On the Laplacian coefficients and Laplacian-like energy of unicyclic graphs with fixed diameter

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Abstract Let G be a graph of order n and let $\Phi(G,\lambda) = det(\lambda I_n - L(G)) = \sum_{k=0}^{n}(-1)^k c_k(G)\lambda^{n-k}$ be the characteristic polynomial of the Laplacian matrix of a graph G. In this paper, we identify the minimal Laplacian coefficients of unicyclic graphs with n vertices and diameter d. Finally, we characterize the graphs with the smallest and the second smallest Laplacian-like energy among the unicyclic graphs with n vertices and fixed diameter d.

Keywords Laplacian coefficients; unicyclic graph; diameter; Laplacian-like energy

AMS Subject Classification 05C50

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1 Introduction

Let $G = (V_G, E_G)$ be a simple undirected graph with n vertices and $L(G) = D(G) - A(G)$ be its Laplacian matrix. The Laplacian polynomial of G is the characteristic polynomial of its Laplacian matrix. That is

$$\Phi(G,\lambda) = det(\lambda I_n - L(G)) = \sum_{k=0}^{n}(-1)^k c_k(G)\lambda^{n-k}.$$

The Laplacian matrix $L(G)$ has non-negative eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ [1]. In particular, we have $c_0(G) = 1, c_1(G) = 2|E(G)|, c_n(G) = 0$ and $c_{n-1}(G) = n\tau(G)$, where $\tau(G)$ is the number of spanning trees of G.

Recently, the study on the Laplacian coefficients attracts much attention. Mohar [2] proved that among all trees of order n. Stevanovic and Ilic [3] showed that among all connected unicyclic graphs of order n. He and Shan [4] proved that among all bicyclic graphs of order n. Pai, Liu and Guo [5] showed that among all connected tricyclic graphs of order n, Ilic, Ilic and Stevanovic[6] verified the Wiener index and Laplacian coefficients of graphs with given diameter or radius.

Motivated by the results in [3-7,11,13] concerning the minimal Laplacian coefficients and Laplacian-like energy of some graphs and the minimal molecular graph energy, this article will characterize the unicyclic graphs with n vertices and diameter d, which minimize Laplacian-like energy.

A unicyclic graph is a connected graph in which the number of vertices equals the number of edges. We will use $\mathscr{U}_n^d$ to denote the set of all the unicyclic graph with n vertices and diameter d.

2 Transformations and Lemmas

In this section, we introduce some lemmas. The Laplacian coefficients $c_k(G)$ of a graph G can be expressed in terms of subtree structures of G by the following result of Kelmans and Chelnokov [8]. Let F be a spanning forest of G with components $T_i, i = 1, 2, \dots, k$ having n_i vertices each, and let $\gamma(F) = \prod_{i=1}^{k} n_i$.

Lemma 2.1([8]) The Laplacian coefficient $c_{n-k}(G)$ of a graph G is given by $c_{n-k}(G) = \sum_{F \in \mathscr{F}_k} \gamma(F)$, where $\mathscr{F}_k$ is the set of all spanning forests of G with exactly k components.

Let $T' = \delta(T, v)$, (see [10] for more details).

Lemma 2.2([10]) Let T be an arbitrary tree, rooted at the center vertex. Let vertex v be on the deepest level of tree T among all branching vertices with degree at least three. Then for the δ-transformation tree $T' = \delta(T, v)$and $0 \leq k \leq n$ holds $c_k(G) \geq c_k(G')$.

Let $C(a_1, \dots, a_{d-1})$ be a caterpillar obtained from a path P_d : $\{v_0, v_1, \dots, v_d\}$ by attaching a_i pendent edges to vertex v_i. For simplicity, $C_{n,d} = C(0, \dots, a_{\lfloor \frac{d}{2} \rfloor}, 0, \dots, 0)$ (see [6] for more details).

