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Study of fullerenes by their Algebraic Properties

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ABSTRACT

The eigenvalues of a graph is the root of its characteristic polynomial. A fullerene F is a 3-connected graphs with entirely 12 pentagonal faces and $n/2$ -10 hexagonal faces, where n is the number of vertices of F. In this paper we investigate the eigenvalues of a class of fullerene graphs.

Keywords: Molecular graph, Adjacency matrix, Eigenvalue, Fullerene.

1. INTRODUCTION

All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. Let $G = (V, E)$ be a simple graph and $W \subseteq V$. Then the induced subgraph by W is the subgraph of G obtained by taking the vertices in W and joining those pairs of vertices in W which are joined in G. Denoted by $G - \{v_1, \ldots, v_k\}$ means a graph obtained by removing the vertices $v_1, \ldots, v_k$ from G and all edges incident to any of them.

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 $\Phi(G,x)$ of graph G was defined as

$$\Phi(G,x) = \det(A(G) - xI).$$

The roots of the characteristic polynomial are named the eigenvalues of graph G and form the spectrum of this graph. If α be an eigenvalue of matrix A, then there exist a vector such as V, in which $A.V = \alpha V$.

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Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $A(G)$, then the energy of G, denoted by $E(G)$, is defined [1, 2] as

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

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 [3].

The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his co-authors [4]. The well-known fullerene, the C_{60} molecule, 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, [5]. 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 and having 12 pentagonal and $(n/2 - 10)$ 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 of fullerene graphs.

2. MAIN RESULTS

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 [6] 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:

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

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

$$\lambda_j = c_0 + c_{n-1}\omega_j + c_{n-2}\omega_j^2 + \cdots + c_1\omega_j^{n-1},\ j = 0 \cdots n-1.$$

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

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

Theorem 1 ([7]). 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 $\left\{U_1^k, \ldots, U_l^k\right\}$ satisfying $B_k U_j^k = \beta_j^k U_j^k$ for $1 \le j \le$ l. Then a complete set of eigenvectors $\{W_1, W_2, \ldots, W_{nl}\}$ for the square matrix

$$A = \begin{bmatrix} A_{11} & A_{12} & \ldots & A_{1l} \\ A_{21} & A_{22} & \ldots & A_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ A_{l1} & A_{l2} & \ldots & A_{ll} \end{bmatrix}$$

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 $\lambda_{\text{(k-1)l+j}} = \beta_j^k$.

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

$$k = j + m_i^{12} (\operatorname{mod} n),$$

for some i.

In this paper by using Theorem 1, we compute the energy of some fullerenes. Consider an infinite class of fullerene with $10n$ vertices, as depicted in Figure 1.

