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On the signless Laplacian coefficients of unicyclic graphs

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ABSTRACT

Let G be a graph of order n and let $Q_G(x) = \sum_{i=0}^{n}(-1)^i p_i(G)x^{n-i}$ be the characteristic polynomial of the signless Laplacian of G. Let $E_{g,n}$ (respectively, $C_g(S_{n-g+1})$) denote the unicyclic graph of order n obtained by a coalescence of a vertex in the cycle C_g with an end vertex (respectively, the center) of the path P_{n-g+1} (respectively, the star S_{n-g+1}). It is proved that for $k = 2, \ldots, n-1$, as G varies over all unicyclic graphs of order n, depending on k and n, the maximum value of $p_k(G)$ is attained at $G = C_n$ or $E_{3,n}$, and the minimum value is attained uniquely at $G = C_4(S_{n-3})$ or $C_3(S_{n-2})$. Except for the resolution of a conjecture on cubic polynomials, the uniqueness issue for the maximization problem is also settled.

1. Introduction

For a (simple) graph G, let $A(G)$ and $D(G)$ be respectively the adjacency matrix and the diagonal matrix of vertex degrees of G. Then $L(G) = D(G) - A(G)$ is the *Laplacian* and $Q(G) = D(G) + A(G)$ is the *signless Laplacian* of G.

The *Laplacian polynomial* (respectively, *signless Laplacian polynomial*) of G, denoted by $L_G(x)$ (respectively, $Q_G(x)$), is the characteristic polynomial of $L(G)$ (respectively, $Q(G)$). Let $c_k(G)$ (respectively,

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$p_k(G)$) ($0 \leqslant k \leqslant n$) be the absolute values of the coefficients of $L_G(x)$ (respectively, $Q_G(x)$), so that

$$L_G(x) = \sum_{k=0}^{n} (-1)^k c_k(G) x^{n-k}$$

and

$$Q_G(x) = \sum_{k=0}^{n} (-1)^k p_k(G) x^{n-k}.$$

Clearly $c_0(G)$ (also, $p_0(G)$) equals 1 and for $1 \leqslant k \leqslant n$, $c_k(G)$ (also, $p_k(G)$) is nonnegative, as $c_k(G)$ (respectively, $p_k(G)$) is equal to the kth elementary symmetric function of the eigenvalues of the positive semidefinite matrix $L(G)$ (respectively, $Q(G)$).

In this paper we consider the problem of maximizing (also, minimizing) the absolute values of the signless Laplacian coefficients $p_k(G)$ (hereafter, referred to simply as the signless Laplacian coefficients) among all unicyclic graphs G of a given order. Work on the corresponding extremal problems for the Laplacian coefficients first began with Gutman and Pavlović [8]. They showed that for all n-vertex trees T we have

$$c_k(S_n) \leqslant c_k(T) \leqslant c_k(P_n), \tag{1.1}$$

where S_n and P_n denote respectively the star and the path on n vertices, for $k = 1, 2, 3, n-3, n-2, n-1, n$, and they conjectured that the inequalities are valid for all integral values of k between 0 and n. The conjecture was established by Zhou and Gutman [16] and an alternative proof was later offered by Mohar [12]. In [14] Stevanović and Ilić extended the extremal problems to unicyclic graphs and proved that for a unicyclic graph G on n vertices, we have $c_k(S'_n) \leqslant c_k(G) \leqslant c_k(C_n)$, where the first inequality is strict if $2 \leqslant k \leqslant n-1$ and G is different from (that is, not isomorphic with) S'_n, and the second inequality is strict if $2 \leqslant k \leqslant n-2$ and $G \neq C_n$. Here S'_n denotes the graph obtained from the star S_n by adding an edge between a pair of pendant vertices and C_n is the cycle on n vertices.

Our interest in the set of conditions

$$p_k(G) \geqslant p_k(H) \quad \big(\text{or} \quad c_k(G) \geqslant c_k(H)\big) \quad \text{for } k = 1, \ldots, n,$$

where G, H are graphs of order n, has been aroused by a classical result of Efroymson, Swartz and Wendroff [6]. They proved that if $(x_1, \ldots, x_n)$ and $(y_1, \ldots, y_n)$ are n-tuples of nonnegative real numbers such that

$$S_k(x_1, \ldots, x_n) \leqslant S_k(y_1, \ldots, y_n) \quad \text{for } k = 1, \ldots, n,$$

then for any real number α with $0 < \alpha \leqslant 1$, we have

$$S_k\big(x_1^\alpha, \ldots, x_n^\alpha\big) \leqslant S_k\big(y_1^\alpha, \ldots, y_n^\alpha\big) \quad \text{for } k = 1, \ldots, n,$$

and, in particular, $\sum_{i=1}^n x_i^\alpha \leqslant \sum_{i=1}^n y_i^\alpha$. Since $p_k(G)$ (respectively, $c_k(G)$) ($1 \leqslant k \leqslant n$) is the kth elementary symmetric function of the signless Laplacian (respectively, Laplacian) eigenvalues of G, by the results of [6], one can readily write down consequences of the above-mentioned set of conditions on the signless Laplacian (or Laplacian) coefficients. For instance, the weak inequality between Laplacian-like energy or incidence energy of different graphs as given in [13, Lemma 2] and [11, Theorem 4.2] respectively are such easy consequences. (However, the conclusions concerning strict inequality seem not direct consequences of the results of [6], as claimed in [11] for the incidence energy, because a statement for the corresponding result for strict inequality cannot be found in [6].)

By the *lollipop graph*, denoted by $E_{g,n}$, we mean the unicyclic graph of order n obtained by a coalescence of a vertex in the cycle C_g with an end vertex of the path P_{n-g+1}. We also denote by $C_g(S_{n-g+1})$ the unicyclic graph of order n obtained by a coalescence of a vertex in the cycle C_g with the center of the star S_{n-g+1}. Note that $C_3(S_{n-2}) = S'_n$.

Below are the main results of this paper:

Theorem 1.1. *Let $n \geqslant 5$ be a positive integer. Let α_n be the unique real root of the cubic polynomial $f_n(x)$ given by*:

$$f_n(x) = 3x^3 + (7 - 10n)x^2 + 2\big(6n^2 - 11n + 8\big)x - \big(4n^3 - 6n^2 - 10n + 24\big).$$

For any positive integer $k = 2, \dots, n-1$, the maximum value of $p_k(G)$, as G varies over all unicyclic graphs of order n, is attained uniquely at $G = C_n$ if $k < \alpha_n$ and uniquely at $G = E_{3,n}$ if $\alpha_n < k$, and precisely at $G = C_n$ and $G = E_{3,n}$ if $k = \alpha_n$ (and α_n is an integer).

Theorem 1.2. *Let $n \geqslant 5$ be a positive integer. For any positive integer $k = 2, \dots, n-1$, the minimum value of $p_k(G)$, as G varies over all unicyclic graphs of order n, is attained uniquely at $G = C_4(S_{n-3})$ for $k = 2, \dots, n-4$ or $k = n-3$ and $n = 5, \dots, 24$ or $k = n-2$ and $n = 5, \dots, 8$, and is attained uniquely at $G = C_3(S_{n-2})$ for $k = n-3$ and $n \geqslant 25$ or $k = n-2$ and $n \geqslant 9$ or $k = n-1$.*

Believing that the optimal graph for the maximization problem is always unique, we pose the following:

Conjecture. *For every positive integer $n \geqslant 5$, the unique real root α_n of the cubic polynomial $f_n(x) := 3x^3 + (7 - 10n)x^2 + 2(6n^2 - 11n + 8)x - (4n^3 - 6n^2 - 10n + 24)$ is never an integer.*

A computer program has been set up to determine the integer i_n that satisfies $f_n(i_n - 1) < 0$ and $f_n(i_n) > 0$. Using the program, we have verified the conjecture for $5 \leqslant n \leqslant 10{,}000$.

In this paper we need a combination of proof techniques, most of which are borrowed from previous work on the extremal problems for the Laplacian coefficients or related topics, but in our treatment we often need more involved and refined arguments.

This paper is organized as follows. In Section 2, we give most of the necessary definitions, notations and background results. In particular, we introduce the known graph-theoretic interpretation of the signless Laplacian coefficients in terms of TU-subgraphs. It is shown that among all unicyclic graph G of order $n \geqslant 5$ the maximum value of $p_{n-1}(G)$ is attained uniquely at $G = E_{3,n}$. In Section 3, we give the second graph-theoretic interpretation of the signless Laplacian coefficients via subdivision graphs and matching polynomials. We introduce the concept of a generalized π-transform and investigate the effects on the matching coefficients of a graph (especially for unicyclic graphs) or of its subdivision graph, upon the application of a generalized π-transformation. In Section 4 and Section 5, we give the proofs for Theorem 1.1 and Theorem 1.2 respectively.

An initial work on the extremal problems over unicyclic graphs of a fixed order for the signless Laplacian coefficients has been carried out recently by Mirzakhah and Kiani [11] — we were not aware of this until near the completion of our work. Making use of the π- and σ-transformations on graphs and the TU-subgraphs description for the signless Laplacian coefficients, they proved that the optimal graphs for the maximization (respectively, minimization) problem are among graphs constructed from a cycle by attaching at each vertex a path (respectively, a star). We could have shortened our proofs a bit in the initial stage of our solution by using their results, but we keep our approach as we expect that the generalized π-transformation will be useful for future study and also our work on the matching coefficients obtained in Section 3 has independent interest.

2. Preliminaries

For a vertex v in a (simple) graph G, denote by $d_G(v)$, or simply $d(v)$, the degree of v in G.

As usual, let C_n, P_n and S_n denote respectively the *cycle*, the *path* and the *star* on n vertices.

The cardinality of a set S is denoted by $|S|$.

The *direct sum* $G_1 \dot{+} G_2$ of vertex-disjoint graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the graph $G = (V, E)$ for which $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$. The characteristic polynomial of (the adjacency matrix of) G is denoted by $P_G(x)$, i.e., $P_G(x) = \det(xI - A(G))$.

Given a graph G and an edge uv of G, we denote by $G - uv$ (respectively, $G - v$) the graph obtained from G by deleting the edge uv (respectively, the vertex v and the edges incident with v). For a subgraph H of G, let $G - H$ denote the subgraph of G induced by vertices not in H.

A connected graph is said to be *unicyclic* if it has as many vertices as edges or, equivalently, if it has a unique cycle. We refer to a unicyclic graph as *odd-unicyclic* or *even-unicyclic*, depending on whether the cycle it contains has odd length or even length. The set of unicyclic graphs of order n with a cycle of length g is denoted by $\mathcal{U}_{g,n}$.

The following nontrivial formula for the Laplacian coefficients of a graph G, due to Kelmans and Chelnokov [10], was invoked in the work of [8] and [14]:

$$c_k(G) = \sum_F \gamma(F) \quad \text{for } k = 1, \ldots, n, \tag{2.1}$$

where the summation runs over all spanning forests F of G with exactly $n-k$ components (or, equivalently, with exactly k edges) and $\gamma(F)$ is the product of the number of vertices in the components of F.

By a *TU-subgraph* of G we mean a spanning subgraph whose components are either trees or odd-unicyclic graphs. If H is a TU-subgraph of G which has as components c odd-unicyclic graphs together with the trees $T_1, T_2, \ldots, T_s$, then the weight $W(H)$ of H is defined by $W(H) = 4^c \prod_{i=1}^s |V(T_i)|$. Equivalently, we let $W(C)$ equal $|V(C)|$ if C is a tree and equal 4 if C is an odd-unicyclic graph, and for a TU-subgraph H define $W(H)$ to be $\prod_C W(C)$, where the product runs through all components C of H.