Lemma 2.3([6]) Among connected acyclic graphs on n vertices and diameter d, caterpillar $C(0, \dots, a_{\lfloor \frac{d}{2} \rfloor}, 0, \dots, 0)$, where $a_{\lfloor \frac{d}{2} \rfloor} = n-d-1$, has minimal Laplacian coefficients c_k, for every $k = 0, 1, \dots, n$.

Let G_{uv} is a α-transform of G, (see [13] for more details).

Lemma 2.4([13]) Let $G_{uv} = \alpha(G)$. Then $c_k(G) \geq c_k(G_{uv})$, with equality if and only if $k \in \{0, 1, n-1, n\}$ when uv is a cut edge or $k \in \{0, 1, n\}$ otherwise.

Let $G_2 =\triangleq \pi_2(G)$, (see [12] for more details).

Lemma 2.5([12]) Let $G_2 = \pi_2(G)$. Then for every $k = 0, 1, \dots, n$, $c_k(G) \geq c_k(G_2)$, with equality if and only if $k \in \{0, 1, n\}$.

Let $G^* = \pi_3(G)$(see [12] for more details).

Lemma 2.6([12]) Let G be a connected unicyclic graph with n vertices, $G^* = \pi_3(G)$. Then for every $k = 0, 1, \dots, n$, $c_k(G) \geq c_k(G^*)$, with equality if and only if $k \in \{0, 1, n-1, n\}$.

3 Main results

For $G \in \mathscr{U}_n^d$, we have $n \geq 3$ and $1 \leq d \leq n-2$. If $d = 1$, then $G \cong C_3$. Therefore, in the following, we assume that $d \geq 2$ and $n \geq 4$.

Let Δ_n^d be an n-vertex graph obtained from a triangle by attaching $n-d-2$ pendent edges and a path of length $\lfloor \frac{d}{2} \rfloor$ at one vertex of the triangle, and a path of length $\lceil \frac{d}{2} \rceil - 1$ to another vertex of the triangle, respectively. Let $\Delta_n^{d'}$ be an n-vertex graph obtained from a triangle by attaching $n-d-2$ pendent edges and a path of length $\lceil \frac{d}{2} \rceil - 1$ at one vertex of the triangle, and a path of length $\lfloor \frac{d}{2} \rfloor$ to another vertex of the triangle, respectively.

Note that if $d = n-2$ or $d \equiv 1 (mod 2)$, then $\Delta_n^d \cong \Delta_n^{d'}$.

Theorem 3.1 Let Δ_n^{2t} and $\Delta_n^{2t'}$ be the two graphs shown in Fig.

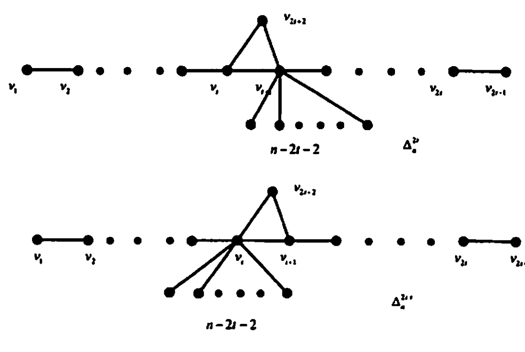

Fig.1 Graphs Δ_n^{2t} and $\Delta_n^{2t'}$

1. Suppose that $2 \leq t \leq \lfloor \frac{n-3}{2} \rfloor$. Then for every $k = 0, 1, \ldots, n$,

$$c_k(\Delta_n^{2t'}) \geq c_k(\Delta_n^{2t}),$$

with equality if and only if $k \in \{0, 1, n-1, n\}$.

Proof. It is easy to see that $c_0(\Delta_n^{2t'}) = c_0(\Delta_n^{2t}) = 1, c_1(\Delta_n^{2t'}) = 2|E(\Delta_n^{2t'})| = 2|E(\Delta_n^{2t})| = c_1(\Delta_n^{2t}), c_n(\Delta_n^{2t'}) = c_n(\Delta_n^{2t}) = 0$, $c_{n-1}(\Delta_n^{2t'}) = n\tau(\Delta_n^{2t'}) = 3n = n\tau(\Delta_n^{2t}) = c_{n-1}(\Delta_n^{2t})$.

