SOME POSETS OF UNICYCLIC GRAPHS BASED ON SIGNLESS LAPLACIAN COEFFICIENTS

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ABSTRACT. Let G be a graph of order n and let $Q(G,x) = \det(xI - Q(G)) = \sum_{i=0}^{n}(-1)^i\zeta_i x^{n-i}$ be the characteristic polynomial of the signless Laplacian matrix of G. We show that the *Lollipop* graph, $L_{n,3}$, has the maximal Q-coefficients, among all unicyclic graphs of order n except C_n. Moreover, we determine graphs with minimal Q-coefficients, among all unicyclic graphs of order n.

1. INTRODUCTION

Throughout this paper we consider simple undirected graphs with n vertices and m edges. Let G be a graph. The vertex set and the edge set of G are denoted by $V(G)$ and $E(G)$, respectively. Let $A(G)$ be the $(0,1)$-adjacency matrix of G. Since $A(G)$ is a symmetric matrix with real entries, its eigenvalues are real. With no loss of generality, we can write them in non-increasing order as $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$. The adjacency characteristic polynomial of the graph G is denoted by $A_G(x) = det(xI - A(G)) = \sum_{i=0}^{n} a_i(G)x^{n-i}$.

A subgraph H of G is called an elementary subgraph if each component of H is either an edge or a cycle. Denote by $c(H)$ and $e(H)$ the number of components in a subgraph H which are cycles and edges, respectively.

Theorem 1.1. [1] *Let G be a graph of order n. Then we have*

$$a_k(G) = \sum(-1)^{k-c(H)-e(H)}2^{c(H)},$$

where the summation is over all the elementary subgraphs H of G with k vertices, $k = 1, 2, \ldots, n$.

Note that for the empty graph, i.e. $G = K_0$, we have $A_G(x) = 1$. An r-matching in a graph G is a set of r edges, such that none of them have a vertex in common, where $r \geq 1$. The number of r-matchings in G is denoted

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by $M(G,r)$. If G is a tree, then $A_G(x) = \sum_{i=0}^{\lfloor n/2 \rfloor}(-1)^i M(G,i)x^{n-2i}$. The following theorem specifies a recurrence relation for $M(G,r)$.

Theorem 1.2. [4] *The number of r-matchings satisfies the following identities:*

(i) $M(G \cup H, r) = \sum_{i=0}^{r} M(G,i)M(H,r-i)$,

(ii) $M(G,r) = M(G-e,r) + M(G-u-v,r-1)$, *if* $e = uv$ *is an edge of* G,

(iii) $M(G,r) = M(G-v,r) + \sum_{u \in N(v)} M(G-v-u,r-1)$, *if* $v \in V(G)$.

Suppose that $D(G) = diag(d_G(v_1), \ldots, d_G(v_n))$ is a diagonal matrix and and $d_G(v)$ denotes the degree of the vertex v in G. Let $L(G) = D(G) - A(G)$ be the Laplacian matrix of G. Related to the Laplacian matrix is the so-called signless Laplacian matrix of G, $Q(G) = D(G) + A(G)$, which has recently been studied (see e.g. [2]). As it is well-known, $L(G)$ and $Q(G)$ are positive semi-definite, and they have the same characteristic polynomial if and only if G is a bipartite graph. The eigenvalues of the matrices $L(G)$ and $Q(G)$ are denoted by $\mu_1(G) \geq \mu_2(G) \geq \ldots \geq \mu_n(G) = 0$ and $\nu_1(G) \geq \nu_2(G) \geq \ldots \geq \nu_n(G) \geq 0$, respectively. The second smallest eigenvalue of $L(G)$, $\mu_{n-1}(G)$, is called the algebraic connectivity of G, and is positive if and only if the graph is connected.

Furthermore, the Laplacian characteristic polynomial of G is denoted by $L_G(x) = det(xI - L(G)) = \sum_{i=0}^{n}(-1)^i \xi_i x^{n-i}$. One may see that the Laplacian coefficient, ξ_{n-k}, can be expressed in terms of subtree structures of G, for $k = 0, 1, \ldots, n$ (see e.g. [1]). Suppose that F is a spanning forest of G with components T_i, $i = 1, 2, \ldots, k$; having n_i vertices each. Let $\gamma(F) = \prod_{i=1}^{k} n_i$. Then we have the following result of Kelmans and Chelnokov.

Theorem 1.3. [1] *The Laplacian coefficient* ξ_{n-k} *of a graph* G *is given by*

$$\xi_{n-k} = \sum_{F \in \mathfrak{F}_k} \gamma(F),$$

where $\mathfrak{F}_k$ *is the set of all spanning forests of* G *with exactly* k *components.*

In particular, we have $\xi_0 = 1$, $\xi_1 = 2m$, $\xi_n = 0$, and $\xi_{n-1} = n\tau(G)$, in which $\tau(G)$ denotes the number of spanning trees of G (see, e.g. [13]).

The characteristic polynomial of the signless Laplacian matrix of G is denoted by $Q_G(x) = det(xI - Q(G)) = \sum_{i=0}^{n}(-1)^i \zeta_i x^{n-i}$. Using the terminology and notation from [2], a spanning subgraph of G whose connected components are trees or odd unicyclic graphs is called a TU-subgraph of G. Suppose that a TU-subgraph H of G contains c odd unicyclic graphs and s trees such as $T_1, \ldots, T_s$. Then the weight of H, $W(H)$, is defined by $W(H) = 4^c \prod_{i=1}^{s} n_i$, in which n_i is the number of the vertices of T_i. Note that if H contains no tree, then $W(H) = 4^c$. According to the following theorem, ζ_i can be expressed in terms of the weight of TU-subgraphs of G.

Theorem 1.4. [2, Theorem 4.4] *Let G be a connected graph. For ζ_i as above, we have $\zeta_0 = 1$ and*

$$\zeta_i = \sum_{H_i} W(H_i), \quad i = 1, \ldots, n;$$

where the summation is over all TU-subgraphs H_i of G with i edges.

