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Research Paper

Spectral properties of fullerene graphs

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Abstract. Fullerenes are polyhedral molecules made of carbon atoms. These graphs have attracted much attention in the chemical and the mathematical literature. In the present paper, we investigate problems concerned with the eigenvalues of fullerene graphs. We obtain new upper bounds for the smallest eigenvalues of fullerenes using bipartite edge-frustration of their related subgraphs.

Keywords: fullerene, eigenvalue, cyclic-k-edge cutset, quotient graph, bipartite edge frustration
Mathematics Subject Classification (2010): Primary 05C90; Secondary 92E10.

1 Introduction

A fullerene is a three connected cubic graph with pentagonal and hexagonal faces satisfying in Euler's formula. The first and the most stable fullerene, namely C_{60}, was discovered by Kroto et al. in 1985 [39, 40]. Euler's theorem says that a fullerene with n vertices has exactly 12 pentagons and $n/2 - 10$ hexagons, where n is a natural number equal or greater than 20 and $n \neq 22$. For more details about mathematical details of fullerene graphs, see references [3, 5, 15, 20, 28–30, 36, 43].

Here, we recall some algebraic definitions that will be used in this paper. Throughout this paper, our notation is standard and mainly taken from [6, 14, 31, 35]. Let G be a simple molecular graph, namely a 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

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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 $\chi(G, \lambda)$ of graph G is defined as

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

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

$$Spec(G) = \{[\lambda_1]^{m_1}, [\lambda_2]^{m_2}, \ldots, [\lambda_r]^{m_r}\},$$

where m_i is the multiplicity of eigenvalue λ_i and $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_r$.

The energy of G is a graph invariant introduced by Gutman [32] as $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$, where λ_i's are all eigenvalues of G, see also [33].

2 Main Results

In this section, we introduce several kinds of infinite families of fullerene graphs and then we investigate some properties of eigenvalues of fullerenes with a trivial cyclic 5-cutset. Here, by applying the interlacing theorem, we find a new bound for the energy of fullerene graphs.

Theorem 2.1. *[6] Let G be a graph with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$ and H be an induced subgraph of G with eigenvalues $\theta_1 \geq \ldots \geq \theta_m$. Then for $i = 1, 2, \ldots, m$, we yield that*

$$\lambda_i \geq \theta_i \geq \lambda_{n-m+i}.$$

Theorem 2.2. *Let H be an induced subgraph of fullerene F with eigenvalues $\theta_1, \ldots, \theta_m$, the eigenvalues of F be $\lambda_1, \ldots, \lambda_n$. Then*

$$\mathcal{E}(F) \geq (3 - \theta_1) + \frac{1}{2}\mathcal{E}(H) + (m - r)|\theta_{r+1}| + (n - m)\lambda_{n-m+r},$$

where r is the number of positive eigenvalues of H and $m = |V(H)|$.

Proof. By using the interlacing theorem, for $1 \leq i \leq m$, we obtain that $\theta_i \leq \lambda_i$. This yields that

$$\begin{aligned}\mathcal{E}(F) &= \sum_{i=1}^{n} |\lambda_i| = 3 + \sum_{i=2}^{r} \lambda_i + \sum_{i=r+1}^{n} |\lambda_i| \geq 3 + \sum_{i=2}^{r} \theta_i + \sum_{i=r+1}^{n} |\lambda_i| \\ &= (3 - \theta_1) + \frac{1}{2}\mathcal{E}(H) + \sum_{i=r+1}^{n} |\lambda_i|.\end{aligned}$$

Again, interlacing theorem implies that $\lambda_{n-m+r+1} \leq \theta_{r+1}$. Consequently,

$$\sum_{i=n-m+r+1}^{n} |\lambda_i| \geq (m - r)|\lambda_{n-m+r+1}| \geq (m - r)|\theta_{r+1}|.$$

Since, $\sum_{i=r+1}^{n-m+r} |\lambda_i| \geq (n - m)\lambda_{n-m+r}$, the assertion follows. □

An equitable partition of a graph G is a partition of the vertex set $V(G)$ into parts $C_1,...,C_s$ such that the number of neighbors lying in C_j of a vertex u in C_i is a constant b_{ij}, independent of u. The orbits of a group action form an equitable partition, but not all equitable partitions come from groups. For example, consider the graph G as depicted in Figure 1. One can easily see that $\{\{1,2,4,5,7,8\},\{3,6\}\}$ is an equitable partition, but clearly it is not the set of orbits under the group action. Equitable partitions give rise to a quotient graph G/π, which is a graph with s cells of π as its vertices and b_{ij} arcs from the ith to the jth cells, see Figure 1. Hence, the entries of the adjacency matrix of the quotient graph G/π are given by $A(G/\pi) = (b_{ij})$.