Now, consider the coefficients $c_{n-k}(G)$ $(k \neq 0, 1, n-1, n)$. Let $\mathscr{F}_k$ and $\mathscr{F}'_k$ be the sets of spanning forests of Δ_n^{2t} and $\Delta_n^{2t'}$ with exactly k components, respectively. Obviously, by the Definition of the spanning forest, the cycle $C = v_t v_{t+1} v_{2t+2} v_t$ satisfies that $C \notin F \in \mathscr{F}_k$ and $C \notin F' \in \mathscr{F}'_k$, where F and F' are the arbitrary forests in $\mathscr{F}_k$ and $\mathscr{F}'_k$, respectively. Now, we distinguish the following three cases.

Case 1. We remove $v_t v_{t+1}$ in Δ_n^{2t} and $\Delta_n^{2t'}$, respectively. We can get T_1 and T'_1, (see fig. 2). Obviously, $T_1 = C(0, 0, \ldots, a_{t-1}, 0, \ldots, 0)$,

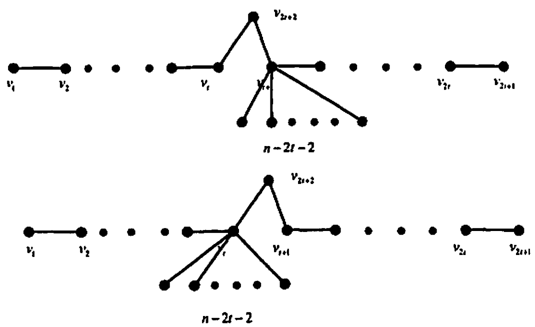

Fig. 2 T_1 *and* T'_1

$T'_1 = C(0, 0, \ldots, a_{t+1}, 0, \ldots, 0)$, where $a_{t-1} = a_{t+1} = n - 2t - 2$. At the same time, the diameters of T_1 and T'_1 are $2t+1$, v_{t+1}, v_{2t+2} are the two central vertices of T_1 and $2t+1$, v_{t+1}, v_{2t+2} are the two central vertices of T'_1, too. By Lemma 2.3, we know for every $k = 0, 1, \ldots, n$,

$$c_k(T_1) \leq c_k(T'_1). \tag{3.1}$$

Case 2. We remove $v_{t+1} v_{2t+2}$ in Δ_n^{2t} and remove $v_t v_{2t+2}$ in $\Delta_n^{2t'}$. We can get T_2 and T'_2. v_{t+1} is the central vertex of T_2 and T'_2, respectively. It is easy to see that $n \geq 2t+2$, and if $n = 2t+3$, we have $T_2 \cong T'_2$. When $n \geq 2t+2$, and $n \neq 2t+3$, we know that $T_2 = \delta(T'_2, v_t)$. Then using Lemma 2.2, we can get that for every $k = 0, 1, \ldots, n$,

$$c_k(T_2) \leq c_k(T'_2). \tag{3.2}$$

Case 3. We remove v_tv_{2t+2} in Δ_n^{2t} and remove $v_{t+1}v_{2t+2}$ in $\Delta_n^{2t'}$. We can get T_3 and T_3'. v_{t+1} is the central vertex of T_3 and T_3', respectively. We know that $T_3 = \delta(T_3', v_t)$. Then using Lemma 2.2, we can get that for every $k = 0, 1, \ldots, n$,

$$c_k(T_3) \le c_k(T_3'). \tag{3.3}$$

From Eqs. (3.1)−(3.3), according to Lemma 2.1, we have that for every $k = 0, 1, \ldots, n$, $c_k(\Delta_n^{2t}) \le c_k(\Delta_n^{2t'})$, with equality if and only if $k \in \{0, 1, n-1, n\}$. □

Let $\nabla_n^d(i)$ $(2 \le i \le d+1)$ be an n-vertex graph obtained from a triangle by attaching $n-d-3$ pendent edges and a path of length $i-1$ at one vertex of the triangle, and a path of length $d-i+1$ to the same vertex of the triangle, respectively (see Fig. 3).