In particular, we have (see, e.g. [2]) $\zeta_0 = 1$, $\zeta_1 = 2m$, and

$$\zeta_2 = 2m^2 - m - \frac{1}{2}\sum_{i=1}^{n} d_i^2. \tag{1}$$

Also, it is easy to check that for trees we have (see e.g. [19])

$$\zeta_i(T) = \xi_i(T) = M(S(T), i), \quad for\ i = 0, 1, \ldots, n.$$

The following relations are well-known (see e.g. [2])

$$I(G)I(G)^t = Q(G), \quad I(G)^t I(G) = A(\mathcal{L}(G)) + 2I_m, \tag{2}$$

where $\mathcal{L}(G)$ is the line graph of G. Since non-zero eigenvalues of $I(G)I(G)^t$ and $I(G)^t I(G)$ are identical, Equation (2) implies that

$$A_{\mathcal{L}(G)}(x) = (x+2)^{m-n} Q_G(x+2). \tag{3}$$

The *subdivision graph* of G, $S(G)$, is the graph obtained by inserting an additional vertex in each edge of G (see, e.g. [1]). So that, its adjacency matrix is of the form

$$\begin{bmatrix} 0 & I(G) \\ I(G)^t & 0 \end{bmatrix}.$$

Hence, by [12, Theorem 1], the adjacency eigenvalues of $S(G)$ are $\pm\sqrt{\nu_i(G)}$, and so we have

$$A_{S(G)}(x) = x^{m-n} Q_G(x^2). \tag{4}$$

The path, the cycle, and the star on n vertices are denoted by P_n, C_n, and S_n, respectively. If $e \in E(G)$, then $G - e$ denotes the subgraph of G with vertex set $V(G)$ and edge set $E(G) \setminus \{e\}$. Also if $v \in V(G)$, then the graph $G - v$ is an induced subgraph of G, obtained from G by deleting the vertex v and all edges incident with it. In addition, a vertex of degree one is called a pendent vertex and a vertex is said to be quasipendent if it is incident to a pendent vertex. For any $v \in V(G)$, let $N_G(v)$ denote the set of all vertices adjacent to v.

In analogy to the following result (Theorem 1.5), in the article [7], Gutman et al. gave a conjecture for Laplacian coefficients, ξ_i, of trees. More precisely, they conjectured that $\xi_i(S_n) \le \xi_i(T) \le \xi_i(P_n)$ where T is a tree on n vertices, for each i $(1 \le i \le n)$.

Theorem 1.5. [5, Proposition 3.2] *Among trees with n vertices, P_n has maximal adjacency coefficients.*

Using connection between ξ_i and the number of i–matchings of the subdivision graph of trees, Zhou et al. proved this conjecture [19]. After that, in [15], it was shown that all Laplacian coefficients of trees are monotone under two transformations called π and σ. As a result, a different proof for the above conjecture was presented. Stevanović et al. in the article [17], generalizing the approach of Mohar on graph transformations [15], showed that the extreme values of the Laplacian coefficients ξ_i $(1 \leq i \leq n)$, among all connected unicyclic graphs of order n, are attained on one side by C_n and on the other side by S_n^+, where S_n^+ denotes the graph consisting of a star and an additional edge.

In the present paper, using graph transformations, we state some results about coefficients of the signless Laplacian characteristic polynomial of graphs, focusing our attention on the unicyclic graphs. As a main result, the above problem is studied for coefficients of the signless Laplacian characteristic polynomial. More precisely, let G be a unicyclic graph of order n and $G \not\cong C_n$, it is shown that, for $0 \leq i \leq n$, $\zeta_i(G) \leq \zeta_i(L_{n,3})$, in which $L_{n,p}$ is the lollipop graph, obtained by attaching a cycle C_p to a pendent vertex of the path P_{n-p}. However, one may check that the Q–coefficients of the graphs C_n and $L_{n,3}$ are not comparable. Moreover, it is shown that $\zeta_i(G) \geq \zeta_i(S_n^+)$, if n is odd, otherwise $\zeta_i(G) \geq \zeta_i(R_n)$, where R_n is C_4 with $n-4$ pendent vertices attached to one of whose vertices and $0 \leq i \leq n$. Finally, we order unicyclic graphs based on their incidence energy.

2. Main Results

Connected graphs in which the number of edges equals the number of vertices are called unicyclic graphs. Therefore, a unicyclic graph is either a cycle or a cycle with trees attached. A unicyclic graph containing an odd cycle (even cycle) is called odd unicyclic (even unicyclic). Let $\mathfrak{U}_{n,g}$ be the set of all unicyclic graphs on n vertices with girth g. If $U \in \mathfrak{U}_{n,g}$, then U consists of the cycle C of length g and a certain number of trees attached to the vertices of C having in total $n-g$ edges. Suppose that the vertices of the cycle C are labeled by $v_1, \ldots, v_g$ such that v_i comes after v_{i-1}. Furthermore, assume that T_i is a rooted tree of order $n_i \geq 1$ attached to v_i. Then we denote U by $C(T_1, \ldots, T_g)$ (see Fig. 1). Now, we have the following corollaries.

Corollary 2.1. [14, Corollary 2.9] *Let $H = G(T_1, \ldots, T_n)$. Then for each $1 \leq k \leq n$ we have*

$$\zeta_i(G(T_1, \ldots, S_{m_k}, \ldots, T_n)) \leq \zeta_i(H) \leq \zeta_i(G(T_1, \ldots, T_{k-1}, P_{m_k}, T_{k+1}, \ldots, T_n)),$$

where $0 \leq i \leq n$; Moreover, both extremal graphs are unique.

Corollary 2.2. [14, Corollary 3.1] *Let $U \in \mathfrak{U}_{n,g}$. Then we have*

$$\zeta_i(C(S_{n_1}, \ldots, S_{n_g})) \leq \zeta_i(U) \leq \zeta_i(C(P_{n_1}, \ldots, P_{n_g})),$$

for $i = 0, 1, \ldots, n$. Moreover, both extremal graphs are unique.

