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On the Difference between Laplacian and Signless Laplacian Coefficients of a Graph and its Applications on the Fullerene Graphs

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Keywords:	Abstract
Fullerene graph,	
Signless Laplacian matrix,	Let $\sum_{i=0}^{n} (-1)^{i} l_{i} x^{n-i}$ and $\sum_{i=0}^{n} (-1)^{i} q_{i} x^{n-i}$ be the char-
Laplacian coefficient	acteristic polynomials of the Laplacian matrix and signless
AMS Subject Classification (2020):	Laplacian matrix of an <i>n</i> -vertex graph, respectively. Let $\alpha_i = q_i - l_i , 0 \le i \le n$. In this paper, we find formulas for some of α_i 's. In particular, we compute α_i 's for some fullerene
05C50; 05C30; 05C07	graphs.
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(Dedicated to the memory of Professor Ali Reza Ashrafi.)

1 Introduction

Let H be an *n*-vertex graph with no loop and parallel edges. The edge set and the vertex set of H are denoted as E(H) and V(H), respectively. We denote by A(H) the adjacency matrix of H. Let $diag(d_{11}, d_{22}, d_{33}, \ldots, d_{nn})$ be the diagonal matrix of vertex degrees of H, denoted by D(H), where d_{ii} is the degree of vertex v_i and L(H) = D(H) - A(H) be the Laplacian matrix of H (see [1–4]). Similarly, the signless Laplacian matrix of a graph H studied in [5, 6], has been defined as Q(H) = D(H) + A(H). Since A(H), L(H) and Q(H) are symmetric matrices with real entries, their eigenvalues are real. We know that L(H) and Q(H) are positive semi-definite, and they have the same eigenvalues if and only if H is bipartite.

The Laplacian and signless Laplacian characteristic polynomials of a graph H are defined by $L_H(t) = det(tI - L(H)) = \sum_{i=0}^n (-1)^i l_i t^{n-i}$ and $Q_H(t) = det(tI - Q(H)) = \sum_{i=0}^n (-1)^i q_i t^{n-i}$,

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respectively. One may see that the Laplacian coefficient, l_i , can be expressed in terms of subtrees of H, for i = 0, 1, ..., n (see [7]). Suppose that F is a spanning subforest of H with connected components $T_1, T_2, ..., T_k$, having $n_1, n_2, ..., n_k$ vertices, respectively. Let $\omega(F) = \prod_{i=1}^k n_i$.

First, we recall the following:

Theorem A ([8, Theorem 7.5]). The coefficients l_i of the polynomial $L_H(t)$ are given by the formula

$$l_i = \sum_F \omega(F),$$

where F is a subforest with i edges.

Using the notation and terminology from [1, 5], a spanning subgraph of a graph H whose connected components are odd unicyclic graphs or trees is called a TU-subgraph of H. Suppose that a TU-subgraph F of H contains t odd unicyclic graphs and s trees T_1, T_2, \ldots, T_s . The weight of F, W(F), is defined by $W(F) = 4^t \prod_{j=1}^s n_j$, in which n_j is $|V(T_j)|$. If F contains no tree, then $W(F) = 4^t$. Based on the next theorem, the coefficients q_j can be expressed in terms of the weight of TU-subgraphs of a graph H.

Theorem B ([5, Theorem 4.4]). For coefficients q_j as above, $q_0 = 1$ and $q_j = \sum_{F_j} W(F_j)$, $j = 1, \ldots, n$, where F_j is a TU-subgraph with j edges.

A fullerene graph is a 3-regular planar graph with only pentagonal and hexagonal faces. A fullerene graph with n carbon atoms, F_n , has $\frac{n}{2} - 10$ hexagons and 12 pentagons.

For the motivation of this paper, we refer to [9-12] concerning the Laplacian coefficients and signless Laplacian coefficients. By calculating the difference between these two coefficients, in the case that one of these polynomial coefficients is available, one can find the other one. Here we investigate $\alpha_i = |q_i - l_i|, 0 \le i \le n$, the difference between Laplacian and signless Laplacian coefficients of some graphs. The notations are taken from [7, 13–16].

