ENERGY AND LAPLACIAN SPECTRUM OF C₄C₈(S) NANOTORI AND NANOTUBE

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The spectrum of a finite graph is by definition the spectrum of the adjacency matrix, that is, its set of eigenvalues together with their multiplicities. The sum of the absolutes of these eigenvalues is the energy of graph. The Laplace spectrum of a finite undirected graph without loops is the spectrum of the Laplace matrix. There are some topological indices related to the Laplacian spectrum. In this paper, using a mathematical model for C₄C₈(S) that introduced in Ref.[26], we write a MATHEMATICA program to compute the energy and Laplacian spectrum of molecular graph of arbitrary C₄C₈(S) nanotori and nanotube.

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1. Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. In recent years there has been considerable interest in the general problem of determining topological indices of nanotubes, nanotori and fullerenes. It has been established, for example, that the Wiener and hyper-Wiener indices of polyhex nanotubes and tori are computable from the molecular graph of these structures. Accordingly, some of the interest has been focused on computing topological indices of these nanostructures.

Let G be a undirected graph without directed and multiple edges, and without loops, the vertex and edge-sets of which are presented by V(G) and E(G), respectively. The adjacency matrix of G is the 0-1 matrix A=A(G)=[a_{ij}] indexed by the vertex set V(G) of G, where a_{ij}=1 when ij is an edge and i \neq j, and 0 otherwise. This matrix characterizes a graph up to isomorphism. It allows the reconstruction of a graph and is a symmetric matrix. The Laplacian matrix of G is the matrix L=L(G)=[l_{ij}] indexed by the vertex set of G, with zero row sums, where \( l_{ij}=-a_{ij} \) for \( i \neq j \). If \( D=D(G)=[d_{ii}] \) is the diagonal matrix, indexed by the vertex set of G such that \( d_{ii} \) is the degree of \( i \), then \( L=D-A \).

The Laplacian matrix is sometimes also called the Kirchhoff matrix of a graph because of its role in the matrix-tree theorem implicit in the work of Kirchhoff. And sometimes \( L(G) \) is called the combinatorial Laplacian, to distinguish it from the normalized Laplacian earlier noted in connection with random walks.

The Laplacian matrix is a real symmetric matrix, so that diagonalization of the Laplacian matrix of a graph (molecule) G with N vertices (atoms) gives N real eigenvalues \( \mu_i(G) \), \( i=1,2,\ldots,N \). The smallest eigenvalue of the Laplacian spectrum is always 0, as a consequence of the special structure of the Laplacian matrix. The sum of these eigenvalues is the trace of \( L \), which is twice the number of edges of G. The uses of the Laplacian matrix, its characteristic polynomial, its eigenspectrum, and related invariants have been explored in chemistry for at least the last decade. There are many problems in physics and chemistry where the Laplacian matrices of graphs and their spectra play the central role. Some of the applications are mentioned in.

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A graph $G$ is called regular of degree $k$, when every vertex has precisely $k$ neighbors. If $G$ is regular of degree $k$, then for every eigenvalue $\theta$ we have $|\theta| \leq k$ and $L(G) = kI - A(G)$. It follows that if $G$ has ordinary eigenvalues $k = \theta_1 \geq \theta_2 \geq \ldots \geq \theta_N$ and Laplace eigenvalues $0 = \mu_1 \leq \mu_2 \leq \ldots \leq \mu_N$, then $\theta_i = k - \mu_i$ for $i = 1, 2, \ldots, N$. Moreover $k$ is the largest eigenvalue of $G$, and its multiplicity equals the number of connected components of $G$.

The Quasi-Wiener index, $W^*$, defined as $W^* = N \sum_{i=2}^{N} \frac{1}{\lambda_i}$, where $\lambda_i$, $i = 2, \ldots, N$ denotes the positive eigenvalues of the Laplacian matrix.

