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On the energy of fullerene graphs

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Abstract. The concept of energy of graph is defined as the sum of the absolute values of the eigenvalues of a graph. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be eigenvalues of graph G, the energy of G is defined as $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$. The aim of this paper is to compute the eigenvalues of two fullerene graphs C_{60} and C_{80}.

Keywords. eigenvalue, fullerene, graph energy.

1 Introduction

By using method of graph theory, we can construct cubic graphs whose faces are pentagons and hexagons. We call these graphs fullerene graphs. The fullerene era started in 1985 by Kroto and his co-athors with the discovery of a stable cluster C_{60} and its interpretation as a cage structure with the familiar shape of a soccer ball, see [22]. The well-known fullerene, the C_{60} molecule (see Figure 1), is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings [23]. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula, $n - m + f = 2$, one can deduce that $(5p + 6h)/3(5p + 6h)/2 + p + h = 2$, and therefore, $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms having 12 pentagonal and

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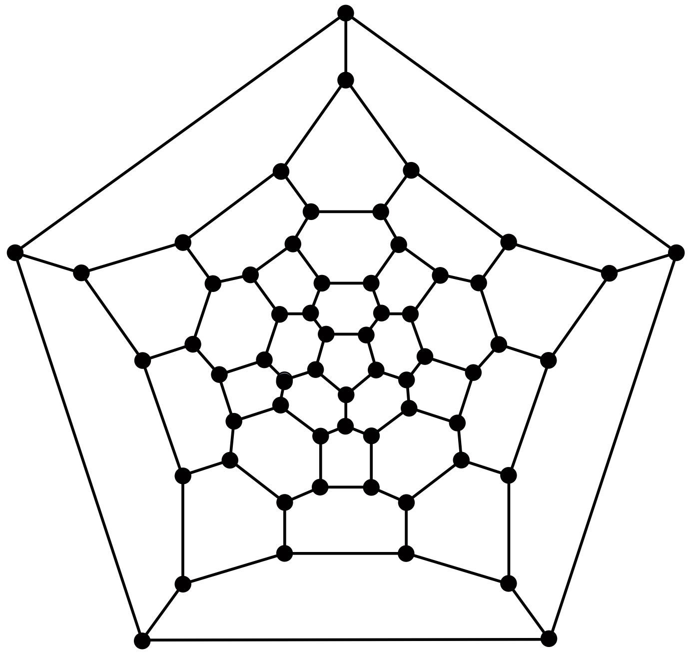

Figure 1. The IPR Fullerene C_{60}.

$(n/2-10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20. The goal of this paper is to compute some new results on the eigenvalues of fullerene graphs. We encourage the interested readers to consult paper [18]. For more information on this topic and more details about mathematics of fullerene graphs see Ref.s [1–11] as well as [16].

2 Definitions and preliminaries

Now we recall some algebraic definitions that will be used in this paper. Throughout this paper, our notation is standard and mainly taken from [12–15, 17, 21]. Let G be a simple molecular graph without directed and multiple edges and without loops. The vertex and edge-sets of G are represented by $V(G)$ and $E(G)$, respectively. The adjacency matrix $A(G)$ of graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that, $a_{ij} = 1$ if v_i and v_j are adjacent and 0 otherwise. The characteristic polynomial of graph G is defined as

$$\chi(G, \lambda) = det(A(G) - \lambda I).$$

The roots of this polynomial are eigenvalues of G and form the spectrum of graph as follows:

$$spec(G) = \{[\lambda_1]^{m_1}, \ldots, [\lambda_1]^{m_s}\},$$

where m_i is the multiplicity of eigenvalue λ_i. If G is a graph on n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of its adjacency matrix, then the energy [20] of G is defined as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