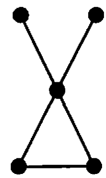


Fig. 1. The graph $C(S_3, S_1, S_1)$

Definition 2.3. *Let G be a connected graph and let $e = uv$ be a non-pendent edge of G not contained in cycles of length 3. Let $G' = \tau(G, u, v)$ denote the graph obtained from G in the following way:*

(1) *Delete the edge e;*
(2) *Identify u and v, and denote the new vertex by w;*
(3) *Add a pendent edge ww' to w;*

We say G' is a τ-Transformation of G at uv.

Theorem 2.4. [17, Theorem 3.2] *Let $G = C(S_{n_1}, S_{n_2}, T_3, \ldots, T_g)$ and let $G' = \tau(G, v_1, v_2)$ be a $\tau-$transformation of a unicyclic graph G. For every $0 \leq i \leq n$ holds $\xi_i(G') \leq \xi_i(G)$, with equality if and only if $i \in \{0, 1, n\}$.*

Theorem 2.5. [18, Theorem 2.2] *Let G be a connected graph and $e = uv$ be a non-pendent edge of G not contained in cycles of length 3. Then $\xi_i(G) \geq \xi_i(\tau(G, u, v))$, for $i = 0, 1, \ldots, n$; with equality if and only if $i \in \{0, 1, n-1, n\}$ when e is a cut edge or $i \in \{0, 1, n\}$ otherwise.*

It is worth mentioning that the previous theorem does not hold for coefficients of the signless Laplacian characteristic polynomial (see Fig. 2). It is easy to check that $Q_G(x) = x^5 - 10x^4 + 34x^3 - 46x^2 + 20x$, and $Q_{G'}(x) = x^5 - 10x^4 + 32x^3 - 42x^2 + 23x - 4$, where G and G' are shown in Fig. 2.

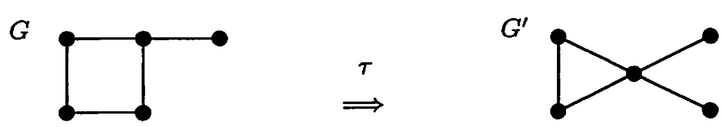


Fig. 2. τ-transformation

We want to generalize the above theorem to the case of Q-coefficient of unicyclic graphs as you see in the following.

Theorem 2.6. [14] *Let G be a graph of order n and size m, then the first derivative of the signless Laplacian characteristic polynomial of G is equal to*

$$xQ'_G(x) = (n - m)Q_G(x) + \sum_{e \in E(G)} Q_{G-e}(x).$$

Consequently, for each $1 \le i \le n$ one may obtain

$$(5) \qquad (m-i)\zeta_i(G) = \sum_{e \in E(G)} \zeta_i(G-e).$$

Remark 2.7. *Let G be a graph of order n. It is easy to check that if n is an even (resp. odd) number, then all non-zero coefficients of the polynomial $Q_G(-x)$ are positive (resp. negative). Hence, if we want to show that a transformation does not decrease the amount of all coefficients, it is enough to prove that for even (resp. odd) n, all non-zero coefficients of the polynomial $Q_{G'}(-x) - Q_G(-x)$ are greater (resp. less) than zero.*

Example 2.8. *Let $G = C_n$ and G' be the graph shown in the below figure, where $n \ge 5$. We want to show that $\zeta_i(G) \ge \zeta_i(G')$, for $1 \le i \le n$.*

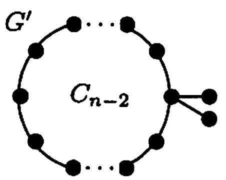


Fig. 3. *The graph G'*

Obviously, we have $\zeta_1(G) = \zeta_1(G') = 2n$ and $\zeta_n(G) = \zeta_n(G') = 4$, if n is odd, otherwise $\zeta_n(G) = \zeta_n(G') = 0$. Also, by Theorem 1.4, $\zeta_{n-1}(G) = n^2 \ge \zeta_{n-1}(G') = 8+n(n-2)$, when $n \ge 5$. So that it is enough to show that for $2 \le i \le n-2$ the claim holds. Using Equation 4, we equivalently show that for $2 \le i \le n-2$, $a_{2i}(S(G)) \ge a_{2i}(S(G'))$. Let $e = uv \in E(S(G))$, and let $e' = u'v'$ be an edge on the cycle in the graph $S(G')$ which is incident with a vertex of degree 4. Applying Theorem 1.2, one may see that

$$\begin{aligned}(-1)^i a_{2i}(S(G)) &= M(S(G)-e,i) + M(S(G)-u-v,i-1)\\ &= M(P_{2n},i) + M(P_{2n-2},i-1),\\ (-1)^i a_{2i}(S(G')) &= M(S(G')-e',i) + M(S(G')-u'-v',i-1).\end{aligned}$$

On the other hand, by Theorem 1.5, we have $M(S(G')-e',i) \le M(S(G)-e,i)$. Also, one may check that the graph $S(G')-u'-v' = 2P_2 \cup P_{2n-6}$ and $S(G)-u-v = P_{2n-2}$. So, the graph $S(G')-u'-v'$ is a spanning subgraph of $S(G)-u-v$, and hence $M(S(G')-u'-v',i-1) \le M(S(G)-u-v,i-1)$. Therefore the claim is proved.

Theorem 2.9. *Let $G = C(S_{n_1}, S_{n_2}, S_{n_3}, T_4, \ldots, T_g)$ be a unicyclic graph on n vertices with girth g, and $G' = \tau(\tau(G, v_1, v_2), v_2, v_3)$ be a τ-transformation of the unicyclic graph $\tau(G, v_1, v_2)$, and $g \ge 5$. Then $\zeta_i(G) \ge \zeta_i(G')$, for each $0 \le i \le n$.*

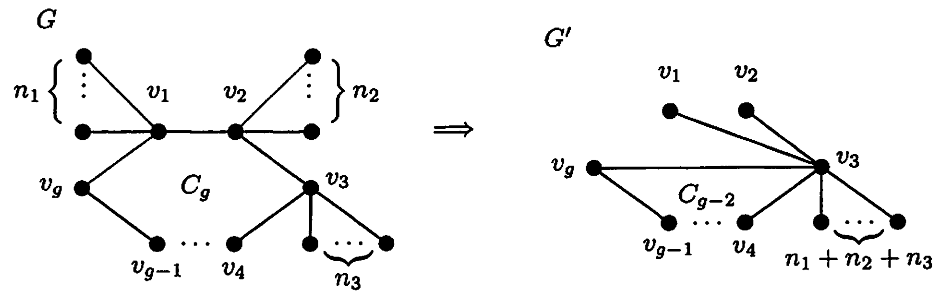


Fig. 4. The graphs G and G'

Proof. Let G be an even unicyclic graph. Since, in this case, two matrices $L(G)$ and $Q(G)$ are similar, the result follows from Theorem 2.4. So, suppose that G is an odd unicyclic graph. Because the graph G' is also an odd unicyclic graph, the signless Laplacian coefficients $\zeta_0(G')=1$, $\zeta_1(G')=2n$, and $\zeta_n(G')=4$ remain the same.