For a graph G of order n, the signless Laplacian coefficients $p_k(G)$ have the following graph-theoretic interpretations (see [5,3]):

$$p_k(G) = \sum_H W(H) \quad \text{for } k = 1, 2, \ldots, n, \tag{2.2}$$

where the summation runs over all TU-subgraphs H of G with k edges. (Note that our definition of $p_k(G)$, which is given at the beginning of Section 1, differs from that as given in [3] or [4] by a factor of $(-1)^k$.)

As an immediate consequence of (2.2) we have the following result, a special case of which has been proved in a different way (and stated somewhat inaccurately) in [11, Theorem 2.1]:

Remark 2.1. Let G be a graph with n vertices and m edges. If H is a proper spanning subgraph with at least one edge, then for any positive integer $k \leqslant n$,

$$p_k(H) \leqslant p_k(G) \text{ and with strict inequality if and only if } 1 \leqslant k \leqslant \min\{m, n\}.$$

The point is, any TU-subgraph of H is necessarily a TU-subgraph of G and there is at least one TU-subgraph of G with k edges which is not a TU-subgraph of H if and only if $1 \leqslant k \leqslant \min\{m, n\}$. By (2.1) a similar remark also holds for the Laplacian coefficients.

Note that the spanning forests of G are precisely TU-subgraphs of G whose components are all trees. So (2.1) and (2.2) imply that every term in the formula for $c_k(G)$ also appears in the formula for $p_k(G)$. So it is expected that the work on the extremal problems for the signless Laplacian coefficients is more involved than that for the Laplacian coefficients.

By definition $p_0(G) = 1$. As simple consequences of formula (2.2), one readily derives the following known basic facts concerning $p_k(G)$ for $k = 1, 2, n-1, n$ (see [3, Corollary 4.5], [4, Proposition 6.1]):

Lemma 2.2.

(i) *For a graph G with m edges,*

$$p_1(G) = 2m \quad \textit{and} \quad p_2(G) = a + \frac{3}{2}m(m-1),$$

where a denotes the number of pairs of nonadjacent edges in G.

(ii) *For $G \in \mathcal{U}_{g,n}$, if G is even-unicyclic, then*

$$p_n(G) = 0 \quad \text{and} \quad p_{n-1}(G) = ng;$$

if G is odd-unicyclic, then

$$p_n(G) = 4 \quad \text{and} \quad p_{n-1}(G) = ng + 4 \sum_{e \in E(G) \setminus E(C)} t_e(G),$$

where C denotes the unique cycle of G and $t_e(G)$ is the order of the unique tree component of the graph $G - e$.

So the unmentioned cases ($k = 0, 1, n$) of Theorem 1.1 and Theorem 1.2 are in fact known: For a unicyclic graph G of order n, $p_1(G)$ is always equal to $2n$, and $p_n(G)$ is equal to 4 if G is odd-unicyclic and equal to 0 if G is even-unicyclic.

Let us recall the definition for a π-transform of a graph, as introduced by Mohar [12] for trees and extended to graphs in general by Stevanović and Ilić [14]. We say that the path $P = u_0u_1u_2 \cdots u_p$ in G is a *pendant path* of length p attached at vertex u_0 if $d_G(u_0) \geqslant 3, d_G(u_p) = 1$ and the internal vertices $u_1, u_2, \ldots, u_{p-1}$ all have degree two. Suppose that $P = u_0u_1u_2 \cdots u_p$ and $Q = u_0v_1v_2 \cdots v_q$ are distinct pendant paths of G attached at u_0 of lengths $p \geqslant 1$ and $q \geqslant 1$ respectively. We call the graph G' obtained from G by relocating the path Q from u_0 to u_p (by deleting the edge u_0v_1 and adding the edge u_pv_1) a *π-transform* of G and denote it by $\pi(G, u_0, P, Q)$.

We call a unicyclic graph a *sun graph* if the tree attached at each vertex of its cycle is a path (possibly of length zero). It is known that every tree can be transformed into a path by a sequence of π-transformations (see [12, Proposition 2.1]). Likewise, if $G \in \mathcal{U}_{g,n}$ is not a sun graph then by applying a sequence of π-transformations we obtain a sun graph $G' \in \mathcal{U}_{g,n}$.

Using Lemma 2.2(ii), one readily shows the following: (1) If G is an odd-unicyclic graph of order n and $G' = \pi(G, u_0, P, Q)$ is a π-transform of G, then $p_{n-1}(G') > p_{n-1}(G)$; and (2) if $G \in \mathcal{U}_{g,n}$ (where g is odd) is a sun graph, different from the lollipop graph $E_{g,n}$, then $p_{n-1}(E_{g,n}) > p_{n-1}(G)$. (We are essentially following the argument given in [4], but we use Fact (1) in place of [4, Lemma 6.2], which, as it stands, is incorrect.)

Also, it is not difficult to show that $p_{n-1}(E_{3,n}) > p_{n-1}(E_{g,n})$ for $g > 3$. Thus, we conclude that among all odd-unicyclic graphs G of order n, the maximum value of $p_{n-1}(G)$ is attained uniquely at $G = E_{3,n}$.

Now by Lemma 2.2(ii), we have

$$p_{n-1}(E_{3,n}) = 3n + 4\big[(n-3) + (n-2) + \cdots + 1\big] = 2n^2 - 7n + 12,$$

and also the maximum value of $p_{n-1}(G)$, as G runs through all even-unicyclic graphs of order n, is attained uniquely at $G = C_n$ (with value n^2) when n is even, and at $G = E_{n-1,n}$ (with value $n(n-1)$) when n is odd. But $2n^2 - 7n + 12 > n^2$ for $n \geqslant 5$, so we obtain:

Remark 2.3. Among all unicyclic graphs G of order $n \geqslant 5$, the maximum value of $p_{n-1}(G)$ is attained uniquely at $G = E_{3,n}$.

3. Matching polynomials

As in the works of Zhou and Gutman [16] and Mohar [12], the subdivision graph and the matching polynomial also play a role in this paper.

Recall that the *subdivision graph* $S(G)$ of a graph G is obtained from G by replacing each of its edges by a path of length 2, or, equivalently, by inserting an additional vertex into each edge of G. We need the following known formula, which provides a link between the signless Laplacian polynomial of G and the characteristic polynomial of its subdivision graph:

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$$P_{S(G)}(x) = x^{m-n} Q_G\big(x^2\big), \tag{3.1}$$

where n, m are respectively the number of vertices and edges of G. (See [11].)

A k-matching in a graph is a set of k edges, no two of which have a vertex in common. The *matching polynomial* of a graph G with n vertices is defined to be

$$M_G(x) = \sum_{k=0}^{\alpha'(G)} (-1)^k m_k(G) x^{n-2k},$$

where $m_0(G) = 1$, $m_k(G)$ denotes the number of k-matchings of G and $\alpha'(G)$ is the matching number of G. (For convenience, we adopt the convention that $m_k(G) = 0$ for $k < 0$ or $k > \alpha'(G)$.)

We will need the following known result, which is a reformulation of the Sachs theorem for the characteristic polynomial of a graph (see [7] or [2]):

Theorem 3.1. *Let $\mathcal{C}$ be the set of subgraphs of G that are regular graphs of degree two. Then*

$$P_G(x) = M_G(x) + \sum_{C \in \mathcal{C}} (-2)^{p(C)} M_{G-C}(x), \tag{3.2}$$

where $p(C)$ denotes the number of components in C; hence, $P_G(x) = M_G(x)$ if and only if G is a forest.

By (3.1) and (3.2) we obtain

Corollary 3.2. *If $G \in \mathcal{U}_{g,n}$, then*

$$p_k(G) = m_k\big(S(G)\big) + (-1)^{g+1} 2 m_{k-g}\big(S(G) - C_{2g}\big) \tag{3.3}$$

for $k = 1, 2, \ldots, n$.

The following known (and pretty obvious) result on matchings (see [7] or [2]) will be used:

Lemma 3.3. *If u, v are adjacent vertices of G, then*

$$m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v)$$

for all nonnegative integers k.

We will also need the following formula, which expresses $m_k(P_n \dot{+} P_m)$ in terms of the binomial coefficients:

Lemma 3.4. *Let m, n be nonnegative integers with at least one positive. For any nonnegative integer $k \leqslant (m+n)/2$,*

$$\sum_{i+j=k} \binom{n-i}{i}\binom{m-j}{j} = m_k(P_n \dot{+} P_m) = \sum_{l=0}^{r} (-1)^l \binom{n+m-k-l}{k-l}, \tag{3.4}$$

where $r = \min\{k, m, n\}$.

Proof. First of all, note that

$$m_i(P_n) = \binom{n-i}{i}, \quad i = 1, 2 \ldots, \left\lfloor \frac{n}{2} \right\rfloor,$$

as $P_{P_n}(x) = M_{P_n}(x)$ and $P_{P_n}(x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i \binom{n-i}{i} x^{n-2i}$ (see [1, p. 73]). The first equality in (3.4) clearly follows because we have $m_k(G_1 \dot{+} G_2) = \sum_{i+j=k} m_i(G_1) m_j(G_2)$ for any vertex-disjoint graphs G_1, G_2.

We are going to establish the second equality by induction on r. The assertion holds when $r = 0$: this is clear if $k = 0$; if $k \geqslant 1$ and one of n, m is 0, then it follows from the above-mentioned formula for $m_i(P_n)$ (noting that $P_0 \dot{+} P_m = P_m$). Now assume that $r \geqslant 1$. In view of Lemma 3.3, by considering the path P_{n+m} with vertex-set $\{v_1, v_2, \ldots, v_{n+m}\}$ and edge-set $\{v_i v_{i+1} \mid i = 1, 2, \ldots, n+m-1\}$, for any nonnegative integer $k \leqslant (m+n)/2$, we have

$$\begin{aligned} m_k(P_{n+m}) &= m_k(P_{n+m} - v_n v_{n+1}) + m_{k-1}(P_{n+m} - v_n - v_{n+1}) \\ &= m_k(P_n \dot{+} P_m) + m_{k-1}(P_{n-1} \dot{+} P_{m-1}); \end{aligned}$$

hence

$$m_k(P_n \dot{+} P_m) = m_k(P_{n+m}) - m_{k-1}(P_{n-1} \dot{+} P_{m-1}) = \binom{n+m-k}{k} - m_{k-1}(P_{n-1} \dot{+} P_{m-1}).$$

On the other hand, by the induction assumption, we have

$$\begin{aligned} m_{k-1}(P_{n-1} \dot{+} P_{m-1}) &= \sum_{l=0}^{r-1} (-1)^l \binom{(n-1)+(m-1)-(k-1)-l}{(k-1)-l} \\ &= \sum_{l=1}^{r} (-1)^{l-1} \binom{n+m-k-l}{k-l}. \end{aligned}$$

So the second equality in (3.4) also follows. □

In the definition of a π-transform of a graph if we replace one of the two attached pendant paths under consideration by a connected graph, we obtain the concept of a generalized π-transform. To give the formal definition, we need the concept of a branch of a connected graph.

We say Q is a *branch* of a connected graph G with root u if Q is a connected induced subgraph of G for which u is the only vertex in Q that has a neighbor not in Q.

Let P and Q be branches of a component of a graph G with a common root u_0, which is also their only common vertex. Assume that P is a path and u_0 has at least one neighbor in G that does not lie on P or Q. Form a graph from G by relocating the branch Q from u_0 to v where v is the other end vertex of the path P (by deleting edges $u_0 w$ and adding new edges vw for every vertex w in Q adjacent to u_0). We refer to the resulting graph as *a generalized π-transform of G* and denote it by $\pi(G, u_0, P, Q)$.

In the proof of our next result we elaborate an argument used in the proof of [12, Theorem 2.2].