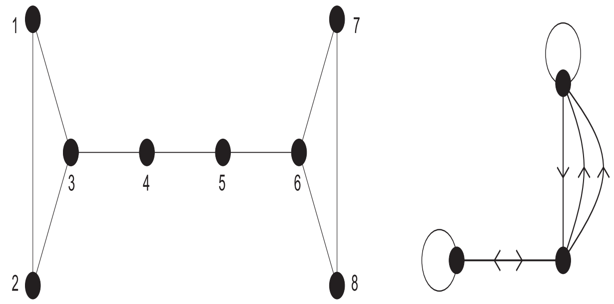


Figure 1. The right graph is the quotient graph of the left graph with an equitable partition $\{\{1,2,7,8\},\{3,6\},\{4,5\}\}$.

Lemma 2.3. *[50] If π is an equitable partition of graph G, then the characteristic polynomial of $A(G/\pi)$ divides the characteristic polynomial of $A(G)$.*

A Jacobi three-matrix is a three-diagonal matrix of order n of the following form

$$\tilde{C} = \begin{pmatrix} a_1 & b_2 & & & \\ c_2 & a_2 & b_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b_n \\ & & & c_n & a_n \end{pmatrix},$$

where $b_i c_i > 0$ for $2 \le i \le n$. Let $P_j, j = 1,2,\cdots,2r$ be the jth order sequential principal submatrix formed by the first j rows and columns of the matrix $\tilde{C} - \lambda I$ and let $P_j(\lambda) = \det(P_j)$. Let $P_0(\lambda) \equiv 1$. It is easy to get that

$$\begin{cases} P_1(\lambda) = a_1 - \lambda, \\ P_i(\lambda) = (a_i - \lambda) P_{i-1}(\lambda) - b_i c_i P_{i-2}(\lambda), \quad i = 2,\cdots,n. \end{cases} \tag{1}$$

Moreover, suppose $\alpha_n(\lambda)$ is the number of pairs, such that two polynomials $P_i(\lambda)$ and $P_{i+1}(\lambda)$ have the same sign for a real number λ, where $i = 0,1,\cdots,n-1$. In [50] it is shown that if $P_i(\lambda) = 0$, then $P_{i-1}(\lambda) \neq 0$.

A set of k edges whose elimination disconnects a graph into two components, each containing a cycle, is called a cyclic-k-edge cutset, and it is called a trivial cyclic-k-cutset if at least one of the resulting two components has a single k-cycle, see [41].

The last author, in a series of papers [1–4, 16–19, 23, 25–27, 37], introduced several infinite classes of fullerenes in order to characterize the fullerene graphs with respect to their symmetry groups. Although, the problem is still as an open problem, but it is a well-known fact that there are only 28 finite groups that arise as symmetry group of a fullerene graph, see [14].

On the other hand, one of the most important problem in the spectral chemical graph theory is to determinate the spectrum of a molecular graph or specially the spectra of fullerene graphs. In [11] the problem is solved for non-classical fullerenes, namely fullerenes with triangles and hexagones. For fullerenes with pentagons and hexagons, the problem is still unsolved, and there are many results concerning fullerene eigenvalues, see [12, 13, 24, 50, 51]. In [50] some eigenvalues of fullerene C_n, where $10 \mid n$, is determined in terms of eigenvalues of related quotient matrix.

Carbon nanotubes are members of the fullerene family. A carbon nanotube ($T_z[m,n]$) consists of a sheet with m rows and n columns of hexagons. Nanotubes can be pictured as sheets of graphite rolled up into a tube as shown in Figure 2. Combining a nanotube $T_z[6,n]$ with two copies of A (Figure 3.) yields the fullerene graph F_{12r}, see Figure 4.

