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ON THE SKEW SPECTRAL MOMENTS OF TREES WITH A GIVEN BIPARTITION

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Abstract. Let G be a simple graph, and $\vec{G}$ be an oriented graph of G with an orientation and skew-adjacency matrix $S(\vec{G})$. Let $\lambda_1(\vec{G}), \lambda_2(\vec{G}), \ldots, \lambda_n(\vec{G})$ be the eigenvalues of $S(\vec{G})$. The number $\sum_{i=1}^{n} \lambda_i^k(\vec{G})$ $(k = 0, 1, \ldots, n-1)$, denoted by $T_k(\vec{G})$, is called the k-th *skew spectral moment* of $\vec{G}$, and $T(\vec{G}) = (T_0(\vec{G}), T_1(\vec{G}), \ldots, T_{n-1}(\vec{G}))$ is the sequence of skew spectral moments of $\vec{G}$. Suppose $\vec{G}_1$ and $\vec{G}_2$ are two digraphs. We shall write $\vec{G}_1 \prec_T \vec{G}_2$ ($\vec{G}_1$ comes before $\vec{G}_2$ in a T-order) if for some k $(1 \le k \le n-1)$, $T_i(\vec{G}_1) = T_i(\vec{G}_2)$ $(i = 0, 1, \ldots, k-1)$ and $T_k(\vec{G}_1) < T_k(\vec{G}_2)$ hold. For two given positive integers p and q with $p \le q$, we denote $\mathscr{T}_n^{p,q} = \{T : T$ is a tree of order n with a (p, q)-bipartition $\}$. In this paper, we discuss T-order among all trees in $\mathscr{T}_n^{p,q}$. Furthermore, the last three trees, in the T-order, underlying graphs among $\mathscr{T}_n^{p,q}$ $(4 \le p \le q)$ are characterized.

1. Introduction

All graphs considered here are finite and simple. Undefined terminology and notation may refer to [1]. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$, respectively. For two vertices x and y $(x \neq y)$, the distance between x and y is the number of edges in a shortest path joining x and y, denoted by $d_G(x, y)$. The girth of a graph is the length of a shortest cycle contained in the graph. We will use $G - x$ or $G - xy$ to denote the graph that arises

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from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$. A *pendant vertex* is a vertex of degree 1. Denote by $PV(T)$ the set of all pendant vertices of T.

A tree is a connected graph of order n with $n-1$ edges. Let $P_n, C_n, K_{1,n-1}$ be a path, a cycle and a star of order n, respectively. Let $U_{n,g}$ be a graph obtained from C_g by attaching $n-g$ pendant vertices to one vertex of C_g. Denote $U_n = U_{n,n-1}$ and $B_n = K_n - e$.

Let $\vec{G}$ be an oriented graph of G with an orientation, which allocates to any edge of G a direction such that the induced graph $\vec{G}$ becomes an oriented graph. Then G is called the underlying graph of $\vec{G}$. The skew-adjacency matrix of $\vec{G}$ is the $n \times n$ matrix $S(\vec{G}) = [s_{ij}]$, where $s_{ij} = 1$ and $s_{ji} = -1$ if $v_i v_j$ is an arc of $\vec{G}$, otherwise $s_{ij} = s_{ji} = 0$. Since $S(\vec{G})$ is skew-symmetric, $iS(\vec{G})$ is Hermitian and so all of the eigenvalues of $iS(\vec{G})$ are real. Thus the eigenvalues of $iS(\vec{G})$ are 0 or pure imaginary and since characteristic polynomial of $S(\vec{G})$ has real coefficients, the eigenvalues occur in complex conjugate pairs, see [2] for details.

In [9], Shader *et al.* studied the relationship between the spectra of a graph G and the skew-spectra of an oriented graph $\vec{G}$ of G. In [8], Hou and Lei characterized of the characteristic polynomial of the skew-adjacency matrix of an oriented graph. Recently the spectra of the skew-adjacency matrices of a graph are considered as a possible way to distinguish adjacency cospectral graphs. So it is reasonable to study the skew spectral moments of a graph.

Let $\vec{G}$ be an oriented graph of G with an orientation, and let $\lambda_1(\vec{G}), \lambda_2(\vec{G}), \ldots, \lambda_n(\vec{G})$ be the eigenvalues of $S(\vec{G})$. The number $\sum_{i=1}^{n} \lambda_i^k(\vec{G})$ $(k = 0, 1, \ldots, n-1)$, denoted by $T_k(\vec{G})$, is called the k-th *skew spectral moment* of $\vec{G}$, and $T(\vec{G}) = (T_0(\vec{G}), T_1(\vec{G}), \ldots, T_{n-1}(\vec{G}))$ is the sequence of skew spectral moments of $\vec{G}$. Suppose $\vec{G}_1$ and $\vec{G}_2$ are two digraphs. We shall write $\vec{G}_1 \prec_T \vec{G}_2$ ($\vec{G}_1$ comes before $\vec{G}_2$ in a T-order) if for some $k (1 \le k \le n-1)$, $T_i(\vec{G}_1) = T_i(\vec{G}_2)$ $(i = 0, 1, \ldots, k-1)$ and $T_k(\vec{G}_1) < T_k(\vec{G}_2)$ hold.

