ON THE SPECTRAL MOMENT OF GRAPHS
WITH GIVEN CLIQUE NUMBER

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ABSTRACT. Let $\mathscr{L}_{n,t}$ be the set of all n-vertex connected graphs with clique number t ($2 \leq t \leq n$). For n-vertex connected graphs with given clique number, lexicographic ordering by spectral moments (S-order) is discussed in this paper. The first $\sum_{i=1}^{\lfloor (n-t-1)/3 \rfloor}(n-t-3i)+1$ graphs with $3 \leq t \leq n-4$, and the last few graphs, in the S-order, among $\mathscr{L}_{n,t}$ are characterized. In addition, all graphs in $\mathscr{L}_{n,n} \bigcup \mathscr{L}_{n,n-1}$ have an S-order; for the cases $t = n-2$ and $t = n-3$, the first three and the first seven graphs in the set $\mathscr{L}_{n,t}$ are characterized, respectively.

1. Introduction. All graphs considered here are finite, simple and connected. For undefined terminology and notation, refer to [**1**]. Let $G = (V_G, E_G)$ be a simple undirected graph with n vertices. $G - v$ and $G - uv$ 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 adding 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 the adjacent vertices of v in G and $d_G(v) = |N_G(v)|$. A *pendant vertex* of G is a vertex of degree 1.

Let G be a simple graph. A clique of G is a subset of vertices such that it induces a complete subgraph of G. We denote the maximum clique size of G by t which is called the *clique number* of G. A *vertex coloring* of a graph $G = (V, E)$ is a map $c : V \to S$ such that $c(v) \neq c(u)$ if v and u are adjacent. The elements of the set S are called the available

colors. We call $\chi(G) := \min\{k : G$ has a k-coloring, a vertex coloring $c : V \to \{1, 2, \ldots, k\}\}$ the *chromatic number* of G.

Let $A(G)$ be the adjacency matrix of a graph G with $\lambda_1(G), \lambda_2(G),$ $\ldots, \lambda_n(G)$ being 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 *kth 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 $G_1 =_s G_2$ if $S_i(G_1) = S_i(G_2)$ for $i = 0, 1, \ldots, n-1$. Similarly, we have $G_1 \prec_s G_2$ (G_1 comes before G_2 in the S-order) if for some k $(1 \le k \le n-1)$, we have $S_i(G_1) = S_i(G_2)$ $(i = 0, 1, \ldots, k-1)$ and $S_k(G_1) < S_k(G_2)$. We shall also write $G_1 \preceq_s G_2$ if $G_1 \prec_s G_2$ 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 refer to [4].

Recently, investigation on S-order of graphs has received increasing attention. For example, 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. Wu and Fan [22] determined the first and the last graphs, in the S-order, of all unicyclic graphs and bicyclic graphs, respectively. Pan, et al., [19] gave the first

$$\sum_{k=1}^{\lfloor (n-t-1)/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right)$$

graphs apart from an n-vertex path, in the S-order, of all trees with n vertices. Wu and Liu [23] determined the last $\lfloor d/2 \rfloor + 1$ graphs, in the S-order, among all n-vertex trees of diameter d $(4 \le d \le n-3)$. Pan, et al., [20] identified the last and the second last graphs, in the S-order, of quasi-trees. Cheng, Liu and Liu identified the last $d + \lfloor d/2 \rfloor - 2$ 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. 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 among the sets of all trees of order n with the largest degree, the leaves number, the independence number and the matching number was also determined, respectively. Li, Zhang and Zhang [12] determined the

first, the second, the last and the second last graphs in the S-order among the set of all graphs with given number of cut edges. Li and Zhang [11] also considered this problem on the n-vertex trees with given bipartition.

On the other hand, there are many Turán-type extremal problems, i.e., given a forbidden graph F, determine the maximal number of edges in a graph on n vertices that does not contain a copy of F. It states that, among n-vertex graphs not containing a clique of size $t+1$, the complete t-partite graph $T_{n,t}$ with (almost) equal parts, which is called the *Turán graph*, has the maximum number of edges. Spectral graph theory has similar Turán extremal problems which determine the largest (or smallest) eigenvalue of a graph not containing a subgraph F. Nikiforov explicitly proposed studying general Turán problems in [12, 16]. For example, he [16] determined the maximum spectral radius of graphs without paths of given length and presented a comprehensive survey on these topics, see [18]. In addition, Sudakov, et al., [21] presented a generalization of Turán theorem in terms of Laplacian eigenvalues, whereas He, et al., [8] gave a generalization of the Turán theorem in terms of signless Laplacian eigenvalues.

Motivated by Turán-type extremal problems, we investigate in this paper the spectral moments of n-vertex graphs with given clique number, which may be regarded as a part of spectral extremal theory. For $2 \le t \le n$, let $\mathscr{L}_{n,t}$ be the set of all n-vertex connected graphs with clique number t. We give the first $\sum_{i=1}^{\lfloor (n-t-1)/3 \rfloor} (n-t-3i) + 1$ graphs with $3 \le t \le n-4$, and the last few graphs, in the S-order, among $\mathscr{L}_{n,t}$. In addition, all graphs in $\mathscr{L}_{n,n} \bigcup \mathscr{L}_{n,n-1}$ have an S-order; for the cases $t = n-2$ and $t = n-3$, the first three and the first seven graphs in the set $\mathscr{L}_{n,t}$ are characterized, respectively. We prove these results in Section 3. According to the relationship between the clique number and the chromatic number of graphs, we study the S-order of graphs with given chromatic number in Section 4. In Section 2, we give some preliminaries which are useful for the proofs of our main results.

2. Preliminaries. Throughout, we denote by P_n, S_n, C_n and K_n a path, a star, a cycle and a complete graph on n vertices, respectively. An *F-subgraph* of G is a subgraph of G, which is isomorphic to the graph F. Let $\phi_G(F)$ (or $\phi(F)$ for short) be the number of all F-subgraphs of G. The notation $G \not\supseteq F$ means that G does not contain F as its

subgraph.

Further on, we will need the following lemmas.

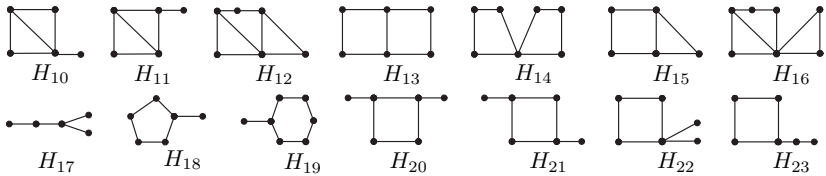**Lemma 2.1** ([20]). *The kth spectral moment of G is equal to the number of closed walks of length k.*

FIGURE 1. Graphs $H_1, H_2, \ldots, H_{22}$ and H_{23}.

Lemma 2.2 ([5]). *Given a connected graph G, $S_0(G) = n$, $S_1(G) = l$, $S_2(G) = 2m$, $S_3(G) = 6t$, where n, l, m and t denote the number of vertices, number of loops, number of edges and number of triangles contained in G, respectively.*

Let $H_1, H_2, \ldots, H_{23}$ be the graphs as depicted in Figure 1, which will be used in Lemma 2.3.

Lemma 2.3. *For every graph G, we have*

(i) $S_4(G) = 2\phi(P_2) + 4\phi(P_3) + 8\phi(C_4)$ ([4]).

(ii) $S_5(G) = 30\phi(C_3) + 10\phi(H_1) + 10\phi(C_5)$ ([4]).

