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ON THE SPECTRAL MOMENT OF GRAPHS WITH K CUT EDGES*

SHUCHAO LI†, HUIHUI ZHANG†, AND MINJIE ZHANG‡

Abstract. Let $A(G)$ be the adjacency matrix of a graph $G$ with $\lambda_1(G)$, $\lambda_2(G)$, \ldots, $\lambda_n(G)$ its eigenvalues in non-increasing order. Call the number $S_k(G) := \sum_{i=1}^n \lambda_i^k(G)$ ($k = 0, 1, \ldots, n-1$) the $k$th spectral moment of $G$. For two graphs $G_1$ and $G_2$, we have $G_1 \prec_i G_2$ if $S_i(G_1) = S_i(G_2)$ for $i = 0, 1, \ldots, k-1$ and $S_k(G_1) < S_k(G_2)$ for some $k \in \{1, 2, \ldots, n-1\}$. Denote by $\mathcal{G}_n^k$ the set of connected $n$-vertex graphs with $k$ cut edges. In this paper, the first, the second, the last and the penultimate graphs, in the $S$-order, are determined among $\mathcal{G}_n^k$, respectively.

Key words. Spectral moment, Cut edge, Clique.

AMS subject classifications. 05C50, 15A18.

1. Introduction. All graphs considered here are finite, simple and connected. Basic terminology and notation may be referred to [1]. Let $G = (V_G, E_G)$ be a simple undirected graph with $n$ vertices. Then $G - v$, $G - uv$ denote the graph obtained from $G$ by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from $G$ by inserting an edge $uv \notin E_G$. For $v \in V_G$, let $N_G(v)$ (or $N(v)$ for short) denote the set of all vertices adjacent to $v$ and $\deg_G(v) = |N_G(v)|$, and $d_G(u, v)$ is the distance between $u$ and $v$. For an edge subset $E$ of $G$, denoted by $G[E]$ the subgraph induced by $E$. A cut edge in a connected graph $G$ is an edge whose deletion results in a disconnected graph. Let $\mathcal{G}_n^k$ be the set of all $n$-vertex graphs, each of which contains $k$ cut edges.

Let $A(G)$ be the adjacency matrix of a graph $G$ with $\lambda_1(G)$, $\lambda_2(G)$, \ldots, $\lambda_n(G)$ its eigenvalues in non-increasing order. The number $\sum_{i=1}^n \lambda_i^k(G)$ ($k = 0, 1, \ldots, n-1$) is called the $k$th spectral moment of $G$, denoted by $S_k(G)$. Let $S(G) = (S_0(G), S_1(G), \ldots, S_{n-1}(G))$ be the sequence of spectral moments of $G$. For two graphs $G_1, G_2$, we shall write $G_1 \succeq G_2$ if $S_i(G_1) = S_i(G_2)$ for $i = 0, 1, \ldots, n-1$. Similarly, we have $G_1 \succeq S G_2$ (if $G_1$ comes before $G_2$ in the $S$-order) if for some $k$ ($1 \leq k \leq n-1$), we have $S_k(G_1) = S_k(G_2)$ ($i = 0, 1, \ldots, k-1$) and $S_k(G_1) < S_k(G_2)$. We shall also write

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$G_1 \preceq_s G_2$ if $G_1 \preceq_s G_2$ or $G_1 = s G_2$. The $S$-order has been used in producing graph catalogs (see [6]), and for a more general setting of spectral moments one may be referred to [5].

Cvetković and Rowlinson [7] studied the $S$-order of trees and unicyclic graphs and characterized the first and the last graphs, in the $S$-order, of all trees and all unicyclic graph with given girth, respectively. Cheng, Liu and Liu [3] identified the last $d + \lfloor \frac{d}{2} \rfloor - 2$ graphs, in the $S$-order, among all $n$-vertex unicyclic graphs of diameter $d$. Cheng and Liu [2] determined the last few graphs, in the $S$-order, among all trees with $n$ vertices and $k$ pendant vertices. Pan et al. [13] gave the first $\sum_{k=1}^{\lfloor \frac{n-k-1}{2} \rfloor} (\lfloor \frac{n-k-1}{2} \rfloor - k + 1)$ graphs apart from an $n$-vertex path, in the $S$-order, of all trees with $n$ vertices. Wu and Fan [16] determined the last and the penultimate graphs, in the $S$-order, of all unicyclic graphs and bicyclic graphs, respectively. Wu and Liu [17] determined the last $\lfloor \frac{d}{2} \rfloor + 1$, in the $S$-order, among all $n$-vertex trees of diameter $d$ ($4 \leq d \leq n - 3$). Pan et al. [14] identified the first and the last graphs, in the $S$-order, of all trees with $n$ vertices and $k$ pendant vertices. Li and Zhang [11] characterized the last four trees, in the $S$-order, among all $n$-vertex trees with a given bipartition. Li and Song [10] identified the last $n$-vertex tree with a given degree sequence in the $S$-order. Consequently, the last trees in the $S$-order in the sets of all trees of order $n$ with the largest degree, the leaves number, the independence number and the matching number were also determined, respectively.

In light of the information available from the related results on the spectral moments of graphs, it is natural to consider this problem on some other class of interesting graphs, and the connected graphs with $k$ cut edges are a reasonable starting point for such a investigation. The $n$-vertex connected graphs with $k$ cut edges have been considered in different fields [8, 12, 15], whereas to our best knowledge, the spectral moments of graphs in $G^k_n$ were, so far, not considered. Here, we identified the first, the second, the last and the penultimate graphs, in the $S$-order, among graphs in $G^k_n$.

Throughout the text, we denote by $P_n$, $K_{1,n-1}$, $C_n$ and $K_n$ the path, star, cycle and complete graph on $n$ vertices, respectively. Let $K^*_1,n$ be a graph obtained from a star $K_{1,n-1}$ by attaching a leaf to one leaf of $K_{1,n-1}$, $U_n$ be a graph obtained from $C_{n-1}$ by attaching a leaf to one vertex of $C_{n-1}$, and $B_4, B_5$ be two graphs obtained from two cycle $C_3, C_3'$ of length 3 by identifying one edge of $C_3$ with one edge of $C_3'$ and identifying one vertex of $C_3$ with one vertex of $C_3'$, respectively; see Fig. 1.1. The join $G \lor H$ of disjoint graphs $G$ and $H$ is obtained by adding an edge from each vertex in $G$ to each vertex of $H$.