There are some results about the (signless Laplacian) spectral moments, see [5], [10] and [12]. Up to now, few results ordering digraphs by the skew spectral moments are obtained. Taghvaee and Fath-Taber [11] studied the T-order of oriented trees and unicyclic graphs and characterized the first and the last digraphs, in a T-order, of all oriented trees and all oriented unicyclic graphs, respectively.

Given a connected bipartite graph G with n vertices, its vertex set can be partitioned into two subsets V_1 and V_2, such that each edge joins a vertex in V_1 and a vertex in V_2. Suppose that V_1 has p vertices and V_2 has q vertices, where $p+q = n$ wtih $p \le q$. Then we say that G has a (p, q)-bipartition. For convenience, let $\mathscr{T}_n^{p,q}$ be the set of all n-vertex trees, each of which has a (p, q)-bipartition.

In light of the information available on the skew spectral moments of graphs, it is nature to consider some other classes of graphs. Trees with a (p, q)-bipartition are a reasonable starting point for such an investigation. In this paper, we order oriented trees with underlying graphs in $\mathscr{T}_n^{p,q}$ $(4 \le p \le q)$. By the T-order, we get the last three oriented trees in $\mathscr{T}_n^{p,q}$ $(4 \le p \le q)$.

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2. **Preliminaries**

In this section, we first give some definitions and lemmas that will be used in the proof of our results. Let $S(\vec{G}) = [s_{ij}]$ be the skew-adjacency matrix of an oriented graph $\vec{G}$ and $W = v_1 v_2 \cdots v_k$ be a walk from v_1 to v_k of G. The sign of W is defined as:

$$sgn(W) = \prod_{i=1}^{k-1} s_{i(i+1)}.$$

Let $w_{ij}^{+}(k)$ and $w_{ij}^{-}(k)$ denote the number of all positive walks and negative walks starting from v_i and terminating at v_j with length k of $\vec{G}$, respectively, see [7] for more details. Gong and Xu [7] obtained the following result on the relationship between the entries of $S^k(\vec{G})$ and the number of walks between any pair of ordered vertices.

Lemma 2.1. [7] *Let $S(\vec{G})$ be the skew-adjacency matrix of an oriented graph $\vec{G}$, and v_i and v_j be two arbitrary vertices of $\vec{G}$. Then*

$$(S^k(\vec{G}))_{ij} = w_{ij}^{+}(k) - w_{ij}^{-}(k).$$

Lemma 2.2. [11] *The k-th skew spectral moment of $\vec{G}$ is the number of closed walks with positive sign of length k minus the number of closed walks with negative sign of length k.*

Let $W = v_1 v_2 \cdots v_k$ be a walk from v_1 to v_k of G. Then $W' = v_k v_{k-1} \cdots v_1$ be a walk from v_k to v_1 of G. When W contains an odd cycle, we have $sgn(W) = -sgn(W')$. So when a walk of length k contains an odd cycle, it doesn't make any contribution to the k-th spectral moment of $\vec{G}$($\vec{G}$ be any oriented graph of G). Hence we just consider walks don't contain odd cycles. In an oriented graph $\vec{G}$, an even cycle is called evenly oriented if for either choice of direction of traversing around C, the number of edges of C directed in the direction of traversal is even. Otherwise C is called oddly oriented. Throughout this paper, we denote C_n^{+} (or resp., C_n^{-}) an evenly (or resp., oddly) oriented even cycle of order n.

We use $\mathscr{U}_5^{+}$ (or resp., $\mathscr{U}_5^{-}$, $\mathscr{B}_4^{+}$, $\mathscr{B}_4^{-}$) to denote the set of digraphs whose underlying graphs is U_5 (or resp., U_5, B_4, B_4), the longest dicycle of which is C_4^{+} (or resp., $C_4^{-}, C_4^{+}, C_4^{-}$). Figure 1 illuminates some digraphs of $\mathscr{U}_5^{+}, \mathscr{U}_5^{-}$, $\mathscr{B}_4^{+}$, $\mathscr{B}_4^{-}$.