Lemma 3.5. *For any graph G, if $G' = \pi(G, u_0, P, Q)$ is a generalized π-transform of G, then $m_k(G') \geqslant m_k(G)$ for every positive integer k, with strict inequality if and only if $2 \leqslant k \leqslant K$, where*

$$\begin{aligned} K = 2 &+ \left\lfloor \frac{p-1}{2} \right\rfloor + \max\bigl\{\alpha'(Q - u_0 - v_i)\colon 1 \leqslant i \leqslant t\bigr\} \\ &+ \max\bigl\{\alpha'(G - P - Q - w)\colon w \in N_G(u_0) \setminus \{u_1, v_1, \ldots, v_t\}\bigr\}, \end{aligned}$$

p being the length of path P, u_1 being the vertex in P adjacent to u_0, $v_1, \ldots, v_t$ being all the vertices in Q adjacent to u_0, and $\alpha'(H)$ being the matching number of H.

Proof. Let P be the path $u_0 u_1 \cdots u_p$ $(p \geqslant 1)$. We first obtain an injective mapping from the set of all matchings of G into the set of all matchings of G'.

For any matching M of G, if $u_{p-1}u_p \notin M$ or $u_0 v_i \notin M$ for each $i = 1, \ldots, t$, then the set of edges in G' corresponding to M, which we denote by M', is clearly a matching of G' (with the same number of edges as M). Let $\mathcal{M}_1$ denote the set of all matchings M' of G' obtained in this way. Note that for any $M' \in \mathcal{M}_1$, exactly one of the following holds: vertex u_p is not covered by M' (which happens when $u_{p-1}u_p \notin M$ and $u_0 v_i \notin M$ for each $i = 1, \ldots, t$), or $u_{p-1}u_p \in M'$ (which happens when $u_{p-1}u_p \in M$

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and $u_0v_i \notin M$ for each $i = 1, \dots, t$), or $u_pv_i \in M'$ for some $i = 1, \dots, t$ and u_0 is not covered by M' (which happens when $u_{p-1}u_p \notin M$ and $u_0v_i \in M$ for some $i = 1, \dots, t$).

If $u_{p-1}u_p \in M$ and $u_0v_i \in M$ for some $i = 1, \dots, t$, then we take M' to be the matching of G' which equals $\{u_iu_{i+1}\colon u_{p-i-1}u_{p-i} \in M\}$ on $E(P)$ and agrees with M on $E(G) \setminus E(P)$ (but replacing edge u_0v_i by u_pv_i). Let $\mathcal{M}_2$ denote the set of all matchings M' of G' obtained in this way. Note that for any $M' \in \mathcal{M}_2$ we have $u_pv_i \in M'$ for some $i = 1, \dots, t$ and $u_0u_1 \in M'$.

It is readily checked that $\mathcal{M}_1 \cap \mathcal{M}_2 = \emptyset$ and $\mathcal{M}_1 \cup \mathcal{M}_2$ consists of all matchings M' of G' that satisfies (exactly) one of the following: u_p is not covered by M'; $u_{p-1}u_p \in M'$; $u_pv_i \in M'$ for some $i = 1, \dots, t$ and either u_0 is not covered by M' or $u_0u_1 \in M'$. Moreover, the correspondence $M \mapsto M'$ is a one-to-one mapping from the set of all matchings of G onto $\mathcal{M}_1 \cup \mathcal{M}_2$. This establishes the inequality $m_k(G') \geqslant m_k(G)$ for every positive integer k.

Note that a matching M' of G' is not in $\mathcal{M}_1 \cup \mathcal{M}_2$ if and only if $u_pv_i \in M'$ for some $i = 1, \dots, t$, u_0 is covered by M' but $u_0u_1 \notin M'$. If w is a neighbor of u_0 in G' other than u_1 — which exists by our assumption on the neighbors of u_0 in G — then clearly $\{u_pv_1, u_0w\}$ is a 2-matching of G' that lies outside $\mathcal{M}_1 \cup \mathcal{M}_2$; hence $m_2(G') > m_2(G)$. So we have $m_k(G') > m_k(G)$ if and only if $2 \leqslant k \leqslant K$, where K is the size of the largest matching of G' that does not belong to $\mathcal{M}_1 \cup \mathcal{M}_2$. To determine K, consider any matching M' of G' that does not belong to $\mathcal{M}_1 \cup \mathcal{M}_2$. Then there exist i, $1 \leqslant i \leqslant t$ and a vertex w of G', adjacent to u_0 and different from u_1, such that edges u_pv_i and u_0w both belong to M'. The remaining edges of M' must lie in the direct sum of the following three graphs: $P_{p-1} : u_1u_2 \cdots u_{p-1}$, $Q - u_0 - v_i$, $G - P - Q - w$, noting that the last two graphs each may have more than one component. Now for the path P_r, $\alpha'(P_r) = \lfloor \frac{r}{2} \rfloor$. So the number of edges in M' is at most $2 + \lfloor \frac{p-1}{2} \rfloor + \alpha'(Q - u_0 - v_i) + \alpha'(G - P - Q - w)$. A matching M' with maximum size that is not in $\mathcal{M}_1 \cup \mathcal{M}_2$ can be found by varying w and v_i. So we have

$$K = 2 + \left\lfloor \frac{p-1}{2} \right\rfloor + \max\{\alpha'(Q - u_0 - v_i)\colon 1 \leqslant i \leqslant t\}$$
$$+ \max\{\alpha'(G - P - Q - w)\colon w \in N_G(u_0) \setminus \{u_1, v_1, \dots, v_t\}\}. \qquad \square$$

It is not difficult to construct a graph G with a generalized π-transform (or even a π-transform) G' such that the numerical quantity K that appears in Lemma 3.5 takes the smallest possible value 2.

Note that for a bipartite graph G with bipartition (V_1, V_2), $\alpha'(G) \leqslant \min\{|V_1|, |V_2|\}$. Our next result says that the preceding inequality becomes an equality if G is a subdivision graph.

Lemma 3.6. *If G is a connected graph of order $n \geqslant 2$, then $\alpha'(S(G))$ equals $n - 1$ if G is a tree and equals n, otherwise. In any case, there is a maximum matching in $S(G)$ that covers any given vertex in $V(G)$.*

Proof. Since the subdivision graph $S(G)$ is a bipartite graph with bipartition $(V(G), E(G))$, clearly $\alpha'(S(G)) \leqslant \min\{|V(G)|, |E(G)|\}$.

First, consider the case when G is a tree. We are going to show that for any given vertex v of G, there is a unique $(n-1)$-matching of $S(G)$ that misses vertex v. [This fact is undoubtedly known (see [15, Lemma 3.1]) and was quoted (without proof) in the proof of [12, Theorem 2.2] — note, however, that the first sentence in the last paragraph of [12, p. 738], as stated, is incorrect. For completeness, we indicate a proof.] For any edge e of G, let v_e denote the vertex inserted into the edge e in the subdivision graph $S(G)$. To give the desired $(n-1)$-matching of $S(G)$, it suffices to specify, for any edge $e \in E(G)$, the edge in the matching that covers vertex v_e. For $e = uw$, we take the desired edge to be v_ew, with $d_G(v, w) > d_G(v, u)$. It is readily checked that the collection of edges obtained in this way forms an $(n-1)$-matching of $S(G)$ that misses vertex v and furthermore it is the only $(n-1)$-matching of $S(G)$ with such property. If u is a given vertex of $S(G)$ that belongs to $V(G)$, take a vertex v of G different from u. By the above, $S(G)$ has an $(n-1)$-matching, and hence a maximum matching, that misses v. This matching clearly covers u.

Now consider the case when G is not a tree. We want to show that $S(G)$ has an n-matching. Note that any n-matching of $S(G')$, where G' is a unicyclic spanning subgraph of G, is also an n-matching of $S(G)$. By removing edges from G, if necessary, hereafter we assume that G is unicyclic. Take any

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edge $e' = uv$ of $E(G)$ that belongs to the cycle of G. Since $G - e'$ is a tree, by what we have done, $S(G - e')$ has an $(n-1)$-matching M' that misses vertex u. Then $M' \cup \{v_{e'}u\}$ is an n-matching of $S(G)$. This proves that a maximum matching of $S(G)$ has size n. Clearly, in this case, every maximum matching covers every vertex of $S(G)$ that belongs to $V(G)$. □

Lemma 3.7. *Let G be a connected graph of order n. If G' is a generalized π-transform of G, then $m_k(S(G)) \leqslant m_k(S(G'))$ for every positive integer k, with strict inequality if and only if $2 \leqslant k \leqslant K$, where K equals $n-2$ if G is a tree and equals $n-1$ if G is a unicyclic graph.*

Proof. Let $G' = \pi(G, u_0, P, Q)$. As can be readily checked, $S(G')$ is a generalized π-transform of $S(G)$ and $S(G') = \pi(S(G), u_0, S(P), S(Q))$. To be specific, let the paths P and $S(P)$ be given by: $P: u_0u_1 \cdots u_p$ $(p \geqslant 1)$ and $S(P): u_0\hat{u}_1u_1\hat{u}_2u_2 \cdots \hat{u}_pu_p$. Let $v_1, \ldots, v_r$ be the vertices in Q adjacent to u_0 and for $i = 1, \ldots, r$, let $\hat{v}_i$ denote the vertex inserted into the edge u_0v_i (respectively, u_pv_i) in $S(G)$ (respectively, $S(G')$).

By Lemma 3.5 and its proof we have $m_k(S(G')) \geqslant m_k(S(G))$ for every positive integer k and with strict inequality if and only if $2 \leqslant k \leqslant K$ where K is the size of the largest matching M' in $S(G')$ with the property that $u_p\hat{v}_i \in M'$ for some $i = 1, \ldots, r$, u_0 is covered by M' but $u_0\hat{u}_1 \notin M'$.

Let R denote the subgraph of G induced by $[V(G) \setminus (V(P) \cup V(Q))] \cup \{u_0\}$. ($G$ can be thought of as a coalescence of its branches P, Q, R at u_0.) Let $q = |V(Q)|$ and let $r = n - p - q$. Then $|V(R)| = r + 1$.

A matching in $S(G')$ with the said property and with the largest possible size can be formed by taking the union of a maximum matching in the path $\hat{u}_1u_1\hat{u}_2u_2 \cdots u_{p-1}\hat{u}_p$, a maximum matching in $S(Q)$ that covers vertex u_0 (but with vertex u_0 replaced by vertex u_p), and a maximum matching in $S(R)$ that covers vertex u_0.

Now a maximum matching in the path $\hat{u}_1u_1\hat{u}_2u_2 \cdots u_{p-1}\hat{u}_p$ has size $p-1$. According to Lemma 3.6, there is a maximum matching in $S(Q)$ (with size $q-1$ if Q is a tree and with size q, otherwise) that covers any given vertex of Q, and a similar statement also holds for $S(R)$.

If G is a tree, then Q and R are also trees. In this case, $K = (p-1) + (q-1) + r = n-2$. If G is unicyclic, then either Q is unicyclic and R is a tree or Q is a tree and R is unicyclic. In any case, $K = p + q + r - 1 = n - 1$. □

Following the notation of [11], we use $C_g(P_{r_1+1}, \ldots, P_{r_g+1})$ to denote the sun graph obtained from the cycle $C_g = v_1v_2 \ldots v_gv_1$ by identifying one end of the path P_{r_i+1} with vertex v_i for $i = 1, \ldots, g$. Note that the lollipop graph $E_{g,n}$ is equal to $C_g(P_{n-g+1}, P_1, \ldots, P_1)$.

Lemma 3.8. *Let n, g be positive integers, $n > g \geqslant 3$. For any $G \in \mathcal{U}_{g,n}$, $m_k(E_{g,n}) \geqslant m_k(G)$ for all positive integers k.*

Proof. If G is not a sun graph, by applying a sequence of π-transformations, we obtain a sun graph H which, by Lemma 3.5, satisfies $m_k(H) \geqslant m_k(G)$ for all positive integers k. Hereafter, we assume that G is a sun graph.