The graph $K^k_n$ is the $n$-vertex graph obtained by attaching $k$ pendant vertices to one vertex of $K_{n-k}$. The graph $P^k_n$ is a graph obtained by identifying one end-vertex of
Let $F$ and $K$ be a graph. An $F$-subgraph of $G$ is a subgraph of $G$ which is isomorphic to the graph $F$. Let $\phi_G(F)$ (or $\phi(F)$) be the number of all $F$-subgraphs of $G$.

**Lemma 1.1** ([4]). The $k$th spectral moment of $G$ is equal to the number of closed walks of length $k$ in $G$.

**Lemma 1.2** ([3], [6], [17]). For every graph $G$, we have

(i) $S_4(G) = 2 \phi(P_2) + 4 \phi(P_3) + 8 \phi(C_4)$;
(ii) $S_5(G) = 30 \phi(C_4) + 10 \phi(U_4) + 10 \phi(C_5)$;
(iii) $S_6(G) = 2 \phi(P_2) + 12 \phi(P_3) + 6 \phi(P_4) + 12 \phi(K_{1,3}) + 12 \phi(U_5) + 36 \phi(B_4) + 24 \phi(B_5) + 24 \phi(C_4) + 48 \phi(C_5) + 12 \phi(C_6)$.

**Lemma 1.3** ([4]). Given a connected graph $G$, $S_3(G) = n, S_1(G) = l, S_2(G) = 2m, S_3(G) = 6l$, where $n, l, m, t$ denote the number of vertices, the number of loops, the number of edges and the number of triangles contained in $G$, respectively.

**Lemma 1.4** ([7]). In the $S$-order of the $n$-vertex unicyclic graphs with girth $g$, the first graph is $U_n^g$ which is obtained by the coalescence of a cycle $C_g$ with a path $P_{n-g+1}$ at one of its end vertices.
2. The last and the penultimate graphs in the S-order among $\varphi^k_n$. In this section, we will determine the last two graphs in the $S$-order among $\varphi^k_n$. Let $E = \{e_1, e_2, \ldots, e_k\}$ be the set of the cut edges of $G \in \varphi^k_n$. Note that $S_2(G) = 2|E_G|$, hence $S_2(G + e) > S_2(G)$. By Lemma 1.3, in order to determine the last graph in the $S$-order among $\varphi^k_n$, it suffices to choose graph $G \in \varphi^k_n$ such that its $S_2(G)$ is as large as possible. So we have the following lemma.

Lemma 2.1. Each component of $G - E$ is a clique.

Theorem 2.2. Of all the connected graphs with $n$ vertices and $k$ cut edges, the last graph in the $S$-order is obtained uniquely at $K^k_n$.

Proof. If $k = 0$, then by Lemma 2.1 we have $\varphi^0_n = \{K_n\}$, our result holds immediately. Therefore, we may assume that $k \geq 1$. Again by Lemma 2.1, we can denote the components of $G - E$ by $K_{a_0}, K_{a_1}, \ldots, K_{a_k}, a_0 + a_1 + \cdots + a_k = n$. Assume, without loss of generality, that $a_0 \geq a_1 \geq a_2 \geq \cdots \geq a_k \geq 1$.

Let $V_i = \{v \in V_{K_{a_i}} : v$ is an endvertex of a cut edge of $G\}$. Choose $G \in \varphi^k_n$ such that $G$ is as large as possible under the order $\preceq_s$. In order to complete the proof, it suffices to show the following facts.

Fact 1. $|V_i| = 1$ for $i = 0, 1, 2, \ldots, k$.

Proof. Suppose to the contrary that there exists $i \in \{0, 1, 2, \ldots, k\}$ such that $|V_i| > 1$. Let $u, u' \in V_{a_i}$, both $u$ and $u'$ are end vertices of the cut edges of $G$. Denote $N_G(u) \setminus N_{K_{a_i}}(u) = \{w_1, w_2, \ldots, w_s\}$ and $N_G(u') \setminus N_{K_{a_i}}(u) = \{z_1, z_2, \ldots, z_l\}$. It is routine to check that $s \geq 1, l \geq 1$. Let

$$G^* = G + \{u'z_1, u'z_2, \ldots, u'z_l\} + \{uz_1, uz_2, \ldots, uz_l\}.$$ 

Then, $G^* \in \varphi^k_n$.

On the one hand, $S_i(G) = S_i(G^*)$ for $i = 0, 1, 2, 3$. On the other hand, $\phi_G(P_2) = \phi_G'(P_2), \phi_G(C_1) = \phi_G'(C_4)$. By Lemma 1.2(i),

$$S_4(G) - S_4(G^*) = 4(\phi_G(P_3) - \phi_G'(P_3)) = 4\left(\binom{s}{2} + \binom{l}{2} - \left(\binom{s + l}{2}\right)\right) = -4sl < 0.$$ 

This implies that $G \prec_s G^*$, a contradiction. Therefore, $|V_i| = 1$ for $0 \leq i \leq k$.

Fact 2. $G \in \mathcal{H}^k_n$.

Proof. If not, then there exists a cut edge $u_0u_i \in E$ such that $u_i$ is the endvertex
of another cut edge(s). Let
\[ |N_G(u_i) \setminus (N_{K_{a_i}}(u_i) \cup \{u_0\})| = l, \quad |N_G(u_0) \setminus (N_{K_{a_0}}(u_0) \cup \{u_i\})| = s. \]

It is straightforward to check that \( l \geq 1 \) and \( s \geq 0 \).