Let $\Lambda(x)=xQ'_G(x)-xQ'_{G'}(x)$. According to Equation (5), we obtain

$$\begin{aligned}\Lambda(x) &= xQ'_G(x)-xQ'_{G'}(x)\\ &= \sum_{i=0}^{n-1}(-1)^i(n-i)(\zeta_i(G)-\zeta_i(G'))x^{n-i}\\ &= \sum_{e\in E(G)} Q_{G-e}(x)-\sum_{e'\in E(G')} Q_{G'-e'}(x).\end{aligned}$$

We must show that all non-zero coefficients of the polynomial $\Lambda(-x)$, for even (resp. odd) n are positive (resp. negative). Equivalently, we prove that all non-zero coefficients of the polynomial $Q_{G-e}(-x)-Q_{G'-e'}(-x)$ for even (resp. odd) n are positive (resp. negative), where $e\in E(G)$ and e' is the corresponding edge in G', i.e.

$$\begin{aligned}
e=v_1v_2 &\longleftrightarrow e'=v_1v_3,\\
e=v_1v_g &\longleftrightarrow e'=v_3v_g,\\
e=v_1w &\longleftrightarrow e'=v_3w,\ \forall w\in N(v_1)\setminus\{v_2,v_g\};\\
e=v_2w &\longleftrightarrow e'=v_3w,\ \forall w\in N(v_2)\setminus\{v_1,v_3\};
\end{aligned}$$

and $e=e'$ for the other edges. Furthermore, this correspondence is an injection.

By induction on n, we prove this claim. By Example 2.8, one may see that for $n=g$ the assertion holds. So, suppose that $n\geq g+1$. Thus, the following cases occur:

Case i: If $e\notin\{v_1v_2,v_2v_3\}$, then let e' is whose corresponding edge in G'. If e is contained in the cycle, then $G-e$ is a tree, so that by Theorem 2.5

we are done. Otherwise, the unicyclic connected component of the graph $G-e$ is of order less than n. Then, by induction hypothesis, all non-zero coefficients of the polynomial $Q_{G-e}(-x)-Q_{G'-e'}(-x)$, for even (resp. odd) n are positive (resp. negative).

Case ii: If $e=v_1v_2$, then whose corresponding edge is $e'=v_1v_3 \in E(G')$. In this case, in a straightforward manner, we show that $\zeta_i(G-e) \geq \zeta_i(G'-e')$, for $2 \leq i \leq n-1$. Let $\omega(G,e)$ be the set of all TU-subgraphs of $G-e$ with i edges and let $\omega(G',e')$ be the set of all TU-subgraphs of $G'-e'$ with i edges. Consider $H' \in \omega(G',e')$. If $\widehat{e}=v_3v_g \notin E(H')$, then the following hold:

• If $v_2v_3 \in E(H')$. Suppose that H' has the tree component T, such that T contains the vertices v_2, v_3, and $a \geq 0$ pendent vertices in $N_G(v_1)$. Let $c=|V(T)|-a$, where $c \geq 2$. Moreover, H' contains an isolated vertex v_1. Therefore, $W(H')=(a+c)N$, for some constant value N. Let $H \in \omega(G,e)$ obtained from H' by removing a edges incident with pendent vertices in $\Big(V(T)\cap N_G(v_1)\Big)\setminus\{v_2\}$ and joining them to the vertex v_1, and also removing the edges incident with pendent vertices in $\Big(V(T)\cap N_G(v_2)\Big)\setminus\{v_3\}$, and joining them to v_2. One may check that $W(H)=(a+1)cN > W(H')$. Moreover, this correspondence is obviously an injection.

• If $v_2v_3 \notin E(H')$. Suppose that H' has tree component T, such that T contains the vertex v_3, $a \geq 0$ pendent vertices in $N_G(v_1)$, and $b \geq 0$ pendent vertices in $N_G(v_2)$. Let $c=|V(T)|-a-b$, where $c \geq 1$. Moreover, H' contains two isolated vertices v_1 and v_2. Therefore, $W(H')=(a+b+c)N$, for some constant value N. Let $H \in \omega(G,e)$ obtained from H' by removing a edges incident with pendent vertices in $V(T)\cap N_G(v_1)$ and joining them to the vertex v_1, and also removing b edges incident with pendent vertices in $V(T)\cap N_G(v_2)$, and joining them to v_2. One may check that $W(H)=(a+1)(b+1)cN \geq W(H')$. Moreover, this correspondence is obviously an injection.

So, assume that $\widehat{e}=v_3v_g \in E(H')$, then the following occur:

(1) Let U be the an odd unicyclic component of H' which contains the edges $\widehat{e}$ and v_2v_3. Moreover, H' contains an isolated vertex v_1. So, $W(H')=4N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. It is easy to check that, $W(H)=(|V(U)|+1)N \geq 4N=W(H')$, because the girth of U is greater than or equal to 3, so that $|V(U)|+1 \geq 4$. Moreover, this correspondence is obviously an injection.