(iii) $S_6(G) = 2\phi(P_2) + 12\phi(P_3) + 6\phi(P_4) + 12\phi(K_{1,3}) + 12\phi(H_2) + 36\phi(H_3) + 24\phi(H_4) + 24\phi(C_3) + 48\phi(C_4) + 12\phi(C_6)$ ([23]).

(iv) $S_7(G) = 126\phi(C_3) + 84\phi(H_1) + 28\phi(H_7) + 14\phi(H_5) + 14\phi(H_6) + 112\phi(H_3) + 42\phi(H_{15}) + 28\phi(H_8) + 70\phi(C_5) + 14\phi(H_{18}) + 14\phi(C_7)$.

(v) $S_8(G) = 2\phi(P_2) + 28\phi(P_3) + 32\phi(P_4) + 8\phi(P_5) + 72\phi(K_{1,3}) + 16\phi(H_{17}) + 48\phi(K_{1,4}) + 168\phi(C_3) + 64\phi(H_1) + 464\phi(H_3) + 384\phi(H_4) + 96\phi(H_{15}) + 96\phi(H_{10}) + 48\phi(H_{11}) + 80\phi(H_{12}) + 32\phi(H_{16}) + 264\phi(C_4) + 24\phi(H_9) + 112\phi(H_2) + 16\phi(H_{23}) + 16\phi(H_{20}) + 16\phi(H_{21}) + 32\phi(H_{22}) + 32\phi(H_{13}) + 32\phi(H_{14}) + 528\phi(K_4) + 96\phi(C_6) + 16\phi(H_{19}) + 16\phi(C_8)$.

Proof.

(iv) By Lemma 2.1, we note that vertices that belong to a closed walk of length 7 induce in G a subgraph isomorphic to C_3, H_1, H_7, H_5, H_6, H_3, H_{15}, H_8, C_5, H_{18}, C_7. By using `matlab`, we can obtain the number of closed walks of length 7 which span these subgraphs is 126, 84, 28, 14, 14, 112, 42, 28, 70, 14 and 14, respectively, then (iv) follows.

(v) By Lemma 2.1, we note that vertices that belong to a closed walk of length 8 induce in G a subgraph isomorphic to P_2, P_3, P_4, P_5, $K_{1,3}$, H_{17}, $K_{1,4}$, C_3, H_1, H_3, H_4, H_{15}, H_{10}, H_{11}, H_{12}, H_{16}, C_4, H_9, H_2, H_{23}, H_{20}, H_{21}, H_{22}, H_{13}, H_{14}, K_4, C_6, H_{19}, C_8. By using `matlab`, we can obtain that the number of closed walks of length 8 which span these subgraphs is 2, 28, 32, 8, 72, 16, 48, 168, 64, 464, 384, 96, 96, 48, 80, 32, 264, 24, 112, 16, 16, 16, 32, 32, 32, 528, 96, 16 and 16, respectively. Then (v) follows immediately. $\square$

A connected subgraph H of G is called a *tree-subgraph* (or *cycle-subgraph*) if H is a tree (or contains at least one cycle). Let H be a proper subgraph of G; we call H an *effective graph* for $S_k(G)$ if H contains a closed walk of length k. Set $\mathscr{T}_k(G) = \{T : T$ is a tree-subgraph of G with $|E_T| \leq k/2\}$; $\mathscr{T}'_k(G) = \{W : W$ is a cycle-subgraph of G with $|E_W| \leq k\}$; $\mathscr{A}_k(G) = \{T : T$ is a tree-subgraph of G, and it is an effective graph for $S_k(G)\}$; $\mathscr{A}'_k(G) = \{W : W$ is a cycle-subgraph of G and it is an effective graph for $S_k(G)\}$. It is easy to see that $\mathscr{A}_k(G) \cap \mathscr{A}'_k(G) = \emptyset$. By Lemma 2.1, we have:

Proposition 2.4. *Given a graph G, the set of all effective graphs for $S_k(G)$ is $\mathscr{A}_k(G) \cup \mathscr{A}'_k(G)$. In particular, if k is odd, then $\mathscr{A}_k(G) = \emptyset$.*

Lemma 2.5 ([23]). *Let G be a non-trivial connected graph with $u \in V_G$. Suppose that two paths of lengths $a, b\,(a \geq b \geq 1)$ are attached to G by their end vertices at u, respectively, to form $G^*_{a,b}$. Then $G^*_{a+1,b-1} \prec_s G^*_{a,b}$.*

Let G and H be two graphs with $u \in V_G$ and $v \in V_H$. We shall denote by $Gu \cdot vH$ the graph obtained from G and H by identifying u and v.

Lemma 2.6 ([23]). *Let G and H be two non-trivial connected graphs with u and $v \in V_G$ and $w \in V_H$. If $d_G(u) < d_G(v)$, then $Gu \cdot wH \prec_s Gv \cdot wH$.*

3. On the S-order among $\mathscr{L}_{n,t}$. In this section, we study the S-order among $\mathscr{L}_{n,t}$ $(2 \leq t \leq n)$. In view of Lemma 2.2, the first few graphs in the S-order among $\mathscr{L}_{n,2}$ must be n-vertex trees. Fortunately, on the other hand, Pan, et al., [19] identified the first

$$\sum_{k=1}^{\lfloor n-1/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

graphs, in the S-order, of all trees with n vertices; these

$$\sum_{k=1}^{\lfloor n-1/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

trees are also the first

$$\sum_{k=1}^{\lfloor n-1/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

graphs in the S-order among $\mathscr{L}_{n,2}$. We will not repeat it here.

A graph $G \not\supseteq F$ on n vertices with the largest possible number of edges is called *extremal* for n and F; its number of edges is denoted by $\mathrm{ex}(n, F)$. The following theorem tells us the Turán graph $T_{n,t}$ is indeed extremal for n and K_{t+1}, and as such unique.

Theorem 3.1 (Turán 1941). *For all integers t, n with $t > 1$, every graph $G \not\supseteq K_{t+1}$ with n vertices and $\mathrm{ex}(n, K_{t+1})$ edges is a $T_{n,t}$.*

Theorem 3.2. *For all integers t, n with $t > 1$, every graph $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}\}$, one has $G \prec_s T_{n,t}$.*

Proof. Note that, for graph $G \in \mathscr{L}_{n,t} \setminus \{T_{n,t}\}$, one has

$$S_i(G) = S_i(T_{n,t}), \quad i = 0, \ 1.$$

By Lemma 2.2 and Theorem 3.1, we have

$$S_2(G) = 2|E_G| < 2|E_{T_{n,t}}| = S_2(T_{n,t}).$$

Hence, $G \prec_s T_{n,t}$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ □

Now assume that $(V_1, V_2, \ldots, V_t)$ is a partition of $T_{n,t}$ with $n = kt + r$ ($0 \le r < t$), where $|V_i| = k$ if $i = 1, 2, \ldots, t - r$ and $|V_i| = k + 1$ otherwise. For $u, v \in V_{T_{n,t}}$, let

- $T_{n,t}^1$ be the graph obtained by deleting the edge uv from $T_{n,t}$, where $u \in V_i, v \in V_j, 1 \le i \ne j \le t - r$;

- $T_{n,t}^2$ be the graph obtained by deleting the edge uv from $T_{n,t}$, where $u \in V_i, v \in V_j, 1 \le i \le t - r$ and $t - r + 1 \le j \le t$;

- $T_{n,t}^3$ be the graph obtained by deleting the edge uv from $T_{n,t}$, where $u \in V_i, v \in V_j, t - r + 1 \le i \ne j \le t$.