2 Main results

In this section, we compute the number of some subgraphs of a given graph and then investigate the difference between Laplacian and signless Laplacian coefficients associated with them. We define the *odd girth* of a graph H, Og(H), as the minimum odd integer k such that C_k is a cycle with k vertices in H and denote the number of subgraphs of H isomorphic to a subgraph F by N(F).

Theorem 2.1. Let H be a graph and Og(H) = k. Then $\alpha_i = 0, i = 1, 2, ..., k - 1$ and $\alpha_k = 4N(C_k)$.

Proof. By Theorems A and B,

$$\begin{array}{lll} \alpha_i & = & \displaystyle\sum_{\substack{F \ is \ a \ TU-subgraph \\ with \ i \ edges}} W(F) - & \displaystyle\sum_{\substack{F \ is \ a \ subforest \\ with \ i \ edges}} \omega(F) \\ & = & \displaystyle\sum_{\substack{F \ is \ a \ TU-subgraph \\ containing \ at \ least \ one \ odd \ cycle}} W(F). \end{array}$$

Since there is no *TU*-subgraph with *i* edges for i = 1, 2, ..., k-1 in H, $\alpha_1 = \alpha_2 = ... = \alpha_{k-1} = 0$. A *TU*-subgraph with *k* edges and at least one cycle is an odd cycle with *k* vertices and W(F) = 4. Thus $\alpha_k = 4N(C_k)$.



Figure 1: Some unicyclic graphs.

In the next result, we calculate α_i , $1 \le i \le 5$, for the fullerene graph. This result can also be obtained using the results of [6, 16].

Corollary 2.2. For the fullerene graph F_n , $\alpha_i = 0$, $1 \le i \le 4$, and $\alpha_5 = 48$.

Proof. By definition, one has $W(C_5) = 4$ and $N(C_5) = 12$. Therefore, $\alpha_5 = 48$.

Theorem 2.3. Let H be an m-edges graph and Og(H) = k. Let C_k^j , $j = 1, 2, ..., N(C_k)$ be cycles in H with k vertices. Then

$$\alpha_{k+1} = 8mN(C_k) - 4\sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j),$$

where v_i^j is *i*-th vertex in C_k^j .

Proof. The *TU*-subgraphs with k+1 edges in *H* are isomorphic to *A* in Figure 1 and *A'*, where *A'* is the union of C_k and an edge. One can see that W(A) = 4, $N(A) = \sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j) - 2kN(C_k)$ and W(A') = 8, $N(A') = (m+k)N(C_k) - \sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j)$. Now by the proof of

Theorem 2.1,

$$\begin{aligned} \alpha_{k+1} &= \sum_{\substack{H \text{ is a } TU-subgraph \ containing \ at \ least} \\ W(H) \\ &= 4N(A) + 8N(A') \\ &= 4(\sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j) - 2kN(C_k)) \\ &+ 8((m+k)N(C_k) - \sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j)) \\ &= 8mN(C_k) - 4\sum_{j=1}^{N(C_k)} \sum_{i=1}^k d(v_i^j), \end{aligned}$$

as desired.

Corollary 2.4. Let H be an r-regular and m-edges graph and Og(H) = k. Let C_k^j , $j = 1, 2, \ldots, N(C_k)$, be cycles in H with k vertices. Then $\alpha_{k+1} = (8m - 4rk)N(C_k)$. In particular, $\alpha_6(F_n) = 144n - 720$.

Proof. Since H is r-regular, the degree of each vertex is r. So, by Theorem 2.3 we have

$$\alpha_{k+1} = 8mN(C_k) - 4rkN(C_k) = (8m - 4rk)N(C_k)$$

Since F_n is a 3-regular graph, m = 3/2n and $\alpha_6(F_n) = 144n - 720$.

In the following lemma, $Ni(C_k) = \{x \in V(H) \mid v_i x \in E(H)\}$, *m* denotes the cardinality of E(H) and $s(x) = \sum_{xy \in E(H)} d(y)$.