First suppose that \( s \geq 1 \). In this case, let
\[ G^* = G - \{u_i z : z \in N_G(u_i) \setminus (N_{K_{a_i}}(u_i) \cup \{u_0\})\} \]
\[ + \{u_0 z : z \in N_G(u_0) \setminus (N_{K_{a_0}}(u_0) \cup \{u_i\})\}. \]

It is easy to see that \( G^* \in \mathcal{K}_n^k \). Note that \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \) and \( \phi_G(P_2) = \phi_{G^*}(P_2) \), \( \phi_G(C_4) = \phi_{G^*}(C_4) \).

\[ S_4(G) - S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) = 4(l(a_i - 1) - l(a_0 - 1) - l) \]
\[ = 4(l(a_i - a_0) - s) < 0, \]

which leads to the contradiction that \( G \prec_s G^* \).

Now suppose \( s = 0 \). Then, there exists a cut edge \( u_i u_j \in E \) such that \( u_j \) is an endvertex of another cut edge(s). Let \( |N_G(u_j) \setminus (N_{K_{a_j}}(u_j) \cup \{u_i\})| = p \). It is straightforward to check that \( p \geq 1 \). Let
\[ G^* = G - \{u_j z : z \in N_G(u_j) \setminus (N_{K_{a_j}}(u_j) \cup \{u_i\})\} \]
\[ + \{u_i w : w \in N_G(u_i) \setminus (N_{K_{a_i}}(u_i) \cup \{u_0\})\} \]
\[ + \{u_0 w : w \in N_G(u_0) \setminus (N_{K_{a_0}}(u_0) \cup \{u_i\})\}. \]

It is easy to see that \( G^* \in \mathcal{K}_n^k \). Note that \( S_i(G) = S_i(G^*) \), \( i = 0, 1, 2, 3 \) and \( \phi_G(P_2) = \phi_{G^*}(P_2) \), \( \phi_G(C_4) = \phi_{G^*}(C_4) \). Hence,

\[ S_4(G) - S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) \]
\[ = 4l(a_i - 1) + p(a_j - 1) - 4p(l - 1) - 4p(l + p)(a_0 - 1) \]
\[ = 4l(a_i - a_0) + p(a_j - a_0) - pl < 0. \]

The last inequality follows from \( a_i \leq a_0, a_j \leq a_0 \) and \( pl > 0 \). Hence, we obtain that \( G \prec_s G^* \), a contradiction. Therefore, \( G \in \mathcal{K}_n^k \). \( \square \)

By Fact 2, we can assume that \( u_0 u_j \in E, 1 \leq j \leq k \).

**Fact 3.** \( a_1 = a_2 = \cdots = a_k = 1 \).

**Proof.** Suppose the contrary that there exists a \( j \in \{1, 2, \ldots, k\} \) such that \( a_j > 1 \). By Fact 2, we have \( G = K(a_0, \{a_1, \ldots, a_{j-1}, a_j, a_{j+1}, \ldots, a_k\}) \). Now we consider \( G^* = K(a_0 + a_j - 1, \{a_1, \ldots, a_{j-1}, 1, a_{j+1}, \ldots, a_k\}) \). It is easy to see that \( G^* \in \mathcal{K}_n^k \).
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Note that $S_i(G) = S_i(G^*)$, $i = 0, 1$ and

$$S_2(G) - S_2(G^*) = 2(a_j - 1) - 2(a_j - 1)a_0 = 2(a_j - 1)(1 - a_0) < 0,$$

i.e., $G$ $\prec_s$ $G^*$, a contradiction. Therefore, $a_j = 1$ for $j = 1, 2, \ldots, k$. □

In view of Fact 3, we have $a_0 = n - k$. Hence, $G = K(n - k, \{1, 1, \ldots, 1\})$, i.e.,

$G \cong K_{\frac{n}{k}}^k$, as desired. □

In the rest of this section, we are to determine the penultimate graph in the $S$-order among $\mathcal{G}_n^k$. Let $E = \{e_1, e_2, \ldots, e_k\}$ be the set of the cut edges of $G \in \mathcal{G}_n^k$.

Delete an edge, say $xy$, from $K_n$ and denote the resulting graph by $G_1$. Let $G_2$ be a graph obtained from $G_1$ by attaching a pendant vertex to one vertex, say $r$, of $G_1$ with $r \neq x, y$. Let $G_3 = K(n - k, \{1, 1, \ldots, 1\}) - uw + vw$, where $uw$ is a cut edge of $K(n - k, \{1, 1, \ldots, 1\})$ and $u, v$ are in the subgraph $K_{n-k}$ with $u \neq v$. It is easy to see that among $\mathcal{G}_n^0$, $K_n$ (resp., $G_1$) is the last (resp., the penultimate) graph in the $S$-order, while among $\mathcal{G}_n^4$ with $n \geq 5$, based on $S_2(G)$, the penultimate graph in the $S$-order must be a graph obtained from $K_n^1$ deleting a non-cut edge, say $e$, from $K_n^1$. Denote the resulting graph by $G'$ if $e$ has a common vertex with the cut edge in $K_n^1$ and by $G_2$ otherwise. Note that $S_4(G_2) = S_4(G')$ for $i = 0, 1, 2, 3$ and $\phi_{G_2}(P_2) = \phi_{G'}(P_2)$, $\phi_{G_2}(C_4) = \phi_{G'}(C_4)$. Hence, by Lemma 1.2(i),

$$S_4(G') - S_4(G_2) = 4(\phi_{G'}(P_3) - \phi_{G_2}(P_3)) = -40,$$

i.e., $G' \prec_s G_2$. Hence, among $\mathcal{G}_n^1$ with $n \geq 5$, $G_2$ is the penultimate graph in the $S$-order. In what follows we only consider $k \geq 2$.

**Theorem 2.3.** Among $\mathcal{G}_n^k$ with $2 \leq k \leq n - 1$, the penultimate graph in the $S$-order is $G_3$ if $k \in \{2, 3, \ldots, n - 2\}$ and $K_{n-1}^k$ otherwise, where $G_3$ is defined as above.