(2) Let U be the an odd unicyclic component of H' which contains the edge $\widehat{e}$ and $a \geq 0$ pendent vertices adjacent to v_2 in the graph G. Also, suppose that $v_2v_3 \notin E(H')$. Therefore, H' contains two isolated vertices v_1 and v_2. So, $W(H') = 4N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. It is easy to check that, $W(H) = (|V(U)| - a + 1)(a+1)N \geq 4N = W(H')$, because the girth of U is greater than or equal to 3, thus $|V(U)| - a + 1 \geq 4$. Moreover, this correspondence is obviously an injection.

(3) Let T be the tree component of H' which contains the edges $\widehat{e}$ and v_2v_3. Suppose that T contains $a \geq 0$ pendent vertices in $N_G(v_1)$. Also, H' contains an isolated vertex v_1. Obviously, by removing the edge $\widehat{e}$ from T, two subtrees of order c and $d + a$ are obtained, where $c \geq 1$ and $d \geq 2$. So, $W(H') = (a + c + d)N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. It is easy to check that, $W(H) = (a+c+1)dN \geq W(H')$, where $c \geq 1$ and $d \geq 2$. Moreover, this correspondence is obviously an injection.

(4) Let T be the tree component of H' which contains the edges $\widehat{e}$ and $v_2v_3 \notin E(T)$. Suppose that T contains $a \geq 0$ and $b \geq 0$ pendent vertices, which are adjacent to v_1 and v_2 in the graph G, respectively. Moreover, H' contains two isolated vertices v_1 and v_2. Obviously, by removing the edge $\widehat{e}$ from T, two subtrees of order c and $d + a + b$ are obtained, where $c, d \geq 1$. So, $W(H') = (a+b+c+d)N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. It is easy to check that, $W(H) = (a + c + 1)(b + 1)dN \geq W(H')$, where $c, d \geq 1$. Moreover, this correspondence is obviously an injection.

Case iii: If $e = v_2v_3 = e'$. In this case, in a straightforward manner, we show that $\zeta_i(G-e) \geq \zeta_i(G'-e')$, for $2 \leq i \leq n-1$. Consider $H' \in \omega(G', e')$.

If $\widehat{e} = v_3v_g \notin E(H')$, then the following hold:

• If $v_1v_3 \in E(H')$. Suppose that H' has tree component T, such that T contains the vertices v_1, v_3, and $a \geq 0$ pendent vertices in $N_G(v_1)$ and $b \geq 0$ pendent vertices in $N_G(v_2)$. Let $c = |V(T)| - a - b - 1$, where $c \geq 1$ because of $v_3 \in V(T)$. Moreover, H' contains an isolated vertex v_2. Therefore, $W(H') = (a + b + 1 + c)N$, for some constant value N. Let $H \in \omega(G,e)$ obtained from H' by removing a edges incident with pendent vertices in $V(T)\cap N_G(v_1)$ and joining them to the vertex v_1, and removing b edges incident with pendent vertices in $\big(V(T)\cap N_G(v_2)\big)\setminus\{v_1\}$, and joining them to v_2, and also removing the edge v_1v_3 and adding the edge v_1v_2. One may check that $W(H) = (a+b+2)cN \geq (a+b+1+c)N = W(H')$, because of $c \geq 1$. Moreover, this correspondence is obviously an injection.

• If $v_1v_3 \notin E(H')$. Suppose that H' has tree component T, such that T contains the vertex v_3, and $a \geq 0$ pendent vertices in $N_G(v_1)$, and $b \geq 0$ pendent vertices in $N_G(v_2)$. Let $c = |V(T)| - a - b$, where $c \geq 1$. Moreover, H' contains two isolated vertices v_1 and v_2. Therefore, $W(H') = (a + b + c)N$, for some constant value N. Let $H \in \omega(G, e)$ obtained from H' by removing a edges incident with pendent vertices in $V(T) \cap N_G(v_1)$ and joining them to the vertex v_1, and also removing b edges incident with pendent vertices in $V(T)\cap N_G(v_2)$, and joining them to v_2. One may check that $W(H) = (a + 1)(b + 1)cN \geq W(H')$. Moreover, this correspondence is obviously an injection.

So, suppose that $\widehat{e} \in E(H')$, then the following occur:

(1) Let U be an odd unicyclic component of H' which contains the edges $\widehat{e}$ and v_1v_3. Furthermore, H' contains an isolated vertex v_2. So, $W(H') = 4N$, for some constant value N. Suppose that $H \in \omega(G, e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edges v_1v_3 and v_3v_g and adding the edges v_1v_2 and v_1v_g. It is easy to check that, $W(H) = (|V(U)|+1)N \geq W(H')$. Moreover, this correspondence is obviously an injection.

(2) Let U be the an odd unicyclic component of H' which contains the edge $\widehat{e}$ and $a \geq 0$ pendent vertices adjacent to v_2 in the graph G. Also, suppose that $v_1v_3 \notin E(H')$. Therefore, H' contains two isolated vertices v_1 and v_2. Obviously, $W(H') = 4N$, for some constant value N. Suppose that $H \in \omega(G, e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. Let $c = |V(U)| - a$. It is easy to check that, $W(H) = (c + 1)(a + 1)N \geq 4N = W(H')$, because the girth of U is greater than or equal to 3, so that $|V(U)| - a = c \geq 3$. Moreover, this correspondence is obviously an injection.

(3) Let T be the tree component of H' which contains the edges $\widehat{e}$ and v_1v_3. Suppose that T contains $a \geq 0$ pendent vertices $N_G(v_2)$. Moreover, H' contains an isolated vertex v_2. Obviously, by removing the edges $\widehat{e}$ from T, two subtrees of order c and $d + a$ are obtained, where $c \geq 1$ and $d \geq 2$. So, $W(H') = (a + c + d)N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edges v_1v_3 and v_3v_g and adding the edges v_1v_2 and v_1v_g. It is easy to check that, $W(H) = (a+c+1)dN \geq W(H')$, where $c \geq 1$ and $d \geq 2$. Moreover, this correspondence is obviously an injection.