Lemma 2.5. For a graph H, let Og(H) = k, $N(C_k) = 1$ and $V(C_k) = \{v_1, v_2, \ldots, v_k\}$. For the subgraphs A, B, C and D of H depicted in Figure 1, the following assertions hold:

(i) $N(A) = \sum_{i=1}^{k} d(v_i) - 2k.$ (ii) $N(B) = \frac{1}{2} \sum_{0 < i < j < k+1} (d(v_i) - 2)(d(v_j) - 2).$ (iii) $N(C) = \sum_{i=1}^{k} s(v_i) + 2k - 3 \sum_{i=1}^{k} d(v_i).$ (iv) $N(D) = \frac{1}{2} \sum_{i=1}^{k} (d(v_i) - 2)(d(v_i) - 3).$ (v) If E is the union of C_k and P_3 , then N(E) is $\frac{1}{2} \sum d(u_i)(d(u_i) - 1) + \frac{1}{2} \sum (d(u_i) - 1)(d(u_i))$

$$\frac{1}{2} \sum_{u_i \notin Ni(C_k) \cup V(C_k)} d(u_i)(d(u_i) - 1) + \frac{1}{2} \sum_{u_i \in Ni(C_k) \setminus V(C_k)} (d(u_i) - 1)(d(u_i) -$$

(vi) If A' is the union of A and K_2 , then

$$N(A') = N(A)(m - (1 + k)) - N(C) - 2N(B) - 2N(D)$$

2).

(vii) If C' is the union of C_k and K_2 , then

$$N(C') = m + k - \sum_{i=1}^{k} d(v_i).$$

(viii) If C'' is the union of C_k and $2K_2$ (the union of two K_2), then

$$N(C'') = \frac{1}{2}(N(C')(m - (1 + k)) - 2N(E) - N(C) - N(A')).$$

Proof. To count the number of subgraphs isomorphic to A, in H, we consides the number of neighborhoods of $V(C_k)$ excluding $V(C_k)$. Then

$$N(A) = \sum_{i=1}^{k} (d(v_i) - 2) = \sum_{i=1}^{k} d(v_i) - 2k.$$

To get the number of subgraphs isomorphic to B, in H, we choose $d(v_i) - 2$ ways an edge joint to v_i and $d(v_j) - 2$ ways an edge joint to v_j , then

$$N(B) = \frac{1}{2} \sum_{0 < i < j < k+1} (d(v_i) - 2)(d(v_j) - 2).$$

To determine the number of subgraphs isomorphic to C in H, we need to count the number of paths P_3 joint to vertex v_i in $V(C_k)$. Essentially, we count the total number of neighbors of v_i^j except v_i , where v_i^j is a neighbor of v_i and does not belong to the cycle. Then

$$N(C) = \sum_{i=1}^{k} s(v_i) + 2k - 3\sum_{i=1}^{k} d(v_i).$$

The number of subgraphs isomorphic to D in H is $\sum_{i=1}^{k} \binom{d(v_i) - 2}{2}$. Thus

$$N(D) = \frac{1}{2} \sum_{i=1}^{k} (d(v_i) - 2)(d(v_i) - 3)$$

Note that N(E) is the number of selections of P_3 in $G \setminus \{v_1, \ldots, v_k\}$. Then

$$N(E) = \sum_{u_i \notin Ni(C_k) \cup V(C_k)} {d(u_i) \choose 2} + \sum_{u_i \in Ni(C_k) \setminus V(C_k)} {d(u_i) \choose 2}$$

= $\frac{1}{2} \sum_{u_i \notin Ni(C_k) \cup V(C_k)} d(u_i)(d(u_i) - 1)$
- $\frac{1}{2} \sum_{u_i \in Ni(C_k) \setminus V(C_k)} (d(u_i) - 1)(d(u_i) - 2).$

We can select N(A)(m-k-1) ways subgraph A and an edge. Now by removing undesirable states, we have

$$N(A') = N(A)(m - (1 + k)) - N(C) - 2N(B) - 2N(D).$$

Also N(C') is the number of selection in $H \setminus \{v_1, \ldots, v_k\}$. Thus

$$N(C') = m + k - \sum_{i=1}^{k} d(v_i).$$

We can choose C' and an edge with N(C')(m - (1 + k)) ways. Now by removing undesirable states, we have

$$N(C'') = \frac{1}{2}(N(C')(m - (1 + k)) - 2N(E) - N(C) - N(A')).$$

In the following, we calculate α_{k+2} based on subgraphs presented in Lemma 2.5.