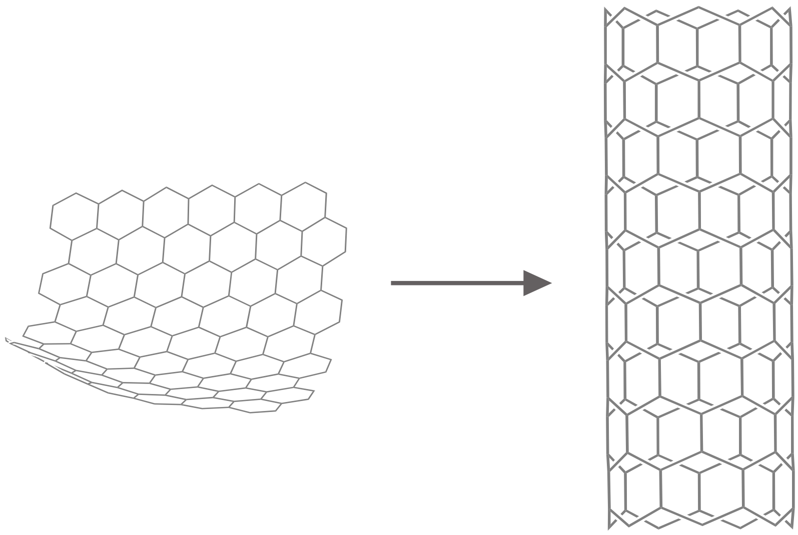


Figure 2. A zig-zag hexagonal sheet and a nanotube structures, in general.

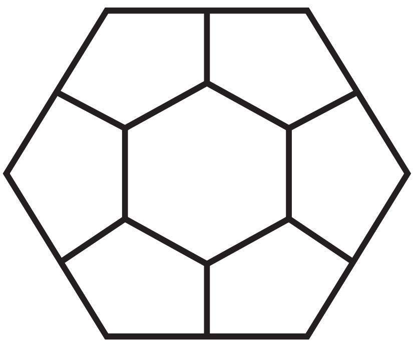


Figure 3. The cap A as a subgraph of F_{12r}.

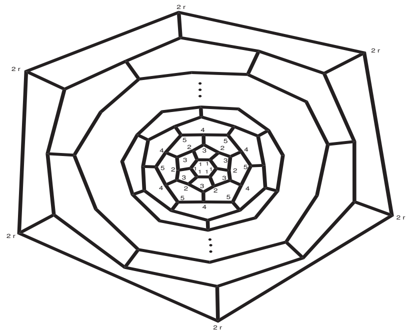


Figure 4. The partition the vertex set of fullerene graph F_{12r}.

Here, by using the method of [50], we conclude the following theorem about the eigenvalues of a fullerene with a trivial cyclic 6-cutset. The vertex set of this fullerene graph can be composed to vertex sets $V_1, \ldots, V_{r+1}$ in which $|V_1| = \ldots = |V_{r+1}| = 6$ and they are the vertices of the inner and outer hexagons. Also, for $i = 2, \ldots r$, we have $|V_i| = 12$. These subsets are called the levels or the layers of this fullerene graph, see [21]. Clearly, by this way the number of vertices of this graph is $12r$ and thus we denote this class of fullerenes by F_{12r}.

Theorem 2.4. *Consider the fullerene graph F_{12r}. Then*

1. *1 is one of its eigenvalues and $\lambda_{l+1}(F) \geq 1$, where the related quotient matrix is of order $2l(l \geq 3)$, and*
2. *F has $2l-2$ eigenvalues that can be grouped in pairs $\{-\mu, \mu\}$, where $1 < \mu < 3$.*

Proof. An equitable partition of F_{12r} is given in Figure 4. Let $\tilde{A}_1$ be the quotient matrix of the quotient graph F_{12r}. Then

$$\tilde{A}_1 = \begin{pmatrix} 2\,1 & & & & & \\ 1\,0\,2 & & & & & \\ & 2\,0\,1 & & & & \\ & & 1\,0\,2 & & & \\ & & & \ddots & & \\ & & & & 2\,0\,1 & \\ & & & & & 1\,2 \end{pmatrix}.$$

By using Eq. 1, we obtain

$$P_j(\lambda) = (\lambda^2 - 5)P_{j-2}(\lambda) - 4P_{j-4}(\lambda), \quad 4 \leq j \leq 2l-1.$$