In particular, if $t = n - 1$ then $|V_1| = |V_2| = \cdots = |V_{n-2}| = 1$ and $|V_{n-1}| = 2$. In this case, for convenience, we assume that $V_i = \{v_i\}$ for $i = 1, 2, \ldots, n - 2$ and $V_{n-1} = \{v_{n-1}, u\}$. Let

$$T_i := T_{n,n-1} - \{uv_1, uv_2, \ldots, uv_{i-1}, uv_i\},$$

where $i = 1, 2, \ldots, n - 3$. It is straightforward to check that $\mathscr{L}_{n,n-1} = \{T_{n,n-1}, T_1, T_2, \ldots, T_{n-3}\}$.

Theorem 3.3. *Among the set of graphs $\mathscr{L}_{n,t}$ with $3 \le t \le n - 1$.*

(i) *If $n = t + 1$, then all graphs in the set $\mathscr{L}_{n,n-1}$ have the following S-order: $T_{n-3} \prec_s T_{n-4} \prec_s \cdots \prec_s T_i \prec_s \cdots \prec_s T_2 \prec_s T_1 \prec_s T_{n,n-1}$.*

(ii) *If $n = kt$ with $3 \le t \le n/2$, then for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}$.*

(iii) *If $n = kt + 1$ with $3 \le t \le n/2$, then for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1, T_{n,t}^2\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}^2 \prec_s T_{n,t}$.*

(iv) *If $n = kt + r$ with $3 \le t \le n/2$, $r = t - 1$ or $(n + 1)/2 \le t \le n - 2$, then for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^2, T_{n,t}^3\}$ one has $G \prec_s T_{n,t}^2 \prec_s T_{n,t}^3 \prec_s T_{n,t}$.*

(v) *If $n = kt + r$ with $4 \le t \le n/2$, $2 \le r \le t - 2$, then for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1, T_{n,t}^2, T_{n,t}^3\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}^2 \prec_s T_{n,t}^3 \prec_s T_{n,t}$.*

Proof.

(i) It follows directly by Lemma 2.2.

(ii) For all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1\}$, by Lemma 2.2, $S_i(G) = S_i(T_{n,t}^1) = S_i(T_{n,t}^2)$ for $i = 0, 1$. Note that $n = kt$ with $3 \leq t \leq n/2$; hence, by the definition of $T_{n,t}^1$, it is the unique graph in $\mathscr{L}_{n,t}$ satisfying the number of its edges equals to $|E_{T_{n,t}}| - 1$ which implies that, for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1\}$, we have $|E_G| < |E_{T_{n,t}^1}|$, i.e., $S_2(G) < S_2(T_{n,t}^1) < S_2(T_{n,t})$. Hence, (ii) holds.

(iii) For any $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1, T_{n,t}^2\}$, one has $S_i(G) = S_i(T_{n,t}^1) = S_i(T_{n,t}^2)$ for $i = 0, 1$. By the definition of $T_{n,t}^1, T_{n,t}^2$, we know they are just the two graphs in $\mathscr{L}_{n,t}$ satisfying $|E_{T_{n,t}^1}| = |E_{T_{n,t}^2}| = |E_{T_{n,t}}| - 1$, which implies that, for all $G \in \mathscr{L}_{n,t} \backslash \{T_{n,t}, T_{n,t}^1, T_{n,t}^2\}$, we have $|E_G| < |E_{T_{n,t}^1}| = |E_{T_{n,t}^2}|$, i.e., $S_2(G) < S_2(T_{n,t}^1) = S_2(T_{n,t}^2) < S_2(T_{n,t})$. In order to complete the proof, it suffices to show $S_3(T_{n,t}^1) < S_3(T_{n,t}^2)$. In fact,

$$S_3(T_{n,t}^1) - S_3(T_{n,t}^2) = 6(\phi_{T_{n,t}^1}(C_3) - \phi_{T_{n,t}^2}(C_3)) = -6 < 0.$$

Hence, (iii) holds.

(iv) and (v) can be proved by a similar discussion as in the proof of (iii). We omit the procedure here.

$\square$

In the following, we are to determine the first few graphs, in the S-order, among $\mathscr{L}_{n,t}$ $(3 \leq t \leq n - 1)$. Let $J_1, J_2, \ldots, J_{10}$ be the n-vertex graphs as depicted in Figure 2.
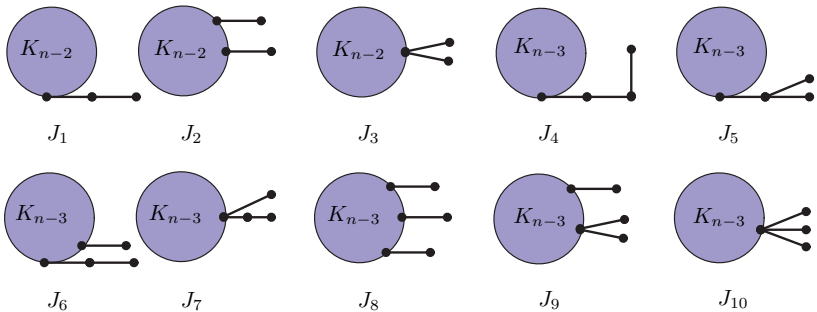

FIGURE 2. n-vertex graphs $J_1, J_2, \ldots, J_{10}$.

Theorem 3.4. *Among the set of all graphs* $\mathscr{L}_{n,t}$.

  (i) *If* $t = n - 2 \geq 3$, *the first three graphs, in the S-order, among* $\mathscr{L}_{n,n-2}$ *are* $J_1 \prec_s J_2 \prec_s J_3$.

  (ii) *If* $t = n - 3 \geq 3$, *the first seven graphs, in the S-order, among* $\mathscr{L}_{n,n-3}$ *are* $J_4 \prec_s J_5 \prec_s J_6 \prec_s J_7 \prec_s J_8 \prec_s J_9 \prec_s J_{10}$.

  Proof.

  (i) For all $G \in \mathscr{L}_{n,n-2} \setminus \{J_1, J_2, J_3\}$, one has not only $S_k(G) = S_k(J_1) = S_k(J_2) = S_k(J_3)$ for $k = 0, 1$ but also $|E_G| > |E_{J_1}| = |E_{J_2}| = |E_{J_3}|$; hence, $S_2(J_1) = S_2(J_2) = S_2(J_3) < S_2(G)$, i.e., $J_i \prec_s G$ for $i = 1, 2, 3$. By Lemma 2.6, we have $J_1 \prec_s J_2 \prec_s J_3$, Therefore, (i) holds.

  (ii) For all $G \in \mathscr{L}_{n,n-3} \setminus \{J_4, J_5, J_6, J_7, J_8, J_9, J_{10}\}$, one has $S_k(G) = S_k(J_4) = \cdots = S_k(J_{10})$ for $k = 0, 1$ and $|E_G| > |E_{J_4}| = \cdots = |E_{J_{10}}|$. Hence, $S_2(J_4) = S_2(J_5) = \cdots = S_2(J_{10}) < S_2(G)$, i.e., $J_i \prec_s G$ for $i = 4, 5, \ldots, 10$. It is easy to see that $S_3(J_4) = S_3(J_5) = \cdots = S_3(J_{10})$.