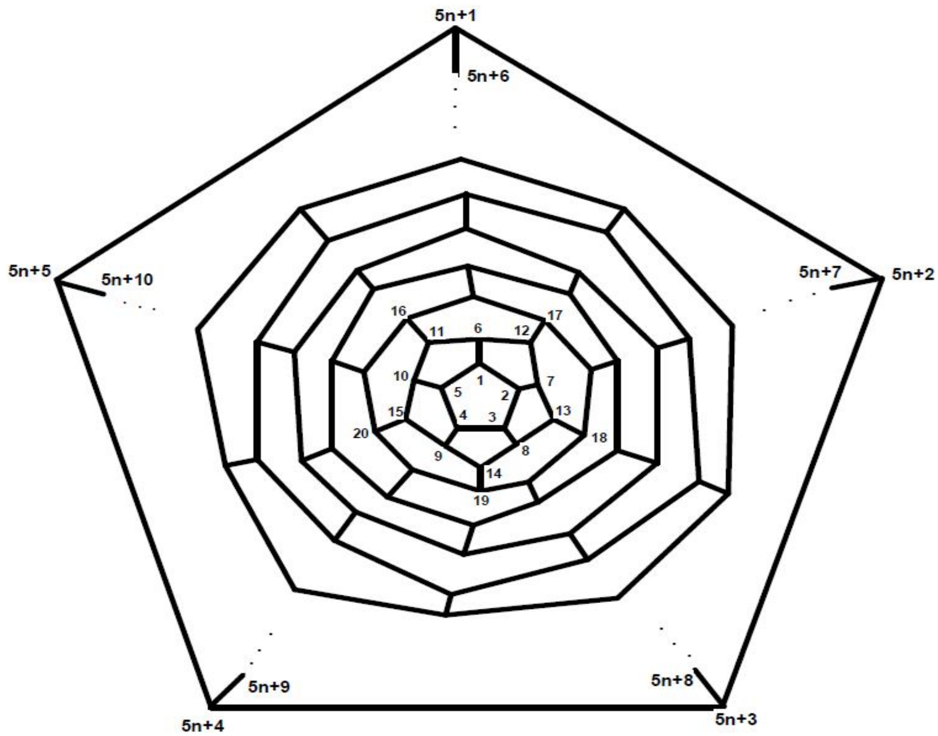

Figure 1. The Schlegel Diagram of C_{10n}.

The first member of this class of fullerenes is C_{20} and the second member of these class has exactly 30 vertices see Figure 2. In [7], Lee and his co – authors computed its eigenvalues. Here we compute the eigenvalues of this class of fullerenes for n = 3, 6 and in continuing we introduce the general form of its adjacency matrix by means of block matrix. Let $\alpha = 1.309 - 0.9511i$, $\overline{\alpha} = 1.309 + 0.9511i$, $\beta = 0.191 - 0.5878i$, $\overline{\beta} = 0.191 + 0.5878i$, $x = 0.618$ $x = 0.618$ and $y = -1.618$. According to Lee et al. Theorem, one can see that the block form of adjacency matrix of C_{30} is as follows:

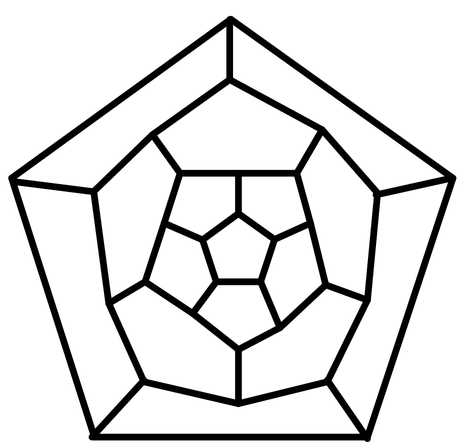

Figure 2. The Schlegel diagram of C_{30}.

$$A(C_{30}) = \begin{bmatrix} A(C_5) & I & 0 & 0 & 0 & 0 \\ I & 0 & M^t & 0 & 0 & 0 \\ 0 & M & 0 & 0 & 0 & I \\ 0 & 0 & 0 & A(C_5) & I & 0 \\ 0 & 0 & 0 & I & 0 & M^t \\ 0 & 0 & I & 0 & M & 0 \end{bmatrix}$$

So the matrices B_i, i = 1, 2, 3, 4 in Theorem 1 are as follows:

$$B_1 = \begin{bmatrix} x & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & \bar{\alpha} & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & x & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & \bar{\alpha} \\ 0 & 0 & 1 & 0 & \alpha & 0 \end{bmatrix}, B_2 = \begin{bmatrix} y & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & \bar{\beta} & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & y & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & \bar{\beta} \\ 0 & 0 & 1 & 0 & \beta & 0 \end{bmatrix}, B_3 = \begin{bmatrix} y & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & \beta & 0 & 0 & 0 \\ 0 & \bar{\beta} & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & y & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & \beta \\ 0 & 0 & 1 & 0 & \bar{\beta} & 0 \end{bmatrix},$$

$$B_4 = \begin{bmatrix} x & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha & 0 & 0 & 0 \\ 0 & \bar{\alpha} & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & x & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & \alpha \\ 0 & 0 & 1 & 0 & \bar{\alpha} & 0 \end{bmatrix}, B_5 = \begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 0 & 2 & 0 \end{bmatrix}.$$