The eigenvalues of the Laplacian matrix are used in calculating the number of spanning trees, $t(G)$, in graph. We know that if $G$ be an undirected graph with Laplacian matrix $L(G)$ and eigenvalues $0 = \mu_1 \leq \mu_2 \leq \ldots \leq \mu_N$, then the number of spanning trees of $G$, equals $^3 t(G) = \frac{N}{\prod_{i=2}^{N} \mu_i}$. Moreover Mohar defined two topological indices, $TI_1$ and $TI_2$ on the ground of Laplacian spectrum $TI_1 = 2N \log(Q/N) \sum_{i=2}^{N} \frac{1}{\mu_i}$ and $TI_2 = \frac{4}{(N \mu_2)}$, where $Q$ is the number of edges.

The eigenvalues of adjacency matrix $A(G)$ are called eigenvalues of graph $G$ $^4$. Following Ivan Gutman $^{22}$, the energy, $E(G)$, of a molecular graph $G$ is defined to be the sum of the absolutes of the eigenvalues of $G$. We encourage the reader to consult papers $^{22-24}$ and references therein for background material as well as basic computational techniques.

A $C_4C_8$ net is a trivalent decoration made by alternating squares $C_4$ and octagons $C_8$. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation$^5$. Optimized $C_4C_8$ net covering a nanotube is illustrated in Figure 1. A nanotorus is a nanotube whose ends are connected.
2. Results and discussions

Description of molecular graphs of nanotori and nanotubes

A carbon nanotorus may be described as a long rolled-up graphite sheet bent around to the form of torus. Let $G_1=TRC_4C_8(S)[p,q]$ and $G_2=TUC_4C_8(S)[p,q]$ be the molecular graphs of $C_4C_8(S)$ nanotorus and nanotube, in which $p$ and $q$ are the number of octagons in vertical and horizontal directions, respectively, Figure 2. Note that the graph $G_1$ has exactly $8pq$ vertices and is a $3$-regular graph and so the Laplacian matrix of this graph is $L(G_1)=3I-A(G_1)$ where $I$ is the $8pq \times 8pq$ identity matrix. Arezoomand and Taeri proved that the set $\{\alpha, \beta, \gamma, \delta\} \in \mathbb{Z}^4 | \beta + \gamma + \delta \in \{0,1\}, \alpha + \gamma + \delta \in \{0,1\}$ is a mathematical model for vertices of $C_4C_8(S)$ lattice and the mapping $\{(i,j) \in \mathbb{Z}_n \times \mathbb{Z}_n : \sum_{(i,j)} a_{ij} = \sum_{(i,j)} b_{ij} \}$ is a distance function on the set of lattice vertices and gives us the minimum distance between two vertices $u$ and $v$. We assume that $a_{ij}$ denotes $(i,j)$-entry of two-dimensional lattice of $G_2$ as shown in Figure 2. We put the origin point $O$ at the $a_{41}$ and consider the vectors $e_0, e_1, e_2, e_3$.

Consider the points $a=a_{11}, b=a_{21}, c=a_{31}, d=a_{41}=O, e=a_{12}, f=a_{22}, g=a_{32}$ and $h=a_{42}$. It is easy to see that every point of $G_2$ can be constructed by a translation of these points in two directions $v=2e_1-e_2+e_3$ and $w=2e_1-e_2-e_3$. This is the content of lemma below.

Lemma 1. Assume that $a_{ij}, 1 \leq i \leq 4p$ and $1 \leq j \leq 2q$, denotes the $(i,j)$-entry of the two-dimensional lattice of $G_2$, as shown in the Fig.2, in our model we have

$$a_{ij} = \begin{cases} a^1_{ij} & i \equiv 1 \text{(mod 4)}, j \text{ odd or } i \equiv 3 \text{(mod 4)}, j \text{ even} \\ a^2_{ij} & i \equiv 1 \text{(mod 4)}, j \text{ even or } i \equiv 3 \text{(mod 4)}, j \text{ odd} \\ a^3_{ij} & i \equiv 2 \text{(mod 4)}, j \text{ odd or } i \equiv 0 \text{(mod 4)}, j \text{ even} \\ a^4_{ij} & i \equiv 2 \text{(mod 4)}, j \text{ even or } i \equiv 0 \text{(mod 4)}, j \text{ odd} \end{cases}$$