Theorem 2.6. Let G be a triangle free graph, Og(G) = k, $N(C_k) = 1$ and $V(C_k) = \{v_1, \ldots, v_k\}$. Then

$$\alpha_{k+2} = 12N(B) - 4N(C) + 12N(D) - 16N(E) + 8N(C')(m-k-1) - 8N(A)(m-k-1).$$

Proof. The *TU*-subgraphs with k + 2 edges and at least one cycle are isomorphic to B, C, D, A' and C''. By the definition of the weight of subgraphs, we have W(B) = W(C) = W(D) = 4 and W(A') = 8. Then by the proof of Theorem 2.1,

$$\begin{aligned} \alpha_{k+2} &= \sum_{\substack{H \text{ is a } TU-subgraph \ containing \ at \ least}\\ &= 4N(B) + 4N(C) + 4N(D) + 8N(A') + 16N(C'')\\ &= 4N(B) + 4N(C) + 4N(D) + 8\Big(N(A)(m-k-1) - N(C)\\ &- N(B) - N(D)\Big) + 16\left[\frac{1}{2}\Big(N(C')(m-k-1) - 2N(E)\\ &- N(C) - N(A)(m-k-1) + N(C) + 2N(B) + 2N(D)\Big)\right]\\ &= 12N(B) - 4N(C) + 12N(D) - 16N(E)\\ &+ 8N(C')(m-k-1) - 8N(A)(m-k-1),\end{aligned}$$

as desired.

Corollary 2.7. Let H be an r-regular graph, Og(H) = k, k > 3 and $N(C_k) = 1$. Then α_{k+2} is given by

$$12k^{2}r^{2} - 4knr^{2} + 2n^{2}r^{2} - 40k^{2}r + 8kr^{2} - 8nr^{2} + 40k^{2} + 4kr + 4nr + 6r^{2} - 30r + 36.$$

Proof. By Lemma 2.5, for the r-regular graph H, we have

$$N(B) = k((r-1)^{2}(k-1),$$

$$N(C) = k(r^{2}-3r-2),$$

$$N(D) = 1/2(r-2)(r-3),$$

$$N(E) = 1/2(r-1)(nr-3kr+4k),$$

$$N(A) = kr-2k,$$

$$N(C') = (m+k-kr)(m-k-1).$$

Then, by Theorem 2.6, we have $\alpha_{k+2} = 12k^2r^2 - 4knr^2 + 2n^2r^2 - 40k^2r + 8kr^2 - 8nr^2 + 40k^2 + 4kr + 4nr + 6r^2 - 30r + 36.$

Theorem 2.8. For the graph F_n , we have

$$\alpha_7 = 4N(A) + 4N(B) + 8N(C) + 8N(D) + 16N(E),$$

where A, B, \ldots, N are depicted in Figure 4.



Figure 2: TU-subgraphs with 7 edges in a Fullerene.



Figure 3: TU-subgraphs with 8 edges in a grpah.

Proof. Note that the TU-subgraphs with 7 edges and a cycle in F_n are isomorphic to subgraphs depicted in Figure 2. Therefore, we get $\alpha_7 = 4N(A) + 4N(B) + 8N(C) + 8N(D) + 16N(E)$. Then by the proof of Theorem 2.1, the assertion holds.