Let $G = C_g(P_{r_1+1}, \ldots, P_{r_g+1})$. We proceed by induction on t, where $t = |\{i \mid r_i > 0\}|$, i.e., the number of nontrivial pendant paths of G. Since $n > g$, clearly $t \geqslant 1$. If $t = 1$, then $G = E_{g,n}$ and there is nothing to show. So suppose that $t > 1$ and assume that the result is valid for a sun graph with less than t nontrivial pendant paths. Without loss of generality, assume that $r_1 > 0$ and let $u_0u_1u_2 \cdots u_{r_1}$ be a pendant path of G of length r_1, with u_0 lying on the cycle of G. By Lemma 3.3, for any $1 \leqslant k \leqslant n$, we have

$$\begin{aligned} m_k(G) &= m_k(G - u_0u_1) + m_{k-1}(G - u_0 - u_1) \\ &= m_k\big(C_g(P_1, P_{r_2+1}, \ldots, P_{r_g+1}) \dot{+} P_{r_1}\big) \\ &\quad + m_{k-1}\big(\big(C_g(P_1, P_{r_2+1}, \ldots, P_{r_g+1}) - u_0\big) \dot{+} P_{r_1-1}\big). \end{aligned}$$

Now let w and w' denote respectively the unique vertices lying on the pendant path of $E_{g,n}$ that are at distance r_1 and $r_1 - 1$ from the unique pendant vertex of $E_{g,n}$. By Lemma 3.3 again, we have

$$m_k(E_{g,n}) = m_k\big(E_{g,n} - ww'\big) + m_{k-1}\big(E_{g,n} - w - w'\big)$$
$$= m_k(E_{g,n-r_1} \dot{+} P_{r_1}) + m_{k-1}(E_{g,n-r_1-1} \dot{+} P_{r_1-1}).$$

Since $C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}), E_{g,n-n_1} \in \mathcal{U}_{g,n-n_1}$ and $C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1})$ has one fewer nontrivial pendant paths than $C_g(P_{r_1+1}, \dots, P_{r_g+1})$, by the induction hypothesis,

$$m_k(E_{g,n-r_1}) \geqslant m_k\big(C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1})\big) \quad \text{for every positive integer } k.$$

But $m_k(G_1 \dot{+} G_2) = \sum_{i+j=k} m_i(G_1)m_j(G_2)$ for any vertex-disjoint graphs G_1, G_2, so we have $m_k(E_{g,n-r_1} \dot{+} P_{r_1}) \geqslant m_k(C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}) \dot{+} P_{r_1})$ for every positive integer k. On the other hand, by applying Lemma 3.3 to $E_{g,n-r_1-1}$ (by taking uv to be one of the two edges in the cycle incident with the vertex at which the pendant path is attached), we obtain

$$m_k(E_{g,n-r_1-1}) = m_k(P_{n-r_1-1}) + m_{k-1}(P_{n-r_1-1-g} \dot{+} P_{g-2}) \geqslant m_k(P_{n-r_1-1}).$$

Since $C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}) - u_0$ is a tree of order $n - n_1 - 1$ and every such tree can be transformed into the path P_{n-n_1-1} by a sequence of π-transformations, by Lemma 3.5, for every positive integer k, we have $m_k(P_{n-n_1-1}) \geqslant m_k(C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}) - u_0)$ and so $m_k(E_{g,n-r_1-1}) \geqslant m_k(P_{n-r_1-1}) \geqslant m_k(C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}) - u_0)$. Hence

$$m_{k-1}(E_{g,n-r_1-1} \dot{+} P_{r_1-1}) \geqslant m_{k-1}\big(\big(C_g(P_1, P_{r_2+1}, \dots, P_{r_g+1}) - u_0\big) \dot{+} P_{r_1-1}\big).$$

We can now conclude that $m_k(E_{g,n}) \geqslant m_k(G)$ for every positive integer k. □

Lemma 3.9. *Let n, g be positive integers, $n > g \geqslant 3$. For any $G \in \mathcal{U}_{g,n}$, $G \neq E_{g,n}$, we have $m_k(S(E_{g,n})) > m_k(S(G))$ for $k = 2, \dots, n-1$.*

Proof. In view of Lemma 3.7, it suffices to consider the case when G is a sun graph. Since $S(E_{g,n}) = E_{2g,2n}$, by Lemma 3.8 we have the weak inequalities $m_k(S(G)) \leqslant m_k(S(E_{g,n}))$ for $k = 2, \dots, n-1$. To obtain the strict inequalities, we need to elaborate the argument given in the proof of Lemma 3.8.

Let $G = C_g(P_{r_1+1}, \dots, P_{r_g+1})$. Then $S(G) = C_{2g}(P_{2r_1+1}, P_1, P_{2r_2+1}, P_1, \dots, P_{2r_g+1}, P_1)$. Since G is not a lollipop graph, G has at least two nontrivial pendant paths. Say, $r_1 \geqslant 1$, and let the pendant path of $S(G)$ of length $2r_1$ be attached to the cycle of $S(G)$ at vertex u_0. By the argument given in the proof of Lemma 3.8 one can show that for every positive integer k,

$$m_k\big(S(G)\big) = m_k\big(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \dots, P_{2r_g+1}, P_1) \dot{+} P_{2r_1}\big)$$
$$+ m_{k-1}\big(\big(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \dots, P_{2r_g+1}, P_1) - u_0\big) \dot{+} P_{2r_1-1}\big),$$
$$m_k\big(S(E_{g,n})\big) = m_k(E_{2g,2n}) = m_k(E_{2g,2n-2r_1} \dot{+} P_{2r_1}) + m_{k-1}(E_{2g,2n-2r_1-1} \dot{+} P_{2r_1-1}).$$

and

$$m_k(E_{2g,2n-2r_1} \dot{+} P_{2r_1}) \geqslant m_k\big(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \dots, P_{2r_g+1}, P_1) \dot{+} P_{2r_1}\big).$$

To complete the proof, we are going to show that

$$m_{k-1}(E_{2g,2n-2r_1-1} \dot{+} P_{2r_1-1})$$
$$> m_{k-1}\big(\big(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \dots, P_{2r_g+1}, P_1) - u_0\big) \dot{+} P_{2r_1-1}\big)$$

for $2 \leqslant k \leqslant n-1$.

For any positive integer i, we have

$$m_i(E_{2g,2n-2r_1-1}) = m_i(P_{2n-2r_1-1}) + m_{i-1}(P_{2n-2r_1-2g-1} \dot{+} P_{2g-2}) \geqslant m_i(P_{2n-2r_1-1}),$$

where the inequality is strict if and only if $m_{i-1}(P_{2n-2r_1-2g-1} \dot{+} P_{2g-2}) > 0$. As $\alpha'(P_{2n-2r_1-2g-1} \dot{+} P_{2g-2}) = \alpha'(P_{2n-2r_1-2g-1}) + \alpha'(P_{2g-2}) = n - r_1 - 2$, so the said inequality is strict if and only if $i \leqslant n - r_1 - 1$. Now for any positive integer $k \leqslant n-1$, there is at least one pair of nonnegative integers

i, j with $i + j = k - 1$ such that $m_i(E_{2g,2n-2r_1-1})m_j(P_{2r_1-1}) > m_i(P_{2n-2r_1-1})m_j(P_{2r_1-1})$. For instance, $(i, j) = (k - r_1, r_1 - 1)$ is one such pair. Note also that for every positive integer i, we have

$$m_i(P_{2n-2r_1-1}) \geqslant m_i\bigl(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \ldots, P_{2r_g+1}, P_1) - u_0\bigr),$$

because the tree $C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \ldots, P_{2r_g+1}, P_1) - u_0$ can be transformed into the path P_{2n-2r_1-1} by a sequence of π-transformations, if it is not already a path.

So for every positive integer k, $2 \leqslant k \leqslant n - 1$, we have

$$\begin{aligned}
&m_{k-1}(E_{2g,2n-2r_1-1} \dot{+} P_{2r_1-1}) \\
&\quad = \sum_{i+j=k-1} m_i(E_{2g,2n-2r_1-1})m_j(P_{2r_1-1}) \\
&\quad > \sum_{i+j=k-1} m_i(P_{2n-2r_1-1})m_j(P_{2r_1-1}) \\
&\quad \geqslant \sum_{i+j=k-1} m_i\bigl(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \ldots, P_{2r_g+1}, P_1) - u_0\bigr)m_j(P_{2r_1-1}) \\
&\quad = m_{k-1}\bigl(C_{2g}(P_1, P_1, P_{2r_2+1}, P_1, \ldots, P_{2r_g+1}, P_1) \dot{+} P_{2r_1-1}\bigr). \qquad \square
\end{aligned}$$

Recently, Gutman and Wagner [9] defined the *matching energy* ME(G) of a graph G to be the sum of the absolute values of the zeros of its matching polynomial. As a digression, we would like to point out that the results obtained in this section can be applied to the study of matching energy of a graph. For instance, in view of Lemma 3.5 and the equivalent definition for ME(G) given by the following integral formula:

$$\mathrm{ME}(G) = \frac{2}{\pi}\int_0^\infty \frac{1}{x^2}\ln\Bigl[\sum_{k\geqslant 0} m_k(G)x^{2k}\Bigr]dx, \tag{3.5}$$

it is clear that we have the following result, which contains [9, Lemma 9] as a special case:

Theorem 3.10. *If G' is a generalized π-transform of G, then* ME$(G') >$ ME(G).

4. Proof of Theorem 1.1

We begin with a result which says that the signless Laplacian coefficients $p_k(G)$ are monotone under generalized π-transformations.

Theorem 4.1. *Let G be a graph of order n. For any generalized π-transform G' of G, we have $p_k(G) \leqslant p_k(G')$ for $k = 0, \ldots, n$. When G is connected, we have $p_k(G) < p_k(G')$ if and only if either $k = 2, \ldots, n - 1$ and G is nonbipartite, or $k = 2, \ldots, n - 2$ and G is bipartite.*

Proof. Let $G' = \pi(G, u_0, P, Q)$. Let P be the path $u_0u_1 \cdots u_p$ and let R be the subgraph of G induced by vertices not in P or Q, together with vertex u_0. Note that G is a coalescence of the nontrivial connected graphs P, Q and R at u_0.

For any TU-subgraph H of G, we denote by H' the corresponding TU-subgraph of G'. In view of the graph-theoretic interpretation of the signless Laplacian coefficients in terms of TU-subgraphs, it suffices to show that for any $k = 1, \ldots, n$, the sum $\sum_H (W(H') - W(H))$, where H runs over all TU-subgraphs of G with k edges, is always nonnegative and when G is connected, the sum is positive if and only if k is in certain range.

Consider an arbitrary TU-subgraph H of G with k edges. If H does not contain any of the edges in Q that are incident with u_0, then $H' = H$ and the contribution of $W(H') - W(H)$ to the required sum is zero. So hereafter we assume that H contains at least one of those edges. There are two

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possible cases: (i) u_0 and u_p, and hence all vertices of P, belong to the same component of H; (ii) u_0 and u_p belong to different components of H.

When (i) happens, clearly the component of H' and that of H containing u_0 have the same number of vertices, and they are both odd-unicyclic or trees. Furthermore, the remaining components are shared by H and H'. So we have $W(H') = W(H)$.

