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Energy of Certain Planar Graphs

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Abstract - The energy E(G) of a graph G is the sum of the absolute values of the eigenvalues of G of its adjacency matrix. The Laplacian energy LE(G) of a graph G is the sum of absolute values of its Laplacian eigenvalues. In this paper, we provide a MATLAB program,to calculate the energy and Laplacian energy of certain planar graphs namely n-regular caterpillar and Necklace.

Keywords: Energy, Laplacian energy,n-regular caterpillar, Necklace.

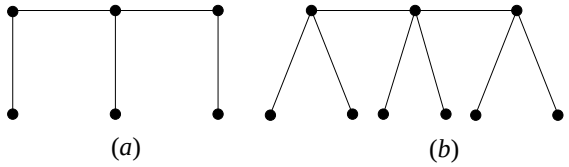
I. INTRODUCTION

For an *n*-vertex graph *G* with adjacency matrix *A* whose eigenvalues are $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, the energy $E(G)$ is $\sum_{i=1}^{n}|\lambda_i|$. The concept "*Graph Energy*" was introduced by Gutman[12] based on H*ü*ckel Molecular Orbital Theory(total π-electron energy). The characteristics of $E(G)$ are discussed in [1, 2,5,6, 7,14,18]. If $D(G)$, $A(G)$ are the diagonal matrix of degree and adjacency matrix of a graph*G*,then the Laplacian matrix L(G) of *G* is$D(G)$-$A(G)$. The Laplacian eigenvalues of *G* are the eigenvalues $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G) = 0$ of $L(G)$. For a graph *G*, the Laplacian energy $LE(G)$ is $\sum_{i=1}^{n}\left|\lambda_i - \frac{2m}{n}\right|$ where *m* is the number of edges of *G* and $\frac{2m}{n}$is the average degree of a vertex of *G*[3, 8,9,15, 16,17,19,20, 22].

A planar graph is a graph that can be drawn in the plane without any of its edges crossing. Otherwise it means that its edges intersect only at the vertices.Planar graphs are applied in various fields.In electronics, integrated circuits are designed in such a way that there are no cross connections or all the components in one layer of a chip are arranged so that it forms a planar graph [4].

In chemistry, atoms and bonds of molecular graphs are represented by vertices and edges respectively.The eigenvalues (and eigenvectors) associated with a molecular graphs provide information on the structure of chemical compounds. Graph Spectra can be used to derive topological indices such as resonance energy, molecular orbital energy and topology of π-electron systems.Partition function, inertial tensor of any polymer chains can be derived from spectra of Laplacian matrix[10, 11,21].

II. *N*-REGULAR CATERPILLAR*CT*(*N, M*)



(*a*) (*b*)

Figure 1: (*a*) 1-regular caterpillar, (b) 2-regular caterpillar

A *caterpillar* is a tree with the property that removal of its end points leaves a path. *n*-regular caterpillar is obtained by attaching *m* pendant edge to each vertex of the path P_n. It is denoted by *CT*(*n*, *m*) where *n* and *m* denote the number of vertices on path and number of pendant edges respectively.

The adjacency matrix of*n*-regular caterpillar is

$$A = \begin{pmatrix} B & I & I & . & . & . & I \\ I & O & O & . & . & . & O \\ I & O & . & & & & . \\ . & . & & . & & & . \\ . & . & & & . & & . \\ . & . & & & & . & . \\ I & O & O & . & . & . & O \end{pmatrix}$$

Where

$$B = \begin{pmatrix} 0 & 1 & 0 & . & . & . & 0 \\ 1 & 0 & 1 & . & . & . & 0 \\ 0 & 1 & 0 & 1 & & & . \\ . & . & 1 & 0 & . & & . \\ . & . & & . & . & . & . \\ . & . & & & . & . & 1 \\ 0 & 0 & . & . & . & 1 & 0 \end{pmatrix},$$

I is the identity matrix of order *n*×*n* and *O* is the zero matrix of order *n*×*n*.

The following MATLAB program generates the adjacency matrix of *n*-regular caterpillar and calculates its energy.

```
function[]=energycater(n,m)
A=zeros((m+1)*n);
for i=1:n-1
        A(i,i+1)=1;
        A(i+1,i)=1;
end
for j=1:n
  for i=j+n:n:(m+1)*n
        A(j,i)=1;
        A(i,j)=1;
  end
end
A
eigenvaluesofcater=eig(A)
energy=sum(abs(eigenvaluesofcater))
```

Proof of correctness of the program

It is easyto understand that the first 'for loop'in the MATLAB program generates the block *B* in the adjacency matrix. The $(i, j)^{th}$ entries of the block *B* represent the adjacency of the path on *n*-vertices.The second and third 'for loop' together generate the identity matrix alongside and below the block *B*. The entries in the identity matrix represent the adjacency of pendant vertices with vertices of pathP_m. To generate the Lalacian matrix let *B* = – (*A*) then degree matrix is formulated which is diagonal