Now interlacing theorem yields that $\lambda_{l+1}(F) \geq \lambda_{l+1}(\tilde{A}_1) = 1$ and thus we yield part (a). Similar to the proof of [50, Theorem 4.1], it holds

$$\det(\tilde{A}_1 - \lambda I) = (3-\lambda)(1-\lambda)(a_1^2 - \lambda^2)(a_2^2 - \lambda^2)\ldots(a_{l-1}^2 - \lambda^2),$$

where a_i's are integers. This completes the proof of the second claim. □

In Figures 5, 6, one can check that the first level is an equitable partition. The vertices of the second layer is decomposed to two equitable partitions, namely the vertices which are labeled by 2 and 3. Hence, the vertices of each level are divided to two equitable partitions except the first and the last level. This means that the total number of such partitions is $2r$, where $r+1$ is the number of layers.

Another class of fullerene graphs is the fullerene graph $A_{20(r-1)}$ as depicted in Figure 5.

Theorem 2.5. *The spectrum of fullerene graph $A_{20(r-1)}$ (r is even) includes the integers $\{-1,1,3\}$.*

Proof. Consider the equitable partition of $A_{20(r-1)}$ as given in Figure 5 and suppose $\tilde{A}_2$ is the quotient matrix obtained from $A_{20(r-1)}$. By using Eq. 1, we obtain $P_0(\lambda) \equiv 1$, $P_1(\lambda) = 2-\lambda$, $P_2(\lambda) = \lambda^2 - 2\lambda - 1$ and $P_3(\lambda) = -\lambda^3 + 3\lambda^2 + \lambda - 5$. Also, for $4 \leq i \leq 2r-3$, we conclude

$$\begin{cases} P_i(\lambda) = (-\lambda)P_{i-1}(\lambda) - P_{i-2}(\lambda) & , \quad i \text{ is even} \\ P_i(\lambda) = (-\lambda)P_{i-1}(\lambda) - 4P_{i-2}(\lambda) & , \quad i \text{ is odd} \end{cases}. \tag{2}$$

Also, we have $P_{2r}(1) = P_{2r-1}(1) - P_{2r-2}(1)$, where $P_1(1) = 1$, $P_2(1) = -2$ and $P_3(1) = -2$. Let t be even and $4 \leq t \leq 2r-4$. Eq. 2 implies that $P_t(1) = P_{t+1}(1) = (-2)^{\frac{t}{2}}$. So we get that $p_{2r-2}(1) = -p_{2r-4}(1) = -(-2)^{r-2}$ and also $P_{2r-1}(1) = -p_{2r-2}(1) - 2p_{2r-3}(1)$, which yields that $P_{2r-1}(1) = -(-2)^{r-2}$. Then $P_{2r}(1) = 0$ and so $\lambda = 1$ is an eigenvalue of $\tilde{A}_2$. Now we prove that -1 is also an eigenvalue of $\tilde{A}_2$. By Eq. 1, we have $P_{2r}(-1) = 3P_{2r-1}(-1) - P_{2r-2}(-1)$, where $P_2(-1) = 2$ and $P_3(-1) = -2$. By using Eq. 2, we conclude that $P_t(-1) = -P_{t+1}(-1) = (-1)^{\frac{t}{2}+1}2^{\frac{t}{2}}$, where t is an even number and $4 \leq t \leq 2r-4$. So, we get

$$\begin{aligned} P_{2r-2}(-1) &= 2p_{2r-3}(-1) - p_{2r-4}(-1) = -2^{\frac{t}{2}+1}(-1)^{r-1} - 2^{\frac{t}{2}}(-1)^{r-1} \\ &= -3(-1)^{r-1}2^{r-2}, \end{aligned}$$

and

$$\begin{aligned} P_{2r-1}(-1) &= p_{2r-2}(-1) - 2p_{2r-3}(-1) = -3(-1)^{r-1}2^{r-2} + 2(-1)^{r-1}2^{r-2} \\ &= -2^{r-2}(-1)^{r-1}. \end{aligned}$$

This means that $P_{2r}(-1) = 0$ and so -1 is an eigenvalue of $\tilde{A}_2$.

$$\tilde{A}_2 = \begin{pmatrix} 2\,1 & & & & & & & & \\ 1\,0\,2 & & & & & & & & \\ & 1\,1\,1 & & & & & & & \\ & & 1\,0\,2 & & & & & & \\ & & & 2\,0\;\;1 & & & & & \\ & & & & \ddots & & & & \\ & & & & & 2\;\;0\,1 & & & \\ & & & & & & 1\,1\,1 & & \\ & & & & & & & 2\,0\,1 & \\ & & & & & & & & 1\,2 \end{pmatrix}.$$