(4) Let T be the tree component of H' which contains the edges $\widehat{e}$ and $v_1v_3 \notin E(T)$. Suppose that T contains $a \geq 0$ and $b \geq 0$ pendent vertices which are adjacent to v_1 and v_2 in the graph G, respectively. Also, H' contains two isolated vertex v_1 and v_2. Obviously, by removing the edge $\widehat{e}$ from T, two subtrees of order c and $d+a+b$ are obtained. So, $W(H') = (a+b+c+d)N$, for some constant value N. Suppose that $H \in \omega(G,e)$ obtained from H' by removing the edges of pendent vertices u and w adjacent to v_3 where $u \in N_G(v_1)$ and $w \in N_G(v_2)$, and joining them to v_1 and v_2, respectively, and also removing the edge v_3v_g and adding the edge v_1v_g. It is easy to check that, $W(H') \leq W(H) = (a+1)(b+c+1)dN$, where $c, d \geq 1$. Moreover, this correspondence is obviously an injection.

Hence, in all cases it is proved that all non-zero coefficients of the polynomial $\Lambda(-x)$ for even (resp. odd) n are positive (resp. negative), and this completes the proof. □

Lemma 2.10. *Let $G = C(S_{n_1}, S_{n_2}, \ldots, S_{n_g})$ be a unicyclic graph on n vertices with girth g, and $G' = C(S_{n-g+1}, S_1, \ldots, S_1)$, where $\sum_{i=1}^{g} n_i = n$, and $n_i \geq 1$. Then $\zeta_i(G') \leq \zeta_i(G)$, for $0 \leq i \leq n$.*

Proof. Let $H = S(G)$ and $H' = S(G')$. We claim that $M(H,r) \geq M(H',r)$, for $1 \leq r \leq [\frac{n}{2}]$. We prove this by induction on n. Let $n = g+2$, and let H be the graph shown in the below figure.

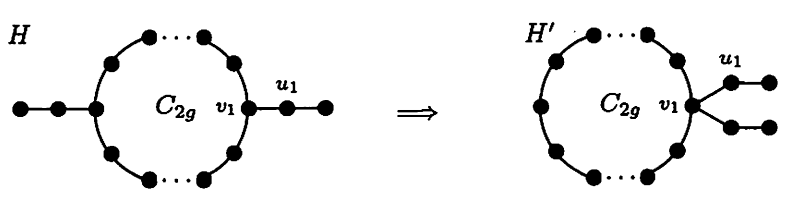


Fig. 5. The graphs H and H'

By Theorem 1.2, we have

$$\begin{aligned} M(H,r) &= M(H - v_1u_1, r) + M(H - v_1 - u_1, r-1), \\ M(H',r) &= M(H' - v_1u_1, r) + M(H' - v_1 - u_1, r-1). \end{aligned}$$

Obviously, $H - v_1u_1 = H' - v_1u_1$, then $M(H - v_1u_1, r) = M(H' - v_1u_1, r)$. Moreover, the graph $H' - v_1 - u_1$ is a proper spanning subgraph of $H - v_1 - u_1$, then $M(H' - v_1 - u_1, r-1) \leq M(H - v_1 - u_1, r-1)$. So suppose that $n \geq g+3$. Let $v \in V(H)$ be a cycle vertex of degree greater than 2, and $u \in V(H)$ be the quasipendent neighbor of v and $u', v' \in V(H')$ be the corresponding vertices. Applying Theorem 1.2 to the edges uv and $u'v'$, we obtain

$$\begin{aligned} M(H,r) &= M(H-uv,r) + M(H-u-v,r-1), \\ M(H',r) &= M(H'-u'v',r) + M(H'-u'-v',r-1). \end{aligned}$$

Clearly, $H' - u' - v'$ is the proper spanning subgraph of $H - u - v$ and so $M(H' - u' - v', r-1) \leq M(H - u - v, r-1)$. On the other hand, by induction hypothesis, we have $M(H' - u'v', r) \leq M(H - uv, r)$. Thus, the claim is proved.

Next, to prove lemma, let $\Delta_i(G)$ be the set of all elementary subgraphs of $S(G)$ with $2i$ vertices which have cycle component. Consequently, Theorem 1.1 follows that

$$\begin{aligned} a_{2i}(S(G)) &= (-1)^i M(S(G), i) + \sum_{L \in \Delta_i(G)} (-1)^{i+g-1} 2 \\ &= (-1)^i M(S(G), i) + (-1)^{i+g-1} 2 |\Delta_i(G)|. \end{aligned}$$

$$\begin{aligned} a_{2i}(S(G')) &= (-1)^i M(S(G'), i) + \sum_{L \in \Delta_i(G')} (-1)^{i+g-1} 2 \\ &= (-1)^i M(S(G'), i) + (-1)^{i+g-1} 2 |\Delta_i(G')|. \end{aligned}$$

Obviously, we have $|\Delta_i(G)| = |\Delta_i(G')|$. Also, according to the claim $M(S(G), i) \geq M(S(G'), i)$. Therefore, Equation (4) implies that $\zeta_i(G) = |a_{2i}(S(G))| \geq \zeta_i(G') = |a_{2i}(S(G'))|$. So, we are done. □

Corollary 2.11. *Let $U \in \mathfrak{U}_{n,g}$. Then for $0 \leq i \leq n$ we have*

(i) If g is an odd number, then $\zeta_i(U) \geq \zeta_i(S_n^+)$;

(ii) If g is an even number, then $\zeta_i(U) \geq \zeta_i(R_n)$, where R_n is C_4 with $n-4$ pendent vertices attached to one of whose vertices.

Proof. This is an immediate result of Corollary 2.2 and Theorem 2.9 and the previous lemma. □

Furthermore, one may check that the Q-coefficients of two graphs S_n^+ and R_n, in the previous corollary are not comparable, for $n \leq 6$ see Appendix. More precisely, it is easy to see that $\zeta_n(S_n^+) = 4 > \zeta_n(R_n) = 0$. On the other hand, $\sum_{i=1}^n d^2_{S_n^+}(v_i) = n^2 - n + 6$ and also $\sum_{i=1}^n d^2_{R_n}(v_i) = n^2 - 3n + 12$. Thus, by Equation 1, we have $\zeta_2(S_n^+) < \zeta_2(R_n)$, for $n \geq 4$.