The eigenvalues of B_1 are $-2.3214, -1.5118, 0.1487, 0.7180, 1.7908$ and 2.1418, repectively. These values for B_2 are $-2.1631, -2.1189, -1.1218, 0.1316, 0.6668$ and 1.3693, 1.3693, respectively. The eigenvalues of B_3 are $-2.1631, -2.1189, -1.1218, 0.1316, 0.6668$ and, respectively. These values for B_4 are $-2.3214, -1.5118, 0.1487, 0.7180, 1.7908$ and 2.1418, respectively. Finally one can see that the eigenvalues of B_5 are $-2.6458, -1.7321, 1, 1.7321, 2.6458$ and 3, , respectively. By using Theorem 1, the spectrum of C_{30} is as follows:

Eigenvalues	**Multiplicity**	**Eigenvalues**	**Multiplicity**
0.6668	2	-2.6458	1
0.7180	2	-2.3214	2
1	1	-2.1631	2
1.3693	2	-2.1189	2
1.7321	1	-1.7321	1
1.7908	2	-1.5118	2
2.4118	2	-1.1218	2
2.6458	1	0.1316	2
3	1	0.1478	2

This implies the energy of this graph is 45.7038. Consider now the fullerene graph C_{60}, depicted in figure 3. The block form of its adjacency matrix is as follows:

$$A(C_{60}) = \begin{bmatrix} W & V^t \\ V & W \end{bmatrix}, \text{ where}$$

$$W = \begin{bmatrix} A(C_5) & I & 0 & 0 & 0 & 0 \\ I & 0 & M^t & 0 & 0 & 0 \\ 0 & M & 0 & I & 0 & 0 \\ 0 & 0 & I & 0 & M^t & 0 \\ 0 & 0 & 0 & M & 0 & I \\ 0 & 0 & 0 & 0 & I & 0 \end{bmatrix} \text{ and } V = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & M \end{bmatrix}.$$

So, B_1, …, B_5 and their eigenvalues are as follows:

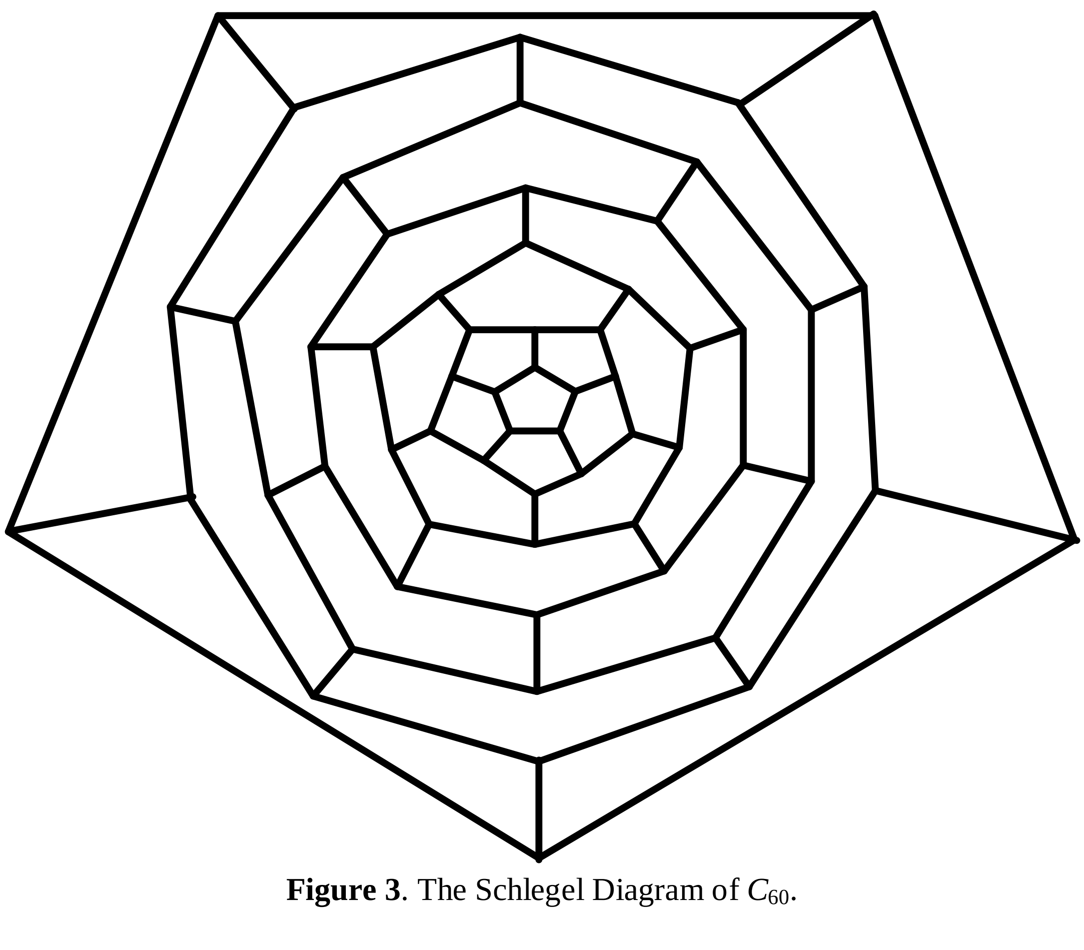

Figure 3. The Schlegel Diagram of C_{60}.

$$B_1 = \begin{bmatrix} x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} \\ 0 & 0 & 0 & 0 & 0 & 0 & x & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\alpha} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad Eigenvalues(B_1) = \begin{cases} -2.5384 \\ -2.3055 \\ -1.9369 \\ -1.4637 \\ -0.9453 \\ 0.3 \\ 0.4425 \\ 1.1082 \\ 1.6180 \\ 2.0439 \\ 2.3600 \\ 2.5532 \end{cases}$$

$$B_2 = \begin{bmatrix} y & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \overline{\beta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \overline{\beta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} \\ 0 & 0 & 0 & 0 & 0 & 0 & y & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\beta} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \overline{\beta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad Eigenvalues\ of\ B2 = \begin{Bmatrix} -2.1427 \\ -2.1424 \\ -1.5330 \\ -1.3055 \\ -0.9828 \\ -0.6180 \\ 0.2410 \\ 0.3763 \\ 0.7879 \\ 1.1287 \\ 1.3935 \\ 1.5609 \end{Bmatrix}$$

$$B_3 = \begin{bmatrix} y & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \overline{\beta} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{\beta} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \beta \\ 0 & 0 & 0 & 0 & 0 & 0 & y & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \beta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \overline{\beta} & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \mathit{Eigenvalues\ of\ B3} = \left\{ \begin{matrix} -2.1427 \\ -2.1424 \\ -1.5330 \\ -1.3055 \\ -0.9828 \\ -0.6180 \\ 0.2410 \\ 0.3763 \\ 0.7879 \\ 1.1287 \\ 1.3935 \\ 1.5609 \end{matrix} \right\}$$

$$B_4 = \begin{bmatrix} x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \overline{\alpha} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{\alpha} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 & 0 & 0 & x & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \overline{\alpha} & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \mathit{Eigenvalues\ of\ B4} = \left\{ \begin{matrix} -2.5384 \\ -2.3055 \\ -1.9369 \\ -1.4637 \\ -0.9453 \\ 0.3 \\ 0.4425 \\ 1.1082 \\ 1.6180 \\ 2.0439 \\ 2.3600 \\ 2.5532 \end{matrix} \right\}$$

$$B_5 = \begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \ Eigenvalues\ of\ B5 = \begin{Bmatrix} -2.9093 \\ -2.6458 \\ -2.2361 \\ -1.7321 \\ -1.2393 \\ 1 \\ 1.2393 \\ 1.7321 \\ 2.2361 \\ 2.6458 \\ 2.9093 \\ 3 \end{Bmatrix}.$$

