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Counting the number of spanning trees of graphs

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ABSTRACT

A spanning tree of graph G is a spanning subgraph of G that is a tree. In this paper, we focus our attention on (n,m) graphs, where $m = n$, $n + 1$, $n + 2$, $n + 3$ and $n + 4$. We also determine some coefficients of the Laplacian characteristic polynomial of fullerene graphs.

Keywords: Spanning tree, Laplacian eigenvalue, fullerene.

1. INTRODUCTION

Throughout this paper all graphs are simple. A (n,m) graph is a graph with n vertices and m edges. A spanning tree in a graph G is a tree that has the same vertex set as G. The study of the number of spanning trees $\tau(G)$ in a graph has an old history and has been very active since, counting the number is interesting, and it has different practical applications in different fields. For example, this number can be characterized the reliability of a network in physics, see [2, 4–7] for more details.

A famous theoretical result on finding the number is the matrix tree theorem [9] which expresses the number of spanning trees in terms of the determinant of Laplacian matrix of the graph. But, counting the number of spanning trees by this method is difficult for large graphs [1, 7, 12]. Due to this reason, there have paid much attention to deriving explicit and possibly simple formulas for certain special classes of graphs. For example, for the complete graph K_n, Cayley's tree formula [8] states that $\tau(K_n) = n^{n-2}$.

In the next section we compute the number of spanning trees of $(n, n + i)$ graphs, where i=0, 1, 2, 3, 4. Finally in section 3, we determine the Laplacian coefficients of fullerene graphs. Throughout this paper, our notation is standard and mainly taken from [3, 11].

2. RESULTS AND DISCUSSION

The aim of this section is enumerating of spanning trees for $(n, n + i)$ graphs, where $i = 0$ …, 4. For example, consider the graphs G, H depicted in Figure 1. It is easy to see that $\tau(G) = 97$ and $\tau(H) = 183$. At the first step, let G be a unicycle graph. One can see that by removing any edge of the cycle, the resulted graph is a spanning tree and so we conclude that:

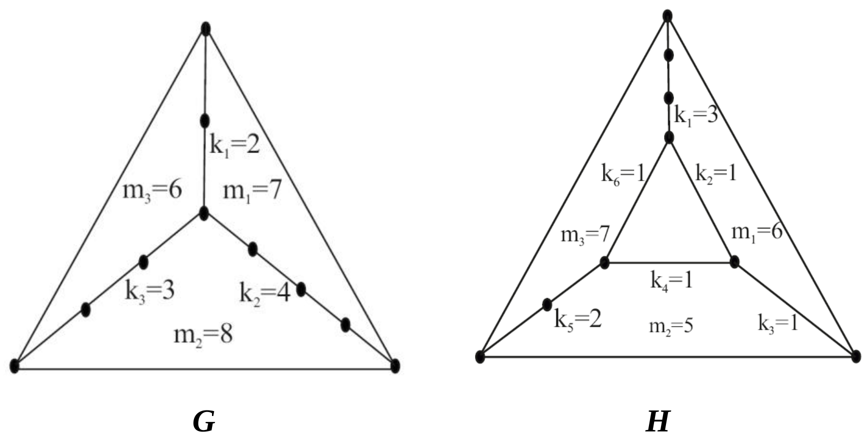

Figure 1. The Graph G and H.

Theorem 1. If G be a (n, n) graph, then $\tau(G)=n$.

Now, consider a $(n, n+1)$ graph as depicted in Figure 2. In this case we have two classes of graphs. One of them can obtained by joining two cycles by a path on $k+ 1$ vertices, Figure 2(1) and the second is a Θ – graph, see Figure 2(2). In both cases we have:

Theorem 2. If G be a $(n, n+1)$ graph, then $\tau(G) = m_1m_2 - k^2$.

Proof. Let G be isomorphic with a bicycle graph as depicted in Figure 2(1), where two cycles are connected by a path with $k + 1$ vertices. In this case, G has exactly two cycles such as C_1 and C_2 and by removing two edges (one edge from C_1 and another from C_2) we can construct a spanning tree. Let m_1 and m_2 are the number of edges of mentioned cycles, respectively. Then $\tau(G) = m_1 - k(m_2 - k) + k(m_1+m_2 - 2k) = m_1m_2 - k^2$. By this method for the second class of $(n, n+1)$ graphs, we get again the above formula.

