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APPLICATIONS OF THE MATRIX PACKAGE MATLAB IN COMPUTING THE HOSOYA POLYNOMIAL OF Zig−Zag NANOTUBES

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The Hosoya polynomial of a molecular graph G is defined as $W(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G. In this paper an algorithm for computing the Hosoya polynomial of zig-zag nanotubes are given.

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1. Introduction

Nanostructured materials have received a lot of attention because of their novel properties. Nanotubes are an important category of one-dimensional nanostructured materials can be prepared from carbon.[1]

A topological index is a real number that is derived from molecular graphs of chemical compounds. Such numbers based on the distances in a graph are widely used for establishing relationships between the structure of molecules and their physico-chemical properties. The distance between atoms of a molecular graph is the length of a minimal path connecting them. The Wiener index was the first distance based topological index introduced early by Harold Wiener.[2] It is defined as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. We encourage the reader to consult papers[3,4] and references therein, for further study on the topic.

We now recall some algebraic notations that will be used in the paper. Suppose G is a graph and e is an edge of G. If e connects the vertices u and v then we write e = uv. Let d(u,v) denote the distance between vertices u and v in G. The Hosoya polynomial of G is defined as $W(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G.[5] Suppose $V(G) = \{v_1, \ldots, v_n\}$ and $M = [d_{ij}]$ denotes the distance matrix of G, where $d_{ij} = d(v_i,v_j)$. Then one can see that $W(G) = 1/2\sum_{i,j}d_{ij}$ and $W(G,x) = 1/2\sum_{i,j} x^{d_{ij}}$.

The problem of computing topological indices of nanostructures is introduced firstly by Diudea and his co-authors.[6-11] He takes the armchair, zig-zag and $TUC_4C_8(R/S)$ nanotubes into consideration and computed the Wiener index of these nanomaterials. The second author of this paper computed the Wiener index of a polyhex and $TUC_4C_8(R/S)$ nanotubes and nanotori.[12-18] In this paper we continue this program to compute the Hosoya polynomial of these nanomaterials. Our notation is standard and mainly taken from the book of Trinajestic[19] and papers by Taeri and his co-authors [20-22]

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2. Main results

In this section we derive an exact formula for the Hosoya polynomial of zig−zag polyhex nanotubes, Figures 1−4. Since $d/dx(W(G,x))|_{x=1} = W(G)$, the Wiener index of these nanomaterials are also computed.

Choose two base vertices v(1,1) and u(1,1) from the 2–dimensional lattice of T = $TUVC_6[m,n]$, Figure 2, where m is the number of rows and n is the number of zig-zags, Figure 3. Assume that $D_{u(1,1)}$ is distance between vertex u(1,1) and all vertices of T. This defines two matrix for the base vertices denoted by $D_{v(1,1)} = [d_{ij}^{v(1,1)}]$ and $D_{u(1,1)} = [d_{ij}^{u(1,1)}]$. Define three matrices $A^{u(1,1)}_{m\times(n/2+1)} = [a_{ij}]$, $A^{v(1,1)}_{m\times(n/2+1)} = [c_{ij}]$ and $B_{(n/2+1)\times n} = [b_{ij}]$ as follows:

Table 1. $A^{u(1,1)}$

i = 1		j = 1	j = 2	**For Other Values of i and j** ⇒	$a_{ij} = a_{i1}$ when j is odd
		$a_{11} = 0$	$a_{12} = 1$		
i > 1	i is even	$a_{i1}=a_{(i-1)1}+1$	$a_{i2}=a_{(i-1)1}+1$		$a_{ij} = a_{i2}$ when j is even
	i is odd	$a_{i1}=a_{i2}+1$	$a_{i2}=a_{(i-1)2}+1$		