where

$$a^1_{ij} = (j-1) e_0 + (i-3)/2 e_1 + (7-i+2j)/4 e_2 + (3-i+2j)/4 e_3,$$

$$a^2_{ij} = (j-1) e_0 + (i-3)/2 e_1 + (9-i+2j)/4 e_2 + (1-i+2j)/4 e_3,$$

$$a^3_{ij} = (j-1) e_0 + (i-4)/2 e_1 + (8-i+2j)/4 e_2 + (-i+2j)/4 e_3,$$

$$a^4_{ij} = (j-1) e_0 + (i-4)/2 e_1 + (6-i+2j)/4 e_2 + (2-i+2j)/4 e_3.$$

Proof. It is easy to see that the lattice points of $G_2$ lie in $\bigcup \bigcup \ldots \bigcup T_h$, where

$T_1 = \{a + (i-1)/4 w + (j-1/2) v | i \equiv 1 \text{ (mod 4), } j \text{ odd} \}$

$T_2 = \{e + (i-1)/4 w + (j-1/2) v | i \equiv 1 \text{ (mod 4), } j \text{ even} \}$

$T_3 = \{b + (i-2)/4 w + (j-1/2) v | i \equiv 2 \text{ (mod 4), } j \text{ odd} \}$

$T_4 = \{f + (i-2)/4 w + (j-1/2) v | i \equiv 2 \text{ (mod 4), } j \text{ even} \}$

$T_5 = \{c + (i-3)/4 w + (j-1/2) v | i \equiv 3 \text{ (mod 4), } j \text{ odd} \}$

$T_6 = \{g + (i-3)/4 w + (j-1/2) v | i \equiv 3 \text{ (mod 4), } j \text{ even} \}$

$T_7 = \{d + (i-4)/4 w + (j-1/2) v | i \equiv 0 \text{ (mod 4), } j \text{ odd} \}$

$T_8 = \{h + (i-4)/4 w + (j-1/2) v | i \equiv 0 \text{ (mod 4), } j \text{ even} \}$

By considering the coordinates of the points $a, b, c, d, e, f, g, h$ and the vectors $v, w$ we can see that the relation (1) holds.

Note that in the $C_4C_8(S)$ net the nearest neighbors of vertex $v=(v_1,v_2,v_3,v_4)$ are

$$v_1 = (v_1 + \epsilon_1(v), v_2, v_3, v_4)$$

$$v_2 = (v_1, v_2 + \epsilon_2(v), v_3, v_4)$$

$$v_3 = (v_1, v_2, v_3 + \epsilon_3(v), v_4 + \epsilon_3(v))$$

where

$$\epsilon_1(v) = (-1)^{v_1+v_2+v_3+v_4},$$

$$\epsilon_2(v) = (-1)^{v_1+v_2+v_3+v_4}.$$
\[\mathcal{E}_{31}(v) = \begin{cases} \mathcal{E}_2(v) & \text{if } v_2 + v_3 + v_4 = v_1 + v_3 - v_4 \\ 0 & \text{otherwise} \end{cases}\]

\[\mathcal{E}_{32}(v) = \begin{cases} \mathcal{E}_2(v) & \text{if } v_2 + v_3 + v_4 \neq v_1 + v_3 - v_4 \\ 0 & \text{otherwise} \end{cases}\]

By above notations, it is obvious that if we fix \(p\) and \(q\), then \(V(G_1)=V(G_2)\) and \(E(G_1)=E(G_2)\) \(\cup \{a_{ij}a_{4p,j} | 1 \leq j \leq 2q\}\).

By the geometry of nanotori we have

\[a^1_{i,j} = a_{i,2q} \quad \text{(and so } a^2_{i,j} = a_{i,1}) \quad \text{when } i=2 \text{ or } 3 \pmod{4}\]

\[a^3_{i,j} = a_{4p,j} \quad \text{(and so } a^4_{i,j} = a_{4p,j}) \quad \text{for all } j.\]

Note that we can compute the other neighbors of these vertices and all of neighbors of other vertices by relations (1).