**Proof.** Choose $G \in \mathcal{G}_n^k \setminus \{K_n^k\}$ such that it is as large as possible according to $\preceq_s$. Denote the components of $G - E$ by $U_0, U_1, U_2, \ldots, U_k$. We are to show that each of the components is a complete graph. In fact, if there exists a $U_i$ which is not a complete graph, i.e., $U_i$ contains two vertices $x, y$ satisfying $xy \notin E_{U_i}$. Let $G' = G + xy$. If $G' \nsubseteq K_n^k$, it is easy to see that $G \prec_s G'$, a contradiction. If $G' \cong K_n^k$, then at least one of $x$ and $y$ is not an endvertex of a cut edge of $G$, without loss of generality, assume that $x$ is not an end vertex of a cut edge of $G$, delete a cut edge of $G'$ and connect the isolated vertex with $x$ by an edge; denote the resulting graph by $G''$. Then we have $S_0(G) = S_0(G''), S_1(G) = S_1(G'')$ and $S_2(G) < S_2(G'')$. Hence, $G \prec_s G''$, a contradiction. Therefore, we may denote the components of $G - E$ by
Let $V_i = \{v \in V_{K_n} : v$ is an endvertex of a cut edge of $G\}$. In order to complete the proof, it suffices to show the following facts.

**Fact 1.** If $a_0 = 1$, then $|V_i| = 1$ for any $i \in \{0, 1, \ldots, k\}$; if $a_0 \geq 3$, then $|V_0| = 2$, $|V_{i}| = 1$, $i \in \{1, 2, \ldots, k\}$.

**Proof.** Note that $G \not \cong K_n^k$, we consider the following possible cases.

*Case 1.* $|V_i| = 1$ for $i = 0, 1, 2, \ldots, k$. In this case let $V_i = \{u_i\}$, $i \in \{0, 1, \ldots, k\}$, First we consider $G \in \mathcal{X}_n^k$. We are to show that $a_1 = 3, a_2 = 1$.

In fact, note that $G \in \mathcal{X}_n^k \setminus \{K_n^k\}$, hence $a_1 \geq 3$; otherwise, $a_1 = 2$, which implies that $G$ contains at least $k + 1$ cut edges, a contradiction. If $a_1 > 3$, we consider graph $G^* := K(a_0 + 1, \{a_1 - 1, a_2, \ldots, a_k\})$ in $\mathcal{X}_n^k \setminus \{K_n^k\}$. Note that $S_i(G) = S_i(G^*)$ for $i = 0, 1$ and $S_2(G) - S_2(G^*) = 2(a_1 - 1 - a_0) = 0$. $G \preceq G^*$, a contradiction. Therefore, $a_1 = 3$.

If $a_2 > 1$, we consider graph $G' := K(a_0 + a_2 - 1, \{3, 1, a_3, \ldots, a_k\}) \in \mathcal{X}_n^k \setminus \{K_n^k\}$. Note that $S_i(G) = S_i(G')$ for $i = 0, 1$ and $S_2(G) - S_2(G') = 2(a_2 - 1 - (a_2 - 1)a_0) = 2(2 - a_0) < 0$. Hence, by Lemma 1.2(i), $S_3(G) < S_3(G^*)$. Thus, $G \preceq G^*$, a contradiction. Therefore, $G \not \in \mathcal{X}_n^k$.

Now consider the case $G \not \in \mathcal{X}_n^k$. It is easy to see that the edge induced graph $G[E]$ is a tree which is not isomorphic to $K_{1,k}$. Hence, partition $V_{G[E]}$ into $D^1(G[E]) \cup D^2(G[E]) \cup D^3(G[E]) \cup \cdots$, where $D^i(G[E]) = \{u \in V_{G[E]} : d_{G[E]}(u, u_0) = i\}$, $i = 1, 2, 3, \ldots$ It is easy to see that $D^2(G[E]) \neq \emptyset$.

If $D^3(G[E]) \neq \emptyset$, that is to say, there exists $u \in D^2(G[E])$ such that $d_{G[E]}(u) \geq 2$, then choose $u_i$ from $D^i(G[E])$ such that $u_i$ is adjacent to $u_0$ and $u$. Let $W := N_{G[E]}(u_i) \setminus \{u_0\}$. As $u \in W$, we have $W \neq \emptyset$. Consider

$$G^* = G - \{u_iw : w \in W\} + \{u_0w : w \in W\}.$$
Then it is routine to check that \( G^* \in \mathcal{G}_n^k \setminus \{K_n^k\} \). Note that \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \) and \( \phi_G(P_2) = \phi_{G^*}(P_2), \phi_G(C_4) = \phi_{G^*}(C_4) \). Hence, by Lemma 1.2(i), we have

\[
S_4(G) = S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) = 4[(a_1 - a_0) - st],
\]

where \( s = |W| \geq 1 \) and \( t = |N_G[S](u_0) \setminus \{u_i\}| \geq 0 \). Note that \( a_1 \leq a_0 \). Hence, if \( a_1 < a_0 \), then for all \( t \geq 0 \) we have \( (a_1 - a_0) - st < 0 \), which implies that \( G \prec_s G^* \), a contradiction. If \( a_1 = a_0 \), then for all \( t \geq 1 \) we have \( (a_1 - a_0) - st < 0 \), which implies that \( G \prec_s G^* \), a contradiction. If \( a_1 = a_0 \) and \( t = 0 \), then \( G^* \cong G \). Hence, it suffices to consider \( D^3(G[\bar{E}]) = \emptyset \) and \( d_{G[\bar{E}]}(u_0) > 1 \). Furthermore, as \( G \notin \mathcal{X}_n^k \), we have \( D^4(G[\bar{E}]) \neq \emptyset \) and for each \( u \in D^2(G[\bar{E}]) \), \( u \) is a leaf of \( G[\bar{E}] \) (otherwise, \( D^3(G[\bar{E}]) \neq \emptyset \), a contradiction).