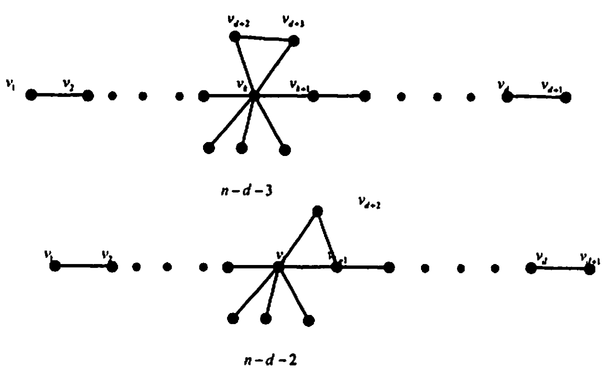

Fig.3 $\nabla_n^d(i)$ and $\Delta_n^d(i)$

Let $\Delta_n^d(i)$ $(2 \le i \le d+1)$ be an n-vertex graph obtained from a triangle by attaching $n-d-2$ pendent edges and a path of length $i-1$ at one vertex of the triangle, and a path of length $d-i$ to another vertex of the triangle, respectively (see Fig. 3). Note that if $i = 2$ or $i = d$, then $\Delta_n^d(i) \cong \nabla_n^d(i)$. And when $3 \le i \le d-1$, $\Delta_n^d(i) = \nabla_n^d(i) - v_{d+2}v_{d+3} + v_{d+2}v_{i+1}$.

Theorem 3.2 Suppose that $3 \le i \le d-1$. Then for every $k =$

$0, 1, \ldots, n$,

$$c_k(\nabla_n^d(i)) \geq c_k(\Delta_n^d(i)),$$

with equality if and only if $k \in \{0, 1, n-1, n\}$.

Proof. It is easy to see that $c_0(\nabla_n^d(i)) = c_0(\Delta_n^d(i)) = 1, c_1(\nabla_n^d(i)) = 2|E(\nabla_n^d(i))| = 2|E(\Delta_n^d(i))| = c_1(\Delta_n^d(i)), c_n(\nabla_n^d(i)) = c_n(\Delta_n^d(i)) = 0$, $c_{n-1}(\nabla_n^d(i)) = n\tau(\nabla_n^d(i)) = 3n = n\tau(\Delta_n^d(i)) = c_{n-1}(\Delta_n^d(i))$.

Now, consider the coefficients $c_{n-k}(G)$ $(k \neq 0, 1, n-1, n)$. Let $\mathscr{F}_k$ and $\mathscr{F}'_k$ be the sets of spanning forests of $\nabla_n^d(i)$ and $\Delta_n^d(i)$ with exactly k components, respectively. Let $F \in \mathscr{F}_k$ and T be the component of F. If $v_{d+2}v_{d+3} \in E(T)$, we define F' with $V(F) = V(F')$ and $E(F') = E(F) - v_{d+2}v_{d+3} + v_{d+2}v_{i+1}$. By the definition of spanning forest, we know that $v_i \notin V(T)$.

Let S contain $a \geq 1$ in the paths $P = v_{i+1}, \ldots, v(i+p)(1 \leq p \leq d-i+1)$. Assume the orders of the components of F different from T and S are $n_1, n_2, \ldots n_{k-2}$. We have

$$\gamma(F) - \gamma(F') = [2a - 1(a+1)] \prod_{i=1}^{k-2} n_i = (a-1) \prod_{i=1}^{k-2} n_i = (a-1)N,$$

where $N = \prod_{i=1}^{k-2} n_i$.

It is easy to see that $a \geq 1$, so $(a-1)N \geq 0$. Since at least one vertex is in P, there exists one forest F such that $a > 1$, and then $(a-1)N > 0$, i.e. $\gamma(F) > \gamma(F')$.