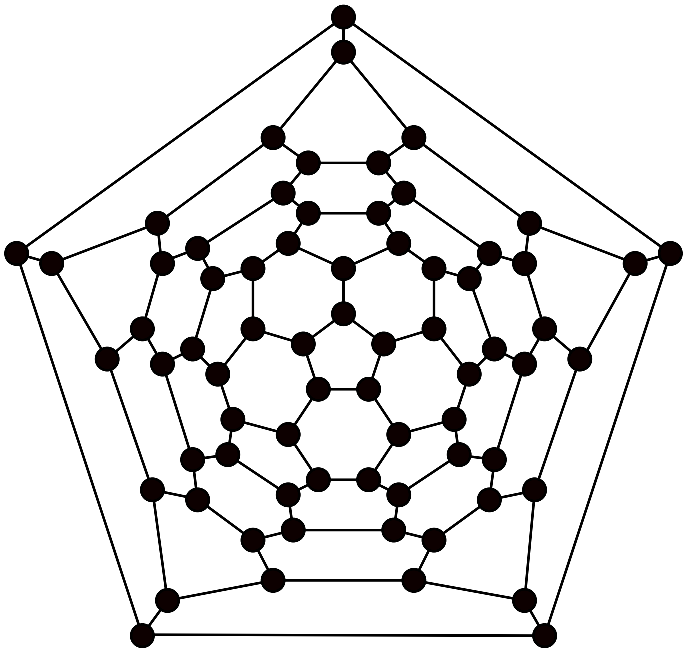

Figure 2. The IPR Fullerene C_{70}.

In theoretical chemistry, the energy is a graph parameter stemming from the Hückel molecular orbital approximation for the total π-electron energy. So, the graph energy has some specific chemical interests and has been extensively studied [19].

Example 2.1. Consider the fullerene C_{70} as depicted in Figure 2. This fullerene is one of the most famous member of the fullerenes, since in this graph all pentagons are isolated. In other words, this fullerene obeys in the Isolated Pentagon Rule (**IPR**). This class of fullerenes is the most stable and many of mathematician work on **IPR** fullerenes.

The eigenvalues of this fullerenes are reporeted in Table 1. Hence, one can see that the energy of this fullerene is

$$\mathcal{E}(C_{70}) = 109.$$

The aim of this paper is to propose a method for computing the energy of fullerene graphs by means of block matrices. Notice that according a result from the seminal paper of Gutman [20], the energy and graph energy for molecules with bipartite molecular graphs are the same, but fullerenes are not bipartite.

3 Main Results

A bijection σ on V with this property that $e = uv$ is an edge if and only if $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E, is called an automorphism of graph G. The set of all automorphisms of G under the composition of mappings forms a group denoted by $Aut(G)$.

A circulant matrix is a matrix where each row vector is rotated one element to the right relative to the preceding row vector. In other words, a circulant matrix [23] is specified by one vector c which appears as the first column of C. The remaining columns of C are each cyclic permutations of the vector c with offset equal to the column index. The last row of C is the vector c, in reverse order and the remaining rows are each cyclic permutations of the last row. In general, an $n \times n$ circulant matrix C takes the following form:

$$C = \begin{pmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \cdots & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & \ddots & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{pmatrix}.$$

The eigenvectors of a circulant matrix are given by

$$v_j = (1, \omega_j, \omega_j^2, \ldots, \omega_j^{n-1})^T, \ j = 0, 1, \ldots, n-1,$$

where, $\omega_k = e^{\frac{2k\pi}{n} i}$ are the n-th roots of unity and $i^2 = 1$. The corresponding eigenvalues are then given by

$$\lambda_j = c_0 + c_{n-1}\omega_j + \cdots + c_1 \omega_j^{n-1}, \ j = 0, \ldots, n-1.$$

Let A and B be matrices of dimensions $n \times m$ and $n' \times m'$, respectively. Then their tensor product is an $nn' \times mm'$ matrix with block forms

$$A \otimes B = [a_{ij} B].$$

Theorem 3.1. ([24]) *Let A_{ij}, $1 \le i, j \le l$ be square matrices of order n that have the complete set of eigenvectors $\{V_1, \ldots, V_n\}$ with $A_{ij} V_k = \alpha_{ij}^k$. Let also $B_k = [\alpha_{ij}^k]$, $1 \le k \le n$ be square matrices of order l, each with a complete set of eigenvectors $\{U_1^k, \ldots, U_l^k\}$ satisfying $B_k U_j^k = \beta_k U_j^k$ for $1 \le j \le l$. Then a complete set of eigenvectors $\{W_1, \ldots, W_{nl}\}$ for the square matrix*

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1l} \\ A_{21} & A_{22} & \cdots & A_{21} \\ \vdots & \vdots & \ddots & \vdots \\ A_{l1} & A_{l2} & \cdots & A_{ll} \end{pmatrix}$$

is given by $W_{(k-1)l+j} = U_j^k \otimes V_k$ for $k = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, l$. The corresponding eigenvalues are $\lambda_{(k-1)l+j} = \beta_j^k$.

