rows of vertices and edges are repeated alternatively; we denote the number of this repetition by q. In each period, there are $16p$ vertices and

$2p$ vertices are joined to the end of the graph and hence the number of vertices in this nanotube is equal to $16pq + 2p$.

The following program is the same as the last program.

```
p:=4; q:=3:# (for example)
n:=16*p*q+2*p;
N:=[];
K1:=[1..5*p];
V1:=[2..5*p-1];
for i in V1 do
 if i mod 5=1 then N[i]:=[i-1,i+1,(i-1)*(6/5)+1+5*p];
  elif (i mod 5) in [0,2] then N[i]:=[i-1,i+1];
   i mod 5=3 then N[i]:=[i-1,i+1,(i-3)*(6/5)+3+5*p];
    elif i mod 5=4 then N[i]:=[i-1,i+1,(i-4)*(p/6)+5+5*p];fi;
od;
N[1]:=[2,5*p,5*p+1];N[5*p]:=[1,5*p-1];
k:=[5*p+1..16*p*q];
k2:=Filtered(k,i-> i mod (16*p) in [1..5*p]);
for i in k2 do
 x:=i mod (16*p);
 if x mod 5=1 then N[i]:=[i-1,i+1,(x-1)*(6/5)+1+i-x+5*p];
  elif x mod 5=2 then N[i]:=[i-1,i+1,i-5*p+1];
   elif x mod 5=3 then N[i]:=[i-1,i+1,(x-3)*(6/5)+3+i-x+5*p];
    elif x mod 5=4 then N[i]:=[i-1,i+1,(x-4)*(6/5)+5+i-x+5*p];
     elif x mod 5=0 then N[i]:=[i-1,i+1,i-5*p];fi;
 if x=1 then N[i]:=[i+1,i-1+5*p,i+5*p];fi;
 if x=5*p then N[i]:=[i-1,i-5*p,i-5*p+1];fi;
od:
k3:=Filtered(k,i-> i mod(16*p) in [5*p+1..11*p]);
for i in k3 do
 x:=(i-5*p) mod (16*p);
 if x mod 6=1 then N[i]:=[i-1,i+1,(x-1)*(5/6)+i-x-5*p+1];
  elif x mod 6=2 then N[i]:=[i-1,i+1,(x-2)*(5/6)+2+i-x-6*p];
   elif x mod 6=3 then N[i]:=[i-1,i+1,(x-3)*(5/6)+3+i-x-5*p];
    elif x mod 6=4 then N[i]:=[i-1,i+1,(x-4)*(5/6)+4+i-x+6*p];
     elif x mod 6=5 then N[i]:=[i-1,i+1,(x-5)*(5/6)+4+i-x-5*p];
      elif x mod 6=0 then N[i]:=[i-1,i+1,x*(5/6)+1+i-x+6*p];fi;
 if x=1 then N[i]:=[i+1,i+6*p-1,i-5*p];fi;
 if x=6*p then N[i]:=[i-1,i+1,i-6*p+1];fi;
od;
k4:=Filtered(k,i-> i mod (16*p) in Union ([11*p+1..16*p-1],[0]));
for i in k4 do
```

```
  x:=(i-11*p) mod (16*p);
    if x mod 5=1 then N[i]:=[i-1,i+1,(x-1)*(6/5)+i-x-6*p];
      elif x mod 5=2 then N[i]:=[i-1,i+1,(x-2)*(6/5)+2+i-x-6*p];
        elif x mod 5=3 then N[i]:=[i-1,i+1,i-1+5*p];
          elif x mod 5=4 then N[i]:=[i-1,i+1,(x-4)*(6/5)+4+i-x-6*p];
            elif x mod 5=0 then N[i]:=[i-1,i+1,i+5*p];fi;
  if x=1 then N[i]:=[i-1,i+1,i-1+5*p];fi;
  if x=5*p then N[i]:=[i-1,i-5*p+1,i+5*p];fi;
od;
K5:=[16*p*q+1..n];
for i in K5 do
  x:=i-16*p*q;
if x mod 2=0 then
        y:=(5/2)*x+16x*p*q-5*p;
      else y:=(5/2)*(x-1)+3+16*p*q-5*p;fi;
    N[i]:=[y];
    N[y][3]:=i;
od;
w:=0;
D:=[];
for i in [1..n] do
    D[i]:=[];
    u:=[i];
    D[i][1];=N[i];
    u:=Union(u,D[i][1]);
    w:=w+Size(D[i][1]);
s:=1; t:=1;
while s <> 0 do
    D[i][t+1]:=[];
    for j in D[i][t] do
      for m in Difference (N[j],u) do
        AddSet(D[i][t+1],m);
      od;
    od;
u:=Union(u,D[i][t+1]);
w:=w+(t+1)*Size(D[i][t+1]);
if D[i][t+1]=[] then s:=0;
    fi;
  t:=t+1;
  od;
od;
w:=w/2;# (This value is equal to Wiener index of the graph)
```

Table 3. The Wiener index of $HAC_5C_6C_7[p,q]$ nanotube

p	q	n	w
2	1	36	2462
3	2	102	32814
4	3	200	176880
5	3	250	309175
6	4	396	972096
7	7	798	5744963
2	3	100	35114
3	4	198	187338
3	5	246	343242
4	6	392	1063944
4	7	456	1627936
8	8	1040	11130768

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