If $v_{d+2}v_{d+3} \notin E(T)$, we define $E(F') = E(F)$, so $\gamma(F) = \gamma(F')$.

Therefore, by using Lemma 2.1, we get $c_k(\nabla_n^d(i)) \geq c_k(\Delta_n^d(i))$, with equality if and only if $k \in \{0, 1, n-1, n\}$. This completes the proof of Theorem 3.2. □

Let U_0 be the unicyclic graph of order $d+2$ shown in Fig. 6. Let $U_0(p_2, \ldots, p_d, p_d + 2)$ be a graph of order n obtained from U_0 by attaching p_i pendent vertices to each $v_i \in V(U_0) \backslash \{v_1, v_{d+1}\}$, respec-

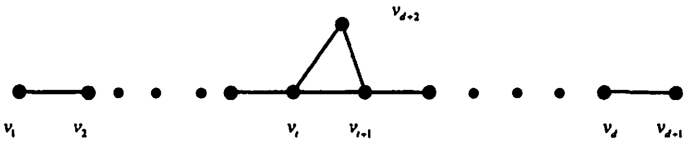

Fig.4 Graph U_0

tively, where $p_{d+2} = 0$ when $k = 1$ or $k = d$. Denote

$$\widetilde{\mathscr{U}_n^d} = \{U_0(p_2, \ldots, p_d, p_{d+2}) : \sum_{i=2}^{d} p_i + p_{d+2} = n - d - 2\}$$

and $\overline{\mathscr{U}}_n^d = \{U_0(0, \ldots, 0, p_i, 0, \ldots, 0) : p_i \geq 0\}$.

Theorem 3.3 Let $G \in \widetilde{\mathscr{U}_n^d} \backslash \overline{\mathscr{U}}_n^d$. Then there is a graph $G^* \in \overline{\mathscr{U}}_n^d$ such that for every $k = 0, 1, \ldots, n$,

$$c_k(G) \geq c_k(G^*),$$

with equality if and only if $k \in \{0, 1, n-1, n\}$.

Proof. Suppose $G \in \widetilde{\mathscr{U}_n^d} \backslash \overline{\mathscr{U}}_n^d$. If $p_{d+2} \geq 1$, such that $v_{d+2}u_1, v_{d+2}u_2, \ldots, v_{d+2}u_{p_{d+2}}$ are pendent edges incident with v_{d+2}. Let $G^* = G - v_{d+2}u_1 - v_{d+2}u_2 - \ldots - v_{d+2}u_{p_{d+2}} + v_{i+1}u_1 + v_{i+1}u_2 + \ldots + v_{i+1}u_{p_{d+2}}$. It is easy to see that $c_0(G^*) = c_0(G) = 1, c_1(G^*) = 2|E(G^*)| = 2|E(G)| = c_1(G), c_n(G^*) = c_n(G) = 0$, $c_{n-1}(G^*) = n\tau(G^*) = 3n = n\tau(G) = c_{n-1}(G)$.

Now, consider the coefficients $c_{n-k}(G)$ $(k \neq 0, 1, n-1, n)$. Let $\mathscr{F}_k$ and $\mathscr{F}_k^*$ be the sets of spanning forests of G and G^* with exactly k components, respectively. Obviously, by the Definition of the spanning forest, the cycle $C = v_i v_{i+1} v_{d+2} v_i$ satisfies that $C \notin F \in \mathscr{F}_k$ and $C \notin F^* \in \mathscr{F}_k^*$, where F and F^* are the arbitrary forests in $\mathscr{F}_k$ and $\mathscr{F}_k^*$, respectively. The next proof is similar to the proof of Theorem 3.1. Then we have that $c_k(G) \geq c_k(G^*)$.

When $p_{d+2} = 0$, let $2 \leq r \leq i$ be the smallest index such that $a_r > 0$, and let $i + 2 \leq s \leq d$ be the largest index such that $a_s > 0$.