Lemma 2.9. Let G be a graph with girth at least 7, Og(G) = k, $N(C_k) = 1$, $V(C_k) = \{v_1, \ldots, v_k\}$ and $Ni(v_i) - V(C_k) = \{v_i^1, \ldots, v_i^{d_i-2}\}$. Then the number of TU- subgraphs of the type shown in Figure 3 is as follows:

$$\begin{split} 1)N(1) &= \sum_{i=1}^{k} \binom{d_{i}-2}{3}, \\ 2)N(2) &= \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{k} \binom{d_{i}-2}{2} (d_{j}-2), \\ 3)N(3) &= \sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} (d(v_{i}^{j})-1)(d_{i}-3), \\ 4)N(4) &= \sum_{1 \leq i < j < r \leq k} (d_{i}-2)d_{j}-2)(d_{r}-2), \\ 5)N(5) &= \sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} (S(v_{i}^{j})-d(v_{i}^{j})-d_{i}+1), \\ 6)N(6) &= \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{k} \sum_{r=1}^{d_{i}-2} (d(v_{i}^{r})-1)(d_{j}-2), \\ 7)N(7) &= \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{k} \sum_{r=1}^{d_{i}-2} (d(v_{i}^{r})-1)(d_{j}-2), \\ 8)N(8) &= [\sum_{i=1}^{k} \binom{d_{i}-2}{2}](m-k-2)-3N(1)-N(3)-N(7), \\ 9)N(9) &= [\sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} (d(v_{i}^{j})-1)](m-k-2)-N(3)-N(7)-2N(6) \\ 10)N(10) &= \sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} \sum_{v_{i} \notin V(C_{k})} \binom{d_{i}}{2} + \sum_{v_{i} \in V(C_{k}), v_{i} \neq v_{i}^{i}} \binom{d_{i}-1}{2}], \\ 11)N(11) &= \sum_{v_{i} \notin V(C_{k})} \binom{d_{i}}{3} + \sum_{v_{i} \in V(C_{k})_{i}} \binom{d_{i}-1}{3}, \\ 12)N(12) &= N_{G-V(C_{k})}(P_{4}), \\ 13)N(13) &= N_{G-V(C_{k})}(P_{3})(m-k-2) \\ &= 3N(11) - 2N(12) - N(5) - N(6) - N(10), \\ 14)N(14) &= \sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} m(G-C'_{ij}, 2), \\ 15)N(15) &= m(G-V(C_{k}), 3), \end{split}$$

where m(G, r) is the number of r-matching in G.

Proof. 1) it is enough to choose three edges outside the cycle from each vertex on the cycle. 2)Suppose *i* and *j* are selected. In $\binom{d_i-2}{2}(d_j-2)$ ways, two edges from v_i and one edge from v_j can be selected. Thus $N(2) = \sum_{i=1}^k \sum_{j=1, j \neq i}^k \binom{d_i-2}{2}(d_j-2)$.

3)In $(d(v_i^j) - 1)(d_i - 3)$ ways, a path of length 2 and an edge from vertex v_i can be chosen. Then $N(3) = \sum_{i=1}^{k} \sum_{j=1}^{d_i-2} (d(v_i^j) - 1)(d_i - 3).$

4) To prove this relation, it is enough to note that an edge can be selected from vertex v_i exactly in $(d_i - 2)$ ways.

5) To count such subgraphs, we count the number of paths of length 3 connected to v_i , which is equal to $(S(v_i^j) - d(v_i^j) - d_i + 1)$. So $N(5) = \sum_{i=1}^k \sum_{j=1}^{d_i-2} (S(v_i^j) - d(v_i^j) - d_i + 1)$. 6) Two edges must be selected from each neighboring vertex of C_k . As a result, we have

(b) Two edges must be selected from each neighboring totel of \mathcal{O}_{k} . The end of $N(6) = \sum_{i=1}^{k} \sum_{j=1}^{d_{i}-2} {d(v_{i}^{j})-1 \choose 2}$. ($d(v_{i}^{r}) - 1$) paths of length 2 starting from vertex v_{i} to v_{i}^{r} and $(d(v_{j}) - 2)$ edge start from vertex v_{j} . So $N(7) = \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{d_{i}-2} (d(v_{i}^{r}) - 1)(d_{j} - 2)$. 8) We count the number of these subgraphs using principle of inclusion and exclusion. The

number of subgraphs C_k with two pendant edge and an edge is $\left[\sum_{i=1}^k \binom{d_i-2}{2}\right](m-k-2)$. Undesirable states are subgraphs of types 1, 3 and 7.