Figure 2. All Bicyclic Graphs.

Here, we consider a (n, $n + 2$) graph. There are six classes of graphs in this case, see Figure 3. In this case the graph G is a tricycle graph or a Θ – graph and it has three cycles such as C_1, C_2 and C_3. By removing exactly three edges from G, a spanning tree can be resulted. To explain our method, let m_1, m_2 and m_3 be the number of edges of the cycles of G, respectively. The following conditions hold:

1. The graph G is composed of three cycles separated by two paths as depicted in Figure 3(1).
2. The graph G is composed of three cycles separated by three paths, see Figure 3(2).
3,4. The graph G is composed of two subgraphs H, K connected by a path of length k and H is isomorphic with graph of Figure 2(2).
5. A graph isomorphic with Figure 3(5).
6. A graph isomorphic with Figure 3(6).

By using the notations of Theorem 2, we have:

Theorem 3. If G be a (n, n+2) graph, then one of the following holds:

$$\tau(G)=\begin{cases} m_1m_2m_3 & \text{if condition } 1,2 \text{ hold} \\ (m_1m_2-k^2)m_3 & \text{if condition } 3,4 \text{ hold} \\ m_1m_2m_3-m_1k_2^2-m_1k_1^2 & \text{if condition } 5 \text{ hold} \\ m_1m_2m_3-2k_1k_2k_3-m_1k_3^2-m_2k_1^2-m_3k_2^2 & \text{if condition } 6 \text{ hold} \end{cases}$$

Proof. The proof of the first claim is clear. For the third and fourth claims note that a spanning tree can be constructed by removing an edge from the cycle and two edges from theta –subgraph by this condition that the resulted graph always be connected. So, one can see that in these cases

$$\tau(G) = (m_1m_2 - k^2)m_3.$$

For the fifth case we have:

$$\tau(G) = (m_1 - k_1)(m_2 - k_1 - k_2)(m_3 - k_2) + k_1(m_1 - k_1)(m_3 - k_2) + k_2(m_1 - k_1)(m_3 - k_2) + k_2(m_1 - k_1)(m_2 - k_1 - k_2) + k_1(m_3 - k_2)(m_2 - k_1 - k_2) + k_1k_2[(m_1 - k_1) + (m_2 - k_1 - k_2) + (m_3 - k_2)] = m_1m_2m_3 - m_1k_2^2 - m_3k_1^2.$$

Finally, for the sixth case by using the last conditions we have:

$$\tau(G) = (m_1 - k_1 - k_2)(m_2 - k_2 - k_3)(m_3 - k_1 - k_3) + k_1k_2(m_2 + m_3 - k_1 - k_2 - 2k_3) + k_1k_3(m_1 + m_2 - k_1 - 2k_2 - k_3) + k_2k_3(m_1 + m_3 - 2k_1 - k_2 - k_3) + k_1(m_2 - k_2 - k_3) \times (m_1 + m_3 - 2k_1 - k_2 - k_3) + k_2(m_3 - k_1 - k_3)(m_1 + m_2 - k_1 - 2k_2 - k_3) + k_3(m_1 - k_1 - k_2)(m_2 + m_3 - k_1 - k_2 - 2k_3) + k_1k_2(m_1 - k_1 - k_2) + k_1k_3(m_3 - k_1 - k_3) + k_2k_3(m_2 - k_2 - k_3) = m_1m_2m_3 - 2k_1k_2k_3 - m_1k_3^2 - m_2k_1^2 - m_3k_2^2.$$