If there exists \( u_i \in D^2(G[\bar{E}]) \) such that \( d_{G[\bar{E}]}(u_i) \geq 3 \), then move \( d_{G[\bar{E}]}(u_i) - 2 \) pendant edges to \( u_0 \) and denote the resulting graph by \( G^* \). It is easy to see that \( G^* \in \mathcal{G}_n^k \setminus \{K_n^k\} \). Note that \( s := d_{G[\bar{E}]}(u_i) - 2 \geq 1 \), \( q := d_{G[\bar{E}]}(u_0) - 1 \geq 1 \), \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \) and \( \phi_G(P_2) = \phi_{G^*}(P_2), \phi_G(C_4) = \phi_{G^*}(C_4) \). Hence, by Lemma 1.2(i), we have

\[
S_4(G) = S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) = 4[s(a_i - 1) - s(a_0 - 1) - sq] = 4s(a_i - a_0 - q) < 0.
\]

We arrive at the contradiction that \( G \prec_s G^* \). Hence, it suffices to consider that, in the edge induced graph \( G[\bar{E}] \), each of the non-pendant vertices in \( D^2(G[\bar{E}]) \) is of degree 2 and \( d_{G[\bar{E}]}(u_0) \geq 3 \).

For convenience, let \( W = \{ u : u \in D^2(G[\bar{E}]), d_{G[\bar{E}]}(u) = 2 \} \). It is easy to see that \( W \neq \emptyset \). If \( |W| \geq 2 \), choose \( u \in W \) such that its unique neighbor in \( G[\bar{E}] \) is a leaf, say \( u' \). Let

\[
G^* = G - uu' + u_0u'.
\]

Then \( G^* \in \mathcal{G}_n^k \setminus \{K_n^k\} \). Since \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \) and \( \phi_G(P_2) = \phi_{G^*}(P_2), \phi_G(C_4) = \phi_{G^*}(C_4) \),

\[
\phi_G(P_3) - \phi_{G^*}(P_3) = (a_i - 1) - (a_0 - 1) - p = a_i - a_0 - p < 0.
\]

This gives the contradiction \( S_4(G) - S_4(G^*) < 0 \), i.e., \( G \prec_s G^* \). Hence, \( |W| = 1 \).

By a similar argument as in the proof of Fact 3 in Theorem 2.2, we obtain that \( a_0 = n - k, a_1 = a_2 = \cdots = a_k = 1 \). If \( a_0 = 1 \), then \( k = n - 1 \), i.e., the penultimate graph is obtained uniquely at \( K_{1,n-1}^* \). It is obvious that \( a_0 \neq 2 \). Hence, if \( a_0 \geq 3 \), then
implies that $S \leq G$ contradicts $\phi$. Fact 3.

Let $x \in N_{K_{m}}$. Consider $G^* = G - \{uu'\} + \{xu\}$. Then $G^* \in \mathcal{G}_n^k \setminus \{K_n^k\}$. Note that $S_i(G) = S_i(G^*)$ for $i = 0, 1, 2, 3, \phi_G(P_2) = \phi_G(C_4) = \phi_G(C_4)$ and $\phi_G(P_2) - \phi_G(P_3) = 1 - (a_0 - 1) = 2 - a_0 < 0 (a_0 \geq 3)$. $S_4(G) - S_4(G^*) < 0$, i.e., $G \prec_s G^*$, a contradiction.

Case 2. There is a $V_i$ such that $|V_i| \geq 3, i \in \{0, 1, \ldots, k\}$

Consider two distinct vertices, say $u_i'$ and $u_i''$, in $V_i$. Let $G^* = G - \{u_i'u : u \in N_G(u_i') + \{u_i''u : u \in N_G(u_i')\}\}$. It is easy to see that $G^* \in \mathcal{G}_n^k \setminus \{K_n^k\}$. Note that $S_i(G) = S_i(G^*)$, $i = 0, 1, 2, 3$, $\phi_G(P_2) = \phi_G(C_4) = \phi_G(C_4)$ and $\phi_G(P_3) - \phi_G(P_3) = -|N_G(u_i')||N_G(u_i')| < 0$. $S_4(G) - S_4(G^*) < 0$, which contradicts $G \prec_s G^*$.

Case 3. max $|V_i| : i = 0, 1, 2, \ldots, k = 2$.

If there exists a $V_i$ with $|V_i| = \{u_i, u_i'\}, i \in \{1, 2, \ldots, k\}$, where $u_i$ is adjacent to $u_0 \in V_0$, then let

$$G^* = G - \{u_i : x \in V_{K_{m}}\} + \{xy : y \in V_{K_{m}}, x \in V_{K_{m}} \setminus \{u_i\}\}.$$ 

It is easy to see that $G^* \in \mathcal{G}_n^k \setminus \{K_n^k\}$. Note that $S_i(G) = S_i(G^*)$ for $i = 0, 1$ and $S_2(G) - S_2(G^*) = 2(a_i - 1) - 2(a_i - 1)a_0 = 2(a_i - 1)(1 - a_0) < 0$. Hence, $S_2(G) < S_2(G^*)$, which contradicts $G \prec_s G^*$. Therefore, $|V_i| = 1$ for $i = 1, 2, \ldots, k$ which implies that $|V_0| = 2$.

This completes the proof of Fact 1. \[ \]

By Fact 1, we can assume that $u_0, u_0' \in V_0$. Hence, in what follows, we assume that $a_0 \geq 3$.

Fact 2. $a_1 = a_2 = \cdots = a_k = 1$.

Proof. By a similar argument as in the proof of Fact 3 in Theorem 2.2, we can get $a_0 = n - k, a_1 = a_2 = \cdots = a_k = 1$. \[ \]

Fact 3. $G \cong G_3$, where $G_3 = K(n - k, \{1, 1, \ldots, 1\}) - u_0u_k + u_0'u_k$, where $u_0u_k$ is a cut edge and $u_0' \in V_{K_{m}} \setminus \{u_0\}$.

Proof. Note that if $G$ has just two cut edges, then it is easy to see that $G \cong G_3$ defined as above. Hence, in what follows, we assume that $G$ contains at least three cut edges.