We will apply this theorem to the case where all blocks in the adjacency matrix are ciculant matrices. An l - level circulant is one whose adjacency matrix has an $l \times l$ block form A, all A_{ij} being circulant. For example, a 2- level circulant,

$$G = C_n(\{n_i^1\}, \{n_i^2\}, \{m_i^{12}\}),$$

would consist of two vertex sets $S_1 = \{v_1, \ldots, v_n\}$ and $S_2 = \{w_1, \ldots, w_n\}$ such that

a) G induces circulants $C_n(\{n_i^1\})$ and $C_n(\{n_i^2\})$ on S_1 and S_2, respectively.

b) Edges between the two circulants are of the form $v_i w_k$, where $k = j + m_i^{12}\ (mod\ n)$, for some i.

The aim of this section is to compute some bounds for eigenvalues of fullerene graphs. It is a well-known fact that for a regular graph of valency r, all eigenvalues such as λ, belong to interval $[-r, r]$, see [17]. In this paper, by using Theorem 3.1, we compute the energy of fullerene C_{80}, as depicted in Figure 1. The symmetric group of this fullerene is isomorphic with icosahedral group I_h and with the following adjacency matrix:

$$\begin{pmatrix}
A(C_5) & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
I & 0 & I & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I & 0 & K^t & 0 & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I & K & 0 & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & I & 0 & 0 & I & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I & 0 & 0 & 0 & I & K^t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & I & I & 0 & 0 & L^t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & I & K & 0 & 0 & 0 & L^t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & L & 0 & 0 & 0 & I & K^t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & L & 0 & 0 & I & I & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & I & 0 & 0 & 0 & I & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K & I & 0 & 0 & I & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & K & I & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & K^t & 0 & I & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & I & 0 & I \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & A(C_5)
\end{pmatrix},$$

where $K = [[0,1,0,0,0]]$ and $L = [[0,0,1,0,0]]$. For computing the eigenvalues of C_{80}, we use Theorem 3.1. First, we compute the eigenvalues of K, K^t, L and $A(C_5)$. Suppose $\alpha = 0.31 + 0.9i$, $\overline{\alpha} = 0.31 - 0.9i$ $\beta = -0.81 + 0.59i$, $\overline{\beta} = -081 - 59i$, then $x = 0.62$, $y = -1.62$. On the other hand, let

$$B_1 = \begin{pmatrix}
2&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
1&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0 \\
0&1&0&1&0&1&0&0&0&0&0&0&0&0&0&0 \\
0&1&1&0&1&0&0&0&0&0&0&0&0&0&0&0 \\
0&0&0&1&0&0&1&1&0&0&0&0&0&0&0&0 \\
0&0&1&0&0&0&1&1&0&0&0&0&0&0&0&0 \\
0&0&0&0&1&1&0&0&1&0&0&0&0&0&0&0 \\
0&0&0&0&1&1&0&0&0&1&0&0&0&0&0&0 \\
0&0&0&0&0&0&1&0&0&0&1&1&0&0&0&0 \\
0&0&0&0&0&0&0&1&0&0&1&1&0&0&0&0 \\
0&0&0&0&0&0&0&0&1&1&0&0&0&1&0&0 \\
0&0&0&0&0&0&0&0&1&1&0&0&1&0&0&0 \\
0&0&0&0&0&0&0&0&0&0&0&1&0&1&1&0 \\
0&0&0&0&0&0&0&0&0&0&1&0&1&0&1&0 \\
0&0&0&0&0&0&0&0&0&0&0&0&1&1&0&1 \\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&2
\end{pmatrix}.$$

Then the eigenvalues of B_1 are as reported in Table 1.

m	Eigen	m	Eigen
1	3	1	2.08
1	2.47	1	-2.69
1	-1.93	2	1
1	1.46	2	-1
1	2.82	2	.62
1	-1.2	2	-1.6

Table 1. The eigenvalues of B_1.