Now we treat Case (ii). Let U denote the component of H that contains vertex u_0. Let a denote the number of vertices in U, other than u_0, that are in Q, let b denote the number of vertices in U that are in P, counting u_0, and let d denote the number of vertices in U, other than u_0, that are in R. Also assume that the component of H that contains u_p has c vertices. (We will use the notations $U(H), a(H), b(H), c(H)$ and $d(H)$ when we need to emphasize the dependence on H.) By the given assumptions, we have $a, b, c \geqslant 1$ and $d \geqslant 0$. In this case, all components of H are also components of H', except for the components U and the path $u_{p-c+1} \cdots u_p$.

First, consider the subcase when U is odd-unicyclic. Clearly, $W(H) = 4cN$, where N is the product of the weights of the common components of H and H'. (If there is no such component, set $N = 1$.) Also, $W(H')$ equals $4(a+c)N$ or $4(b+d)N$, depending on whether the cycle of U is in R or in Q. If the cycle of U is in R, then $W(H') - W(H)$ equals $4aN$ and is always positive. If the cycle is in Q, then the difference $W(H') - W(H)$ equals $4(b+d-c)N$, which can be positive, negative or zero, depending on the values of b, c, d. We are going to group such differences into partial sums in an appropriate way so that each partial sum is nonnegative. Let $\mathcal{H}$ denote the set of all TU-subgraphs H of G with k edges that possess the following properties: u_0 and u_p belong to different components of H; the component $U(H)$ is odd-unicyclic; the subgraph of $U(H)$ induced by vertices that are in Q is odd-unicyclic and fixed (so that $a(H)$ is equal to a fixed positive integer a); the subgraph of $U(H)$ induced by vertices that are in R is a fixed tree (so that $d(H)$ is equal to a fixed nonnegative integer d); $b(H), c(H)$ are positive integers such that $b(H) + c(H)$ equals a fixed positive integer M, $2 \leqslant M \leqslant p+1$; and lastly, the components of H other than $U(H)$ and the one containing u_p, if any, are also fixed (so that $N(H)$ is equal to a fixed positive integer N). Noting that there is a one-to-one correspondence between $\mathcal{H}$ and the set of ordered pairs (b, c) of positive integers with $b + c = M$, we have

$$\sum_{H \in \mathcal{H}} \bigl(W\bigl(H'\bigr) - W(H)\bigr) = \sum_{b=1}^{M-1} 4(b+d-c)N = 4dN(M-1),$$

where the second equality follows from $\sum_{b=1}^{M-1} b = \sum_{b=1}^{M-1} c$, as $b + c = M$. Clearly, the sum is zero if $d = 0$ and is positive if $d \geqslant 1$.

Now we consider the subcase when U is a tree. We have $W(H) = (a+b+d)cN$ and $W(H') = (a+c)(b+d)N$ for some positive integer N, and so $W(H') - W(H) = a(b+d-c)N$. Let $\tilde{\mathcal{H}}$ denote the set of all TU-subgraphs H of G with k edges, defined in a way similar to that for $\mathcal{H}$, except that now we require $U(H)$ to be a tree instead of being odd-unicyclic. Then we have

$$\sum_{H \in \tilde{\mathcal{H}}} \bigl(W\bigl(H'\bigr) - W(H)\bigr) = aN \sum_{b=1}^{M-1} (b+d-c) = aN \sum_{b=1}^{M-1} (2b+d-M) = adN(M-1).$$

Since $M \geqslant 2$, the sum is zero for $d = 0$ and is positive for $d \geqslant 1$.

Now it should be clear that we have the weak inequalities $p_k(G') \geqslant p_k(G)$ for $k = 1, \ldots, n$.

A careful examination of the above argument shows that for a fixed k, the strict inequality $p_k(G') > p_k(G)$ holds if and only if G has a TU-subgraph H with k edges such that u_0 and u_p belong to different components of H and $a(H), d(H)$ are both positive integers (equivalently, the component $U(H)$ contains a vertex in Q and a vertex in R, both different from u_0).

Hereafter, we assume, in addition, that G is connected.

Take any spanning tree F of G. Clearly $F - u_0u_1$ is a TU-subgraph of G with $n-2$ edges which has the following properties: the vertices u_0, u_p lie in different components and we have $a(F - u_0u_1), d(F - u_0u_1) \geqslant 1$. For each $k = 2, \ldots, n-3$, by removing edges from $F - u_0u_1$ appropriately, we obtain a TU-subgraph H of G with k edges that satisfies $a(H), d(H) \geqslant 1$. This establishes the strict inequality $p_k(G) < p_k(G')$ for $k = 2, \ldots, n-2$. On the other hand, it is readily seen that there is no TU-subgraph of G with one edge or with n edges that has the desired properties. So we always have $p_1(G) = p_1(G')$ and $p_n(G) = p_n(G')$.

When G is nonbipartite, we can find an odd-unicyclic spanning subgraph E of G. Then $E - u_0u_1$ is a TU-subgraph with $n-1$ edges that has the desired properties. So in this case we have $p_{n-1}(G) < p_{n-1}(G')$.

On the other hand, when G is bipartite, every TU-subgraph with $n-1$ edges must be a spanning tree and hence contains P as a subgraph. In this case there is no TU-subgraph of G with $n-1$ edges that has the desired properties. Thus, we have $p_{n-1}(G) = p_{n-1}(G')$. □

If the connectedness assumption on G is dropped, then the last part of the preceding theorem no longer holds. This is because, if G is disconnected and if G has too many components that are trees, then G and any generalized π-transform G' cannot have a TU-subgraph with $n-2$ edges, and so we have $p_{n-2}(G) = p_{n-2}(G') = 0$.

In Theorem 4.1, if the generalized π-transform $G' = \pi(G, u_0, P, Q)$ is such that P, Q are paths, then we recover [11, Lemma 2.5]. Our above proof is an elaboration (and correction) of the argument given in [11]. As another immediate corollary of the theorem we have the following:

Corollary 4.2. *Let G be a unicyclic graph of order n and let $G' = \pi(G, u_0, P, T)$ be a generalized π-transform of G, where P is a path and T is a tree. If G is odd-unicyclic then*

$$p_k(G) < p_k\big(G'\big) \quad \text{for } k = 2, \ldots, n-1.$$

If G is even-unicyclic, then

$$p_k(G) < p_k\big(G'\big) \quad \text{for } k = 2, \ldots, n-2.$$

Lemma 4.3. *Let $G \in \mathcal{U}_{g,n}$ be an odd-unicyclic graph. If $G \neq E_{g,n}$, then*

$$p_k(G) < p_k(E_{g,n}), \quad k = 2, \ldots, n-1.$$

Proof. In view of Corollary 4.2, we may assume that $G = C_g(P_{r_1+1}, \ldots, P_{r_g+1})$. By (3.3) we need only show that

$$m_k\big(S(G)\big) + 2m_{k-g}\big(S(G) - C_{2g}\big) < m_k\big(S(E_{g,n})\big) + 2m_{k-g}\big(S(E_{g,n}) - C_{2g}\big)$$

for $k = 2, \ldots, n-1$. For every such k, by Lemma 3.9 we have $m_k(S(E_{g,n})) > m_k(S(G))$. On the other hand, we also have $m_{k-g}(S(E_{g,n}) - C_{2g}) \geqslant m_{k-g}(S(G) - C_{2g})$, because

$$S(G) - C_{2g} = P_{2r_1} \dot{+} P_{2r_2} \dot{+} \cdots \dot{+} P_{2r_g}, \qquad S(E_{g,n}) - C_{2g} = P_{2n-2g},$$
$$2n - 2g = 2r_1 + 2r_2 + \cdots + 2r_g,$$

and in general, it is true that $m_j(P_{n_1+n_2}) \geqslant m_j(P_{n_1} \dot{+} P_{n_2})$. So we are done. □

To compare the values $p_k(E_{g,n})$ (when n, k are fixed and g varies), we will need the following explicit expression for $p_k(E_{g,n})$.

Lemma 4.4. *For any positive integers g, n, $3 \leqslant g \leqslant n$ and any integer $k = 1, \ldots, n$, we have*

$$p_k(E_{g,n}) = \binom{2n-k}{k} + \sum_{l=0}^{r} (-1)^l \binom{2n-1-k-l}{k-1-l} + (-1)^{g+1} 2 \binom{2n-g-k}{k-g}, \tag{4.1}$$

where $r = \min\{k-1, 2(n-g), 2(g-1)\}$.

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Proof. Let $E_{g,n}$ consist of the cycle $C_g = v_1 v_2 \cdots v_g v_1$ together with the pendant path $P = v_g u_1 u_2 \cdots u_{n_g}$ (where $n_g = n - g$) attached at v_g. We denote by $\hat{v}_i$ $(1 \leqslant i \leqslant g)$ the vertex in $S(E_{g,n})$ that subdivides the edge $v_i v_{i+1}$ (where v_{g+1} is taken to be v_1) and by $\hat{u}_i$ $(1 \leqslant i \leqslant n-g)$ the vertex that subdivides the edge $u_{i-1}u_i$ (where u_0 is taken to be v_g). By applying Lemma 3.3 (with $G = S(E_{g,n}), u = v_g$ and $v = \hat{v}_g$) and Lemma 3.4, we have

$$\begin{aligned} m_k\big(S(E_{g,n})\big) &= m_k(P_{2n}) + m_{k-1}(P_{2(n-g)} \dot{+} P_{2g-2}) \\ &= \binom{2n-k}{k} + \sum_{l=0}^{r} (-1)^l \binom{2n-1-k-l}{k-1-l}, \end{aligned}$$

where $r = \min\{k-1, 2(n-g), 2(g-1)\}$. On the other hand, since $S(E_{g,n}) - C_{2g} = P_{2(n-g)}$, we also have $m_{k-g}(S(E_{g,n}) - C_{2g}) = \binom{2n-g-k}{k-g}$. So, in view of (3.3), our assertion follows. $\square$

Lemma 4.5. *Let $n \geqslant 5$ be a positive integer. Let α_n be the (unique) real root of the cubic polynomial $f_n(x)$ given by:*

$$f_n(x) = 3x^3 + (7 - 10n)x^2 + 2\big(6n^2 - 11n + 8\big)x - \big(4n^3 - 6n^2 - 10n + 24\big).$$

For any positive integer $k = 2, \ldots, n-1$, the maximum value of $p_k(E_{g,n})$, as g runs through all integers between 3 and n (inclusive), is attained at $g = n$ if $k \leqslant \alpha_n$ and at $g = 3$ if $\alpha_n \leqslant k \leqslant n-1$. Moreover, the maximum is always attained uniquely except when $k = \alpha_n$.

Proof. By Remark 2.3 we have $p_{n-1}(E_{3,n}) > p_{n-1}(E_{g,n})$ for $g = 4, 5, \ldots, n$. Hereafter, we assume that $2 \leqslant k \leqslant n-2$.

According to (4.1), $p_k(E_{g,n})$ is the sum of three parts, namely,

$$\binom{2n-k}{k}, \qquad \sum_{l=0}^{r(g)} (-1)^l \binom{2n-1-k-l}{2(n-k)} \quad \text{and} \quad (-1)^{g+1} 2\binom{2n-g-k}{2(n-k)},$$

where $r(g) = \min\{k-1, 2(n-g), 2(g-1)\}$. (We have deliberately rewritten the binomial coefficients $\binom{2n-1-k-l}{k-1-l}$ and $\binom{2n-g-k}{k-g}$ as $\binom{2n-1-k-l}{2(n-k)}$ and $\binom{2n-g-k}{2(n-k)}$ respectively.) Note that the first part is independent of G. The second part is a partial sum of the finite alternating series $\sum_{l=0}^{k-1} (-1)^l \binom{2n-1-k-l}{2(n-k)}$, and clearly the partial sums $S_i := \sum_{l=0}^{i} (-1)^l \binom{2n-1-k-l}{2(n-k)}$ $(i = 0, \ldots, k-1)$ of this alternating series satisfy

$$S_1 < S_3 < S_5 < \cdots < S_{k-1} < \cdots < S_4 < S_2 < S_0,$$

as its terms have decreasing magnitude. The third part is a term of the finite sequence $(-1)^{g+1} 2\binom{2n-g-k}{2(n-k)}$, $g = 3, \ldots, n$, and it is readily seen that the first term of this sequence is strictly greater than the remaining terms, provided that $k \geqslant 3$ (when $k = 1$ or 2, all terms in the sequence are zero). So the inequality $p_k(E_{g,n}) > p_k(E_{3,n})$ holds only if $r(g) < r(3)$. The value of $r(3)$ varies with n and k. For technical reasons, we deal with the cases $k = 2, 3, 4$ separately first.