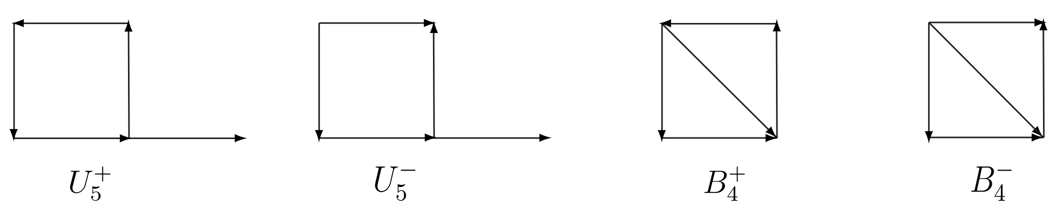

FIGURE 1. Some oriented graphs $\vec{U}_5$ and $\vec{B}_4$.

Let F be a graph. An F-subgraph of G is a subgraph of G which isomorphic to the graph F. Let $\phi_G(F)$ (or $\phi(F)$) be the number of all F-subgraphs of G.

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It is easy to see that $T_0(\vec{G}) = n$, and if k is odd, then $T_k(\vec{G}) = 0$. Taghvaee and Fath-Taber [11] gave the skew spectral moments $T_k(\vec{G})$ for $k = 2, 4, 6$, respectively.

Lemma 2.3. [11] *Let $\vec{G}$ be an oriented graph. Then we have*

(i) $T_2(\vec{G}) = -2\phi(P_2)$;

(i) $T_4(\vec{G}) = 2\phi(P_2) + 4\phi(P_3) + 8\phi((C_4^+) - \phi(C_4^-))$;

(iii) $T_6(\vec{G}) = -2\phi(P_2) - 12\phi(P_3) - 6\phi(P_4) - 12\phi(K_{1,3}) + 12(\phi(U_5^-) - \phi(U_5^+)) + 12(\phi(B_4^-) - \phi(B_4^+)) + 24\phi(C_3) + 48(\phi(C_4^-) - \phi(C_4^+)) + 12(\phi(C_6^+) - \phi(C_6^-))$.

3. T-order and operations of graphs

In this section, we will show some transformations of a graph and prove that the T-order of a digraph is monotonic on these transformations.

Operation I. Assume that u, v, w are three distinct vertices of a tree T, such that $uv \in E(T)$, $d(u) = 1$, $d(w) \geq d(v)$ and $d_T(v, w) = 2$. Let T_1 be the graph obtained from T by deleting the edge uv and adding the edge uw,

$$T_1 = T - uv + uw.$$

We say that T_1 is obtained from T by Operation I.

Note 1. If T is in $\mathscr{T}_n^{p,q}$, T_1 is obtained from T by Operation I, then T_1 is also in $\mathscr{T}_n^{p,q}$.

Lemma 3.1. *Let T_1 be obtained from T by Operation I. Then $\vec{T} \prec_T \vec{T}_1$.*

Proof. Since $\phi_T(P_2) = \phi_{T_1}(P_2)$, by Lemma 2.3 (i), we have $T_2(\vec{T}) = T_2(\vec{T}_1)$. Note that $T_i(\vec{T}) = T_i(\vec{T}_1)$ ($i = 0, 1, 2, 3$). Thus we consider the 4-th skew spectral moment of $\vec{T}$ and $\vec{T}_1$, respectively. By Lemma 2.3, we only need to compare $\phi(P_3)$ of T and T_2. We have

$\phi_{T_1}(P_3) - \phi_T(P_3) = \binom{d(w)+1}{2} + \binom{d(v)-1}{2} - \binom{d(w)}{2} - \binom{d(v)}{2} = d(w) - d(v) + 1 > 0.$

By Lemma 2.3 (ii),

$T_4(\vec{T}_1) - T_4(\vec{T}) = 4[\phi_{T_1}(P_3) - \phi_T(P_3)] = 4(d(w) - d(v) + 1) > 0,$

i.e., $\vec{T} \prec_T \vec{T}_1$. Hence Lemma 3.1 is true. □

Operation II. Let uw be an edge of a tree U and $d(w) \geq 2$. Let T be obtained from U and the star $K_{1,k+1} (k \geq 2)$ by identifying u with a pendant vertex of $K_{1,k+1}$ whose center is v. Let T_2 be the graph obtained from T by deleting all edges vz and adding all edges wz, where $z \in W = N_T(v) \backslash \{u\}$,

$$T_2 = T - \{vz : z \in W\} + \{wz : z \in W\}$$

and we say T_2 is obtained from T by Operation II.

Note 2. If T is in $\mathscr{T}_n^{p,q}$, T_2 is obtained from T by Operation II, then T_2 is also in $\mathscr{T}_n^{p,q}$.