Let also

$$B_2 = \begin{pmatrix}
x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \overline{\alpha} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & \alpha & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \overline{\beta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & \alpha & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 1 & \overline{\alpha} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\alpha} & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x
\end{pmatrix}.$$

Then the eigenvalues of B_2 are as reported in Table 2. For matrix

m	Eigen	m	Eigen	m	Eigen
1	-2.7	1	2.47	1	1.46
1	-2.65	1	0.2739	1	0.62
1	-2.2	1	2.08	2	-1.62
1	-1.93	1	1.91		
1	-0.71	1	1		
1	-1	1	1.38		

Table 2. The eigenvalues of B_2.

$$B_3 = \begin{pmatrix}
y & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \overline{\beta} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & \beta & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & \overline{\beta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & \beta & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 1 & \overline{\beta} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \beta & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\beta} & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & y
\end{pmatrix},$$

then the eigenvalues of B_3 are as reported in Table 3.

m	Eigen	m	Eigen	m	Eigen
1	-2.7	1	2.47	1	1.46
1	-2.65	1	0.2739	1	0.62
1	-2.2	1	2.08	2	-1.62
1	-1.93	1	1.91		
1	-0.71	1	1		
1	-1	1	1.38		

Table 3. The eigenvalues of B_3.

For matrix

$$B_4 = \begin{pmatrix}
y & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \beta & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & \overline{\beta} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & \overline{\beta} & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 1 & \beta & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\beta} & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \beta & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & y
\end{pmatrix},$$

the eigenvalue are reported in Table 4.

m	Eigen	m	Eigen	m	Eigen
1	-2.7	1	2.47	1	1.46
1	-2.65	1	0.2739	1	0.62
1	-2.2	1	2.08	2	-1.62
1	-1.93	1	1.91		
1	-0.71	1	1		
1	-1	1	1.38		

Table 4. The eigenvalues of B_4.

Finally, consider the matrix

$$B_5 = \begin{pmatrix} x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \alpha & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \overline{\alpha} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \overline{\alpha} & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 0 & 0 & 0 & 1 & \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\alpha} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x \end{pmatrix}.$$

The spectrum of B_5 is as follows:

$$Spec(B_5) = \{[-2.65],[2.82],[2.47],[-2.20],[-1.93],[-1.20],[-1],$$

$$[-0.71],[1.91],[0.27],[1.46],[1.37],[1],[-1.62],[0.62]^2\}.$$

Hence, by using Theorem 3.1, the eigenvalues of C_{80} are as reported in Table 5.

This yields that the energy of this fullerene graph is

$$\mathcal{E}(C_{80}) = 125.1.$$

Concluding Remarks The energy of a fullerene is not the summation of the absolute values of the eigenvalues but twice the summation of the first $n/2$ eigenvalues in non-increasing order. Computing the energy of fullerene graphs is very difficult problem and there are many papers concerning with estimating the eigenvalues of fullerene graphs. In this paper, by using Sagan methods for determining the eigenvalues of cyclic matrix, we computed the energy of IPR fullerene C_{80}. The same approach we used here could be applied to other

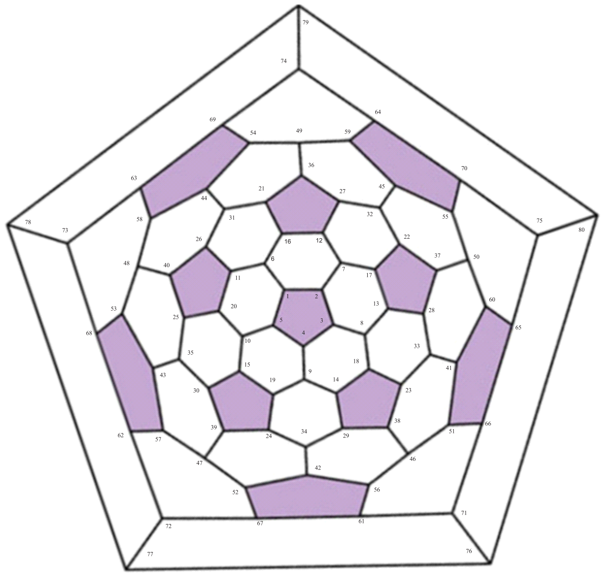

Figure 3. Fullerene graph C_{80} with symmetric group I_h.

m	Eigen	m	Eigen	m	Eigen
3	-1.2	4	1.38	1	3
8	-1.62	6	1	3	2.82
5	-1.93	8	0.62	5	2.47
4	-2.2	4	0.27	3	2.08
4	-2.65	4	-0.71	4	1.91
3	-2.7	6	-1	5	1.46

Table 5. Eigenvalues of icosahedral fullerene C_{80}.

fullerene graphs. Estimating the energy of fullerene graphs were also computed in some earlier papers such as [12].

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