So its spectrum is as follows:

Eigenvalues	**Multiplicity**	**Eigenvalues**	**Multiplicity**
1.2393	1	-1.2393	1
1.3935	2	-0.9828	2
1.5609	2	-0.9453	2
1.6180	2	-0.6180	2
1.7321	1	0.2410	2
2.0439	2	0.3	2
0.3763	2	-2.1424	2
0.4425	2	-1.9369	2
0.7879	2	-1.7321	1
1	1	-1.5330	2
1.1082	2	-1.4637	2
1.1287	2	-1.3055	2
-2.9093	1	2.2361	1
-2.6458	1	2.3600	2
-2.5384	2	2.5532	2
-2.3055	2	2.6458	1
-2.2361	1	2.9093	1
-2.1427	2	3	1

So, its energy is 93.1814. In general, one can see that the adjacency matrix of this class of fullerenes is as follows:

i) n is odd

$$\begin{bmatrix}
A(C_5) & I & & & & & & & & & & & & \\
I & 0 & Mt & & & & & & & & & & & \\
 & M & 0 & I & & & & & & & & & & \\
 & & I & 0 & Mt & & & & & & & & & \\
 & & & M & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & Mt & & & & & & & \\
 & & & & & M & 0 & & & & & & & I \\
 & & & & & & & A(C_5) & I & & & & & \\
 & & & & & & & I & 0 & Mt & & & & \\
 & & & & & & & & M & 0 & I & & & \\
 & & & & & & & & & I & 0 & Mt & & \\
 & & & & & & & & & & M & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & Mt \\
 & & & & & & I & & & & & & M & 0
\end{bmatrix},$$

ii) n is even

$$\begin{bmatrix}
A(C_5) & I & & & & & & & & & & & & \\
I & 0 & M^t & & & & & & & & & & & \\
 & M & 0 & I & & & & & & & & & & \\
 & & I & 0 & M^t & & & & & & & & & \\
 & & & M & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & I & & & & & & & \\
 & & & & & I & 0 & & & & & & & M^t \\
 & & & & & & & A(C_5) & I & & & & & \\
 & & & & & & & I & 0 & M^t & & & & \\
 & & & & & & & & M & 0 & I & & & \\
 & & & & & & & & & I & 0 & M^t & & \\
 & & & & & & & & & & M & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & I \\
 & & & & & & M & & & & & & I & 0
\end{bmatrix}.$$

and then according to Theorem 1 the block matrices $B_1, B_2, \ldots, B_5$ are $2n \times 2n$ as follows:

i) n is odd

$$
B_1 = \begin{bmatrix}
x & 1 & & & & & & & & & & & & \\
1 & 0 & \bar{\alpha} & & & & & & & & & & & \\
 & \alpha & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \bar{\alpha} & & & & & & & & & \\
 & & & \alpha & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & \bar{\alpha} & & & & & & & \\
 & & & & & \alpha & 0 & & & & & & & 1 \\
 & & & & & & & x & 1 & & & & & \\
 & & & & & & & 1 & 0 & \bar{\alpha} & & & & \\
 & & & & & & & & \alpha & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \bar{\alpha} & & \\
 & & & & & & & & & & \alpha & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & \bar{\alpha} \\
 & & & & & & 1 & & & & & & \alpha & 0
\end{bmatrix},
$$

$$
B_2 = \begin{bmatrix}
y & 1 & & & & & & & & & & & & \\
1 & 0 & \bar{\beta} & & & & & & & & & & & \\
 & \beta & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \bar{\beta} & & & & & & & & & \\
 & & & \beta & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & \bar{\beta} & & & & & & & \\
 & & & & & \beta & 0 & & & & & & & 1 \\
 & & & & & & & y & 1 & & & & & \\
 & & & & & & & 1 & 0 & \bar{\beta} & & & & \\
 & & & & & & & & \beta & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \bar{\beta} & & \\
 & & & & & & & & & & \beta & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & \bar{\beta} \\
 & & & & & & 1 & & & & & & \beta & 0
\end{bmatrix},
$$