Table 2. $A^{v(1,1)}$

i = 1		j = 1	j = 2	**For Other Values of i and j** ⇒	$c_{ij} = c_{i1}$ when j is odd
		$c_{11} = 0$	$c_{12} = 1$		
i > 1	i is even	$c_{i1}=c_{i2}+1$	$c_{i2}=c_{(i-1)2}+1$		$c_{ij} = c_{i2}$ when j is even
	i is odd	$c_{i1}=c_{(i-1)1}+1$	$c_{i2}=c_{i1}+1$		

We now define a new matrix $B_{m\times(n/2+1)}$, as $b_{i1} = i-1$, $1 \le i \le m$, and $b_{ij}=b_{i(j-1)}+1$ for other entries. From these matrices, one can compute matrices $D_{u(1,1)}$ and $D_{v(1,1)}$ as follows:

$$d_{ij}^{u(1,1)} = \begin{cases} \max(a_{ij}, b_{ij}) & 1 \le j \le n/2+1 \\ d_{i(n-j+2)}^{u(1,1)} & j > n/2+1 \end{cases},$$

$$d_{ij}^{v(1,1)} = \begin{cases} \max(a_{ij}, c_{ij}) & 1 \le j \le n/2+1 \\ d_{i(n-j+2)}^{v(1,1)} & j > n/2+1 \end{cases}.$$

Set $D_{u(1,1)} = [\Delta_i^{u(1,1)}]_{1\le i\le m}$ and $D_{v(1,1)} = [\Delta_i^{v(1,1)}]_{1\le i\le m}$, such that Δ_i denotes the i^{th} row of the matrix. We also assume that the first row of $D_{u(1,1)}$ and $D_{v(1,1)}$ are as follows:

$$[d_{u(1,1)}^{u(1,1)}, d_{v(1,2)}^{u(1,1)}, d_{u(1,2)}^{u(1,1)}, \cdots, d_{v(1,n/2)}^{u(1,1)}, d_{u(1,n/2)}^{u(1,1)}, d_{v(1,1)}^{u(1,1)}],$$
$$[d_{v(1,1)}^{v(1,1)}, d_{u(1,1)}^{v(1,1)}, d_{v(1,2)}^{v(1,1)}, d_{u(1,2)}^{v(1,1)} \cdots, d_{v(1,n/2)}^{v(1,1)}, d_{u(1,n/2)}^{v(1,1)}].$$

Suppose $D_{u(i,1)}$ and $D_{v(i,1)}$ are distance matrices associated to the i^{th} row of T. Then,

$$D_{u(i,1)} = \begin{bmatrix} \Delta_i^{v(1,1)} \\ \vdots \\ \Delta_2^{v(1,1)} \\ \Delta_1^{u(1,1)} \\ \\ \Delta_{m-i+1}^{u(1,1)} \end{bmatrix}, \quad D_{v(i,1)} = \begin{bmatrix} \Delta_i^{u(1,1)} \\ \vdots \\ \Delta_2^{u(1,1)} \\ \Delta_1^{v(1,1)} \\ \\ \Delta_{m-i+1}^{v(1,1)} \end{bmatrix}.$$

Notice that matrices associated to other columns of T are the same as the first one, Figure 3. Furthermore, two matrices $D_{u(i,j)}$ and $D_{v(i,j)}$ are obtained by replacement of the columns of $D_{u(i,1)}$ and $D_{v(i,1)}$, respectively. To compute the Hosoya polynomial of T, it is enough to count the equal entries of the distance matrix of T. But, the entries of the i^{th} row of these matrices $(1 < i \leq m)$ are appear $2n(m - i+1)$ times, and the entries of the first row are appear nm times. Suppose $D_{u(1,1)} = [d_{ij}^{u(1,1)}]$ and $D_{v(1,1)} = [d_{ij}^{v(1,1)}]$. So, we achieve two polynomials for vertices u and v, as follows:

$$W_u(T,x) = \frac{1}{2} n\left[\left(m\sum_{j=1}^{n} x^{d_{ij}^{u(1,1)}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1)\left(\sum_{j=1}^{n} x^{d_{ij}^{u(1,1)}} \right)\right)\right]$$
$$W_v(T,x) = \frac{1}{2} n\left[\left(m\sum_{j=1}^{n} x^{d_{ij}^{v(1,1)}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1)\left(\sum_{j=1}^{n} x^{d_{ij}^{v(1,1)}} \right)\right)\right]$$