Lemma 3.2. *Let T_2 be obtained from T by Operation II. Then $\vec{T} \prec_T \vec{T}_2$.*

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Proof. As the proof of Lemma 3.1, we get $T_i(\vec{T}) = T_i(\vec{T_2})$ $(i = 0, 1, 2, 3)$. Thus we consider the 4-th skew spectral moment of $\vec{T}$ and $\vec{T_2}$, respectively. By Lemma 2.3, we only need to compare $\phi(P_3)$ of T and T_2. We have

$\phi_{T_2}(P_3) - \phi_T(P_3) = \binom{d(w)+k}{2} - \binom{d(w)}{2} - \binom{k+1}{2} = k(d(w) - 1) > 0.$

By Lemma 2.3 (ii),

$T_4(\vec{T_2}) - T_4(\vec{T}) = 4[\phi_{T_2}(P_3) - \phi_T(P_3)] = 4k(d(w) - 1) > 0,$

i.e., $\vec{T} \prec_T \vec{T_2}$. Hence Lemma 3.2 is true. □

Lemma 3.3. *Let T be the tree as depicted in Operation II, and let T' be the tree obtained from T by deleting all edges $vv_i (i = 1, 2, \ldots, k-1)$ and adding all edges $wv_i (i = 1, 2, \ldots, k-1)$. Assume that w_1 is in $N_T(w)\backslash\{u\}$.*

(i) *If $d_T(w) > 2$, then $\vec{T} \prec_T \vec{T'}$;*
(ii) *If $d_T(w) = 2$ and $d_T(w_1) \geq 2$, then $\vec{T'} \prec_T \vec{T}$;*
(iii) *If $d_T(w) = 2$ and $d_T(w_1) = 1$, then $\vec{T} =_T \vec{T'}$.*

Proof. Note that $T_i(\vec{T}) = T_i(\vec{T'})$ $(i = 0, 1, 2, 3)$. We have

$$\phi_{T'}(P_3) - \phi_T(P_3) = (k-1)(d_T(w) - 2).$$

If $d_T(w) > 2$, then we get $\phi_T(P_3) < \phi_{T'}(P_3)$. Hence we have $T_4(\vec{T}) < T_4(\vec{T'})$, i.e., $\vec{T} \prec_T \vec{T'}$. This completes the proof of (i).

If $d_T(w) = 2$, then we get $\phi_T(P_3) = \phi_{T'}(P_3)$. In view of Lemma 2.3 (ii), we see that

$$T_6(\vec{T'}) - T_6(\vec{T}) = -6(k-1)(d_T(w_1) - 1).$$

If $d_T(w_1) \geq 2$, then we get $T_6(\vec{T'}) < T_6(\vec{T})$, i.e., $\vec{T'} \prec_T \vec{T}$. This completes the proof of (ii).

If $d_T(w_1) = 1$, then $T \cong T'$, i.e., $\vec{T} =_T \vec{T'}$. This completes the proof of (iii). □

4. The last three oriented trees in the T-order among $\mathscr{T}_n^{p,q}$

In this section, we determine the last three trees, in the T-order, whose underlying graphs among the set $\mathscr{T}_n^{p,q}(4 \leq p \leq q)$.

For convenience, let $B_{p,q}^{k,l}$, $D_{p,q}^{k,l}(k, l \geq 0)$ be the trees as depicted in Figure 2, where the degree of u is no less than of v. In particular, $B_{p,q}^{0,0} \cong D_{p,q}^{0,0}$.

Let $T_{n,d}(p_1, \ldots, p_{d-1})$ be a tree of order n created from a path $P_{d+1} = v_0v_1 \cdots v_{d-1}v_d$ by attaching p_i $(p_i \geq 0)$ pendant vertices to v_i $(i = 1, 2, \ldots, d-1)$, respectively, where $n = d + 1 + \sum_{i=1}^{d-1} p_i$.

Theorem 4.1. Let $T \in \mathscr{T}_n^{p,q}$, then one has $\vec{T} \preceq_T \vec{B}_{p,q}^{0,0}$ with equality if and only if $T \cong B_{p,q}^{0,0}$.

Proof. Choose an oriented tree $\vec{T}$, which underlying graph T with a (p, q)-bipartition such that it is as large as possible with respect to the T-order. Suppose $diam(T) = d$, and $P = v_0v_1 \cdots v_{d-1}v_d$ is the longest path of T. Hence, in order to complete the proof, it suffices to show the following claim.

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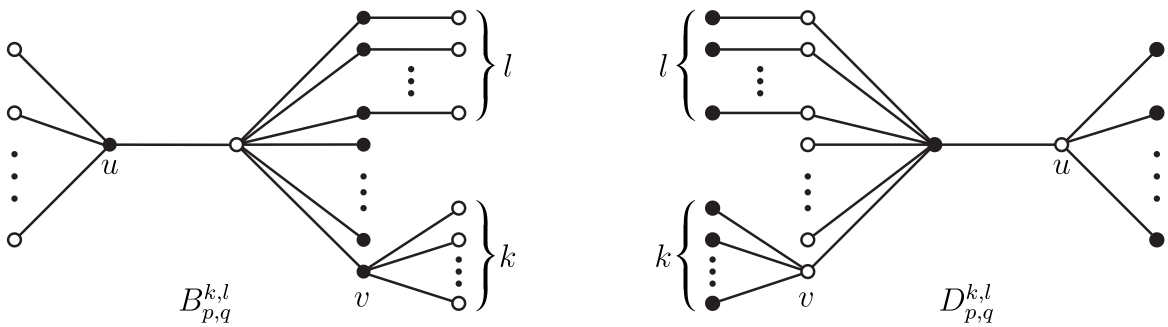

FIGURE 2. The construction of $B^{k,l}_{p,q}$ and $D^{k,l}_{p,q}$.