$$B_3 = \begin{bmatrix}
y & 1 & & & & & & & & & & & & \\
1 & 0 & \beta & & & & & & & & & & & \\
 & \bar{\beta} & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \beta & & & & & & & & & \\
 & & & \bar{\beta} & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & \beta & & & & & & & \\
 & & & & & \bar{\beta} & 0 & & & & & & & 1 \\
 & & & & & & & y & 1 & & & & & \\
 & & & & & & & 1 & 0 & \beta & & & & \\
 & & & & & & & & \bar{\beta} & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \beta & & \\
 & & & & & & & & & & \bar{\beta} & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & \beta \\
 & & & & & & 1 & & & & & & \bar{\beta} & 0
\end{bmatrix},$$

$$B_4 = \begin{bmatrix}
x & 1 & & & & & & & & & & & & \\
1 & 0 & \alpha & & & & & & & & & & & \\
 & \bar{\alpha} & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \alpha & & & & & & & & & \\
 & & & \bar{\alpha} & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & \alpha & & & & & & & \\
 & & & & & \bar{\alpha} & 0 & & & & & & & 1 \\
 & & & & & & & x & 1 & & & & & \\
 & & & & & & & 1 & 0 & \alpha & & & & \\
 & & & & & & & & \bar{\alpha} & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \alpha & & \\
 & & & & & & & & & & \bar{\alpha} & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & \alpha \\
 & & & & & & 1 & & & & & & \bar{\alpha} & 0
\end{bmatrix},$$

$$B_5 = \begin{bmatrix}
2 & 1 & & & & & & & & & & & & \\
1 & 0 & 2 & & & & & & & & & & & \\
 & 2 & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & 2 & & & & & & & & & \\
 & & & 2 & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & 2 & & & & & & & \\
 & & & & & 2 & 0 & & & & & & & 1 \\
 & & & & & & & 2 & 1 & & & & & \\
 & & & & & & & 1 & 0 & 2 & & & & \\
 & & & & & & & & 2 & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & 2 & & \\
 & & & & & & & & & & 2 & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & 2 \\
 & & & & & & 1 & & & & & & 2 & 0
\end{bmatrix}.$$

ii) n is even

$$B_1 = \begin{bmatrix}
x & 1 & & & & & & & & & & & & \\
1 & 0 & \bar{\alpha} & & & & & & & & & & & \\
 & \alpha & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \bar{\alpha} & & & & & & & & & \\
 & & & \alpha & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & 1 & & & & & & & \\
 & & & & & 1 & 0 & & & & & & & \bar{\alpha} \\
 & & & & & & & x & 1 & & & & & \\
 & & & & & & & 1 & 0 & \bar{\alpha} & & & & \\
 & & & & & & & & \alpha & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \bar{\alpha} & & \\
 & & & & & & & & & & \alpha & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & 1 \\
 & & & & & & \alpha & & & & & & 1 & 0
\end{bmatrix},$$

$$B_2 = \begin{bmatrix}
y & 1 & & & & & & & & & & & & \\
1 & 0 & \bar{\beta} & & & & & & & & & & & \\
 & \beta & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \bar{\beta} & & & & & & & & & \\
 & & & \beta & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & 1 & & & & & & & \\
 & & & & & 1 & 0 & & & & & & & \bar{\beta} \\
 & & & & & & & y & 1 & & & & & \\
 & & & & & & & 1 & 0 & \bar{\beta} & & & & \\
 & & & & & & & & \beta & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \bar{\beta} & & \\
 & & & & & & & & & & \beta & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & 1 \\
 & & & & & & \beta & & & & & & 1 & 0
\end{bmatrix},$$