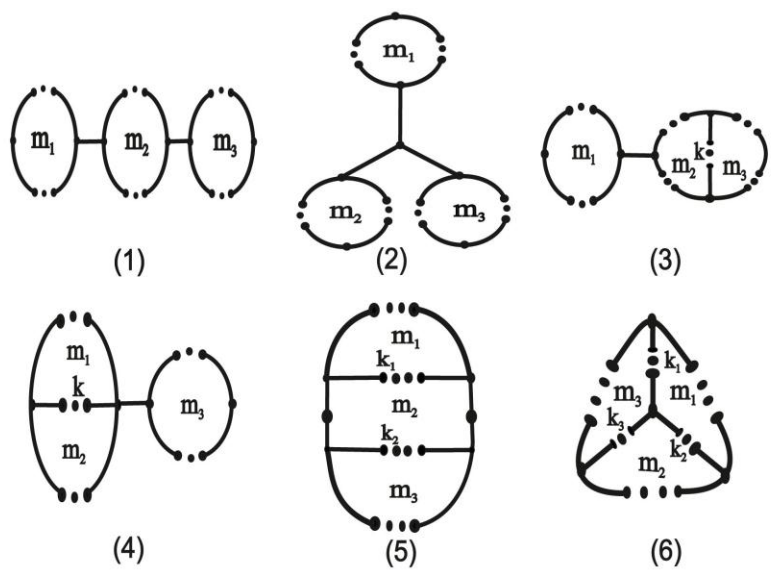

Figure 3. All Tricycle Graphs.

We continue our method for $(n, n + 3)$ graphs to compute the number of spanning trees. It is a longsome work to see that in this case, there are 22 classes of graphs. We enumerate these classes by numbers 1, …, 24, see Figure 4. However, similar to the last theorems we can compute the number of spanning trees. Hence, we have the following theorem without proof:

Theorem 4. If G be a $(n, n+3)$ graph, then one of the following cases hold:

- for graph 4(1): $\tau(G) = m_1m_2m_3m_4$
- for graph 4 (2): $\tau(G) = m_1m_2m_3m_4$
- for graph 4 (3): $\tau(G) = m_1m_4(m_2m_3 - k_2)$
- for graph 4 (4): $\tau(G) = m_1m_4(m_2m_3 - k_2)$
- for graph 4 (5): $\tau(G) = m_1m_4(m_2m_3 - k_2)$
- for graph 4 (6): $\tau(G) = m_1m_2(m_3m_4 - k_2)$
- for graph 4 (7): $\tau(G) = m_1m_2(m_3m_4 - k_2)$
- for graph 4 (8): $\tau(G) = m_3m_4(m_1m_2 - k_2)$
- for graph 4 (9): $\tau(G) = m_3m_4(m_1m_2 - k_2)$
- for graph 4 (10): $\tau(G) = (m_1m_2 - k_1^2)(m_3m_4 - k_2^2)$
- for graph 4 (11): $\tau(G) = (m_1m_2 - k_1^2)(m_3m_4 - k_2^2)$
- for graph 4 (12): $\tau(G) = (m_1m_2 - k_1^2)(m_3m_4 - k_2^2)$
- for graph 4 (13): $\tau(G) = (m_1m_2m_3 - m_1k_2^2 - m_3k_1^2)m_4$
- for graph 4 (14): $\tau(G) = (m_1m_2m_3 - m_1k_2^2 - m_3k_1^2)m_4$
- for graph 4 (15): $\tau(G) = (m_1m_2m_3 - m_1k_2^2 - m_3k_1^2)m_4$
- for graph 4 (16): $\tau(G) = (m_1m_2m_3 - 2k_1k_2k_3 - m_1k_3^2 - m_2k_1^2 - m_3k_2^2)m_4$
- for graph 4 (17): $\tau(G) = (m_1m_2m_3 - 2k_1k_2k_3 - m_1k_3^2 - m_2k_1^2 - m_3k_2^2)m_4$
- for graph 4 (18): $\tau(G) = (m_1m_2m_3 - 2k_1k_2k_3 - m_1k_3^2 - m_2k_1^2 - m_3k_2^2)m_4$
- for graph 4 (19): $\tau(G) = (m_1m_2m_3 - 2k_1k_2k_3 - m_1k_3^2 - m_2k_1^2 - m_3k_2^2)m_4$
- for graph 4 (20): $\tau(G) = (m_1 - k_1)(m_2 - k_1 - k_2)(m_3 - k_2 - k_3)(m_4 - k_3) +$