Claim 1. $T \cong T_{n,d}(p_1, \ldots, p_{d-1})$.

Assume otherwise. Then $PV(T)\backslash \bigcup_{i=1}^{d-1} N(v_i) \neq \emptyset$. Choose $w_1 \in PV(T)\backslash \bigcup_{i=1}^{d-1} N(v_i)$, such that $d(w_1, P) = max\{d(w, P)|w \in PV(T)\backslash \bigcup_{i=1}^{d-1} N(v_i)\}$. Let $uw_1 \in E(T)$, and $N(u) \cap PV(T) = W$, $d(u, u') = 2$. When $|W| = 1$, let $T_1 = T - uw_1 + u'w_1$; when $|W| \geq 2$, let $T_2 = T - \{uz : z \in W\} + \{u'z : z \in W\}$. By Lemma 3.1 or 3.2, we have $\vec{T} \prec_T \vec{T_1}$ or $\vec{T} \prec_T \vec{T_2}$, a contradiction to the choice of $\vec{T}$. This completes the proof of Claim 1.

Note that $T \cong T_{n,d}(p_1, \ldots, p_{d-1})$. Using Operations I and II, $d-3$ times, we get that $T \cong B^{0,0}_{p,q}$. This completes the proof of Theorem 4.1. □

Theorem 4.2. For any $T \in \mathscr{T}_n^{p,q}\backslash\{B^{0,0}_{p,q}\}$ with $4 \leq p \leq q$, one has $\vec{T} \preceq_T \vec{B}^{0,1}_{p,q}$ with equality if and only if $T \cong B^{0,1}_{p,q}$.

Proof. For any $\vec{T}$, $T \in \mathscr{T}_n^{p,q}\backslash\{B^{0,0}_{p,q}\}$, from the proof of Theorem 4.1, it is easy to see that T can be transformed into $B^{0,0}_{p,q}$ by carrying Operations I and II, repeatedly. Let $\mathscr{A}_1$ denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $B^{0,0}_{p,q}$ by carrying Operation I once, and let $\mathscr{A}_2$ denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $B^{0,0}_{p,q}$ by carrying Operation II once. It follows from Lemma 3.1 and 3.2 that the second last tree, in the T-order, whose underlying graphs among $\mathscr{T}_n^{p,q}$ must be in $\mathscr{A}_1 \cup \mathscr{A}_2$.

By the definitions of $\mathscr{A}_1$ and $\mathscr{A}_2$, it is routine to check that $\mathscr{A}_1 = \{B^{0,1}_{p,q}, D^{0,1}_{p,q}\}$(in particular, if $p = q$ then $B^{0,1}_{p,q} \cong D^{0,1}_{p,q}$, hence $\mathscr{A}_1 = \{B^{0,1}_{p,q}\}$), $\mathscr{A}_2 = \{B^{k,0}_{p,q}, 2 \leq k \leq \lfloor\frac{p-1}{2}\rfloor\} \cup \{D^{k,0}_{p,q}, 2 \leq k \leq \lfloor\frac{q-1}{2}\rfloor\}$. Note that $B^{0,1}_{p,q}$ can be obtained from $B^{k,0}_{p,q}$ by using Operation I $(k-1)$ times. By Lemma 3.1, we have $\vec{B}^{k,0}_{p,q} \prec_T \vec{B}^{0,1}_{p,q}$ for $2 \leq k \leq \lfloor\frac{p-1}{2}\rfloor$. Similarly, we have $\vec{D}^{k,0}_{p,q} \prec_T \vec{D}^{0,1}_{p,q}$ for $2 \leq k \leq \lfloor\frac{q-1}{2}\rfloor$.

Hence if $p = q$ then $\vec{B}^{0,1}_{p,q}$ is just the second last tree, in the T-order, underlying graphs among $\mathscr{T}_n^{p,q}$ for $p \geq 4$. So in what follows we consider $p < q$.