$\square$

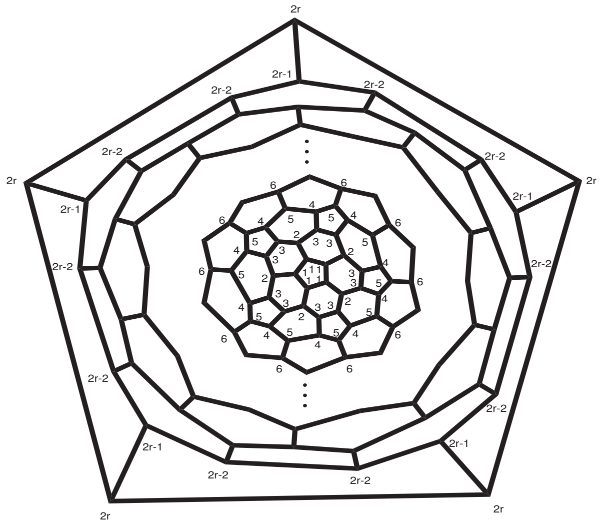


Figure 5. The partition of the vertex set of fullerene graph $A_{20(r-1)}$, r is even.

One can find that the multiplicity of both eigenvalues -1 and 1 of fullerene graph $A_{20(r-1)}$(r is even) is $r-3$ and this graph has no symmetric eigenvalues except -1 and 1.

Theorem 2.6. *Consider the fullerene graph $B_{10(r+2)}$ (r is even), as depicted in Figure 6. Then $\{1,3\}$ are eigenvalues of $B_{10(r+2)}$.*

Proof. An equitable partition of fullerene $B_{10(r+2)}$(r is even) is given in Figure 6. Let $\tilde{A}_3$ be the quotient matrix related to $B_{10(r+2)}$. Similar to the proof of last theorem, one can see that $P_0(\lambda) \equiv 1$, $P_1(\lambda) = 2-\lambda$, $P_2(\lambda) = \lambda^2 - 2\lambda - 1$ and $P_3(\lambda) = -\lambda^3 + 3\lambda^2 + \lambda - 5$. Let $4 \leq i \leq 2r-3$, by Eq. 1, we have $P_{2r}(1) = P_{2r-1}(1) - P_{2r-2}(1)$, where $P_1(1) = 1$, $P_2(1) = -2$ and $P_3(1) = -2$. On the other hand, $P_t(1) = P_{t+1}(1) = 2(-1)^{\frac{t}{2}}$, where t is even and $4 \leq t \leq 2r-4$. Hence, $P_{2r-2}(1) = -p_{2r-4}(1) = 2(-1)^{r-1}$ and

$$\begin{aligned} P_{2r-1}(1) &= -p_{2r-2}(1) - 2p_{2r-3}(1) = -2(-1)^{r-1} - 4(-1)^{r-2} \\ &= -2(-1)^{r-1} + 4(-1)^{r-1}. \end{aligned}$$

Then $P_{2r}(1) = 0$, which yields that $\lambda = 1$ is an eigenvalue of $\tilde{A}_3$.

$$\tilde{A}_3 = \begin{pmatrix} 2\,1\,0 & & & & & \\ 1\,0\,2 & & & & & \\ 0\,1\,1 & 1 & & & & \\ 0\,0\,1 & 1 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 1 & 1\,0\,0 \\ & & & & 1 & 1\,1\,0 \\ & & & & & 2\,0\,1 \\ & & & & & 1\,2 \end{pmatrix}.$$