  $k_1(m_3 - k_2 - k_3)(m_4 - k_3)[(m_1 - k_1) + (m_2 - k_1 - k_2)] + k_2(m_1 - k_1)(m_4 - k_3) \times [(m_2 - k_1 - k_2) + (m_3 - k_2 - k_3)] + k_3(m_2 - k_1 - k_2)(m_1 - k_1)[(m_3 - k_2 - k_3) + (m_4 - k_3)] + k_1k_3[(m_1 - k_1)(m_4 - k_3) + (m_1 - k_1)(m_3 - k_2 - k_3) + (m_2 - k_1 - k_2)(m_4 - k_3) + (m_2 - k_1 - k_2)(m_3 - k_2 - k_3)] + k_1k_2(m_4 - k_3)[(m_1 - k_1) + (m_2 - k_1 - k_2) + (m_3 - k_2 - k_3)] + k_2k_3(m_1 - k_1)[(m_2 - k_1 - k_2) + (m_3 - k_2 - k_3) + (m_4 - k_3)] + k_1k_2k_3[(m_1 - k_1) + (m_2 - k_1 - k_2) + (m_3 - k_2 - k_3) + (m_4 - k_3)] =$
  $m_1m_2m_3m_4 + k_1^2k_3^2 - k_1^2m_3m_4 - k_2^2m_1m_4 - k_3^2m_1m_2.$

- for graph 4 (21): $\tau(G) = (m_1 - k_1 - k_2)(m_2 - k_2 - k_3)(m_3 - k_3 - k_4)(m_4 - k_1 - k_4) + k_1(m_2 - k_2 - k_3)(m_3 - k_3 - k_4)[(m_1 - k_1 - k_2) + (m_4 - k_1 - k_4)] + k_2(m_3 - k_3 - k_4)$

$$(m_4 - k_1 - k_4) [(m_1 - k_1 - k_2) + (m_2 - k_2 - k_3)] + k_3(m_1 - k_1 - k_2) (m_4 - k_1 - k_4) [(m_2 - k_2 - k_3) + (m_3 - k_3 - k_4)] + k_4(m_1 - k_1 - k_2) (m_2 - k_2 - k_3) [(m_3 - k_3 - k_4) +(m_4 - k_1 - k_4)] + k_1k_2(m_3 - k_3 - k_4)[(m_1 - k_1 - k_2)+(m_2 - k_2 - k_3) + (m_4 - k_1 - k_4)] + k_1k_3[(m_1 - k_1 - k_2)(m_2 - k_2 - k_3) + (m_1 - k_1 - k_2) (m_3 - k_3 - k_4) + (m_2 - k_2 - k_3) (m_4 - k_1 - k_4) + (m_3 - k_3 - k_4)(m_4 - k_1 - k_4)] + k_1k_4(m_2 - k_2 - k_3) [(m_1 - k_1 - k_2) + (m_3 - k_3 - k_4) + (m_4 - k_1 - k_4)] + k_2k_3(m_4 - k_1 - k_4)[(m_1 - k_1 - k_2) + (m_2 - k_2 - k_3) + (m_3 - k_3 - k_4)] + k_2k_4[(m_1 - k_1 - k_2) (m_3 - k_3 - k_4) + (m_1 - k_1 - k_2) (m_4 - k_1 - k_4) + (m_2 - k_2 - k_3)(m_3 - k_3 - k_4) + (m_2 - k_2 - k_3) (m_4 - k_1 - k_4)] + k_3k_4(m_1 - k_1 - k_2) [(m_2 - k_2 - k_3) + (m_3 - k_3 - k_4) + (m_4 - k_1 - k_4)]+(k_1k_2k_3+k_1k_3k_4+k_1k_2k_4)(m_1 - k_1 - k_2) + (m_2 - k_2 - k_3) + (m_3 - k_3 - k_4) + (m_4 - k_1 - k_4) = m_1m_2m_3m_4 - 2k_1k_2k_3k_4 + k_1^2k_3^2 - k_1 k_3^2 + k_2^2 k_4^2 + k_1 k_3^2 (m_2 + m_3) - k_1 k_4^2 m_2 - k_1^2 m_2m_3 - k_4^2 m_1m_2 - k_3^2 m_1m_4 - k_2^2 m_3m_4 - k_1k_2 k_3^2 + k_1k_2 k_4^2 + k_1k_3 k_4^2 + (k_1k_2k_3 - k_1k_2k_4 - k_1k_3k_4)m_3 + (k_1k_4 - k_1k_3)m_2m_3.$$