In order to complete the proof, it suffices to compare $\vec{B}^{0,1}_{p,q}$ with $\vec{D}^{0,1}_{p,q}$. By Lemma 2.3, we have $T_i(\vec{B}^{0,1}_{p,q}) = T_i(\vec{D}^{0,1}_{p,q})$ for $i = 0, 1, 2, 3$. We have

$$\phi_{B^{0,1}_{p,q}}(P_3) - \phi_{D^{0,1}_{p,q}}(P_3) = \binom{p-1}{2} + \binom{q}{2} + 1 - \binom{p}{2} - \binom{q-1}{2} - 1 = q - p > 0,$$

by Lemma 2.3 (ii), $T_4(\vec{B}^{0,1}_{p,q}) - T_4(\vec{D}^{0,1}_{p,q}) = 4(\phi_{B^{0,1}_{p,q}}(P_3) - \phi_{D^{0,1}_{p,q}}(P_3)) > 0$, i.e., $\vec{D}^{0,1}_{p,q} \prec_T \vec{B}^{0,1}_{p,q}$. Theorem 4.2 is true. □

For convenience, let $C^k_{p,q}$, $E^k_{p,q} (1 \le k \le q-2)$ be the trees as depicted in Figure 3. It is easy to see that $C^k_{p,q}$, $E^k_{p,q} \in \mathscr{T}^{p,q}_n$.

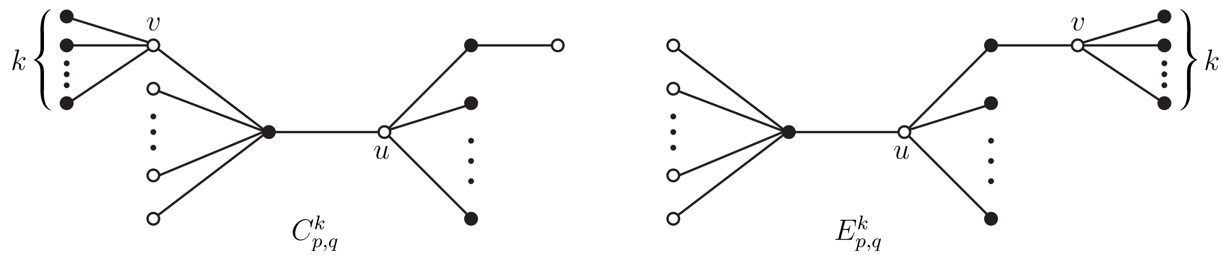

FIGURE 3. The construction of $C^k_{p,q}$ and $E^k_{p,q}$.

Theorem 4.3. Let p and q be positive integers with $4 \le p \le q$.
(i) For any $T \in \mathscr{T}^{p,q}_n \backslash \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$ with $p = q$, we have $\vec{T} \preceq_T \vec{B}^{2,0}_{p,q}$ with equality if and only if $T \cong B^{2,0}_{p,q}$.
(ii) For any $T \in \mathscr{T}^{p,q}_n \backslash \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$ with $p < q$, if $p \ge \frac{q+4}{2}$, then we have $\vec{T} \preceq_T \vec{D}^{0,1}_{p,q}$ with equality if and only if $T \cong D^{0,1}_{p,q}$; if $p < \frac{q+4}{2}$, then we have $\vec{T} \preceq_T \vec{B}^{2,0}_{p,q}$ with equality if and only if $T \cong B^{2,0}_{p,q}$.

Proof. For any $\vec{T}$, $T \in \mathscr{T}^{p,q}_n \backslash \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$, by a similar discussion as in the proof of Theorem 4.2, T can be transformed into $B^{0,0}_{p,q}$ (respectively, $B^{0,1}_{p,q}$)by carrying the Operations I and II, repeatedly. Let $\mathscr{B}_1$ denote the set of all trees in $\mathscr{T}^{p,q}_n$ which can be transformed into $B^{0,1}_{p,q}$ by carrying Operation I once, and let $\mathscr{B}_2$ denote the set of all trees in $\mathscr{T}^{p,q}_n$ which can be transformed into $B^{0,1}_{p,q}$ by carrying Operation II once. It follows from Lemma 3.1 and 3.2 that, if $p < q$ then the third last tree, in the T-order, whose underlying graph among $\mathscr{T}^{p,q}_n$ must be in $\{D^{0,1}_{p,q}\} \cup \mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2$, where $\mathscr{A}_2$ is defined in the proof of Theorem 4.2. Note that if $p = q$, then $B^{0,1}_{p,q} \cong D^{0,1}_{p,q}$. Hence the third last tree, in the T-order, whose underlying graph among $\mathscr{T}^{p,q}_n$ must be in $\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2$.

By the definition of $\mathscr{B}_1$ and $\mathscr{B}_2$, it is routine to check that

$$\mathscr{B}_1 = \{B^{2,0}_{p,q}, B^{0,2}_{p,q}, C^1_{p,q}, E^1_{p,q}\},$$

$$\mathscr{B}_2 = \{C^k_{p,q} : 2 \le k \le q-2\} \cup \{E^k_{p,q} : 2 \le k \le q-2\} \cup \{B^{k,1}_{p,q} : 2 \le k \le \lfloor \frac{p-2}{2} \rfloor\}.$$

We obtained (based on Lemma 3.1) that

$$\vec{B}^{k,1}_{p,q} \prec_T \vec{B}^{k-1,1}_{p,q} \prec_T \cdots \prec_T \vec{B}^{1,1}_{p,q} \cong \vec{B}^{0,2}_{p,q}.$$

We first show the following Claims.