□

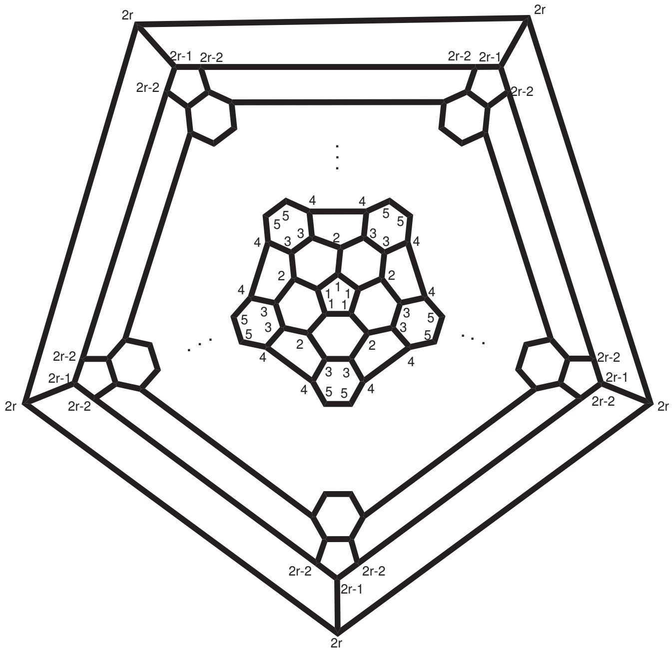


Figure 6. The partition of the vertex set of fullerene graph $B_{10(r+2)}$, r is even.

3 Integral Fullerene Graphs

In this section, we focus on integral fullerenes, namely fullerenes whose all eigenvalues are integer.

Proposition 3.1. *Every fullerene graph has more than five distinct eigenvalues.*

Proof. The smallest fullerene is C_{20} with diameter 5 and the other have diameter greater than 5. This completes the proof. □

The k-th spectral moment of a graph is defined as $S_k = \sum_{i=1}^{n} \lambda_i^k$ and it is equal to the number of closed walk of length k in G. Knowing $S_0, \cdots, S_{n-1}$, we can compute the eigenvalues of G.

Lemma 3.2. *[20] Let F be a fullerene on n vertices with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Then $S_1 = 0$, $S_2 = 2m$, $S_3 = 0$ and $S_4 = 15n$.*

Theorem 3.3. *There is no integral fullerene.*

Proof. Suppose F is an integral fullerene. Then by Proposition 3.1, it must has at least six distinct eigenvalues and by Perron-Frobenius Theorem [6] all of them are in the interval $(-3,3]$. This means that $Spec(F) = \{[3]^1, [2]^{m_1}, [1]^{m_2}, [0]^{m_3}, [-1]^{m_4}, [-2]^{m_5}\}$. Clearly by Lemma

3.2 and substituting these values in k-th spectral moment of F, we obtain

$$\begin{aligned}
&3 + 2m_1 + m_2 - m_4 - 2m_5 = 0,\\
&9 + 4m_1 + m_2 + m_4 + 4m_5 = 3n,\\
&27 + 8m_1 + m_2 - m_4 - 8m_5 = 0,\\
&81 + 16m_1 + m_2 + m_4 + 16m_5 = 15n,\\
&1 + m_1 + m_2 + m_3 + m_4 + m_5 = n.
\end{aligned}$$

Solving above equations yields a contradiction which means that it has not a solution and we are done. □

4 Bipartite spanning subgraph of fullerene

The graph G is called bipartite if the vertex set V can be partitioned into two disjoint subsets V_1 and V_2 such that all edges of G have one endpoint in V_1 and one in V_2. Bipartite edge frustration of a graph G denoted by $\varphi(G)$ is the minimum number of edges that need to be deleted to obtain a bipartite spanning subgraph. It is easy to see that $\varphi(G) = 0$ if and only if G is bipartite. It is a well-known fact that a graph G is bipartite if and only if G does not have an odd cycle. By Euler's formula, every fullerene has 12 pentagonal faces and so it is not bipartite. Here by $\lambda_n(F)$, we mean the smallest eigenvalue of fullerene F.

Theorem 4.1. *[12] Let F be a fullerene graph on n vertices. Then*

$$\lambda_n(F) \leq -3 + \frac{4}{n}\varphi(F).$$

Theorem 4.2. *[12] If F is a fullerene graph on n vertices, then*

$$\lambda_n(F) \leq -3 + 8\sqrt{\frac{3}{5n}}. \tag{3}$$

Theorems 4.1 and 4.2 show that $\lambda_n(F_n)$ tends to -3 if n gets sufficiently large. In the appendix, all eigenvalues of fullerene graphs $B_{10(r+2)}$ and $A_{20(r-1)}$ are listed, respectively.