- for graph 4 (22): $k_2 + k_4 + k_6 = m_4$ and so

$$\tau(G) = (m_1 - k_1 - k_2 - k_3) (m_2 - k_3 - k_4 - k_5) (m_3 - k_1 - k_5 - k_6)(k_2 + k_4 + k_6) + (m_1 - k_1 - k_2 - k_3) (m_2 - k_3 - k_4 - k_5) [(k_2 + k_4) (k_1 + k_5 + k_6) + k_6(k_1 + k_5)] + (m_1 - k_1 - k_2 - k_3) (m_3 - k_1 - k_5 - k_6)[(k_2 + k_6) (k_3 + k_4 + k_5) + k_4(k_3 + k_5)] + (m_2 - k_3 - k_4 - k_5) (m_3 - k_1 - k_5 - k_6)[(k_4 + k_6)(k_1 + k_2 + k_3) + k_2(k_1 + k_3)] + [(m_1 - k_1 - k_2 - k_3) + (m_2 - k_3 - k_4 - k_5) + (m_3 - k_1 - k_5 - k_6)] k_2 kk_6 + [(m_1 - k_1 - k_2 - k_3) + (m_2 - k_3 - k_4 - k_5) +(m_3 - k_1 - k_5 - k_6)] (k_2 + k_4 + k_6) \times (k_1k_3+ k_3k_5 + k_1k_5) + [(m_1 - k_1 - k_2 - k_3) + (m_2 - k_3 - k_4 - k_5) + (m_3 - k_1 - k_5 - k_6)] [k_2k_6(k_3 + k_5) + k_4k_6(k_1 + k_3) + k_2k_4(k_1 + k_5)] = m_1m_2m_3m_4 - m_2m_4 k_1^2 - m_2m_3 k_2^2 - m_3m_4 k_3^2 - m_1m_3 k_4^2 - m_1m_4 k_5^2 - m_1m_2 k_6^2 - 2m_1k_4k_5k_6 - 2m_2k_1k_2k_6 - 2m_3k_2k_3k_4 - 2m_4k_1k_3k_5 - 2k_1k_2k_4k_5 - 2k_2k_3k_5k_6 - k_1k_3k_4k_6 + k_1^2k_4^2 + k_2^2k_5^2 + k_3^2 k_6^2 .$$