The contribution of the last term on the right side of (4.1) is zero if $k < g$ and, in particular, if $k = 2$. So it is obvious that the maximum value of $p_2(E_{g,n})$, as g varies, is attained uniquely at $g = n$. Then $E_{g,n} = C_n$.

When $k = 3$, $r(g)$ equals 2 if $3 \leqslant g \leqslant n-1$ and equals 0 if $g = n$. So the maximum value of $p_3(E_{g,n})$ is attained at $g = 3$ or $g = n$. Now we have

$$p_3(E_{3,n}) - p_3(E_{n,n}) = \sum_{l=1}^{2} (-1)^l \binom{2n-4-l}{2-l} + 2\binom{2n-6}{0} = 8 - 2n < 0$$

as $n \geqslant 5$. So the maximum value of $p_3(E_{g,n})$ is attained uniquely at $g = n$.

When $k=4$, $r(g)$ equals 0 if $g=n$, equals 2 if $g=n-1$ and equals 3 if $3 \leqslant g \leqslant n-2$. So the maximum value of $p_4(E_{g,n})$ as g varies between 3 and n is attained at $g=3, n-1$ or n. In view of Lemma 2.2, by calculations we have

$$p_4(E_{3,5})=27, \qquad p_4(E_{4,5})=20 \quad \text{and} \quad p_4(E_{5,5})=25.$$

Hence the maximum value of $p_4(E_{g,5})$ is attained uniquely at $g=3$.

When $n \geqslant 6$, the last term in the expression for $p_4(E_{n,n})$ (also, $p_4(E_{n-1,n})$) as given by (4.1) is equal to zero. So, in this case, we clearly have $p_4(E_{n-1,n}) < p_4(E_{n,n})$, and the maximum value of $p_4(E_{g,n})$ must be attained at $g=3$ or $g=n$. By calculation we have

$$p_4(E_{3,n}) - p_4(E_{n,n}) = -2n^2 + 19n - 43 < 0.$$

Hence, for $n \geqslant 6$, the maximum value of $p_4(E_{g,n})$ is attained uniquely at $g=n$.

Summarizing what we have done so far, for $k=2,3,4$, $\max_g p_k(E_{g,n})$ is attained uniquely at $g=n$, except that $\max_g p_4(E_{g,5})$ is attained uniquely at $g=3$.

When $k \geqslant 5$, we have $r(3)=4=r(n-2)<r(g)$ for $4 \leqslant g \leqslant n-3$, $r(n-1)=2$ and $r(n)=0$. Note that $\binom{2n-g-k}{2(n-k)}=0$. Since $k \leqslant n-2$, $\binom{2n-g-k}{2(n-k)}=0$ for $g=n-1, n-2$. In other words, the last term in the expression for $p_k(E_{n-1,n})$ (also, for $p_k(E_{n,n})$) is equal to zero. Hence $p_k(E_{n,n}) > p_k(E_{n-1,n})$ and the maximum value of $p_k(E_{g,n})$ is attained only at $g=3$ or $g=n$. Now $p_k(E_{3,n}) - p_k(E_{n,n})$ equals

$$2\binom{2n-3-k}{k-3} + \sum_{l=1}^{4}(-1)^l \binom{2n-1-k-l}{k-1-l},$$

and after some calculations it becomes

$$f_n(k)\frac{\binom{2n-k-4}{k-3}}{(n-k)(2n-k-4)(k-2)},$$

where $f_n(x)$ is the given cubic polynomial. As $5 \leqslant k \leqslant n-2$, it is readily checked that $\frac{\binom{2n-k-4}{k-3}}{(n-k)(2n-k-4)(k-2)} > 0$. So $p_k(E_{3,n})$ is greater than, equal to, or less than $p_k(E_{n,n})$, depending on whether $f_n(k)$ is greater than, equal to, or less than 0. Note that for $n \geqslant 5$, $f_n(x)$ is a strictly increasing cubic polynomial function, as the discriminant of the derivative of $f_n(x)$, which equals $-4(8n^2-58n+95)$, is negative. It follows that when $n \geqslant 6$, for $5 \leqslant k \leqslant n-1$, $\max_g p_k(E_{g,n})$ is attained at $g=n$ if $k \leqslant \alpha_n$ and at $g=3$ if $k \geqslant \alpha_n$, and, moreover, the maximum is always attained uniquely except when $k=\alpha_n$. By what we have done at the beginning, the preceding conclusion also holds for $k=2,3,4$, because for $n \geqslant 6$ we have $\alpha_n > 4$ as $f_n(4) < 0$.

At the beginning we have also proved that $\max_g p_k(E_{g,5})$ is attained uniquely at $g=5$ if $k=2,3$ and at $g=3$ if $k=4$. Since $3 < \alpha_5 < 4$ (as $f_5(3) < 0$ and $f_5(4) > 0$), our result also holds for $n=5$. □

Proof of Theorem 1.1. By Lemma 4.3 if $G \in \mathcal{U}_{g,n}$ is odd-unicyclic and if $G \neq E_{g,n}$, then $p_k(G) < p_k(E_{g,n})$ for $k=2,\ldots,n-1$. So, among all odd-unicyclic graphs G of order n, the maximum value of $p_k(G)$ is attained only when G is a lollipop graph.

Note that for $1 \leqslant k \leqslant n-1$, every TU-subgraph of C_n with k edges is a spanning forest. So by (2.1) and (2.2) we have $p_k(C_n) = c_k(C_n)$ for $k=1,\ldots,n-1$.

If $G \in \mathcal{U}_{g,n}$ is even-unicyclic, then G is bipartite and for $k=2,\ldots,n-2$ by Stevanović and Ilić [14] we have

$$p_k(G) = c_k(G) \leqslant c_k(C_n) = p_k(C_n),$$

where the inequality becomes equality if and only if $G = C_n$.

Thus, the maximum value of $p_k(G)$ as G varies over all unicyclic graphs of order n is always attained among lollipop graphs and by Lemma 4.5 our result follows. □

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5. Proof of Theorem 1.2

First, we recall the definition of a σ-transformation, as introduced by Mohar [12] for trees and extended to general graphs by Stevanović and Ilić [14].

Let w be a vertex of degree $p+1$ in a graph G, which is not a star, such that $wv_1, \dots, wv_p$ are pendant edges incident with w and v_0 is the neighbor of w distinct from $v_1, \dots, v_p$. We call the graph G' obtained from G by removing edges $wv_1, \dots, wv_p$ and adding new edges $v_0v_1, \dots, v_0v_p$ a σ-transform of G and we write $G' = \sigma(G, w)$. It is easy to see if G' is a σ-transform of G then G is a generalized π-transform of G'; indeed, we have, $G = \pi(G', v_0, P, Q)$, where P is the path P_2: v_0w and Q is the star on vertices $v_0, v_1, \dots, v_p$ with center v_0.

The following is an immediate consequence of Corollary 4.2.

Theorem 5.1. *Let $G \in \mathcal{U}_{g,n}$ be a unicyclic graph and let $G' = \sigma(G, w)$ be a σ-transform of G. If G is odd-unicyclic, then*

$$p_k(G) > p_k(G') \quad \text{for } k = 2, \dots, n-1.$$

If G is even-unicyclic, then

$$p_k(G) > p_k(G') \quad \text{for } k = 2, \dots, n-2.$$

Let $C_g(S_{r_1+1}, \dots, S_{r_g+1})$ denote the unicyclic graph which consists of the cycle $C_g = v_1v_2 \cdots v_gv_1$ together with r_i pendant edges attached at vertex v_i for $i = 1, \dots, g$, where $r_1, \dots, r_g$ are nonnegative integers. We write $C_g(S_{n-g+1}, S_1, \dots, S_1)$ simply as $C_g(S_{n-g+1})$.

It is known that every tree which is not a star can be transformed into a star by a sequence of σ-transformations (see [12, Proposition 3.1]). Likewise, every unicyclic graph with cycle length g can be transformed into a graph of the form $C_g(S_{r_1+1}, \dots, S_{r_g+1})$ by applying a sequence of σ-transformations, if the graph is not already of such form.

By Theorem 5.1 if $G \in \mathcal{U}_{g,n}$ is an odd-unicyclic (respectively, even-unicyclic) graph and if G is not of the form $C_g(S_{r_1+1}, \dots, S_{r_g+1})$ then there exists a graph $G' \in \mathcal{U}_{g,n}$ of such form such that $p_k(G) > p_k(G')$ for $k = 2, \dots, n-1$ (respectively, for $k = 2, \dots, n-2$). To compare the values of $p_k(G)$ between odd-unicyclic (or even-unicyclic) graphs G of the form $C_g(S_{r_1+1}, \dots, S_{r_g+1})$ we need the concept of a double τ-transform of a unicyclic graph. Before giving the definition, we first recall the definition of a τ-transform of a unicyclic graph, as introduced by Stevanović and Ilić [14].

An edge e of a graph G is said to be *contracted* if it is deleted and its ends are identified.

Let v and w be two neighboring vertices on the cycle of a unicyclic graph G with degrees $p+2$ and $q+2$ respectively such that there are p pendant edges incident with v and q pendant edges incident with w (where p, q are nonnegative integers). The graph G' obtained from G by contracting edge vw and adding a new pendant edge to vertex v is called a *τ-transform* of G and is denoted by $\tau(G, v, w)$.

Let u, v and w be three consecutive vertices on the cycle of a unicyclic graph G with degrees $p+2$, $q+2$ and $r+2$ respectively such that there are p (respectively, q, r) pendant edges incident with u (respectively, v, w). The graph G' obtained from G by contracting edges uv and vw and adding two new pendant edges uv and uw to vertex u is called a *double τ-transform of G* and is denoted by $\tau(G, u, v, w)$.

Theorem 5.2. *If $G \in \mathcal{U}_{g,n}$ $(g \geqslant 5)$ is an odd-unicyclic graph of the form $C_g(S_{r_1+1}, \dots, S_{r_g+1})$ and $G' \in \mathcal{U}_{g-2,n}$ is a double τ-transform of G, then*

$$p_k(G) > p_k(G') \quad \text{for } k = 2, \dots, n-1.$$

Proof. Let $C = v_1v_2 \cdots v_gv_1$ be the cycle of G. Without loss of generality, assume that $G' = \tau(G, v_1, v_2, v_3)$. There is a natural one-to-one correspondence between the edges of G and those of G'. (Under this correspondence, the edges v_2v_3, v_2u, v_3v of G, where u, v do not lie on C, correspond respectively to the edges v_1v_3, v_1u and v_1v of G'.) This correspondence between edges induces a one-to-one correspondence between TU-subgraphs of G with k edges and TU-subgraphs of G' with k edges. Note that, since G (also, G') is odd-unicyclic, every spanning subgraph of G (respectively, G') is a TU-subgraph of G (respectively, G'). We first show that if H is a TU-subgraph of G and H' is the corresponding TU-subgraph of G' then $W(H) \geqslant W(H')$. We also examine when the strict inequality holds.