Further on, by Lemma 2.3 (i)–(ii), we have

$$(3.1) \qquad S_4(J_4) = 2|E_{J_4}| + 8\phi_{J_4}(C_4)$$
$$+ 4\left[(n-4)\binom{n-4}{2} + \binom{n-3}{2} + 2\binom{2}{2}\right],$$

$$(3.2) \qquad S_4(J_5) = 2|E_{J_5}| + 8\phi_{J_5}(C_4)$$
$$+ 4\left[(n-4)\binom{n-4}{2} + \binom{n-3}{2} + \binom{3}{2}\right],$$

$$(3.3) \qquad S_4(J_6) = 2|E_{J_6}| + 8\phi_{J_6}(C_4)$$
$$+ 4\left[(n-5)\binom{n-4}{2} + 2\binom{n-3}{2} + \binom{2}{2}\right].$$

By (3.1) and (3.2), we have $S_4(J_4) - S_4(J_5) = -4 < 0$; hence, $J_4 \prec_s J_5$. Similarly, we can show that $J_6 \prec_s J_7, J_8 \prec_s J_9 \prec_s J_{10}$.

By (3.2) and (3.3), we have $S_4(J_5) - S_4(J_6) = -4(n-6)$. If $n > 6$, obviously we have $S_4(J_5) - S_4(J_6) < 0$, i.e., $J_5 \prec_s J_6$ for $n > 6$. If $n = 6, S_4(J_5) - S_4(J_6) = 0$, whereas $S_5(J_5) - S_5(J_6) = 10(\phi_{J_5}(H_1) - \phi_{J_6}(H_1)) = -10 < 0$, i.e., $J_5 \prec_s J_6$ for $n = 6$, we hence

obtain that $J_5 \prec_s J_6$ for $n \geq 6$. Similarly, we can also show that $J_7 \prec_s J_8$ for $n \geq 6$.

Therefore, we obtain $J_4 \prec_s J_5 \prec_s J_6 \prec_s J_7 \prec_s J_8 \prec_s J_9 \prec_s J_{10} \prec_s G$ for $G \in \mathscr{L}_{n,n-3} \setminus \{J_4, J_5, J_6, J_7, J_8, J_9, J_{10}\}$, as desired.   □
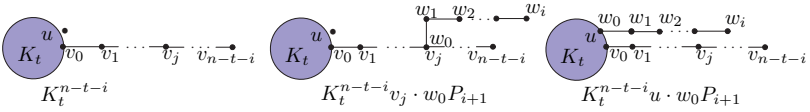

FIGURE 3. Graphs K_t^{n-t-i}, $K_t^{n-t-i}v_j \cdot w_0 P_{i+1}$ and $K_t^{n-t-i}u \cdot w_0 P_{i+1}$ with some vertices labeled.

Given a path $P_{i+1} = w_0 w_1 w_2 \ldots w_i$, set $G_j^i := K_t^{n-t-i} v_j \cdot w_0 P_{i+1}$ and $H^i := K_t^{n-t-i}u \cdot w_0 P_{i+1}$ (see Figure 3), where $3 \leq t \leq n-2$, $0 \leq j \leq n-t-2i$ and $1 \leq i \leq \lfloor (n-t)/2 \rfloor$.

Theorem 3.5. *Among the set of all graphs $\mathscr{L}_{n,t}$ with $3 \leq t \leq n-4$, the first*

$$\sum_{i=1}^{\lfloor (n-t-1)/3 \rfloor} (n-t-3i) + 1$$

graphs, in the S-order, are

$$K_t^{n-t} \prec_s G_{n-t-2}^1 \prec_s G_{n-t-3}^1 \prec_s \cdots$$
$$\prec_s G_3^1 \prec_s G_2^1 \prec_s G_{n-t-4}^2 \prec_s G_{n-t-5}^2 \prec_s \cdots \prec_s G_3^2 \prec_s \cdots$$
$$\prec_s G_{n-t-2i}^i \prec_s G_{n-t-2i-1}^i \prec_s \cdots$$
$$\prec_s G_{i+1}^i \prec_s G_{n-t-2(i+1)}^{i+1} \prec_s \cdots \prec_s G_{\lfloor n-t-1/3 \rfloor+1}^{\lfloor n-t-1/3 \rfloor}.$$

Proof. Note that, for any connected graph G, one has $G \prec_s G + e$, where $e \notin E_G$. Hence, for $3 \leq t \leq n-4$, the first graph in the S-order among $\mathscr{L}_{n,t}$ is obtained from K_t by attaching some trees to the vertices of K_t; in view of Lemma 2.6, the first few graphs in the S-order among $\mathscr{L}_{n,t}$ is just the kite graph K_t^{n-t}. Furthermore, it suffices for us to

consider the set of graphs

$\mathscr{A} = \{G : G$ is an n-vertex graph obtained by attaching
some trees to K_t such that G contains just two pendant vertices$\}$.

It is easy to see that $\mathscr{A}$ is a subset of $\mathscr{L}_{n,t}$ and

$$\mathscr{A} = \left\{ G_j^i : 0 \leq j \leq n - t - 2i, \ 1 \leq i \leq \left\lfloor \frac{n-t}{2} \right\rfloor \right\}$$
$$\bigcup \left\{ H^i : 1 \leq i \leq \left\lfloor \frac{n-t}{2} \right\rfloor \right\}. \qquad \square$$

We first show the following claims.

Claim 3.6. $G_j^i \prec_s H^{i'} \prec_s G_0^{i''}$, where $1 \leq j \leq n - t - 2i$, $1 \leq i \leq \lfloor (n - t - 1)/2 \rfloor$, $1 \leq i', i'' \leq \lfloor (n - t)/2 \rfloor$.

Proof of Claim 3.6. Note that $1 \leq j \leq n - t - 2i$, $1 \leq i \leq \lfloor (n - t - 1)/2 \rfloor$, $1 \leq i', i'' \leq \lfloor (n - t)/2 \rfloor$, $S_k(H^{i'}) = S_k(G_j^i) = S_k(G_0^{i''})$ for $k = 0, 1, 2, 3$. By Lemma 2.3 (i), we have

$$(3.4) \qquad S_4(H^{i'}) = 2m(H^{i'}) + 8\phi_{H^{i'}}(C_4)$$
$$+ 4 \left[(t - 2) \binom{t-1}{2} + 2 \binom{t}{2} + n - t - 2 \right],$$

$$(3.5) \qquad S_4(G_j^i) = 2m(G_j^i) + 8\phi_{G_j^i}(C_4)$$
$$+ 4 \left[(t - 1) \binom{t-1}{2} + \binom{t}{2} + \binom{3}{2} + n - t - 3 \right],$$

$$(3.6) \qquad S_4(G_0^{i''}) = 2m(G_0^{i''}) + 8\phi_{G_0^{i''}}(C_4)$$
$$+ 4 \left[(t - 1) \binom{t-1}{2} + \binom{t+1}{2} + n - t - 2 \right].$$

Note that $\phi_{H^{i'}}(C_4) = \phi_{G_j^i}(C_4) = \phi_{G_0^{i''}}(C_4)$; hence, (3.4)–(3.6) give

$$(3.7) \qquad S_4(G_0^{i''}) - S_4(H^{i'}) = 4, \qquad S_4(H^{i'}) - S_4(G_j^i) = 4(t - 3).$$

In view of (3.7), if $3 < t \leq n - 4$, we obtain $G_j^i \prec_s H^{i'} \prec_s G_0^{i''}$; if $t = 3$, then $S_4(H^{i'}) = S_4(G_j^i) < S_4(G_0^{i''})$ and $S_5(H^{i'}) - S_5(G_j^i) =$

$10\phi_{H^{i'}}(U_4) - 10\phi_{G_j^i}(U_4) = 10 > 0$. Hence, $G_j^i \prec_s H^{i'} \prec_s G_0^{i''}$ for $t = 3$. Therefore, $G_j^i \prec_s H^{i'} \prec_s G_0^{i''}$ for $3 \leq t \leq n - 4$, as desired. □

Claim 3.7. $G_{j+1}^i \prec_s G_j^i$, where $1 \leq i \leq \lfloor (n - t - 1)/2 \rfloor$, $1 \leq j < n - t - 2i$.