Claim 2. The last tree, in the T-order, underlying graphs among $\mathscr{A}_2$ is $\vec{B}^{2,0}_{p,q}$.

In graph $B_{p,q}^{k,0}$, we obtained (based on Lemma 3.1) that

$$\vec{B}_{p,q}^{\lfloor \frac{p-1}{2} \rfloor,0} \prec_T \vec{B}_{p,q}^{\lfloor \frac{p-1}{2} \rfloor-1,0} \prec_T \cdots \prec_T \vec{B}_{p,q}^{k,0} \prec_T \cdots \prec_T \vec{B}_{p,q}^{3,0} \prec_T \vec{B}_{p,q}^{2,0}. \tag{4.1}$$

Similarly, we obtain

$$\vec{D}_{p,q}^{\lfloor \frac{p-1}{2} \rfloor,0} \prec_T \vec{D}_{p,q}^{\lfloor \frac{p-1}{2} \rfloor-1,0} \prec_T \cdots \prec_T \vec{D}_{p,q}^{k,0} \prec_T \cdots \prec_T \vec{D}_{p,q}^{3,0} \prec_T \vec{D}_{p,q}^{2,0}. \tag{4.2}$$

Note that if $p = q$, it is easy to see that $B_{p,q}^{2,0} \cong D_{p,q}^{2,0}$, then Claim 2 is true.

In the following we assume $p < q$. By (4.1) and (4.2), it suffices to compare $\vec{B}_{p,q}^{2,0}$ with $\vec{D}_{p,q}^{2,0}$. In fact, one has $T_i(\vec{B}_{p,q}^{2,0}) = T_i(\vec{D}_{p,q}^{2,0})$ for $i = 0, 1, 2, 3$. Since $\phi_{B_{p,q}^{2,0}}(P_2) = \phi_{D_{p,q}^{2,0}}(P_2) = n - 1$, and

$$\phi_{B_{p,q}^{2,0}}(P_3) - \phi_{D_{p,q}^{2,0}}(P_3) = \binom{p-2}{2} + \binom{q}{2} - \binom{p}{2} - \binom{q-2}{2} = 2(q-p) > 0,$$

by Lemma 2.3 (ii), $T_4(\vec{B}_{p,q}^{2,0}) - T_4(\vec{D}_{p,q}^{2,0}) = 4(\phi_{B_{p,q}^{0,1}}(P_3) - \phi_{D_{p,q}^{0,1}}(P_3)) > 0$, i.e., $\vec{D}_{p,q}^{2,0} \prec_T \vec{B}_{p,q}^{2,0}$. Hence Claim 2 is true.

Claim 3. The last tree, in the T-order, underlying graphs among $\mathscr{B}_1 \cup \mathscr{B}_2$ is $\vec{B}_{p,q}^{2,0}$.

By Lemma 3.3 (i), we have $\vec{C}_{p,q}^{k} \prec_T \vec{C}_{p,q}^{1}$ for $2 \le k < q-2$. By Lemma 3.3 (ii), we have $\vec{C}_{p,q}^{1} \prec_T \vec{C}_{p,q}^{q-2}$. Similarly, we have $\vec{E}_{p,q}^{k} \prec_T \vec{E}_{p,q}^{1}$ for $2 \le k < q-2$ and $\vec{E}_{p,q}^{1} \prec_T \vec{E}_{p,q}^{q-2}$.

The last tree, in the T-order, whose underlying graph among $\mathscr{B}_1 \cup \mathscr{B}_2$ must be in $\{B_{p,q}^{2,0}, B_{p,q}^{0,2}, C_{p,q}^{q-2}, E_{p,q}^{q-2}\}$. Note that $\vec{C}_{p,q}^{q-2}$ and $\vec{E}_{p,q}^{q-2}$ have the same degree sequence, hence by Lemma 2.3, $T_i(\vec{B}_{p,q}^{0,2}) = T_i(\vec{C}_{p,q}^{q-2}) = T_i(\vec{E}_{p,q}^{q-2})$ for $i = 0, 1, 2, 3$. We have

$$\phi_{C_{p,q}^{q-2}}(P_3) - \phi_{B_{p,q}^{0,2}}(P_3) = \binom{p-1}{2} + \binom{q-1}{2} + 2 - \binom{p-2}{2} - \binom{q}{2} - 2 = -(q-p+1) < 0,$$

by Lemma 2.3, $T_4(\vec{C}_{p,q}^{q-2}) - T_4(\vec{B}_{p,q}^{0,2}) < 0$, i.e., $\vec{C}_{p,q}^{q-2} \prec_T \vec{B}_{p,q}^{0,2}$. Similarly, $\vec{E}_{p,q}^{q-2} \prec_T \vec{B}_{p,q}^{0,2}$.