Let H be a TU-subgraph of G with k edges, and let H' be the corresponding TU-subgraph of G'. We divide our discussion into cases.

1°. Suppose that H contains every edge of the cycle C. Then the edges removed from G (respectively, G') to obtain H (respectively, H') are all pendant edges. So in this case H (respectively, H') has precisely one nontrivial component, which is unicyclic. Hence we have $W(H) = W(H') = 4$.

2°. Suppose that $v_1v_2 \notin E(H)$ or $v_2v_3 \notin E(H)$ but all other edges of C are in H. Then H has precisely one or two nontrivial components, each of which is a tree: the component containing v_1 must be nontrivial, and the one containing v_2 can be nontrivial when $v_1v_2, v_2v_3 \notin E(H)$. When H has one nontrivial component, the component must be a tree with k edges. In this case $W(H) = k+1$. When H has two nontrivial components, let r, s be the number of edges in these tree components. Then $r + s = k$ and we have $W(H) = (r + 1)(s + 1) = k + 1 + rs > k + 1$. On the other hand, the only nontrivial component of H' is unicyclic; hence $W(H') = 4$. Since H contains every edge of C other than v_1v_2, v_2v_3, $k \geqslant g - 2 \geqslant 5 - 2 = 3$. It follows that we have $W(H) \geqslant W(H')$. Indeed, in this case the inequality is always strict, except when $g = 5$ and $k = 3$.

3°. Suppose that v_1v_2, v_2v_3 are both edges of H and at least one edge of C does not belong to H. In this case, the components of H (also, of H') are all trees. Also, the component of H containing v_1 has the same number of vertices as the component of H' containing v_1. The other components are shared by H and H'. So we have $W(H) = W(H')$.

4°. Suppose that $v_1v_2 \notin E(H)$, $v_2v_3 \in E(H)$ and at least one other edge of C does not belong to H. In this case the components of H (also, of H') are trees. Let T_1 (respectively, T_2) denote the component of H that contains v_1 (respectively, v_2 and hence also v_3). Also, let T_3 denote the component of H' that contains v_1 (and v_3 but not v_2 as $v_1v_2 \notin E(H)$ and $v_1v_3 \in E(H')$). Note that T_3 is the subgraph in G' corresponding to the edge-induced subgraph of G formed by the edges $E(T_1) \cup E(T_2)$; so we have

$$\begin{aligned} W(T_3) &= \left|V(T_3)\right| = \left|E(T_3)\right| + 1 = \left|E(T_1)\right| + \left|E(T_2)\right| + 1 \\ &= \left|V(T_1)\right| + \left|V(T_1)\right| - 1 \leqslant \left|V(T_1)\right|\left|V(T_2)\right| = W(T_1)W(T_2), \end{aligned}$$

where the inequality follows from the elementary fact that for any real numbers $x, y \geqslant 1$, we have $xy \geqslant x + y - 1$ with equality if and only if $x = 1$ or $y = 1$. The remaining nontrivial components of H and H' (if any) being common, we have $W(H') \leqslant W(H)$, with strict inequality if and only if T_1 has order at least 2.

5°. Suppose that $v_1v_2 \in H$, $v_2v_3 \notin H$ and at least one other edge of C is not in H. The argument is similar to that for 4°.

6°. Suppose that $v_1v_2 \notin E(H)$, $v_2v_3 \notin E(H)$ and at least one other edge of C does not belong to $E(H)$. Let T_1 (respectively, T_2, T_3) denote the component of H containing v_1 (respectively, v_2, v_3). Also, let T_4 denote the component of H' that contains v_1. Then

$$\begin{aligned} W(T_4) &= \left|V(T_4)\right| = \left|V(T_1)\right| + \left|V(T_2)\right| + \left|V(T_3)\right| - 2 \\ &\leqslant \left|V(T_1)\right|\left|V(T_2)\right|\left|V(T_3)\right| = W(T_1)W(T_2)W(T_3). \end{aligned}$$

The remaining nontrivial components of H and H' (if any) being common, we have $W(H) \geqslant W(H')$.

In view of (2.2) we have the inequalities $p_k(G) \geqslant p_k(G')$ for $k = 1, 2, \ldots, n$.

Take $H = G - v_1v_2$. Then H is a TU-subgraph of G with $n - 1$ edges. By 2° we have $W(H) > W(H')$ and so the strict inequality $p_{n-1}(G) > p_{n-1}(G')$ holds.

For any given positive integer $k = 2, \ldots, n - 2$, let H be any TU-subgraph of G with k edges that contains, in particular, the edges v_2v_3 and v_gv_1, but does not contain the edge v_1v_2 and $v_{g-1}v_g$. Then by 4° we have $W(H) > W(H')$ and so the strict inequality $p_k(G) > p_k(G')$ holds. □

With slight modifications, the proof for Theorem 5.2 also yields the following corresponding result for even-unicyclic graphs.

Theorem 5.3. *If $G \in \mathcal{U}_{g,n}$ ($g \geqslant 6$) is an even-unicyclic graph of the form $C_g(S_{r_1+1}, \ldots, S_{r_g+1})$ and $G' \in \mathcal{U}_{g-2,n}$ is a double τ-transform of G, then*

$$p_k(G) > p_k(G') \quad \text{for } k = 2, \ldots, n-1.$$

Theorem 5.2 (also, Theorem 5.3) no longer holds if we replace "double τ-transform" by "τ-transform". For a counter-example, see [11, the paragraph following Theorem 3.2].

Lemma 5.4. *Let $G = C_4(S_{r_1+1}, S_{r_2+1}, S_{r_3+1}, S_{r_4+1})$. Let G' be the graph obtained from G by relocating the r_j pendant edges at vertex v_j to vertex v_i, where $1 \leqslant i, j \leqslant 4$, $i \neq j$. Assume that $r_i, r_j \geqslant 1$. Then for $k = 2, \ldots, n-2$, $p_k(G) \geqslant p_k(G') + 3r_ir_j$ when v_i and v_j are adjacent and $p_k(G) \geqslant p_k(G') + 4r_ir_j$ when v_i and v_j are nonadjacent; and $p_k(G) = p_k(G')$ for $k = 1, n-1$ or n.*

Proof. Let $v_1v_2v_3v_4v_1$ be the cycle of G.

First, we consider the case when v_i, v_j are adjacent vertices of G. Without loss of generality, let $i = 1$ and $j = 2$. Let $v_1u_1, \ldots, v_1u_{r_1}$ denote the pendant edges of G attached to v_1 and $v_2w_1, \ldots, v_2w_{r_2}$ be the pendant edges attached to v_2. We denote by $\hat{u}_i$ ($1 \leqslant i \leqslant r_1$) and $\hat{w}_j$ ($1 \leqslant j \leqslant r_2$) the vertices of $S(G)$ (hence, also of $S(G')$) that subdivide edges v_1u_i and v_2w_j of G (or v_1u_i and v_1w_j of G') respectively. Also, denote by $\hat{v}_i$, $1 \leqslant i \leqslant 4$, the vertex of $S(G)$ (also, of $S(G')$) that subdivides edges v_iv_{i+1}, where v_5 is taken to be v_1.

Let M' be a matching in $S(G')$. By modifying the set of edges in $S(G)$ corresponding to M', we will construct a matching in $S(G)$. There are six subcases to be considered:

1°. If $v_1\hat{w}_j \notin M'$ for $j = 1, \ldots, r_2$ then the set of edges M in $S(G)$ corresponding to M' is clearly a matching in $S(G)$ such that $v_2\hat{w}_j \notin M$ for $j = 1, \ldots, r_2$.

2°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_2$ and v_2 is not covered by M', then the set of edges M in $S(G)$ corresponding to M' is a matching in $S(G)$ for which $v_2\hat{w}_j \in M$ for some $j = 1, \ldots, r_2$, and v_1 is not covered by M.

3°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_2$ and $v_2\hat{v}_1 \in M'$, then we obtain a matching M in $S(G)$ from M' by replacing $v_1\hat{w}_j$ by $v_2\hat{w}_j$ and $v_2\hat{v}_1$ by $v_1\hat{v}_1$.

4°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_2$, $v_2\hat{v}_2 \in M'$ and $v_4\hat{v}_4 \notin M'$, then we obtain a matching M in $S(G)$ from M' by replacing $v_1\hat{w}_j$ by $v_2\hat{w}_j$ and $v_2\hat{v}_2$ by $v_1\hat{v}_4$.

5°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_2$, $v_2\hat{v}_2 \in M'$, $v_4\hat{v}_4 \in M'$ and $v_3\hat{v}_3 \notin M'$, then we obtain a matching M in $S(G)$ from M' by replacing $v_1\hat{w}_j$ by $v_2\hat{w}_j$, $v_2\hat{v}_2$ by $v_1\hat{v}_4$ and $v_4\hat{v}_4$ by $v_4\hat{v}_3$.

6°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_2$, $v_2\hat{v}_2 \in M'$, $v_4\hat{v}_4 \in M'$ and $v_3\hat{v}_3 \in M'$, then we obtain a matching M in $S(G)$ from M' by replacing $v_1\hat{w}_j$ by $v_2\hat{w}_j$, $v_2\hat{v}_2$ by $v_1\hat{v}_4$, $v_4\hat{v}_4$ by $v_4\hat{v}_3$ and $v_3\hat{v}_3$ by $v_3\hat{v}_2$.

It is readily checked that the mapping $M' \mapsto M$ constructed in the above manner is a one-to-one map from the set of all matchings in $S(G')$ into the set of all matchings M in $S(G)$ with the following property: if $v_2\hat{w}_j \in M$ for some $j = 1, \ldots, r_2$ and if v_1 is covered by M then $v_1\hat{v}_1 \in M$ or $v_1\hat{v}_4 \in M$. So a matching M in $S(G)$ is not in the range of this map if and only if $v_2\hat{w}_j \in M$ for some $j = 1, \ldots, r_2$ and $v_1\hat{u}_i \in M$ for some $i = 1, \ldots, r_1$. Any such matching M must have at least two edges and contains at most $n-2$ edges as it must miss vertex $\hat{v}_1$ and one of the vertices $\hat{v}_2$, $\hat{v}_3$ or $\hat{v}_4$. Indeed, it is not difficult to show that for any pair i, j, $1 \leqslant i \leqslant r_1$, $1 \leqslant j \leqslant r_2$, there are precisely three $(n-2)$-matchings in $S(G)$ that contain both of the edges $v_1\hat{u}_i$, $v_2\hat{w}_j$. This shows that for $k = 2, \ldots, n-2$, $m_k(S(G)) - m_k(S(G')) \geqslant 3r_1r_2$ and $m_k(S(G)) = m_k(S(G'))$ for $k = 1, n-1$ or n.

On the other hand, $S(G) - C_8$ and $S(G') - C_8$ are both equal to $(n-4)K_2$. So we have $m_{k-4}(S(G) - C_8) = m_{k-4}(S(G') - C_8)$ for every nonnegative integer k. In view of (3.3) the desired inequalities between $p_k(G)$ and $p_k(G')$ are satisfied.

Now we consider the case when v_i, v_j are not adjacent vertices of G. Without loss of generality, take $i = 1$ and $j = 3$. Let $u_i, \hat{u}_i, i = 1, \ldots, r_1$, $w_j, \hat{w}_j, j = 1, \ldots, r_3$ and $\hat{v}_i, i = 1, 2, 3, 4$ have the obvious meanings.

For any matching M' in $S(G')$, by modifying the set of edges in $S(G)$ corresponding to M', we will construct a matching in $S(G)$. There are six subcases to be considered:

1°. If $v_1\hat{w}_j \notin M'$ for $j = 1, \ldots, r_3$, then the set of edges M in $S(G)$ corresponding to M' is clearly a matching in $S(G)$ such that $v_3\hat{w}_j \notin M$ for $j = 1, \ldots, r_2$.