Proof of Claim 3.7. Note that, for $1 \leq i \leq \lfloor (n - t - 1)/2 \rfloor$, $1 \leq j < j + 1 \leq n - t - 2i$, it is routine to check that $S_k(G_j^i) = S_k(G_{j+1}^i)$, $k \in \{0, 1, 2, 3, 4\}$. In what follows, we consider $k \geq 5$. On the one hand, for $5 \leq k \leq 2j + 3$, it is easy to see that, for any $W \in \mathscr{A}_k'(G_j^i)$, there exists $W' \in \mathscr{A}_k'(G_{j+1}^i)$ such that $W \cong W'$, and vice versa. Hence,

$$(3.8) \qquad \mathscr{A}_k'(G_j^i) = \mathscr{A}_k'(G_{j+1}^i), \quad k = 5, 6, \ldots, 2j + 3.$$

In what follows, we distinguish our discussion in the following two possible cases.

Case 1. $1 \leq j \leq (n - t - i - 1)/2$. In this case, if $5 \leq k \leq 2j + 2$, then for any $T \in \mathscr{A}_k(G_j^i)$, there exists $T' \in \mathscr{A}_k(G_{j+1}^i)$ such that $T \cong T'$ for $5 \leq k \leq 2j + 2$, and vice versa. Note that, if k is odd, then $\mathscr{A}_k(G) = \emptyset$; hence, $\mathscr{A}_{2j+3}(G_j^i) = \mathscr{A}_{2j+3}(G_{j+1}^i) = \emptyset$. Therefore,

$$(3.9) \qquad \mathscr{A}_k(G_j^i) = \mathscr{A}_k(G_{j+1}^i), \quad k = 5, 6, \ldots, 2j + 3.$$

By (3.8), (3.9) and Proposition 2.4, we obtain

$$S_k(G_j^i) = S_k(G_{j+1}^i), \quad k = 5, 6, \ldots, 2j + 3.$$

If $1 \leq j < (n - t - i - 1)/2$, note that $k = 2j + 4$. Then, for any $W \in \mathscr{A}_{2j+4}'(G_j^i)$, there exists $W' \in \mathscr{A}_{2j+4}'(G_{j+1}^i)$ such that $W \cong W'$, and vice versa. Hence, $\mathscr{A}_{2j+4}'(G_j^i) = \mathscr{A}_{2j+4}'(G_{j+1}^i)$. Notice that, for any $T \in \mathscr{A}_{2j+4}(G_j^i)$, $T' \in \mathscr{A}_{2j+4}(G_{j+1}^i)$, it is routine to check

- if $|E_T \cap E_{K_t}| = 0$, then $\phi_{G_j^i}(T) - \phi_{G_{j+1}^i}(T') = \phi_{G_j^i}(P_{j+3}) - \phi_{G_{j+1}^i}(P_{j+3}) = -1$;
- if $|E_T \cap E_{K_t}| = 1$, then $\phi_{G_j^i}(T) - \phi_{G_{j+1}^i}(T') = \phi_{G_j^i}(P_{j+3}) - \phi_{G_{j+1}^i}(P_{j+3}) = t - 1$;
- if $|E_T \cap E_{K_t}| \geq 2$, then $\phi_{G_j^i}(T) - \phi_{G_{j+1}^i}(T') = 0$.

Hence,

$$\begin{aligned}
|\mathscr{A}_{2j+4}(G_j^i)| - |\mathscr{A}_{2j+4}(G_{j+1}^i)| &= \phi_{G_j^i}(T) - \phi_{G_{j+1}^i}(T') \\
&= \phi_{G_j^i}(P_{j+3}) - \phi_{G_{j+1}^i}(P_{j+3}) \\
&= t - 2 \geq 1 > 0.
\end{aligned}$$

By Proposition 2.4, we have

$$\begin{aligned}
S_{2j+4}(G_j^i) - S_{2j+4}(G_{j+1}^i) &= (2j+4)(\phi_{G_j^i}(P_{j+3}) - \phi_{G_{j+1}^i}(P_{j+3})) \\
&= (2j+4)(t-2) > 0,
\end{aligned}$$

which implies that $G_{j+1}^i \prec_s G_j^i$ for $1 \leq j < (n-t-i-1)/2$.

If $j = (n-t-i-1)/2$, by a similar way as above we can obtain that

$$|\mathscr{A}'_{2j+4}(G_j^i)| - |\mathscr{A}'_{2j+4}(G_{j+1}^i)| = 0,$$
$$|\mathscr{A}_{2j+4}(G_j^i)| - |\mathscr{A}_{2j+4}(G_{j+1}^i)| = (t-1) > 0.$$

By Proposition 2.4, we get $S_{2j+4}(G_j^i) > S_{2j+4}(G_{j+1}^i)$, i.e., $G_{j+1}^i \prec_s G_j^i$ holds for $j = (n-t-i-1)/2$.

Case 2. $(n-t-i-1)/2 < j \leq n-t-2i$. Note that $j > (n-t-i-1)/2$, hence $2(n-t-i-j)+1 < 2j+3$. In view of (3.8), we have

$$\mathscr{A}'_k(G_j^i) = \mathscr{A}'_k(G_{j+1}^i), \quad k = 5, 6, \ldots, 2(n-t-i-j)+1.$$

Furthermore, for $5 \leq k \leq 2(n-t-i-j)+1$, we have for all $T \in \mathscr{A}_k(G_j^i)$, there exists $T' \in \mathscr{A}_k(G_{j+1}^i)$ such that $T \cong T'$ and vice versa. Hence,

$$\mathscr{A}_k(G_j^i) = \mathscr{A}_k(G_{j+1}^i), \quad k = 5, 6, \ldots, 2(n-t-i-j)+1.$$

By Proposition 2.4, $S_k(G_j^i) = S_k(G_{j+1}^i)$ holds for $5 \leq k \leq 2(n-t-i-j)+1$. For $k = 2(n-t-i-j+1)$, by a similar discussion as in the proof of Case 1, we can obtain that

$$|\mathscr{A}'_{2(n-t-i-j+1)}(G_j^i)| - |\mathscr{A}'_{2(n-t-i-j+1)}(G_{j+1}^i)| = 0,$$
$$|\mathscr{A}_{2(n-t-i-j+1)}(G_j^i)| - |\mathscr{A}_{2(n-t-i-j+1)}(G_{j+1}^i)| = \phi_{G_j^i}(T) - \phi_{G_{j+1}^i}(T') = 1.$$

By Proposition 2.4, $S_{2(n-t-i-j+1)}(G_j^i) - S_{2(n-t-i-j+1)}(G_{j+1}^i) = 2(n-t-i-j+1) \cdot 1 > 0$. Hence, $G_{j+1}^i \prec_s G_j^i$ holds for $(n-t-i-1)/2 < j \leq n-t-2i$.

By Cases 1 and 2, Claim 3.7 holds. This completes the proof.   □

Claim 3.8. $G_{i+1}^i \prec_s G_{n-t-2(i+1)}^{i+1}$, *where* $1 \leq i < \lfloor (n-t-1)/3 \rfloor$.