Now, let $G = C(P_{n_1}, T_2, \dots, T_g)$, and $w \in V(P_{n_1})$, such that $deg_G w = 1$. Let $G' = \gamma(G, v_1)$ be a graph obtained from G by removing the edge v_1v_2 and adding the edge wv_2. For the definition and other properties of the γ-transformation, the reader is referred to [17].

Theorem 2.12. [17, Theorem 3.1] *Let $G = C(P_{n_1}, T_2, \dots, T_g)$ and $G' = \gamma(G, v_1)$ be a γ-transformation of a connected unicyclic graph G. For every $0 \le i \le n$ holds $\xi_i(G) \le \xi_i(G')$, with equality if and only if $i \in \{0, 1, n\}$.*

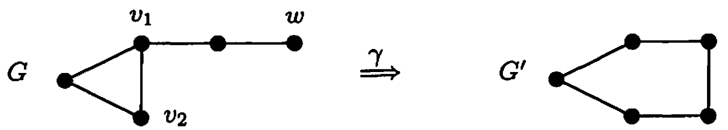


Fig. 6.

In addition, the previous theorem does not hold for the coefficients of the signless Laplacian characteristic polynomial. As we see in Fig. 6, one may check that $Q_G(x) = x^5 - 10x^4 + 34x^3 - 48x^2 + 27x - 4$ and $Q_{G'}(x) = x^5 - 10x^4 + 35x^3 - 50x^2 + 25x - 4$.

Next, we want to obtain an upper bound for the signless Laplacian coefficients of unicyclic graphs. Here, we recall some definitions and theorems from the literature.

Let $C(n, g)$ be the set of all unicyclic graphs obtained from C_g by adding to it $n - g$ pendent vertices. The following lemmas hold for adjacency coefficients of unicyclic graphs.

Lemma 2.13. [11, Lemma 2.4] *Let $G \in \mathfrak{U}_{n,g}$ where $g \not\equiv 0$ (mod 4). Then $|a_i(G)| \le |a_i(L_{n,g})|$, for $i = 1, 2, \dots, n$.*

Lemma 2.14. [11, Lemma 2.5] *Let $G \in \mathfrak{U}_{n,g} \setminus C(n, g)$, where $g \equiv 0$ (mod 4). Then $|a_i(G)| \le |a_i(L_{n,g})|$, for $i = 1, 2, \dots, n$.*

Lemma 2.15. [11, Lemma 3.6] *Let g be an even number, where $n > g$ and $g \ge 8$. Then $|a_i(L_{n,g})| \le |a_i(L_{n,6})|$, for $i = 1, 2, \dots, n$.*

Lemma 2.16. [11, Lemma 3.7] *Let $G \in C(n, g)$ and g be even ($g \ge 8$). Then $|a_i(G)| \le |a_i(L_{n,6})|$, for $i = 1, 2, \dots, n$.*

Accordingly, we have the following corollary.

Corollary 2.17. *Let $U \in \mathfrak{U}_{n,g}$, $n \ge 6$, and $U \ncong C_n$. Then $\zeta_i(U) \le \zeta_i(L_{n,3})$, for $i = 1, 2, \dots, n$.*

Proof. For any $U \in \mathfrak{U}_{n,g}$, one may see that $S(U) \in \mathfrak{U}_{2n,2g}$. So, by Equation (4), we have

$$\zeta_i(U) = |a_{2i}(S(U))|, \text{ for } 1 \le i \le n.$$

Hence, we consider the adjacency coefficients of $S(U)$. Applying Lemmas 2.13, 2.14, 2.15, and 2.16, one may obtain that $|a_{2i}(S(U))| \le |a_{2i}(L_{2n,6})|$. This completes the proof. □

3. An application

The energy of a graph, $\mathcal{E}(G)$, is defined as the sum of the absolute value of its eigenvalues. This concept was introduced by Gutman in [6].

Let A be an n by m matrix with real entries. The singular values of the matrix A are the square root of the eigenvalues of AA^t, where A^t is the transpose of A. If A is a symmetric matrix, then its singular values are the absolute value of its eigenvalues. So, the energy of a graph G is indeed the sum of the singular values of its adjacency matrix [16]. Nikiforov in [16] has extended the concept of graph energy for arbitrary matrices. More precisely, for any $n \times m$ matrix A, the energy of A is defined as the sum of its singular values.

Let $\sigma_1(G), \dots, \sigma_n(G)$ be the singular values of the incidence matrix of the graph G. By Equation (2), it is easy to obtain that $\sigma_i(G) = \sqrt{\nu_i(G)}$. Hence, the incidence energy is defined as $\mathcal{IE}(G) = \sum_{i=1}^{n} \sigma_i(G) = \sum_{i=1}^{n} \sqrt{\nu_i(G)}$ (see [8, 9, 12]). Furthermore, the following theorem holds for the incidence energy of graphs.

Theorem 3.1. [12] *Let G be a graph, then $\mathcal{IE}(G) = \frac{\mathcal{E}(S(G))}{2}$.*

Also the kth elementary symmetric function of the n real numbers $x_1, x_2, \dots, x_n$, $k \le n$, is defined as

$$S_k(x_1, \dots, x_n) = \sum_{S \subseteq \{1,\dots,n\}, |S|=k} \prod_{i \in S} x_i.$$

One may see that

$$\begin{aligned} Q_G(x) &= x^n - S_1(\nu_1, \dots, \nu_n)x^{n-1} + S_2(\nu_1, \dots, \nu_n)x^{n-2} \\ &- \dots \pm S_n(\nu_1, \dots, \nu_n). \end{aligned}$$

So, we have $S_i(\nu_1, \dots, \nu_n) = \zeta_i$. For other properties of elementary symmetric functions, the reader is referred to [1]. We write $(x_1, \dots, x_n) \preceq (y_1, \dots, y_n)$ if $S_k(x_1, \dots, x_n) \le S_k(y_1, \dots, y_n)$, for $1 \le k \le n$, where $x_1, x_2, \dots, x_n, y_1, y_2, \dots, y_n$ are real numbers. Efroymson, Swartz, and Wendroff proved the following theorem.