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matrix of *B*. For all *n*, the first entry*B*(1, 1) and n^{th} entry *B*(*n*, *n*) is taken as *m*+1.The remaining entries between *B*(2, 2) and *B*(*n* – 1, *n* – 1) to be *m*+2 for all *n* and between *B*(*n* + 1, *n* + 1) and *B*((*m*+1)*n*, (*m*+1)*n*) to be 1. At the end, the required Laplacian matrix *B* is obtained.The following MATLAB program provides the Laplacian matrix and Laplacian energy of *n*-regular caterpillar function[]=energylapcater(n,m)

```
A=zeros((m+1)*n);
for i=1:n-1
        A(i,i+1)=1;
        A(i+1,i)=1;
end
for j=1:n
   for i=j+n:n:(m+1)*n
        A(j,i)=1;
        A(i,j)=1;
   end
end
A;
B=-(A);
B(1,1)=m+1;
B(n,n)=m+1;
for i=2:n-1
        B(i,i)=m+2;
end
for i=n+1:(m+1)*n
        B(i,i)=1;
end
B
eigenvaluesoflapcaterenergy=eig(B)
Energy=sum(abs(eigenvaluesoflapcaterenergy))
```

III. K_3^n-NECKLACE

Let $P = v_1, v_2, \ldots v_m$ be a path, for a graphH_i,$P \cup H_i$ has a cut vertexv_i,i =1, 2, …*m*. Then the graph $P \cup (\sum_{i=1}^{m} H_i)$is called a *necklace*. If each H_i is isomorphic to a complete graph K_3 then it is called K_3^n*-necklace*, where *n* denotes multiplicity.

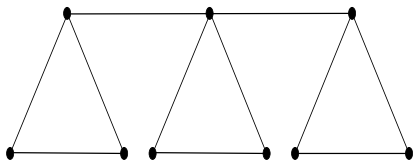

Figure 2: K_3^3-neclace

In general, the adjacency matrix ofK_3^n is

$$A = \begin{pmatrix} B & C & O & . & . & . & O \\ C & B & C & O & & & . \\ O & C & B & C & O & & . \\ . & O & C & . & . & . & . \\ . & & O & . & . & . & O \\ . & & & . & . & . & C \\ O & . & . & . & O & C & B \end{pmatrix}$$

where $B = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

and *O* is the zero matrix of order 3×3.

The following MATLAB program gives the adjacency matrix of necklace and calculates its energy.

```
function[]=energyneck(n)
A=zeros(3*n);
for i=1:3*n-1
        A(i,i+1)=1;
        A(i+1,i)=1;
end
for i=1:n-1
        A(3+(i-1)*3,4+(i-1)*3)=0;
        A(4+(i-1)*3,3+(i-1)*3)=0;
end
for i=1:n
        A(1+(i-1)*3,3+(i-1)*3)=1;
        A(3+(i-1)*3,1+(i-1)*3)=1;
end
for i=1:n-1
        A(1+(i-1)*3,4+(i-1)*3)=1;
        A(4+(i-1)*3,1+(i-1)*3)=1;
End
Aeigenvaluesofenergyneck=eig(A)
Energy=sum(abs(eigenvaluesofenergyneck))
```

The following MATLAB program generates the Laplacian matrix and Laplacian energy of K_3 neclace.

```
function[]=energylapneck(n)
A=zeros(3*n);
for i=1:3*n-1
        A(i,i+1)=1;
        A(i+1,i)=1;
end
for i=1:n-1
        A(3+(i-1)*3,4+(i-1)*3)=0;
        A(4+(i-1)*3,3+(i-1)*3)=0;
end
for i=1:n
        A(1+(i-1)*3,3+(i-1)*3)=1;
        A(3+(i-1)*3,1+(i-1)*3)=1;
end
for i=1:n-1
        A(1+(i-1)*3,4+(i-1)*3)=1;
        A(4+(i-1)*3,1+(i-1)*3)=1;
end
A;
B=-(A)
for i=1:3*n
        B(i,i)=2;
end
for i=1:n-2
        B(4+(i-1)*3,4+(i-1)*3)=4;
end
B(1,1)=3;
B(4+(n-2)*3,4+(n-2)*3)=3;
B
eigenvaluesofenergylapneck=eig(B)
```

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Energy=sum(abs(eigenvaluesofenergylapneck))

IV.CONCLUSION

In this paper, we have provided the MATLAB program to compute the energy $E(G)$ and Laplacian energy $LE(G)$ of n-regular caterpillar $CT(n, m)$ and Neclace K_3^n. The outcomes of this paper are expected to be useful to researchers in the area of molecular graphs.Programsto calculate the energy for various other graphs and their applications are under study.

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