**A MATHEMATICA program for computing the adjacency and Laplacian matrices of \(G_1\) and \(G_2\).**

Now we are ready to write a MATHEMATICA program for computing the adjacency and Laplacian matrices of \(C_4C_8(S)\) nanotori and nanotubes. Using these two important matrices we can compute some topological indices. In the output of our program \(V=V(G_1)=V(G_2)\), \(A1\) and \(A2\) are the adjacency matrices of \(G_1\) and \(G_2\), respectively. Also \(L1\) and \(L2\) are the Laplacian matrices of \(G_1\) and \(G_2\), respectively and \(Eig1, Eig2\) are the set of their eigenvalues. Finally \(D2\) is the degree matrix of \(G_2\).

\[p=4; q=5;(* \text{for example})\]

\[a = \{0, -1, 1, 1\}; b = \{0, -1, 1, 0\}; c = \{0, 0, 1, 0\}; d = \{0, 0, 0, 0\}; e = \{1, -1, 1, 1\}; f = \{1, -1, 0, 0\}; g = \{1, 0, 0, 0\}; h = \{1, 0, 0, 0\}; v = \{2, 0, -1, 1\}; w = \{0, 2, -1, -1\}; V = \{\}\;

For[i=1, i\leq 4p,]

For[j=1, j\leq 2q,]

If[Mod[i,4]==1 && OddQ[j], AppendTo[V, a+(i-1)/4w+(j-1)/2v]];  
If[Mod[i,4]==1 && EvenQ[j], AppendTo[V, e+(i-1)/4w+(j/2-1)v]];  
If[Mod[i,4]==2 && OddQ[j], AppendTo[V, b+(i-2)/4w+(j-1)/2v]];  
If[Mod[i,4]==2 && EvenQ[j], AppendTo[V, f+(i-2)/4w+(j/2-1)v]];  
If[Mod[i,4]==3 && OddQ[j], AppendTo[V, c+(i-3)/4w+(j-1)/2v]];  
If[Mod[i,4]==3 && EvenQ[j], AppendTo[V, g+(i-3)/4w+(j/2-1)v]];  
If[Mod[i,4]==0 && OddQ[j], AppendTo[V, d+(i/4-1)w+(j-1)/2v]];  
If[Mod[i,4]==0 && EvenQ[j], AppendTo[V, h+(i/4-1)w+(j/2-1)v]];  

j++;

i++;

A1 = Table[x[i,j], \{i,1,8p\}, \{j,1,8p\}];

ff[u_, v_] := Sum[Abs[u[[i]] - v[[i]]], \{i,1,4\}];

For[i=1, i\leq 8p,]

For[j=1, j\leq 8p,]

If[ff[V[i], V[j]] == 1, x[i,j] = 1, x[i,j] = 0];

j++;

i++;

For[i=1, i\leq 2q,]

x[i, (8p-2)q+i] = 1;

x[(8p-2)q+i, i] = 1;

i++;

For[i=0, i\leq p-1,]

x[(8i+2)q+1,(8i+4)q] = 1;

x[(8i+4)q,(8i+2)q+1] = 1;

x[(8i+4)q+1,(8i+6)q] = 1;
x[(8i+6)q, (8i+4)q+1]=1;
i++;
A2 = Table[z[i, j], {i, 1, 8p*q}, {j, 1, 8p*q}];
For[i= 1, i ≤ 8p*q, 
  For[j = 1, j ≤ 8p*q, 
    If[ff[V[i]], V[j]] = = 1, z[i, j] = 1, z[i, j] = 0];
  j++;
i++;
For[i = 0, i ≤ p-1 ,
  z[(8i+2)*q+1,(8i+4)*q] = 1;
  z[(8i+4)*q, (8i+2)*q+1] = 1;
  z[(8i+4)*q+1,(8i+6)*q]=1;
  z[(8i+6)*q, (8i+4)*q+1]=1;
i++]
D2 = Table[dd[i, j], {i, 1, 8p*q}, {j, 1, 8p*q}];
B=A2.A2;
For[i = 1, i ≤ 8p*q, 
  For[j = 1, j ≤ 8p*q, 
    If[i= =j, dd[i,j]=B[[i]][[j]], dd[i,j]=0];
  ]
]
L1=3*IdentityMatrix[8p*q] - A1;
L2=D2-A2;
Eig1=Eigenvalues[L1]//N
Eig2=Eigenvalues[L2]//N