Let $N_{G_0}(u_0) = \{u_1, u_2, \ldots, u_m\}$ and $N_{G_0}(u_0)' = \{u_1', u_2', \ldots, u_t'\}$. Without loss of generality, assume that $m \geq t$. Obviously, $t \geq 1$. First we show that $t = 1$. \[ \]
Otherwise, let
\[ G^* = G - \{ u_0''u_2', u_0'u_3', \ldots, u_0''u'_4 \} + \{ u_0'u_2', u_0'u_3', \ldots, u_0''u'_4 \}. \]

It is easy to see that \( G^* \in \mathcal{G}_n^k \setminus K_n^k \). Note that \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \), \( \phi_G(P_2) = \phi_{G^*}(P_2) \), and \( \phi_G(C_4) = \phi_{G^*}(C_4) \). Hence,
\[ S_4(G) - S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) = -4m(t - 1) < 0, \]
which contradicts \( G \bowtie_s G^* \).

Now we are to show that \( m = k - 1 \). If not, there exists a vertex \( u \in \{ u_1, u_2, \ldots, u_m, u'_1, u'_2, \ldots, u'_4 \} \) such that \( d_G[u](u) \geq 2 \). Denote \( N_G[u](u) \setminus \{ u_0, v_0 \} = \{ u_01, u_02, \ldots, u_0s \} \). Let
\[ G^* = G - \{ u_0'1, u_0'2, \ldots, u_0's \} + \{ u_0u_1, u_0u_2, \ldots, u_0u_s \}. \]

It is easy to see that \( G^* \in \mathcal{G}_n^k \setminus K_n^k \). Notice that \( S_i(G) = S_i(G^*) \) for \( i = 0, 1, 2, 3 \), \( \phi_G(P_2) = \phi_{G^*}(P_2) \) and \( \phi_G(C_4) = \phi_{G^*}(C_4) \).
\[ S_4(G) - S_4(G^*) = 4(\phi_G(P_3) - \phi_{G^*}(P_3)) = 4s(a_i - 1) - 4s(m - 1) < 0. \]

The last inequality follows by \( a_i = 1 < n - k = a_0 \) (by Fact 2), and \( m \geq 1, s \geq 1 \). Thus, we are led to the contradiction that \( G \bowtie_s G^* \). So we have \( m = k - 1, t = 1 \), which is equivalent to that \( G \cong G_3 \). \( \square \)

By Facts 1 and 3, Theorem 2.3 holds. \( \square \)

3. The first and the second graphs in the \( S \)-order among \( \mathcal{G}_n^k \). In this section, we determine the first and the second graphs in the \( S \)-order on \( \mathcal{G}_n^k \). Let \( \mathcal{E} = \{ e_1, e_2, \ldots, e_k \} \) be the set of all the cut edges of \( G \in \mathcal{G}_n^k \). Note that if we delete an edge, say \( e \), from a connected graph \( G \), then in the view of \( S_2(G) = 2|E_G| \), we have \( S_2(G) > S_2(G - e) \). In order to determine the first graph in the \( S \)-order among \( \mathcal{G}_n^k \), it suffices to choose the graph such that its size is as small as possible.

**Theorem 3.1.** Of all the connected graphs with \( n \) vertices and \( k \) cut edges, the first graph in the \( S \)-order is obtained uniquely at \( P_n^k \).

**Proof.** Choose \( G \in \mathcal{G}_n^k \) such that it is as small as possible according to the relation \( \bowtie_s \). If \( k = 0 \), then it is easy to see that \( G \cong C_n \) and our result holds. Therefore, we may assume that \( k \geq 1 \). We show the following claim first.

**Claim 1.** \( G \) contains exactly one cycle.

**Proof.** Assume to the contrary that \( G \) contains at least two cycles. If \( G \) contains two cycles \( C^1 \) and \( C^2 \) such that \( C^1 \) and \( C^2 \) have edges in common; see Fig. 3.1(a),...
then let $G^* = G - \{uv, xy\} + ux$ (see Fig. 3.1(b)); if $G$ contains two cycles $C^1$ and $C^2$ such that $C^1$ and $C^2$ have just one vertex in common; see Fig. 3.1(c), then let $G^* = G - \{ux, vx\} + uv$ (see Fig. 3.1(d)). It is routine to check that $G^* \in \mathcal{G}_k^n$ and in each of the above cases one has $S_i(G) = S_i(G^*)$, $i = 0, 1$ and $S_2(G) - S_2(G^*) = 2 > 0$. $G^* \prec_s G$, a contradiction.

If $G$ contains two cycles $C_i = u_0u_1u_2 \cdots u_{i-1}$ and $C_j = v_0v_1v_2 \cdots v_{j-1}$ such that $C_i$ connects $C_j$ by a path $P$, $i \geq 2$. Assume that the endvertices of $P_i$ are $u_0, v_1$, and the vertex, say $u_t$ (resp., $v_m$), on the cycle $C_i$ (resp., $C_j$) in $G$ either is of degree 2 or has subgraph $G_t$ (resp., $H_m$) attached, $0 \leq t \leq l - 1$, $0 \leq m \leq j - 1$. Graph $G$ is depicted in Fig. 3.2. Let

$$G^* = G - \{u_0u_1, v_1v_2, v_0v_1\} + \{u_0v_2, u_1v_0\},$$

then $G^* \in \mathcal{G}_k^n$. Since $S_i(G) = S_i(G^*)$, $i = 0, 1$. We have the contradiction $S_2(G) - S_2(G^*) = 2 > 0$. Therefore, $G$ contains exactly one cycle. 

By Claim 1, we know that $G$ is a unicyclic graph. Note that $G$ contains exactly $k$ cut edges, hence $G$ is an $n$-vertex unicyclic graph with girth $n - k$. By Lemma 1.4 the first graph in the $S$-order among the $n$-vertex unicyclic graph with girth $n - k$ is just the graph $P_k^n$, as desired. 

In the remainder of this section, we determine the second graph in the $S$-order among $\mathcal{G}_k^n$ $(k \geq 3)$.

**Theorem 3.2.** Of all graphs with $n$ vertices and $k$ cut edges, the second graph
in the $S$-order is obtained uniquely at \( \hat{U}_{n}^{k}(k \geq 3) \), where \( \hat{U}_{n}^{k} \) is obtained by attaching two leaves to the pendant vertex of graph \( P_{n-2}^{k-2} \).