Proof of Claim 3.8. By a similar discussion as in the proof of Claims 3.6 and 3.7, we can show that $S_k(G_{i+1}^i) = S_k(G_{n-t-2(i+1)}^{i+1})$ for $0 \leq k \leq 2i+3$ and $S_{2i+4}(G_{n-t-2(i+1)}^{i+1}) - S_{2i+4}(G_{i+1}^i) = 2i + 4 > 0$. Hence, $G_{i+1}^i \prec_s G_{n-t-2(i+1)}^{i+1}$.   □

By Claims 3.6–3.8, we have the following fact.

Fact 3.9. The set $\mathscr{B} := \{K_t^{n-t}, G_{n-t-2}^1, G_{n-t-3}^1, \ldots, G_3^1, G_2^1, G_{n-t-4}^2, G_{n-t-5}^2, \ldots, G_3^2, \ldots, G_{n-t-2i}^i, G_{n-t-2i-1}^i, \ldots, G_{i+1}^i, G_{n-t-2(i+1)}^{i+1}, \ldots, G_{\lfloor (n-t-1)/3 \rfloor+1}^{\lfloor (n-t-1)/3 \rfloor}\}$ consists of $\sum_{i=1}^{\lfloor (n-t-1)/3 \rfloor} (n-t-3i) + 1$ graphs, and they are in the following S-order:

$$K_t^{n-t} \prec_s G_{n-t-2}^1 \prec_s G_{n-t-3}^1 \prec_s \cdots$$
$$\prec_s G_3^1 \prec_s G_2^1 \prec_s G_{n-t-4}^2 \prec_s G_{n-t-5}^2 \prec_s \cdots \prec_s G_3^2 \prec_s \cdots$$
$$\prec_s G_{n-t-2i}^i \prec_s G_{n-t-2i-1}^i \prec_s \cdots$$
$$\prec_s G_{i+1}^i \prec_s G_{n-t-2(i+1)}^{i+1} \prec_s \cdots \prec_s G_{\lfloor (n-t-1)/3 \rfloor+1}^{\lfloor (n-t-1)/3 \rfloor},$$

where $3 \leq t \leq n - 4$.

Claim 3.10. *Among* $\mathscr{A} \setminus \mathscr{B}$, *one has* $G_{\lfloor (n-t)/3 \rfloor}^{\lfloor (n-t)/3 \rfloor} \preceq_s G_j^i$, *where* $1 \leq j \leq n-t-2i$, $j \leq i \leq \lfloor (n-t-1)/2 \rfloor$.

Proof of Claim 3.10. For a fixed j in $\{1, 2, \ldots, n-t-2i\}$, there does not exist G_j^i satisfying $i \geq j > \lfloor (n-t)/3 \rfloor$. By Lemma 2.2, we know $G_j^j \prec_s G_j^i$ for all $1 \leq j \leq \lfloor (n-t)/3 \rfloor$, $j < i \leq \lfloor (n-t-1)/2 \rfloor$. Hence, according to the S-order, the first graph in $\{G_j^j : 1 \leq j \leq \lfloor (n-t)/3 \rfloor\}$ is just the first graph in $\{G_j^i : 1 \leq j \leq n-t-2i, j \leq i \leq \lfloor (n-t-1)/2 \rfloor\}$. In what follows, we are to determine the first graph in the S-order among $\{G_j^j : 1 \leq j \leq \lfloor (n-t)/3 \rfloor\}$.

Note that $1 \leq i+1 \leq \lfloor (n-t)/3 \rfloor - 1$; hence, $1 \leq i+1 \leq (n-t-3)/3$. By a similar discussion as in the proof of Claim 3.6, we have $S_k(G_i^i) = S_k(G_{i+1}^{i+1})$ for $0 \leq k \leq 2i+3$ and $S_{2i+4}(G_i^i) -$

$S_{2i+4}(G_{i+1}^{i+1}) = (2i + 4)(t - 3)$. Hence, if $t > 3$, we obtain that $S_{2i+4}(G_i^i) > S_{2i+4}(G_{i+1}^{i+1})$; if $t = 3$, then $S_{2i+4}(G_i^i) = S_{2i+4}(G_{i+1}^{i+1})$. Furthermore, if $t = 3$, $\mathscr{A}_{2i+5}(G_i^i) = \mathscr{A}_{2i+5}(G_{i+1}^{i+1}) = \emptyset$ and, for all $W \in \mathscr{A}'_{2i+5}(G_i^i)$, $W' \in \mathscr{A}'_{2i+5}(G_{i+1}^{i+1})$, we have $\phi_{G_i^i}(W) - \phi_{G_{i+1}^{i+1}}(W') = 1$. By Proposition 2.4, $S_{2i+5}(G_i^i) - S_{2i+5}(G_{i+1}^{i+1}) \geq 1 > 0$. Hence, we obtain

$$G_{i+1}^{i+1} \prec_s G_i^i, \quad 1 \leq i < \left\lfloor \frac{n-t}{3} \right\rfloor,$$

which implies that $G_{\lfloor(n-t)/3\rfloor}^{\lfloor(n-t)/3\rfloor} \preceq_s G_j^i$ for all $1 \leq j \leq n - t - 2i$, $j \leq i \leq \lfloor (n-t-1)/2 \rfloor$, as desired. $\square$

Claim 3.11.
$$G_{\lfloor(n-t-1)/3\rfloor+1}^{\lfloor(n-t-1)/3\rfloor} \prec_s G_{\lfloor(n-t)/3\rfloor}^{\lfloor(n-t)/3\rfloor}.$$

Proof of Claim 3.11. Note that

$$\left\lfloor \frac{n-t-1}{3} \right\rfloor = \left\lfloor \frac{n-t}{3} \right\rfloor$$

or

$$\left\lfloor \frac{n-t-1}{3} \right\rfloor = \left\lfloor \frac{n-t}{3} \right\rfloor - 1,$$

and, for the latter case, $\lfloor (n-t)/3 \rfloor = (n-t)/3$. Hence, if

$$\left\lfloor \frac{n-t-1}{3} \right\rfloor = \left\lfloor \frac{n-t}{3} \right\rfloor,$$

then let

$$i = j = \left\lfloor \frac{n-t-1}{3} \right\rfloor.$$

By Claim 3.7,
$$G_{\lfloor(n-t-1)/3\rfloor+1}^{\lfloor(n-t-1)/3\rfloor} \prec_s G_{\lfloor(n-t-1)/3\rfloor}^{\lfloor(n-t-1)/3\rfloor},$$

i.e.,
$$G_{\lfloor(n-t-1)/3\rfloor+1}^{\lfloor(n-t-1)/3\rfloor} \prec_s G_{\lfloor(n-t)/3\rfloor}^{\lfloor(n-t)/3\rfloor}.$$

If
$$\left\lfloor \frac{n-t-1}{3} \right\rfloor = \frac{n-t}{3} - 1,$$

by Lemma 2.5,
$$G_{n-t/3}^{(n-t/3)-1} \prec_s G_{n-t/3}^{n-t/3},$$

i.e.,
$$G_{\lfloor (n-t-1)/3 \rfloor+1}^{\lfloor (n-t-1)/3 \rfloor} \prec_s G_{\lfloor (n-t)/3 \rfloor}^{\lfloor (n-t)/3 \rfloor},$$

as desired.