We can apply π_3−transformation to vertex v_r or v_s, and get the graph G^* obtained by moving pendent vertices to the vertex v_{r+1} or v_{s-1} of a path. After applying the algorithm, we finally get the graph $G^* \in \overline{\mathscr{U}}_n^d$. According to Lemma 2.6, we have that for every $k = 0, 1, \ldots, n$ $c_k(G) \geq c_k(G^*)$, with equality if and only if $k \in \{0, 1, n-1, n\}$.

From the above proof, we know there is a graph $G^* \in \overline{\mathscr{U}}_n^d$ such that for every $k = 0, 1, \ldots, n$, $c_k(G) \geq c_k(G^*)$, with equality if and only if $k \in \{0, 1, n-1, n\}$. □

Theorem 3.4 For any graph $G \in \widetilde{\mathscr{U}_n^d}$, $3 \leq d \leq n-2$, we have that for every $k = 0, 1, \ldots, n$,

$$c_k(G) \geq c_k(\Delta_n^d),$$

with equality if and only if $k \in \{0, 1, n\}$.

Proof. By the proof of Theorem 3.3, we have if $p_j > 0$, then $j = i$ or $j = i+1$. Next, we only need to prove that $i = \lceil \frac{d}{2} \rceil$.

Otherwise, without loss of generality, suppose that $i = 2$, we denote the graph H. If $i = \lceil \frac{d}{2} \rceil$, we denote the graph G.

Obviously, $c_0(H) = c_0(G) = 1$, $c_1(H) = c_1(G) = n$, $c_n(H) = c_n(G) = 0$, $c_{n-1}(H) = c_{n-1}(G) = 3n$.

Now, consider the coefficients c_{n-k} $(k \neq 0, 1, n-1, n)$. Let $\mathscr{F}_k$ and $\mathscr{F}_{k_1}$ be the sets of spanning forests of H and G with exactly k components, respectively. Obviously, by the Definition of the spanning forest, the cycle $C_H = v_2 v_3 v_{d+2} v_2$ and $C_G = v_{\lceil \frac{d}{2} \rceil} v_{\lceil \frac{d}{2} \rceil + 1} v_{d+2} v_{\lceil \frac{d}{2} \rceil}$ satisfie that $C_H \notin F \in \mathscr{F}_k$ and $C_G \notin F_1 \in \mathscr{F}_{k_1}$, where F and F_1 are the arbitrary forests in $\mathscr{F}_k$ and $\mathscr{F}_{k_1}$, respectively. The next proof is similar to the proof of Theorem 3.1. □

From the proof of Theorems 3.3 and 3.4, we have

Theorem 3.5 For any graph $G \in \widetilde{\mathscr{U}_n^d} \backslash \{\Delta_n^d\}$ with $d \equiv 0 (mod 2)$ and $4 \leq d \leq n-3$, we have that for every $k = 0, 1, \ldots, n$,

$$c_k(G) \geq c_k(\Delta_n^{d'}),$$

with equality if and only if $k \in \{0, 1, n\}$.

Theorem 3.6 Let G be a graph in $\mathscr{U}_n^d$, $d \geq 1$. Then for every $k = 0, 1, \ldots, n$,

$$c_k(G) \geq c_k(\Delta_n^d),$$

with equality if and only if $k \in \{0, 1, n\}$.

Proof. If $d = 1$, then $G \cong C_3$. If $d = 2$, then $G \cong C_4$, $G \cong C_5$ or $G \cong \Delta_n^2$. Thus, by Lemma 2.4, the result holds for $d = 1, 2$. Therefore, we can assume that $3 \leq d \leq n - 2$.

Choose $G \in \mathscr{U}_n^d$ such that the Laplacian coefficients of G are as small as possible. Let $P = v_1 v_2 \ldots v_{d+1}$ be the induced path of length d and let C_q be the only cycle in G. We first proof the next claim.

Claim: $V(C_q) \cap V(P_d) \neq \emptyset$.