Topological indices and energy of nanotori and nanotube

It is easy to see that |E(G)| = 12pq and so |E(G,j)|=12pq-2q. Note that MATHEMATICA arranges the Laplacian eigenvalues decreasing. So if we append these below lines to the program, then we have numerical values of the topological indices $W^*$, $TI_1$, $TI_2$, the number of spanning trees $t(G), \mu_2$ (as defined in the section 1) and energy of nanotori and nanotube :

(*for nanotori*)
Eig1[[8p*q-1]]
QuasiWiener1 = 8p*q*Sum[1/Eig1[[i]], {i, 1, 8p*q - 1}] 
tG1=Product[1/Eig1[[i]], {i, 1, 8p*q - 1}]/(8p*q) 
TI1G1 =4/3*Sum[1/Eig1[[i]], {i, 1, 8p*q - 1}]
TI2G1 =4/(8p*q*Eig1[[8p*q - 1]])
E1=Eigenvalues[A1]; 
EnG1=Sum[Abs[E1[[i]]],{i,1,8p*q}]/N
(*for nanotube*)
Eig2[[8p*q-1]]
QuasiWiener2=8p*q*Sum[1/Eig2[[i]], {i, 1, 8p*q - 1}] 
tG2=Product[1/Eig2[[i]], {i, 1, 8p*q - 1}]/(8p*q) 
TI1G2=16p*q*Log[4/3]/(8p*q) 
TI2G2=4/(8p*q*Sum[1/Eig2[[i]], {i, 1, 8p*q - 1}]}
respectively, where

\[ E(G_2) = \sum |E_i| \]

\[ E_2 = \text{Eigenvalues}[A_2]; \]

\[ \mu_1 \leq \mu_2 \]

\[ \mu \text{ in Tables 1, 2.} \]

We give a numerical data for these indices, number of spanning trees and energies of the graphs \( G_1 \) and \( G_2 \) in Tables 1, 2. After running our programs, we can guess some conjectures as follows:

**Conjecture 1.** After running our program in many cases for \( p \) and \( q \), we guess that the characteristic polynomial of Laplacian matrix of \( G_1 \) is of the form

\[ f(x) = (x - \mu_1)^{a_1} (x - \mu_2)^{a_2} \cdots (x - \mu_k)^{a_k}, \]

where \( 0 = \mu_1 < \mu_2 < \cdots < \mu_k = 6 \) are distinct eigenvalues of Laplacian matrix with multiplicity \( a_i, 1 \leq i \leq k \), respectively, \( \sum_{i=1}^{k} a_i = |V(G_1)|, a_i = a_{i+1} = 1 \) and for \( 1 \leq j \leq \lfloor k/2 \rfloor \), \( a_{k-j} = a_j \).

**Conjecture 2.** If we fix \( p \) and \( q \), then we have \( E(G_1) > E(G_2) \), where \( E(G) \) is the energy of graph \( G \).
3. Conclusions

In this work, we give a MATHEMATICA program for calculating two important matrices adjacency and Laplacian of arbitrary C_{4C8}(S) nanotorus and nanotubes. Many structural properties of these nanostructures are depending to these matrices. The molecular graph of these structures is given as an algebraic definition. Similarly one can write simple MATHEMATICA program and compute many topological indices related with these matrices, such as Randic index, Zagreb group indices, etc. Moreover according Huckel theory we can equate the eigenvectors of the adjacency matrix for atomic orbitals in the construction of molecular orbitals. Also we can use the eigenvectors for analyze some physico-chemical properties and interesting intra-and intermolecular ordering (for more details see Refs. [27, 28]).

References