By Fact 3.9, Claims 3.10 and 3.11, Theorem 3.5 holds.   □

4. Further results. In this section, we shall study the spectral moments of graphs with given chromatic number. This parameter has a close relationship with the clique number of graphs. Let $\mathscr{M}_{n,\chi}$ be the set of all n-vertex connected graphs with chromatic number χ. Note that $\mathscr{M}_{n,n} = \{K_n\}$; hence, we will only consider $2 \le \chi < n$.

We say that a graph G is *color critical* if $\chi(H) < \chi(G)$ for every proper subgraph H of G. Here, for simplicity, we abbreviate the term "color critical" to "critical." A *t-critical* graph is one that is t-chromatic and critical.

Lemma 4.1 ([9]). *Suppose the chromatic number $\chi(G) = t \ge 4$, and let G be a t-critical graph on more than t vertices (so $G \ne K_t$). Then*

$$|E_G| \ge \left(\frac{t-1}{2} + \frac{t-3}{2(t^2 - 2t - 1)} \right) |V_G|.$$

Lemma 4.2. *For any $G \in \mathscr{M}_{n,t}$ $(4 \le t < n)$,*

$$|E_G| \ge \frac{t(t-1)}{2} + n - t,$$

and the equality holds if and only if G is an n-vertex graph which is obtained from K_t by attaching some trees to K_t.

Proof. In order to determine the lower bound on the size of G in $\mathscr{M}_{n,t}$ $(4 \le t < n)$, it suffices to consider that G is obtained from a t-critical graph G' by attaching some trees to it. If $G' \cong K_t$, our result holds by direct computing; otherwise, consider the function

$$f(x) = \left(\frac{t-1}{2} + \frac{t-3}{2(t^2 - 2t - 1)} \right) x + n - x,$$

where t is a fixed positive integer with $4 \leq t < x$. It is easy to see that

$$f'(x) = \frac{t-1}{2} + \frac{t-3}{2(t^2 - 2t - 1)} - 1 = \frac{t(t-3)(t-2)}{2(t^2 - 2t - 1)} > 0$$

for $t \geq 4$. Hence, $f(x)$ is a strict increasing function in x, where $4 \leq t < x < n$. Together with Lemma 4.1, we have

$$\begin{aligned}
|E_G| &= |E_{G'}| + (n - |V_{G'}|) \\
&\geq \left(\frac{t-1}{2} + \frac{t-3}{2(t^2 - 2t - 1)} \right) |V_{G'}| + (n - |V_{G'}|) \\
&> \left(\frac{t-1}{2} + \frac{t-3}{2(t^2 - 2t - 1)} \right) t + (n - t) \\
&> \frac{t(t-1)}{2} + (n - t).
\end{aligned}$$

This completes the proof. $\qquad\qquad\square$

In order to determine the first few graphs in $\mathscr{M}_{n,2}$, by Lemma 2.2 these graphs must be n-vertex trees. Note that Pan, et al., [19] identified the first

$$\sum_{k=1}^{\lfloor (n-1)/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

graphs, in the S-order, of all trees with n vertices; these

$$\sum_{k=1}^{\lfloor (n-1)/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

trees are also the first

$$\sum_{k=1}^{\lfloor (n-1)/3 \rfloor} \left(\left\lfloor \frac{n-k-1}{2} \right\rfloor - k + 1 \right) + 1$$

graphs in the S-order among $\mathscr{M}_{n,2}$. We will not repeat them here.

For convenience, let $C_n^t := C_n u \cdot v P_{t+1}$, where $u \in V_{C_n}$ and v is an end-vertex of path P_{t+1}.

Theorem 4.3. *Among the set of graphs $\mathscr{M}_{n,3}$ with $n \geq 5$, the first two graphs in the S-order are C_n, C_{n-2}^2 if n is odd and C_{n-1}^1, C_{n-3}^3 otherwise.*

Proof. In order to determine the first two graphs in $\mathscr{M}_{n,3}$ with $n \geq 5$, based on Lemma 2.2 it suffices to consider the n-vertex connected graphs each of which contains a unique odd cycle. Denote the set of such graphs by $\mathscr{U}_n$.

Choose $G \in \mathscr{U}_n$ such that it is as small as possible according to the S-order. On the one hand, G contains a unique odd cycle, say C_t, that is to say, G is obtained by planting some trees to C_t if $t < n$. On the other hand, in view of Lemma 2.6, G is obtained from C_t by attaching a path P_{n-t+1} to it, i.e., $G \in \{C_t^{n-t} : t = 3, 5, \ldots\}$.

If n is odd, then it suffices for us to compare C_n with C_t^{n-t}, where $3 \leq t \leq n - 2$. In fact, $S_i(C_t^{n-t}) - S_i(C_n) = 0$ for $i = 0, 1, 2, 3$. By Lemma 2.3 (i), we have

$$S_4(C_t^{n-t}) - S_4(C_n) = 4(\phi_{C_t^{n-t}}(P_3) - \phi_{C_n}(P_3))$$
$$= 4(n + 1 - n) = 4 > 0.$$

Hence, $C_n \prec_s C_t^{n-t}$. Furthermore, for any C_t^{n-t} with $3 \leq t \leq n - 4$, it is routine to check that $S_i(C_t^{n-t}) = S_i(C_{n-2}^2) = 0$ for $i = 0, 1, 2, 3, 4$. By direct computing (based on Lemma 2.3), we have

$$S_5(C_t^{n-t}) - S_5(C_{n-2}^2) > 0 \quad \text{if } t = 3, \ n \geq 7;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-2}^2) > 0 \quad \text{if } t = 5, \ n \geq 9;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-2}^2) = 0 \quad \text{if } t \geq 7, \ n \geq 11;$$
$$S_6(C_t^{n-t}) - S_6(C_{n-2}^2) = 0 \quad \text{if } t \geq 7, \ n \geq 11;$$
$$S_7(C_t^{n-t}) - S_7(C_{n-2}^2) > 0 \quad \text{if } t = 7, \ n \geq 11;$$
$$S_7(C_t^{n-t}) - S_7(C_{n-2}^2) = 0 \quad \text{if } t \geq 9, \ n \geq 13;$$
$$S_8(C_t^{n-t}) - S_8(C_{n-2}^2) > 0 \quad \text{if } t \geq 9, \ n \geq 13.$$

This gives $C_{n-2}^2 \prec_s C_t^{n-t}$. Therefore, C_n, C_{n-2}^2 are the first two graphs in the S-order among $\mathscr{M}_{n,3}$ for odd n.

If n is even, it suffices to consider the graphs C_t^{n-t} with $3 \leq t \leq n-1$. In fact, for any C_t^{n-t} with $3 \leq t \leq n - 3$, $S_i(C_t^{n-t}) = S_i(C_{n-1}^1)$ for

$i = 0, 1, 2, 3, 4$. By Lemma 2.3, we have

$$S_5(C_t^{n-t}) - S_5(C_{n-1}^1) > 0 \quad \text{if } t = 3, \ n \geq 6;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-1}^1) > 0 \quad \text{if } t = 5, \ n \geq 8;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-1}^1) = 0 \quad \text{if } t \geq 7, \ n \geq 10;$$
$$S_6(C_t^{n-t}) - S_6(C_{n-1}^1) > 0 \quad \text{if } t \geq 7, \ n \geq 10.$$

Hence, we have $C_{n-1}^1 \prec_s C_t^{n-t}$ for $3 \leq t \leq n - 1$.