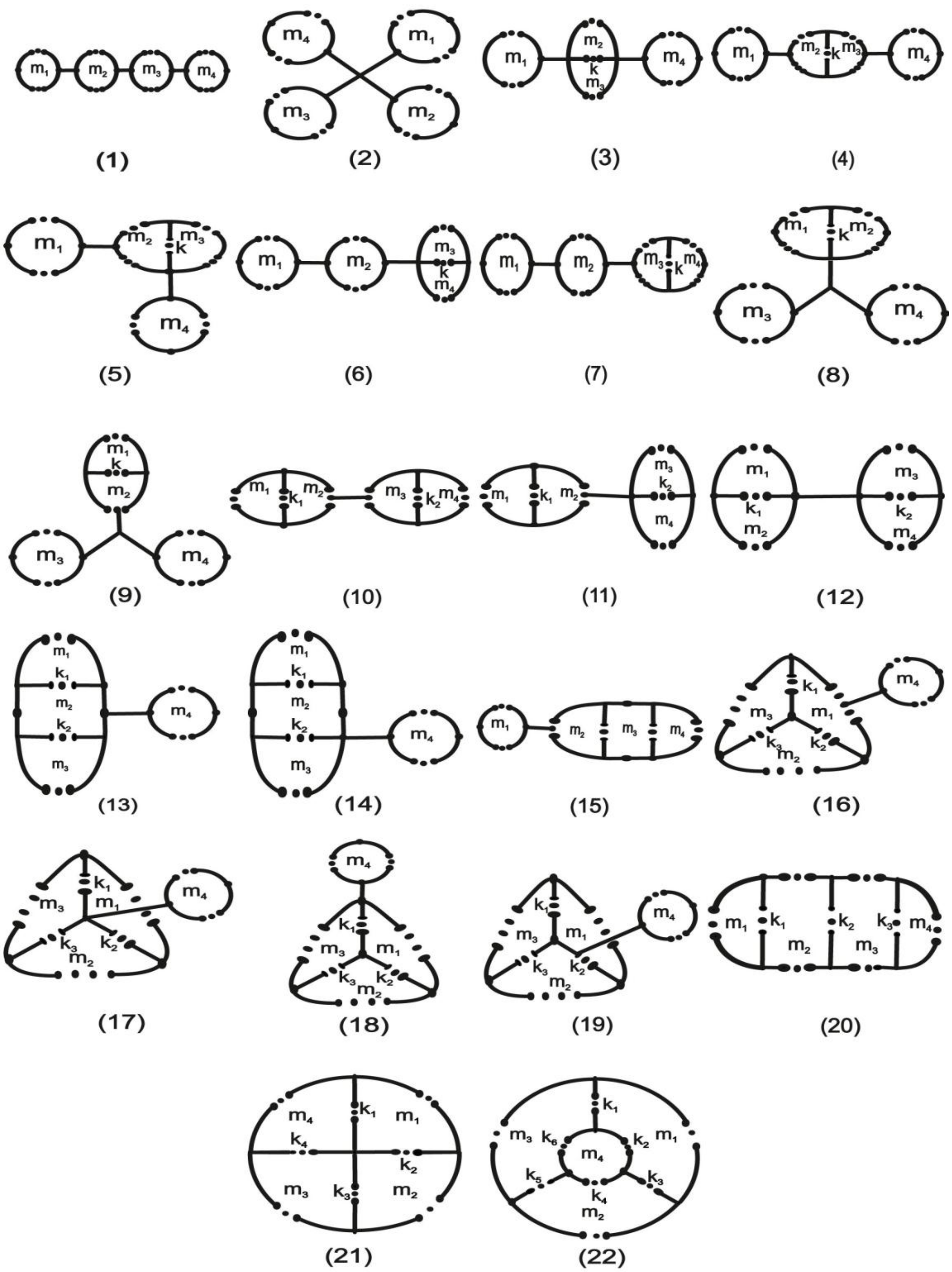

Figure 4. All Four Cycle Graphs.

3. LAPLACIAN COEFFICIENTS OF FULLERENES

By the discovery of the first fullerene molecule, i.eC_{60} by Kroto and his co-authors [10] in 1985, fullerene graphs are considered by many mathematicians in all over the word. The name fullerene was given to cubic carbon molecules in which the atoms are arranged on a sphere in pentagons and hexagons. At first fullerene graphs were defined as 3–regular planar 3–connected graphs whose faces are pentagons and hexagons. We denote a fullerene with n vertices by F_n.

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 $\varphi(G,x)$ of graph G is defined as

$$\varphi(G,x) = \det(x I - A).$$

The roots of the characteristic polynomial are the eigenvalues of graph G and form the spectrum of this graph. The Laplacian matrix of G is the mark $L(G) = [l_{ij}]$ indexed by the vertex set of ,with zero row sums, where $L_{ij} = -a_{ij}$ for $i \neq j$. If $D(G) = [d_{ij}]$ 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 roots of Laplacian characteristic polynomial

$$\psi(G,x) = \det(x I - L).$$

are the Laplacian eigenvalues of graph G. Let the Laplacian characteristic polynomial of fullerene graph F be

$$\psi(F,x) = \sum_{k=0}^{n-1} (-1)^k c_k x^{n-k} = c_0 x^n - \cdots + (-1)^{n-1} c_{n-1} x + (-1)^n c_n .$$

The aim of this section is to determine c_0, c_1, …, c_7, c_{n-1}, c_n. The Laplacian matrix $L(G)$ has non–negative eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$ [11]. By Viettes formula, $c_k = \sigma_k(\mu_1, \mu_2, \ldots, \mu_{n-1})$ is a symmetric polynomial of order $n - 1$. In particular, $c_0 = 1$, $c_1 = 2m$, $c_n = 0$ and $c_{n-1} = n\tau(G)$, where m and $\tau(G)$ denote the number of edges and the number of spanning trees of G, respectively. According to the Temperley's Theorem [3], one can also see that

$$\tau(G) = \frac{\mu_1 \mu_2 \cdots \mu_{n-1}}{n} .$$

If G is a tree, coefficient c_{n-2} is equal to its Wiener number, which is defined as the sum of distances between all pairs of vertices.