**Proof.** Note that if we delete an edge $e$ from a connected graph $G$, then in the view of $S_{2}(G) = 2|E_{G}|$, we have $S_{2}(G) > S_{2}(G - e)$. In order to determine the second graph in the $S$-order among $\mathscr{G}_{n}^{k}$, it suffices to determine the second graph in the $S$-order among the set of all $n$-vertex unicyclic graphs with girth $n - k$; we denote this set by $\mathscr{G}_{n}^{k}$.

Choose $G \in \mathscr{G}_{n}^{k} \setminus \{ P_{n}^{k} \}$ such that it is as small as possible with respect to $\preceq_{1}$. Let $\mathcal{E}$ be the set of $k$ cut edges of $G$. Then $G[\mathcal{E}]$ is a forest. We are to show that $G[\mathcal{E}]$ is a tree. If this is not true, then it is equivalent to that there exist at least two vertices, say $u_{0}, v_{0}$, on the unique cycle contained in $G$ satisfying $d_{G}(u_{0}), d_{G}(v_{0}) \geq 3$.

In the edge induced graph $G[\mathcal{E}]$, consider the tree, say $T_{1}$, containing $u_{0}$. We claim $T_{1}$ is a path. Otherwise, choose a longest path $P = u_{0}u_{1} \cdots u_{p}$ in $T_{1}$ with endvertices $u_{0}$ and $u_{p}$. It is easy to see $\deg(u_{p}) = 1$. If there exists $u_{i}$ with $i \geq 1$ on $P$ such that $d_{G}(u_{i}) = 2$. Choose a vertex $x$ in $N_{G}(u_{i}) \setminus \{ u_{i-1}, u_{i+1} \}$ and let $G^{*} = G - u_{i}x + u_{p}x$, then $G^{*} \in \mathscr{G}_{n}^{k} \setminus \{ P_{n}^{k} \}$. Note that $S_{i}(G) = S_{i}(G^{*})$ for $i = 0, 1, 2, 3$, $\phi_{G}(P_{2}) = \phi_{G^{*}}(P_{2})$, $\phi_{G}(C_{4}) = \phi_{G^{*}}(C_{4})$ and $\phi_{G}(P_{3}) = \phi_{G^{*}}(P_{3}) \geq 1$. Hence, by Lemma 1.2(i), we get the contradiction $S_{i}(G) - S_{i}(G^{*}) > 0$. Hence, each vertex $u_{i}$ on $P$ is of degree 2 in $G$. Hence, if $d_{G}(u_{0}) = 3$, then $T_{1}$ is a path, as desired. If $d_{G}(u_{0}) > 3$, then choose $x$ from $N_{G}(u_{0})$ such that $x$ is not on the cycle and the path $P$ contained in $G$. Let $G^{*} = G - u_{0}x + u_{p}x$. Then $G^{*} \in \mathscr{G}_{n}^{k} \setminus \{ P_{n}^{k} \}$. Notice that $S_{i}(G) = S_{i}(G^{*})$ for $i = 0, 1, 2, 3$, $\phi_{G}(P_{2}) = \phi_{G^{*}}(P_{2})$, $\phi_{G}(C_{4}) = \phi_{G^{*}}(C_{4})$ and $\phi_{G}(P_{3}) - \phi_{G^{*}}(P_{3}) \geq 2$. By Lemma 1.2(i), we get the contradiction $S_{i}(G) - S_{i}(G^{*}) > 0$. By a similar argument, we can also show that, in $G[\mathcal{E}]$, the component contains $v_{0}$ is also a path, say $P^{0}$. For convenience, let $v_{0}^{0}$ be the neighbor of $v_{0}$ on $P^{0}$.

If $|E_{P^{0}}| = 1$, then move the pendant edge from $v_{0}$ to the unique neighbor of $u_{0}$ on the path $P$ and denote the resulting graph by $G^{*}$. It is easy to see that $G^{*} \in \mathscr{G}_{n}^{k} \setminus \{ P_{n}^{k} \}$.

When $k = 3$, by Lemma 1.1, we have $S_{i}(G) \geq S_{i}(G^{*})$ for $i = 0, 1, \ldots, n - 2$ and $S_{n-1}(G^{*}) > S_{n-1}(G^{*})$. Hence, $G^{*} \preceq_{1} G$, a contradiction.

When $k \geq 4$, note that $\phi_{G}(P_{2}) = \phi_{G^{*}}(P_{2})$, $\phi_{G}(C_{4}) = \phi_{G^{*}}(C_{4})$, $\phi_{G}(P_{3}) = \phi_{G^{*}}(P_{3})$, $\phi_{G}(K_{1,3}) = \phi_{G^{*}}(K_{1,3})$, $\phi_{G}(U_{5}) = \phi_{G^{*}}(U_{5})$, $\phi_{G}(B_{4}) = \phi_{G^{*}}(B_{4})$, $\phi_{G}(B_{5}) = \phi_{G^{*}}(B_{5})$, $\phi_{G}(C_{3}) = \phi_{G^{*}}(C_{3})$, $\phi_{G}(C_{6}) = \phi_{G^{*}}(C_{6})$ and $\phi_{G}(P_{4}) = \phi_{G^{*}}(P_{4}) \geq 1$. Hence, by Lemma 1.2(iii), we get that $S_{i}(G) = S_{i}(G^{*})$ for $i = 0, 1, 2, 3, 4, 5$ and $S_{6}(G) - S_{6}(G^{*}) > 0$, a contradiction.