2°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_3$ and v_3 is not covered by M', then the set of edges M in $S(G)$ corresponding to M' is a matching in $S(G)$ for which $v_3\hat{w}_j \in M$ for some $j = 1, \ldots, r_3$, and v_1 is not covered by M.

3°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_3$, $v_3\hat{v}_2 \in M'$ and $v_2\hat{v}_1 \notin M'$, then we obtain a matching M in $S(G)$ from M' by replacing $v_1\hat{w}_j$ by $v_3\hat{w}_j$ and $v_3\hat{v}_2$ by $v_1\hat{v}_1$.

4°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_3$, $v_3\hat{v}_2 \in M'$ and $v_2\hat{v}_1 \in M'$, to obtain M from M' we replace $v_1\hat{w}_j$ by $v_3\hat{w}_j$, $v_3\hat{v}_2$ by $v_1\hat{v}_1$ and $v_2\hat{v}_1$ by $v_2\hat{v}_2$.

5°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_3$, $v_3\hat{v}_3 \in M'$ and $v_4\hat{v}_4 \notin M'$, then we obtain M from M' by replacing $v_1\hat{w}_j$ by $v_3\hat{w}_j$ and $v_3\hat{v}_3$ by $v_1\hat{v}_4$.

6°. If $v_1\hat{w}_j \in M'$ for some $j = 1, \ldots, r_3$, $v_3\hat{v}_3 \in M'$ and $v_4\hat{v}_4 \in M'$, then we obtain M from M' by replacing $v_1\hat{w}_j$ by $v_3\hat{w}_j$, $v_3\hat{v}_3$ by $v_1\hat{v}_4$ and $v_4\hat{v}_4$ by $v_4\hat{v}_3$.

It is readily checked that the mapping $M' \mapsto M$ constructed in the above manner is a one-to-one map from the set of all matchings in $S(G')$ into the set of all matchings M in $S(G)$ with the following property: if $v_3\hat{w}_j \in M$ for some $j = 1, \ldots, r_3$ and if v_1 is covered by M then $v_1\hat{v}_1 \in M$ or $v_1\hat{v}_4 \in M$. Then we can show that for any $i, j, 1 \leqslant i \leqslant r_1, 1 \leqslant j \leqslant r_3$, there are precisely four $(n-2)$-matchings in $S(G)$ that contain both of the edges $v_1\hat{u}_i, v_3\hat{w}_j$ and miss exactly one of the following pairs of vertices: $\hat{v}_1$ and $\hat{v}_3$, $\hat{v}_1$ and $\hat{v}_4$, $\hat{v}_2$ and $\hat{v}_3$, or $\hat{v}_2$ and $\hat{v}_4$. So for $2 \leqslant k \leqslant n-2$, $m_k(S(G)) - m_k(S(G')) \geqslant 4r_1r_3$. On the other hand, we also have $m_{k-4}(S(G) - C_8) = m_{k-4}(S(G') - C_8)$ for every nonnegative integer k. So the desired inequalities between $p_k(G)$ and $p_k(G')$ follow. □

By a similar (but less involved) argument, one can also establish the following:

Lemma 5.5. *Let* $G = C_3(S_{r_1+1}, S_{r_2+1}, S_{r_3+1})$ *and* $G' = C_3(S_{r_1+r_2+1}, S_1, S_{r_3+1})$ $(r_1, r_2 \geqslant 1)$. *Then* $p_k(G) \geqslant p_k(G') + 2r_1r_2$ *for* $k = 2, \ldots, n-2$ *and* $p_k(G) = p_k(G')$ *for* $k = 1, n-1$ *or* n.

Lemma 5.6. *For any positive integer* $n \geqslant 5$, *we have*

(i) $p_k(C_4(S_{n-3})) > p_k(C_3(S_{n-2}))$ *for* $k = 2, \ldots, n-4$;
(ii) $p_{n-3}(C_4(S_{n-3})) > p_{n-3}(C_3(S_{n-2}))$ *for* $n = 5, \ldots, 24$ *and* $p_{n-3}(C_4(S_{n-3})) < p_{n-3}(C_3(S_{n-2}))$ *for* $n \geqslant 25$;
(iii) $p_{n-2}(C_4(S_{n-3})) > p_{n-2}(C_3(S_{n-2}))$ *for* $n = 5, 6, 7, 8$ *and* $p_{n-2}(C_4(S_{n-3})) < p_{n-2}(C_3(S_{n-2}))$ *for* $n \geqslant 9$; *and*
(iv) $p_{n-1}(C_4(S_{n-3})) < p_{n-1}(C_3(S_{n-2}))$.

Proof. By Lemma 2.2(i) $p_2(C_4(S_{n-3})) = 2n - 6 + \frac{3}{2}n(n-1) > n - 3 + \frac{3}{2}n(n-1) = p_2(C_3(S_{n-2}))$.

By Lemma 2.2(ii), we also have

$$p_{n-1}\big(C_3(S_{n-2})\big) = 3n + 4(n-3) = 7n - 12 > 4n = p_{n-1}\big(C_4(S_{n-3})\big),$$

as $n \geqslant 5$.

Hereafter, for convenience, we denote $C_4(S_{n-3})$ and $C_3(S_{n-2})$ by G and G' respectively. It is clear that G' is a τ-transform of G. To be specific, let $C = v_1v_2v_3v_4v_1$ be the cycle of G and assume that $G' = \tau(G, v_1, v_2)$. There is a natural one-to-one correspondence between the edges of G and those of G'. Since G' is odd-unicyclic, every spanning subgraph of G' is a TU-subgraph. But for G, a spanning subgraph is a TU-subgraph if and only if it does not contain the cycle of G as a subgraph.

Let H be a spanning subgraph of G with k edges, and let H' be the corresponding spanning subgraph of G', certainly also with k edges.

1°. If H contains every edge of the cycle C, then H is not a TU-subgraph of G. On the other hand, H' is a TU-subgraph with exactly one nontrivial component, which is odd-unicyclic. So $W(H') = 4$.

Altogether there are $\binom{n-4}{k-4}$ such subgraph H of G. Their contribution to $p_k(G)$ is zero, whereas the total contribution of the corresponding subgraphs H' of G' to $p_k(G')$ is $4\binom{n-4}{k-4}$.

2°. Suppose that $v_1v_2 \notin H$ but all other edges of C belong to H. Then H is a TU-subgraph of G with precisely one nontrivial component, which is a tree with k edges; so $W(H) = k+1$. On the other hand, H' is a TU-subgraph of G' with precisely one nontrivial component, which is odd-unicyclic; so $W(H') = 4$. Altogether there are $\binom{n-4}{k-3}$ such subgraph H of G.

3°. Suppose that $v_1v_2 \in H$ but there is at least one edge of C not in H. In this case, the components of H (also, of H') are trees. Furthermore, the component of H containing v_1 has the same number of vertices as the component of H' containing v_1, and the other components of H and H' (if any) are the same. So in this case we have $W(H) = W(H')$.

4°. Suppose that $v_1v_2 \notin H$ and there is at least one other edge of C not in H. We have the following subcases, depending on which edges of C do not lie on H:

(1) the edges of C that do not lie on H are v_1v_2, v_2v_3; or v_1v_2, v_2v_3, v_3v_4; or all edges of C: then H and H' each have exactly one nontrivial component, which is a tree. So $W(H)$ and $W(H')$ are both equal to $k+1$.

(2) the edges of C not in H are v_1v_2, v_2v_3 and v_1v_4: then H and H' share the same components and we have $W(H) = W(H')$.

(3) the edges of C not in H are v_1v_2 and v_3v_4 or v_1v_2, v_3v_4 and v_4v_1: then H has two nontrivial components, namely, a tree with one edge and a tree with $k-1$ edges; so $W(H) = 2k$. On the other hand, H' has only one nontrivial component, which is a tree with k edges. So $W(H') = k+1$. The number of such H is $\binom{n-4}{k-2} + \binom{n-4}{k-1} = \binom{n-3}{k-1}$.

(4) the edges of C not in H are v_1v_2 and v_1v_4: then H has two nontrivial components, namely, a tree with two edges and a tree with $k-2$ edges, and H' has only one nontrivial component. So we have $W(H) = 3(k-1)$ and $W(H') = k+1$. The number of such H is $\binom{n-4}{k-2}$.

From the above we find that $p_k(G) - p_k(G')$ equals

$$-\binom{n-4}{k-4}(4) + \binom{n-4}{k-3}(k+1-4) + \binom{n-3}{k-1}\bigl(2k-(k+1)\bigr)$$
$$+\binom{n-4}{k-2}\bigl(3(k-1)-(k+1)\bigr),$$

and after further calculations it becomes

$$\frac{(n-4)!}{(k-4)!(n-k-2)!}\left[\frac{n-k-4}{(n-k)(n-k-1)} + \frac{n-3}{(k-2)(k-3)} + \frac{2}{k-3}\right].$$

So $p_k(G) > p_k(G')$ for $3 < k \leqslant n-4$. Note that we also have $p_3(G) > p_3(G')$ as

$$p_3(G) - p_3(G') = 2\binom{n-3}{2} + 2\binom{n-4}{1} > 0.$$

When $k = n-3$, the expression inside the square bracket is $-\dfrac{(n-\frac{29}{2})^2 - \frac{409}{4}}{6(n-5)(n-6)}$. It is readily checked that the latter expression is positive for integers n between 7 and 24 (inclusive) but is negative for integers $n \geqslant 25$. So we have $p_{n-3}(G) > p_{n-3}(G')$ for $n = 7, \dots, 24$ and $p_{n-3}(G) < p_{n-3}(G')$ for $n \geqslant 25$. When $n = 5$, the inequality $p_{n-2}(G) > p_{n-2}(G')$ becomes $p_3(G) > p_3(G')$, which holds as we have already shown that $p_k(G) > p_k(G')$ for $k = 2, \dots, n-4$. Similarly, the inequality $p_{n-3}(G) > p_{n-3}(G')$ also holds for $n = 6$.

When $k = n-2$, the expression inside the square bracket can be written as $-\dfrac{(n-6)^2-5}{(n-4)(n-5)}$. It is readily checked that the latter expression is positive for $n = 6, 7, 8$ and is negative for $n \geqslant 9$. So we have $p_{n-2}(G) > p_{n-2}(G')$ for $n = 6, 7, 8$ (and also for $n = 5$, which has already been done), and $p_{n-2}(G) < p_{n-2}(G')$ for $n \geqslant 9$. □

Proof of Theorem 1.2. By Theorem 5.1 among odd-unicyclic (respectively, even-unicyclic) graphs G, the minimum value of $p_k(G)$ for $k = 2, \dots, n-1$ (respectively, $k = 2, \dots, n-2$) is attained only if G is of the form $C_g(S_{r_1+1}, \ldots, S_{r_g+1})$. By Theorem 5.2 (respectively, Theorem 5.3) for odd (respectively, even) g, among graphs of the form $C_g(S_{r_1+1}, \ldots, S_{r_g+1})$, the minimum value of $p_k(G)$ is attained only if $g = 3$ (respectively, $g = 4$). Then by Lemma 5.5 (respectively, Lemma 5.4) the minimum value of $p_k(G)$ when G varies over graphs of the form $C_3(S_{r_1+1}, S_{r_2+1}, S_{r_3+1})$ (respectively, $C_4(S_{r_1+1}, S_{r_2+1}, S_{r_3+1}, S_{r_4+1})$) is attained at $G = C_3(S_{n-2})$ (respectively, $C_4(S_{n-3})$). So the minimum value of $p_k(G)$ as G varies over all unicyclic graphs of order n is attained at either $C_3(S_{n-2})$ or $C_4(S_{n-3})$, and our result follows from Lemma 5.6. □

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