Lemma 5 [3]. The coefficients of the characteristic polynomial of a graph G satisfy:

- $a_1 = 0$,
- $-a_2$ is the number of edges of G,
- $-a_3$ is twice the number of triangles in G,
- $a_4 = n_a - 2n_b$, where n_a is the number of pairs of disjoint edges in G, and n_b is the number of 4-cycles in G.

Let G be a graph. A subgraph of G whose components are circuits or a complete graph with two vertices is called an elementary subgraph of G.

Lemma 6 [3]. The coefficients of the characteristic polynomial are given by

$$(-1)^i a_i = \sum (-1)^{r(\Lambda)} 2^{s(\Lambda)},$$

where the summation goes on the elementary subgraphs Λ of G with i vertices.

Theorem 7 The coefficients of the Laplacian characteristic polynomial of a fullerene graph F satisfy:

- $c_1 = 3n$,
- $c_2 = 3/2n(3n - 4)$,
- $c_3 = -9/2n^3 + 18n^2 - 18n$,
- $c_4 = 27/8n^4 - 27n^3 + 72n^2 - 129/2n$,
- $c_5 = -81/40n^5 + 27n^4 - 135n^3 + 603/2n^2 - 1278/5n + 24$,
- $c_6 = 81/80\, n^6 - 81/4n^5 + 162n^4 - 2601/4n^3 + 6579/5n^2 - 1154n + 380$,
- $c_7 = -243/560\, n^7 + 243/20\, n^6 - 567/4\, n^5 + 3537/4n^4 - 15606/5n^3 + 30243/5n^2 - 42612/7n + 3840$.

Proof. Let F be a fullerene graph on n vertices and eigenvalues $\lambda_1, \ldots, \lambda_n$. Since a fullerene graph is a 3-regular, then the Laplacian eigenvalues are $\mu_i = 3 - \lambda_i$. This completes the first assertion. For the second part, notice that

$$c_2 = \sum_{i,j} \mu_i \mu_j .$$

But from the first part $\sum_i \mu_i = 3n$. This implies that $(\sum_i \mu_i)^2 = 9n^2$. On the other hand, it is well known fact that

$$\sum_i \mu_i^2 = 2m + \sum_i d_i^2 .$$

This completes the second claim. The coefficient c_3 can be given by

$$c_3 = \sum_{i,j,k} \mu_i \mu_j \mu_k = \sum_{i,j,k} (3-\lambda_i)(3-\lambda_j)(3-\lambda_k).$$

But $\sum_i \lambda_i = 0$ and this completes the proof of part 3.

From Lemma 5(*iv*), $a_4 = n_a - 2n_b$. Since fullerenes haven't 4-cycles, so we should to enumerate all elementary subgraphs with 4 vertices that are pairs of disjoint edges and this value is $m(m - 5)/2$. This means that $a_4 = 3n(3n - 10)/8$ and c_4 can be obtained as follows:

$$c_4 = \sum_{i,j,k,s} \mu_i \mu_j \mu_k \mu_s$$

$$= \sum_{i,j,k,s} [81 - 27(\lambda_i + \lambda_j) - 27(\lambda_r + \lambda_s) + 9\lambda_i\lambda_j + 9\lambda_r\lambda_s$$

$$+ 9(\lambda_i + \lambda_j)(\lambda_r + \lambda_s) - 3\lambda_i\lambda_j(\lambda_r + \lambda_s) - 3\lambda_r\lambda_s(\lambda_i + \lambda_j) + \lambda_i\lambda_j\lambda_k\lambda_s] .$$

Finally, since every fullerene graph has only 12 pentagonal faces, according to Lemma 6, $a_5 = -24$. By using a similar method with the last parts, the fifth Laplacian coefficient can be obtained.

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