If $|E_{P^{0}}| > 1$, then let $G^{*} = G - uv_{0}^{0} + u_{p}v_{0}^{0}$. It is easy to see that $G^{*} \in \mathscr{G}_{n}^{k} \setminus \{ P_{n}^{k} \}$. Note that $\phi_{G}(P_{2}) = \phi_{G^{*}}(P_{2})$, $\phi_{G}(C_{4}) = \phi_{G^{*}}(C_{4})$, $\phi_{G}(P_{3}) = \phi_{G^{*}}(P_{3})$, $\phi_{G}(K_{1,3}) = \phi_{G^{*}}(K_{1,3})$, $\phi_{G}(U_{5}) = \phi_{G^{*}}(U_{5})$, $\phi_{G}(B_{4}) = \phi_{G^{*}}(B_{4})$, $\phi_{G}(B_{5}) = \phi_{G^{*}}(B_{5})$, $\phi_{G}(C_{4}) = \phi_{G^{*}}(C_{4})$.
φ \_G\_C, \phi_C(C_4) = \phi_G\_C, \phi_G(C_6) = \phi_G\_C\_C, and \phi_G(P_4) - \phi_G(P_4) \geq 1. By
Lemma 1.2(iii), we get that \(S_i(G) = S_i(G^*)\) for \(i = 0, 1, 2, 3, 4, 5\) and \(S_6(G) - S_6(G^*) > 0\),
a contradiction.

Therefore, \(G[E]\) is a tree. That is to say, there exists just one vertex, say \(u_0\), on the unique cycle such that \(d_G(u_0) \geq 3\). Choose one of the longest paths, say \(P := u_0u_1 \cdots u_p\), from \(G[E]\). It is easy to see that \(u_p\) is a leaf of \(G\). Furthermore, we have the following claim.

CLAIM 2. The length of \(P\) is \(k - 1\), i.e., \(P := u_0u_1 \cdots u_{k-1}\) and \(G[E]\) is obtained from \(P\) by attaching a leaf to \(u_{k-2}\) of \(P\).

Proof. Note that \(P = u_0u_1 \cdots u_p\) is one of the longest paths of \(G[E]\) and \(u_p\) is a leaf. Hence, we first show that \(d_G(u_0) = 3\). Otherwise, choose \(x\) from \(N_G(u_0)\) such that \(x\) is not on the cycle and the path \(P\) of \(G\). If \(d_G(u_i) \geq 3\) for some \(i \in \{1, 2, \ldots, p - 1\}\), then let \(G^* = G - u_0x + u_p\). Obviously, \(G^* \notin \mathcal{P}_n\). Note that \(S_i(G) = S_i(G^*)\), \(i = 0, 1, 2, 3, \phi_G(P_2) = \phi_G(P_2), \phi_G(C_4) = \phi_G(C_4)\) and \(\phi_G(P_3) = \phi_G(P_3) - 1\). By Lemma 1.2(i), we get the contradiction \(S_i(G) - S_i(G^*) > 0\).

Now we show that \(d_G(u_i) = 2, i = 1, 2, \ldots, p - 2\) and \(d_G(u_{p-1}) = 3\). Note that \(G \not\in \mathcal{P}_n\), there exists at least one vertex \(u_i\) \((1 \leq i \leq p - 1)\) on \(P\) such that \(d_G(u_i) \geq 3\).

If there exists a vertex \(u_i\) \((1 \leq i \leq p - 1)\) on \(P\) such that \(d_G(u_i) \geq 4\), then choose \(x \in N_G(u_i) \setminus \{u_{i-1}, u_{i+1}\}\) and let \(G^* = G - u_0x + u_p\). Obviously, \(G^* \notin \mathcal{P}_n\). Since \(S_i(G) = S_i(G^*)\), \(i = 0, 1, 2, 3\), \(\phi_G(P_2) = \phi_G(P_2), \phi_G(C_4) = \phi_G(C_4)\) and \(\phi_G(P_3) = \phi_G(P_3) - 2\), by Lemma 1.2(i), we have the contradiction \(S_i(G) - S_i(G^*) > 0\).

If \(d_G(u_{p-1}) = 2, d_G(u_i) = 3\) for some \(i \in \{1, 2, \ldots, p - 2\}\), then choose \(z_1\) in \(N_G(u_i) \setminus \{u_{i-1}, u_{i+1}\}\) and let \(G^* = G - u_0z_1 + u_{p-1}z_1\). Then \(G^* \notin \mathcal{P}_n\). Note that \(S_i(G) = S_i(G^*)\), \(i = 0, 1, 2, 3\), \(\phi_G(P_2) = \phi_G(P_2), \phi_G(C_4) = \phi_G(C_4)\) and \(\phi_G(P_3) = \phi_G(P_3) - 1\), \(\phi_G(P_3) = \phi_G(P_3) - 1 > 0\). Hence, by Lemma 1.2(i), we have the contradiction \(S_i(G) - S_i(G^*) > 0\).

If \(d_G(u_{p-1}) = 2, d_G(u_i) = 3\) for some \(i \in \{1, 2, \ldots, p - 2\}\), then choose \(z_1\) in \(N_G(u_i) \setminus \{u_{i-1}, u_{i+1}\}\) and let \(G^* = G - u_0z_1 + u_{p-1}z_1\). Then it is easy to see that \(G^* \notin \mathcal{P}_n\). Note that \(S_i(G) = S_i(G^*)\) for \(i = 0, 1, 2, 3, 4, 5\), \(\phi_G(P_2) = \phi_G(P_2), \phi_G(C_4) = \phi_G(C_4)\) and \(\phi_G(P_3) = \phi_G(P_3)\). Hence, by Lemma 1.2(iii), we get the contradic-
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Hence, \( d_G(u_0) = 3, d_G(u_1) = d_G(u_2) = \cdots = d_G(u_{p-2}) = 2, d_G(u_{p-1}) = 3 \) and \( d_G(u_p) = 1 \). For convenience, let \( N_G(u_{p-1}) \setminus \{u_{p-2}, u_p\} = \{z_0\} \). It is easy to see that \( z_0 \) is a leaf; otherwise \( G[E] \) contains a path \( P' := u_0u_1 \cdots u_{p-1}z_0 \cdots z_t \), where \( z_t \) is a leaf. It is routine to check that the length of \( P' \) is longer than that of \( P \), a contradiction. Therefore, \( d_G(z_0) = 1 \), as desired.

Based on Claim 2, Theorem 3.2 follows immediately.

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