Therefore the Hosoya polynomial of T is as follows:

$$W(T,x) = W_u(T,x) + W_v(T,x)$$

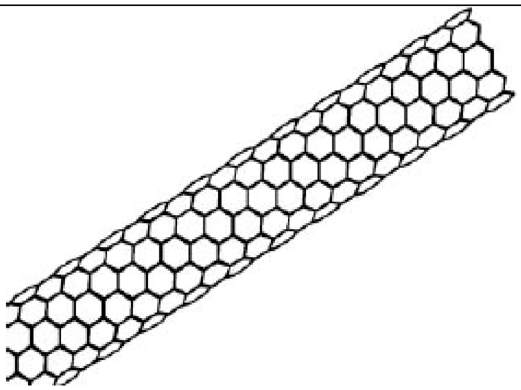

Fig. 1. 3D−Representation of Zig−Zag Nanotubes.

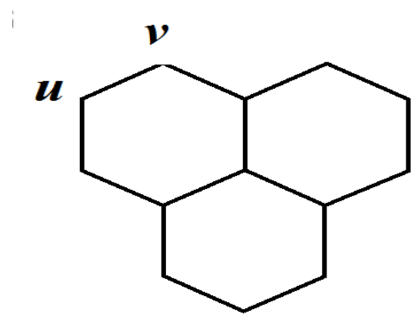

Fig. 2. The Base Vertices of T.

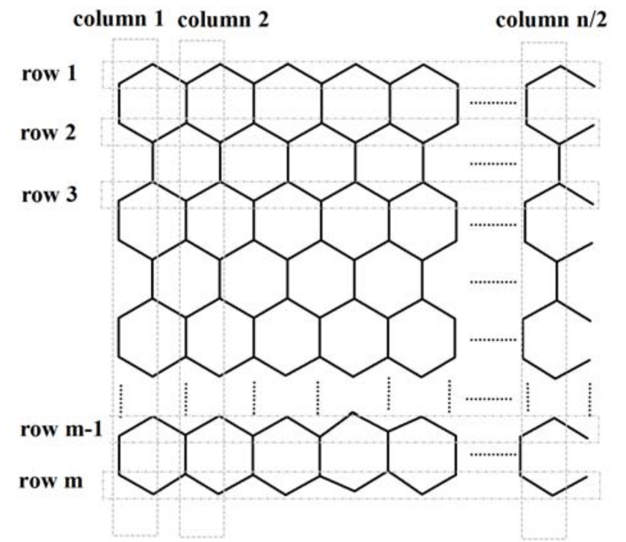

Fig. 3. The 2–Dimensional Lattice of an Arbitrary Zig−Zag Nanotube.

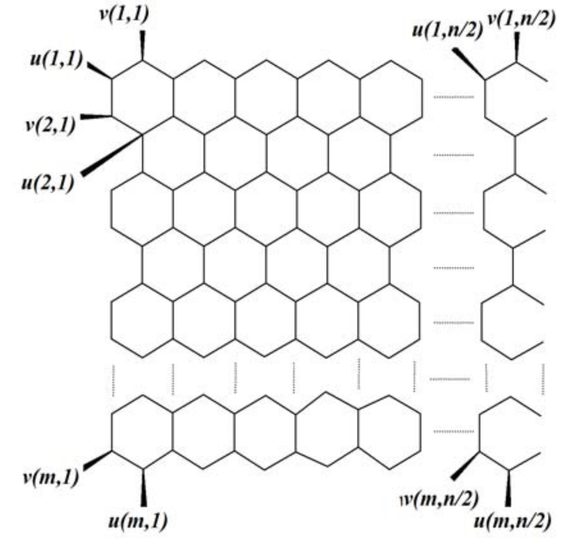

Fig. 4. A Labeling for T.