Otherwise, since G is connected, there exists an path $v_i v_k \cdots v_l$ connecting C_q and P_d, where $v_i \in V(C_q)$, $v_l \in V(P_d)$ and $v_k, \cdots, v_{l-1} \in V(G) \backslash (V(C_q) \cup V(P_d))$. We can get $G_{v_i v_k} = \alpha(G)$, according Lemma 2.4, we have $c_k(G) \geq c_k(G_{v_i v_k})$, a contradiction. Then, $V(C_q) \cap V(P_d) \neq \emptyset$.

Since $V(C_q) \cap V(P_d) \neq \emptyset$, let $C_q = u_1 \cdots u_l v_1 \cdots v_s u_1$ $(s \geq 1)$, where $u_1, \cdots, u_l = V(C_q) \cap V(P_d)$ and $v_1, \cdots, v_s = V(C_q) \backslash V(P_d)$. If $l \geq 2$, we can apply π_2-transformation on C_q as long as $C_q \neq C_3$. According to Lemma 2.5, we have that for every $k = 0, 1, \ldots, n$ $c_k(G) \geq c_k(G^*)$, with equality if and only if $k \in \{0, 1, n-1, n\}$.

Let $P = v_1 v_2 \ldots v_{d+1}$ be the induced path of length d. Every $v_i (2 \leq i \leq d)$ on the path P is a root of a tree T_i with $a_i (a_2 \leq 1, and a_d \leq 1)$ vertices, that does not contain other vertices of P. We apply $\alpha-$transformation on trees $T_2, T_3, \ldots, T_{d-1}$ and the cycle C_q as long as we get the graph $G^* \notin \widetilde{\mathscr{U}_n^d}$ or $G^* \notin \{\nabla_n^d(i) | 2 \leq i \leq d\}$. By Lemma 2.4, it is easy to see that for every $k = 0, 1, \ldots, n$, $c_k(G) \geq c_k(G^*)$, with equality if and only if $k \in \{0, 1, n\}$, and $G^* \in \widetilde{\mathscr{U}_n^d}$.

On the basis of Theorems 3.2 and 3.3, we know that there exists

$G^{**} \in \overline{\mathscr{U}}_n^d$ such that for every $k = 0, 1, \ldots, n$, $c_k(G^*) \geq c_k(G^{**})$, with equality if and only if $k \in \{0, 1, n-1, n\}$. By Theorem 3.4, Theorem 3.6 follows immediately. □

Theorem 3.7 For any graph $G \in \mathscr{U}_n^d \backslash \{\Delta_n^d\}$ with $d \equiv 0(mod2)$ and $4 \leq d \leq n-3$, we have that for every $k = 0, 1, \ldots, n$,

$$c_k(G) \geq c_k(\Delta_n^{d'}),$$

with equality if and only if $k \in \{0, 1, n\}$.

4 Laplacian-like energy of unicyclic graphs with fixed diameter

The Laplacian-like energy of graph G, LEL for short, is defined as follows: $LEL(G) = \sum_{k=1}^{n-1} \sqrt{\mu(k)}$, where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the Laplacian eigenvalues of G. This concept was introduced by Liu and Liu [7], where it was demonstrated it has similar feature as molecular graph energy (for more details see [8]). Stevanović in [9] presented a connection between LEL and Laplacian coefficients.

Theorem 4.1([9]) Let G and H be two graphs with n vertices. If $c_k(G) \leq c_k(H)$ for $k = 1, 2, \cdots, n-1$, then $LEL(G) \leq LEL(H)$. Furthermore, if a strict inequality $c_k(G) < c_k(H)$ holds for some $1 \leq k \leq n-1$, then $LEL(G) < LEL(H)$.

Corollary 4.2. Let G be a graph in $\mathscr{U}_n^d$. Then if $G \not\cong \Delta_n^{d'}$, and $G \not\cong \Delta_n^d$, $LEL(G) > LEL(\Delta_n^{d'}) > LEL(\Delta_n^d)$.

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