Next, we compare C_{n-3}^3 with C_t^{n-t}, where $3 \leq t \leq n - 5$. Obviously, $S_i(C_t^{n-t}) = S_i(C_{n-3}^3)$ for $i = 0, 1, 2, 3, 4$. By Lemma 2.3, we have

$$S_5(C_t^{n-t}) - S_5(C_{n-3}^3) > 0 \quad \text{if } t = 3, \ n \geq 8;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-3}^3) > 0 \quad \text{if } t = 5, \ n \geq 10;$$
$$S_5(C_t^{n-t}) - S_5(C_{n-3}^3) = 0 \quad \text{if } t \geq 7, \ n \geq 12;$$
$$S_6(C_t^{n-t}) - S_6(C_{n-3}^3) = 0 \quad \text{if } t \geq 7, \ n \geq 12;$$
$$S_7(C_t^{n-t}) - S_7(C_{n-3}^3) > 0 \quad \text{if } t = 7, \ n \geq 12;$$
$$S_7(C_t^{n-t}) - S_7(C_{n-3}^3) = 0 \quad \text{if } t \geq 9, \ n \geq 14;$$
$$S_8(C_t^{n-t}) - S_8(C_{n-3}^3) = 0 \quad \text{if } t \geq 9, \ n \geq 14.$$

Hence, in what follows we need compare $S_9(C_{n-3}^3)$ with $S_9(C_t^{n-t})$ for $t \geq 9, n \geq 14$. Note that, by Proposition 2.4, we have $\mathscr{A}_9'(C_t^{n-t}) = \{C_9\}$, $\mathscr{A}_9'(C_{n-3}^3) = \emptyset$, $\mathscr{A}_9(C_t^{n-t}) = \mathscr{A}_9(C_{n-3}^3) = \emptyset$ if $t = 9, \ n \geq 14$. Hence, $S_9(C_t^{n-t}) - S_9(C_{n-3}^3) = 18(\phi_{C_t^{n-t}}(C_9) - 0) = 18 > 0$ if $t = 9$, $n \geq 14$, i.e., $C_{n-3}^3 \prec_s C_t^{n-t}$ in this case.

If $t \geq 11$, $n \geq 16$, then $\mathscr{A}_9'(C_t^{n-t}) = \mathscr{A}_9'(C_{n-3}^3) = \emptyset$, $\mathscr{A}_9(C_t^{n-t}) = \mathscr{A}_9(C_{n-3}^3) = \emptyset$. Hence, $S_9(C_t^{n-t}) = S_9(C_{n-3}^3)$ for $t \geq 11$, $n \geq 16$. Note that $\mathscr{A}_{10}'(C_t^{n-t}) = \mathscr{A}_{10}'(C_{n-3}^3) = \emptyset$,

$$|\mathscr{A}_{10}(C_t^{n-t})| - |\mathscr{A}_{10}(C_{n-3}^3)| = \phi_{C_t^{n-t}}(P_6) - \phi_{C_{n-3}^3}(P_6) = n + 4 - (n + 3) = 1$$

for $t \geq 11$, $n \geq 16$, hence

$$S_{10}(C_t^{n-t}) - S_{10}(C_{n-3}^3) = 10(\phi_{C_t^{n-t}}(P_6) - \phi_{C_{n-3}^3}(P_6)) = 10 > 0,$$

which implies $C_{n-3}^3 \prec_s C_t^{n-t}$ for $3 \leq t \leq n - 5$.

This completes the proof.   □

Note that, for Turán graph $T_{n,t}$, $\chi(T_{n,t}) = t$ and its size attains the maximum among $\mathscr{M}_{n,t}$. Combining with Lemmas 2.2 and 4.2, we have

Theorem 4.4.

(i) *For any graph $G \in \mathscr{M}_{n,t} \setminus \{K_t^{n-t}\}$ with $4 \leq t < n$, one has $K_t^{n-t} \prec_s G$.*

(ii) *For any graph $G \in \mathscr{M}_{n,t} \setminus \{T_{n,t}\}$, where $2 \leq t < n$, one has $G \prec_s T_{n,t}$.*

By Theorem 4.3, the Turán graph $T_{n,t}$ is the last graph in the S-order among $\mathscr{M}_{n,t}$. In view of Lemma 2.2 and Theorem 3.3, the next result follows immediately.

Theorem 4.5. *Among the set of graphs $\mathscr{M}_{n,t}$ with $2 \leq t \leq n-1$,*

(i) *If $n = t+1$, then all graphs in the set $\mathscr{M}_{n,n-1}$ have the following S-order: $T_{n-3} \prec_s T_{n-4} \prec_s \cdots \prec_s T_i \prec_s \cdots \prec_s T_2 \prec_s T_1 \prec_s T_{n,n-1}$.*

(ii) *If $n = kt$ with $3 \leq t \leq n/2$, then for all $G \in \mathscr{M}_{n,t} \setminus \{T_{n,t},\ T_{n,t}^1\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}$.*

(iii) *If $n = kt+1$ with $3 \leq t \leq n/2$, then for all $G \in \mathscr{M}_{n,t} \setminus \{T_{n,t},\ T_{n,t}^1, T_{n,t}^2\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}^2 \prec_s T_{n,t}$.*

(iv) *If $n = kt+r$ with $3 \leq t \leq n/2$, $r = t-1$ or $(n+1)/2 \leq t \leq n-2$, then for all $G \in \mathscr{M}_{n,t} \setminus \{T_{n,t},\ T_{n,t}^2,\ T_{n,t}^3\}$ one has $G \prec_s T_{n,t}^2 \prec_s T_{n,t}^3 \prec_s T_{n,t}$.*

(v) *If $n = kt + r$ with $4 \leq t \leq n/2$, $2 \leq r \leq t-2$, then for all $G \in \mathscr{M}_{n,t} \setminus \{T_{n,t},\ T_{n,t}^1,\ T_{n,t}^2,\ T_{n,t}^3\}$ one has $G \prec_s T_{n,t}^1 \prec_s T_{n,t}^2 \prec_s T_{n,t}^3 \prec_s T_{n,t}$.*

By Theorems 3.4–3.5 and Lemma 4.2, we have

Theorem 4.6.

(i) *For $t = n - 2 \geq 4$, the first three graphs in the S-order in the set $\mathscr{M}_{n,n-2}$ are as follows: $J_1 \prec_s J_2 \prec_s J_3$.*

(ii) *For $t = n - 3 \geq 4$, the first seven graphs in the S-order among the set of graphs $\mathscr{M}_{n,n-3}$ are as follows: $J_4 \prec_s J_5 \prec_s J_6 \prec_s J_7 \prec_s J_8 \prec_s J_9 \prec_s J_{10}$.*

(iii) *For $4 \leq t \leq n-4$, the first $1 + \sum_{i=1}^{\lfloor (n-t-1)/3 \rfloor} (n-t-3i)$ graphs, in the S-order, among the set of graphs $\mathscr{M}_{n,t}$ are as follows*:

$$K_t^{n-t} \prec_s G_{n-t-2}^1 \prec_s G_{n-t-3}^1 \prec_s \cdots$$

$$\prec_s G_3^1 \prec_s G_2^1 \prec_s G_{n-t-4}^2 \prec_s G_{n-t-5}^2 \prec_s \cdots \prec_s G_3^2 \prec_s \cdots$$

$$\prec_s G_{n-t-2i}^i \prec_s G_{n-t-2i-1}^i \prec_s \cdots$$

$$\prec_s G_{i+1}^i \prec_s G_{n-t-2(i+1)}^{i+1} \prec_s \cdots \prec_s G_{\lfloor (n-t-1)/3 \rfloor + 1}^{\lfloor (n-t-1)/3 \rfloor}.$$

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