Theorem 3.2. [3] *If $(x_1, \dots, x_n) \preceq (y_1, \dots, y_n)$, then $\sum_{i=1}^{n} x_i^{\alpha} \le \sum_{i=1}^{n} y_i^{\alpha}$, for any $0 < \alpha \le 1$.*

As a trivial consequence of the Theorem 3.2, we have the following Theorem.

Theorem 3.3. *Let G and G' be two graphs of order n. If $\zeta_i(G) \le \zeta_i(G')$, for $0 \le i \le n$; then $\mathcal{IE}(G) \le \mathcal{IE}(G')$.*

So, the following corollaries hold.

Corollary 3.4. *Let $U = C(T_1, \ldots, T_g)$. Then we have*

$$\mathcal{IE}(C(T_1, \ldots, S_{n_i}, \ldots, T_g)) \leq \mathcal{IE}(U) \leq \mathcal{IE}(C(T_1, \ldots, T_{i-1}, P_{n_i}, T_{i+1}, \ldots, T_g)),$$

for $i = 0, 1, \ldots, n$. Moreover, both extremal graphs are unique.

Proof. Using Corollary 2.1, the result follows. □

Corollary 3.5. *Let $U = C(T_1, \ldots, T_g)$. Then*

$$\mathcal{IE}(C(S_{n_1}, \ldots, S_{n_g})) \leq \mathcal{IE}(U) \leq \mathcal{IE}(C(P_{n_1}, \ldots, P_{n_g})).$$

Moreover, both extremal graphs are unique.

Proof. Using Corollary 2.2, the result follows. □

Theorem 3.6. [10, Thoerem 1.3] For $n = 8, 12, 14$; and $n \geq 16$, $\mathcal{E}(L_{n,6}) > \mathcal{E}(C_n)$.

Corollary 3.7. *Let U be a unicyclic graph of order $n \geq 4$. Then $\mathcal{IE}(U) \leq \mathcal{IE}(C_n)$, if $n = 5$, otherwise $\mathcal{IE}(U) \leq \mathcal{IE}(L_{n,3})$.*

Proof. First, one may check that $\mathcal{E}(C_{10}) \approx 12.9443$ and $\mathcal{E}(L_{10,6}) \approx 12.9321$. So, by Theorem 3.1, we find that $\mathcal{IE}(L_{5,3}) < \mathcal{IE}(C_5)$. Next, for $n \neq 5$, by Theorems 3.6 and 3.1, we obtain that $\mathcal{IE}(L_{n,3}) > \mathcal{IE}(C_n)$. On the other hand, using Corollary 2.17 and Theorem 3.3, we conclude that $\mathcal{IE}(U) \leq \mathcal{IE}(L_{n,3})$, if $U \neq C_n$. This completes the proof. □

Corollary 3.8. *Let $U \in \mathfrak{U}_{n,g}$. Then $\mathcal{IE}(U) \geq \mathcal{IE}(S_n^+)$, where g is an odd number, and $\mathcal{IE}(U) \geq \mathcal{IE}(R_n)$, in which R_n is C_4 with $n-4$ pendent vertices attached to one of whose vertices.*

Proof. This is an immediate consequence of Theorem 3.3 and Corollary 2.11. □

APPENDIX

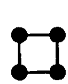
We compute the signless Laplacian characteristic polynomial of unicyclic graphs of order up to 6.

****

$n = 4$

****

1



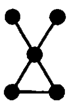
2

1) $x^4 - 8x^3 + 19x^2 - 16x + 4$
2) $x^4 - 8x^3 + 20x^2 - 16x$

****

$n = 5$

****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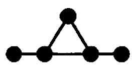
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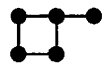
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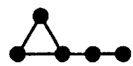
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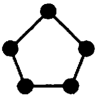
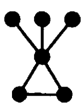

5

1) $x^5 - 10x^4 + 32x^3 - 42x^2 + 23x - 4$
2) $x^5 - 10x^4 + 33x^3 - 44x^2 + 23x - 4$
3) $x^5 - 10x^4 + 34x^3 - 46x^2 + 20x$
4) $x^5 - 10x^4 + 34x^3 - 48x^2 + 27x - 4$
5) $x^5 - 10x^4 + 35x^3 - 50x^2 + 25x - 4$

****

$n = 6$

****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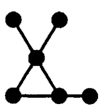
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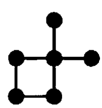
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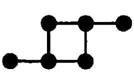
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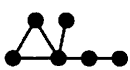
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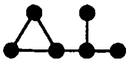
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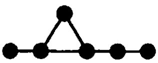
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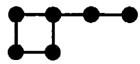
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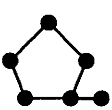
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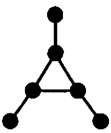
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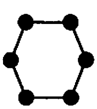
13

1) $x^6 - 12x^5 + 48x^4 - 86x^3 + 75x^2 - 30x + 4$

2) $x^6 - 12x^5 + 50x^4 - 92x^3 + 79x^2 - 30x + 4$
3) $x^6 - 12x^5 + 51x^4 - 96x^3 + 80x^2 - 24x$
4) $x^6 - 12x^5 + 52x^4 - 100x^3 + 84x^2 - 24x$
5) $x^6 - 12x^5 + 51x^4 - 98x^3 + 88x^2 - 34x + 4$
6) $x^6 - 12x^5 + 52x^4 - 102x^3 + 95x^2 - 38x + 4$
7) $x^6 - 12x^5 + 52x^4 - 102x^3 + 92x^2 - 34x + 4$
8) $x^6 - 12x^5 + 53x^4 - 108x^3 + 104x^2 - 42x + 4$
9) $x^6 - 12x^5 + 53x^4 - 106x^3 + 92x^2 - 24x$
10) $x^6 - 12x^5 + 53x^4 - 106x^3 + 95x^2 - 34x + 4$
11) $x^6 - 12x^5 + 51x^4 - 96x^3 + 81x^2 - 30x + 4$
12) $x^6 - 12x^5 + 52x^4 - 100x^3 + 83x^2 - 24x$
13) $x^6 - 12x^5 + 54x^4 - 112x^3 + 105x^2 - 36x$

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