$$B_3 = \begin{bmatrix}
y & 1 & & & & & & & & & & & & \\
1 & 0 & \beta & & & & & & & & & & & \\
 & \bar{\beta} & 0 & 1 & & & & & & & & & & \\
 & & 1 & 0 & \beta & & & & & & & & & \\
 & & & \bar{\beta} & 0 & \ddots & & & & & & & & \\
 & & & & \ddots & \ddots & 1 & & & & & & & \\
 & & & & & 1 & 0 & & & & & & & \beta \\
 & & & & & & & y & 1 & & & & & \\
 & & & & & & & 1 & 0 & \beta & & & & \\
 & & & & & & & & \bar{\beta} & 0 & 1 & & & \\
 & & & & & & & & & 1 & 0 & \beta & & \\
 & & & & & & & & & & \bar{\beta} & 0 & \ddots & \\
 & & & & & & & & & & & \ddots & \ddots & 1 \\
 & & & & & & \bar{\beta} & & & & & & 1 & 0
\end{bmatrix},$$

$$B_4 = \begin{bmatrix} x & 1 & & & & & & & & & & & & \\ 1 & 0 & \alpha & & & & & & & & & & & \\ & \bar{\alpha} & 0 & 1 & & & & & & & & & & \\ & & 1 & 0 & \alpha & & & & & & & & & \\ & & & \bar{\alpha} & 0 & \ddots & & & & & & & & \\ & & & & \ddots & \ddots & 1 & & & & & & & \\ & & & & & 1 & 0 & & & & & & & \alpha \\ & & & & & & & x & 1 & & & & & \\ & & & & & & & 1 & 0 & \alpha & & & & \\ & & & & & & & & \bar{\alpha} & 0 & 1 & & & \\ & & & & & & & & & 1 & 0 & \alpha & & \\ & & & & & & & & & & \bar{\alpha} & 0 & \ddots & \\ & & & & & & & & & & & \ddots & \ddots & 1 \\ & & & & & & \bar{\alpha} & & & & & & 1 & 0 \end{bmatrix},$$

$$B_5 = \begin{bmatrix} 2 & 1 & & & & & & & & & & & & \\ 1 & 0 & 2 & & & & & & & & & & & \\ & 2 & 0 & 1 & & & & & & & & & & \\ & & 1 & 0 & 2 & & & & & & & & & \\ & & & 2 & 0 & \ddots & & & & & & & & \\ & & & & \ddots & \ddots & 1 & & & & & & & \\ & & & & & 1 & 0 & & & & & & & 2 \\ & & & & & & & 2 & 1 & & & & & \\ & & & & & & & 1 & 0 & 2 & & & & \\ & & & & & & & & 2 & 0 & 1 & & & \\ & & & & & & & & & 1 & 0 & 2 & & \\ & & & & & & & & & & 2 & 0 & \ddots & \\ & & & & & & & & & & & \ddots & \ddots & 1 \\ & & & & & & 2 & & & & & & 1 & 0 \end{bmatrix}.$$

B_3

Since B_1, B_4 and B_2, B_3 are conjugated matrix, then Spec(B_1) = Spec(B_4) and Spec(B_2) = Spec(B_3). So, the energy of this class of fullerene can be obtained by the following:

$$E(C_{10n}) = 2E(B_1) + 2E(B_2) + E(B_5).$$

3. CONCLUSIONS

In this paper an efficient method is presented which is useful for computing energy of fullerenes. We applied our method on C_{30} and C_{60} fullerenes. It remains as an open problem what is the energy of C_{10n} fullerenes in general case. We proposed a block matrix of order $2n \times 2n$ for adjacency matrix of C_{10n}. By this matrix we offer five matrices $B_1, \ldots, B_5$ which they are the main blocks of adjacency matrix. So, to obtain eigenvalues of adjacency matrix of this fullerene it is enough to obtain the eigenvalues of B_i, i =1, 2, 3, 4, 5. Then by using Lee Theorem we can obtain the eigenvalues of $A(C_{10n})$ and then the energy of this class of fullerenes.

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