On the other hand, $B_{p,q}^{0,2}$ can be transformed into $B_{p,q}^{2,0}$ by carrying Operation I once, and by Lemma 3.2 we have $\vec{B}_{p,q}^{0,2} \prec_T \vec{B}_{p,q}^{2,0}$. That is to say, $\vec{B}_{p,q}^{2,0}$ is the last tree, in the T-order, underlying graphs among $\mathscr{B}_1 \cup \mathscr{B}_2$. Hence Claim 3 is true.

If $p = q$, by Claim 2 and Claim 3, then $\vec{B}_{p,q}^{2,0}$ is the last tree, in the T-order, underlying graphs among $\mathscr{T}_n^{p,q} \backslash \{B_{p,q}^{0,0}, B_{p,q}^{0,1}\}$. Hence (i) is true.

Now in what follows we assume $p < q$. According to Claim 2 and Claim 3, it suffices to compare $\vec{B}_{p,q}^{2,0}$ with $\vec{D}_{p,q}^{0,1}$ in this case.

By Lemma 2.3, $T_i(\vec{D}_{p,q}^{0,1}) = T_i(\vec{B}_{p,q}^{2,0})$ for $i = 0, 1, 2, 3$. In view of Lemma 2.3, it is routine to check that $\phi_{D_{p,q}^{0,1}}(P_2) = \phi_{B_{p,q}^{2,0}}(P_2) = n - 1$, $\phi_{D_{p,q}^{0,1}}(C_4) = \phi_{B_{p,q}^{2,0}}(C_4) = 0$, and

$$\phi_{D_{p,q}^{0,1}}(P_3) - \phi_{B_{p,q}^{2,0}}(P_3) = \binom{p}{2} + \binom{q-1}{2} + 1 - \binom{p-2}{2} - \binom{q}{2} - 3 = 2p - q - 4.$$

If $p > \frac{q+4}{2}$, then we have $\phi_{D_{p,q}^{0,1}}(P_3) > \phi_{B_{p,q}^{2,0}}(P_3)$. By Lemma 2.3, $T_4(\vec{D}_{p,q}^{0,1}) > T_4(\vec{B}_{p,q}^{2,0})$. So $\vec{B}_{p,q}^{2,0} \prec_T \vec{D}_{p,q}^{0,1}$. Hence in this case $\vec{D}_{p,q}^{0,1}$ is the third last tree, in the T-order, underlying graphs among $\mathscr{T}_n^{p,q}$.

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If $p = \frac{q+4}{2}$, then we have $\phi_{D^{0,1}_{p,q}}(P_3) = \phi_{B^{2,0}_{p,q}}(P_3)$. By Lemma 2.3 (ii), $T_4(\vec{D}^{0,1}_{p,q}) = T_4(\vec{B}^{2,0}_{p,q})$. By direct computing, we have

$$\phi_{D^{0,1}_{p,q}}(P_4) - \phi_{B^{2,0}_{p,q}}(P_4) = [(p-1) + (q-2)(p-1)] - [(p-3)(q-1) + 2(q-1)] = 0.$$

$$\begin{aligned}\phi_{D^{0,1}_{p,q}}(K_{1,3}) - \phi_{B^{2,0}_{p,q}}(K_{1,3}) &= \binom{p}{3} + \binom{q-1}{3} - \binom{p-2}{3} - \binom{q}{3} - 1 \\ &= \frac{-(q-3)^2+1}{4} < 0.\end{aligned}$$

By Lemma 2.3 (iii), $T_6(\vec{D}^{0,1}_{p,q}) > T_6(\vec{B}^{2,0}_{p,q})$. So $\vec{B}^{2,0}_{p,q} \prec_T \vec{D}^{0,1}_{p,q}$. Hence in this case $\vec{D}^{0,1}_{p,q}$ is the third last tree, in the T-order, underlying graphs among $\mathscr{T}^{p,q}_n$.

If $p < \frac{q+4}{2}$, then we have $\phi_{D^{0,1}_{p,q}}(P_3) < \phi_{B^{2,0}_{p,q}}(P_3)$. By Lemma 2.3, $T_4(\vec{D}^{0,1}_{p,q}) < T_4(\vec{B}^{2,0}_{p,q})$. So $\vec{D}^{0,1}_{p,q} \prec_T \vec{B}^{2,0}_{p,q}$. Hence in this case $\vec{B}^{2,0}_{p,q}$ is the third last tree, in the T-order, underlying graphs among $\mathscr{T}^{p,q}_n$. This completes the proof of (ii).

So Theorem 4.3 is true. □

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