9)We count the number of these subgraphs using the principle of inclusion and exclusion. The number of subgraphs C_k with pendant P_3 and an edge is $\left[\sum_{i=1}^k \sum_{j=1}^{d_i-2} (d(v_i^j)-1)\right](m-k-2)$. Undesirable states are subgraphs of types 3, 7 and 6.

10) It is enough to count the number of paths of length 2 that do not have a vertex in common with the c_k and its pendant edge.

11)It is enough to count the number of 4-vertex star subgraphs that do not have a common vertex with the C_k .

12) Clearly, the number of 4-vertex paths in $G - C_k$ must be counted.

13) Clearly, the number of 3-vertex paths in $G - C_k$, is $N_{G-C_k}(P_3)$. Using the principle of inclusion and exclusion, we select a distinct edge from $C_k \cup P_3$. Clearly, Undesirable states are 11, 12, 5, 6 and 10.

14) We count the number of 2-matching in $G - C_{ij}$ where C_{ij} is C_k along with a pendant edge $v_i v_i^j$.

15)We count the number of 3-matching in $G - C_k$.

Theorem 2.10. Let G be a graph with girth at least 7, Og(G) = k, $N(C_k) = 1$, $V(C_k) = 0$ $\{v_1, \ldots, v_k\}$. Then

> $\alpha_{k+3} = 4N(1) + 4N(2) + 4N(3) + 4N(4)$ + 4N(5) + 4N(6) + 4N(7) + 8N(8)+ 8N(9) + 12N(10) + 16N(11) + 16N(12)+ 24N(13) + 8N(14) + 32N(15),

where TU-subgraphs $1, 2, \ldots, 15$ are depicted in Figure 3.

Proof. TU-subgraphs with k+3 edges and a cycle in G are isomorphic to subgraphs depicted in Figure 3. Now we get

W(1) = W(2) = W(3) = W(4) = W(5) = W(6) = W(7) = 4,W(8) = W(9) = W(14) = 8,W(10) = 12, W(11) = W(12) = 16, W(13) = 24, W(15) = 32.Then by the proof of Theorem 2.1, the assertion holds.

We can calculate the eighth Laplacian and signless Laplacian coefficients of fullerene graphs, only for IPR (Isolated Pentagon Rule) fullerenes, and then their difference. However, this method requires pentagonal separation. In the following, a method is presented that does not require this separation.



Figure 4: TU-subgraphs of F_n generated by 8 edges.

Theorem 2.11. For the graph F_n , we have

$$\begin{aligned} \alpha_8 &= 4N(A) + 4N(B) + 4N(C) + 4N(D) \\ &+ 8N(E) + 8N(F) + 16N(G) + 12N(H) \\ &+ 32N(K) + 16N(L) + 24N(M) + 16N(N), \end{aligned}$$

where A, B, \ldots, N are depicted in Figure 4.

Proof. Note that the TU-subgraphs with 8 edges and a cycle in F_n are isomorphic to subgraphs depicted in Figure 3. Now we get

$$\begin{split} W(A) &= W(B) = W(C) = W(D) = 4, \, W(E) = W(F) = 8, \\ W(G) &= 16, \, W(H) = 12, \, W(K) = 32, \, W(L) = 16, \\ W(M) &= 24, \, W(N) = 16. \end{split}$$

Then by the proof of Theorem 2.1, the assertion holds.

48

3 Concluding remarks

In this research, the difference between Laplacian and signless Laplacian coefficients is calculated. Therefore, by calculating one of them, the other becomes available as well. It is recommended to proceed with the calculation of the coefficient α_{k+4} .

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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