In Figure 7, the bipartite edge frustration of some classes of fullerene graphs are shown. Also, by using Theorem 4.1, we give some upper bounds for the smallest eigenvalue of these classes of fullerene graphs. In Theorems 4.3 and 4.4, we give upper bounds for the smallest eigenvalues of fullerenes $A_{20(r-1)}, B_{10(r+2)}, F_{12r}$ and D_{10r} which are better than the bound given in Eq. 3.

Theorem 4.3. *Consider the fullerene graph $F \in \{A_{20(r-1)}, B_{10(r+2)}\}$. Then we have $\varphi(F) = 12$, $\lambda_n(A_{20(r-1)}) \leq -3 + \frac{24}{10(r-1)}$ and $\lambda_n(B_{10(r+2)}) \leq -3 + \frac{48}{10(r+2)}$.*

Proof. It is clear that by removing the edges $e_1, \ldots, e_{12}$ from F, the resulted graph has no odd cycle and consequently is bipartite, see Figure 7. This implies that $\varphi(F) \leq 12$. On the other hand, it is clear that we can not remove less than 12 edges to achieve a bipartite graph and thus $\varphi(F) = 12$ By using Theorem 4.1, we have

$$\lambda_n(A_{20(r-1)}) \leq -3 + \frac{4}{20(r-1)} \times 12 = -3 + \frac{24}{10(r-1)},$$

and

$$\lambda_n(B_{10(r+2)}) \leq -3 + \frac{4}{10(r+2)} \times 12 = -3 + \frac{48}{10(r+2)}.$$

□

Theorem 4.4. *Consider the fullerene graph $F \in \{F_{12r}, D_{10r}\}$. Then we have $\varphi(F) = 6$, $\lambda_n(F_{12r}) \leq -3 + \frac{2}{r}$ and $\lambda_n(D_{10r}) \leq -3 + \frac{24}{10r}$.*

Proof. Similar to the proof of Theorem 4.3, $\varphi(F) = 6$, see Figure 7. Theorem 4.1 shows that

$$\lambda_n(F_{12r}) \leq -3 + \frac{4}{12r} \times 6 = -3 + \frac{2}{r},$$

and

$$\lambda_n(D_{10r}) \leq -3 + \frac{4}{10r} \times 6 = -3 + \frac{24}{10r}.$$

□

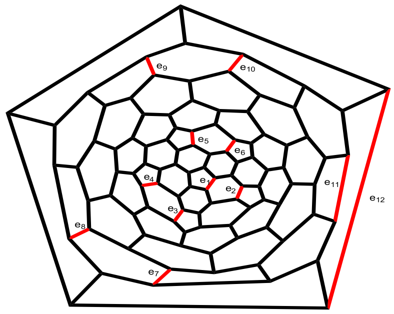
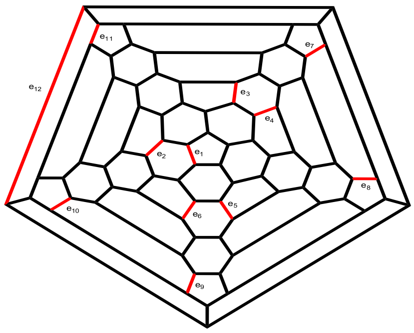
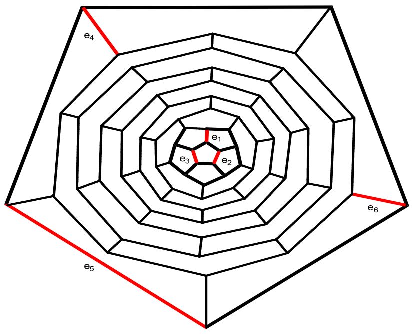
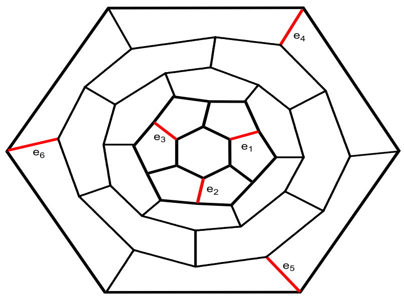
Name	Fullerene graph (F)
a) Fullerene graph $A_{20(r-1)}$ $(r=6)$	
b) Fullerene graph $B_{10(r+2)}$ $(r=6)$	
c) Fullerene graph D_{10r} $(r=6)$	
d) Fullerene graph F_{12r} $(r=2)$	

Figure 7. Bipartite spanning subgraphs of four classes of fullerenes.

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