A MATLAB Program for Computing Hosoya Polynomial of Zig-Zag Nanotubes

```
reply = input('Enter number rows of graph zig-zag (m): ');
m=reply;
reply = input('Enter number columns of graph zig-zag (n): ');
n=reply;
%Au=[a_ij]
au=zeros(m,n/2+1);
au(1,1)=0;
au(1,2)=1;
for i=2:m
    if mod(i,2)==0
         au(i,1)=au(i-1,1)+1;
           au(i,2)=au(i,1)+1;
    else
        au(i,2)=au(i-1,2)+1;
        au(i,1)=au(i,2)+1;
    end
end
    for j=3:n/2+1
        for i=1:m
            if mod(j,2)~=0
                au(i,j)=au(i,1);
            else
                au(i,j)=au(i,2);
            end
        end
    end
%Av=[c_ij]
av=zeros(m,n/2+1);
av(1,1)=0;
av(1,2)=1;
for i=2:m
    if mod(i,2)==0
         av(i,2)=av(i-1,2)+1;
           av(i,1)=av(i,2)+1;
    else
        av(i,1)=av(i-1,1)+1;
        av(i,2)=av(i,1)+1;
    end
end
```

```
    for j=3:n/2+1
        for i=1:m
            if mod(j,2)~=0
                av(i,j)=av(i,1);
            else
                av(i,j)=av(i,2);
            end
         end
    end
%B=[b_ij]
bz=zeros(m,n/2+1);
for i=1:m
    bz(i,1)=i-1;
end
for j=2:n/2+1
    for i=1:m
        bz(i,j)=bz(i,j-1)+1;
    end
end
%Du=[du_ij]
du=zeros(m,n);
  for j=1:n/2+1
      for i=1:m
          du(i,j)=max(au(i,j),bz(i,j));
      end
  end
  for j=n/2+2:n
      for i=1:m
          du(i,j)=du(i,n-j+2);
      end
  end
%Dv=[dv_ij]
dv=zeros(m,n);
  for j=1:n/2+1
      for i=1:m
          dv(i,j)=max(av(i,j),bz(i,j));
      end
  end
  for j=n/2+2:n
      for i=1:m
          dv(i,j)=dv(i,n-j+2);
      end
  end
%in matrix eu we have
eu=zeros(m,max(max(du))+1);
for i=1:m
    for j=1:n
        eu(i,du(i,j)+1)=eu(i,du(i,j)+1)+1;
    end
end

ku=[m,(2*m-2):-2:2];
kku=zeros(m,max(max(du))+1);
for j=1:max(max(du))
    kku(:,j)=ku';
end;
hu=zeros(m,max(max(du))+1);
lu=[m,(2*m-2):-2:2];
for i=1:m
hu(i,:)=1/2*n*(lu(i)*eu(i,:));
end

cu=hu(1,:);
for i=2:m
cu=hu(i,:)+cu;
end
%in matrix ev we have
ev=zeros(m,max(max(dv))+1);
```

```
for i=1:m
    for j=1:n
        ev(i,dv(i,j)+1)=ev(i,dv(i,j)+1)+1;
    end
end

kv=[m,(2*m-2):-2:2];
kkv=zeros(m,max(max(dv))+1);
for j=1:max(max(dv))
    kkv(:,j)=kv';
end;
 hv=zeros(m,max(max(dv))+1);
lv=[m,(2*m-2):-2:2];
for i=1:m
hv(i,:)=1/2*n*(lv(i)*ev(i,:));
end
 cv=hv(1,:);
for i=2:m
cv=hv(i,:)+cv;
end
%W(T)=zeros()
%W(T)=cu+cv;
```

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