

Extremal graphs for the maximum A_α -spectral radius of graphs with order and size

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Abstract

In 1986, Brualdi and Solheid firstly proposed the problem of determining the maximum spectral radius of graphs in the set $\mathcal{H}_{n,m}$ consisting of all simple connected graphs with n vertices and m edges, which is a very tough problem and far from resolved. The A_α -spectral radius of a simple graph of order n , denoted by $\rho_\alpha(G)$, is the largest eigenvalue of the matrix $A_\alpha(G)$ which is defined as $\alpha D(G) + (1 - \alpha)A(G)$ for $0 \leq \alpha < 1$, where $D(G)$ and $A(G)$ are the degree diagonal and adjacency matrices of G , respectively. In this paper, if r is a positive integer, $n > 30r$ and $n - 1 \leq m \leq rn - \frac{r(r+1)}{2}$, we characterize all extremal graphs which have the maximum A_α -spectral radius of graphs in the set $\mathcal{H}_{n,m}$. Moreover, the problem on A_α -spectral radius proposed by Chang and Tam [T.-C. Chang and B.-T. Tam, Graphs of fixed order and size with maximal A_α -index. Linear Algebra Appl. 673 (2023), 69-100] has been solved.

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1 Introduction

In this paper, we only consider finite undirected graphs without multiple edges or loops. Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Denote by $|V(G)| = n$ and $|E(G)| = m$ the number of vertices and edges of G , respectively. Let $N_G(u)$ be the set of

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vertices which are adjacent to u in G , if there is no ambiguous, we denote by $N(u)$ for simplify. Moreover, denote by $d_i = d_G(v_i)$ the degree of vertex v_i for $i = 1, 2, \dots, n$. For two distinct vertices $u, v \in V(G)$, if u is adjacent to v then denote $u \sim v$, or for short uv ; if u is not adjacent to v then denote $u \not\sim v$. For $uv \notin E(G)$, let $G + uv$ be the graph which is obtained from G by adding the new edge uv . For $uv \in E(G)$, let $G - uv$ be the graph which is obtained from G by deleting the edge uv .

The adjacency matrix of a simple graph G is the $n \times n$ matrix $(a_{ij})_{n \times n}$, where $a_{ij} = 1$ if v_i is adjacent to v_j , and 0 otherwise. Moreover, the largest eigenvalue of $A(G)$ is usually called the spectral radius of G . For given two positive integers n and $m \geq n - 1$, let $\mathcal{H}_{n,m}$ be the set of all connected graphs of order n with size m , and let $\mathcal{G}_{n,m}$ be the set of all graphs of order n with size m . In 1986, Brualdi and Solheid [5] firstly proposed the following problem:

Problem 1.1. [5] *For given two positive integers n and $m \geq n - 1$, determine the maximum spectral radius of graphs in $\mathcal{H}_{n,m}$ and characterize all extremal graphs which attain the maximum value.*

Further, for $n \leq m \leq n + 5$, Brualdi and Solheid [5] characterized all graphs which have the maximum spectral radius in $\mathcal{H}_{n,m}$. Later, in 1988, for a given positive integer $r \geq 3$ and $m = n + r$, Cvetković and Rowlinson [12] proved that $S_{n,m}$ is the unique graph with maximum spectral radius in $\mathcal{H}_{n,m}$ for sufficiently large n (the definition of $S_{n,m}$ is given in Section 2). In 1991, for $m = n + \binom{r}{2} - 1$ with positive integer r , Bell [2] determined all graphs which have maximum spectral radius in $\mathcal{H}_{n,m}$. However, up to now, for given any two integers n and $m \geq n - 1$, Problem 1.1 is far from being completely resolved and seems to be very tough.

In 2017, Nikiforov [21] introduced the A_α -matrix of a simple graph G which is defined to be $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$, where $\alpha \in [0, 1)$. The largest eigenvalues of $A_\alpha(G)$ is denoted by $\rho_\alpha(G)$, which is called the A_α -spectral radius of G . If G is connected, there exists a unique positive eigenvector corresponding to $\rho_\alpha(G)$, which is called the Perron vector of A_α . Notice that $A_0(G) = A(G)$ and $A_{\frac{1}{2}}(G) = \frac{1}{2}Q(G)$, where $Q(G)$ is the signless Laplacian matrix of G . Hence Problem 1.1 may be generalized to the following problem.

Problem 1.2. *Determine all graphs which have the maximum A_α -spectral radius in $\mathcal{H}_{n,m}$.*

Nikiforov, Pastén, et al. [22] proved that the star graph S_n is the unique graph maximizing the A_α -spectral radius in $\mathcal{H}_{n,n-1}$. Recently, Li, Tam, et.al. in [19] have made significant progress on Problem 1.2.

Theorem 1.3. [19] *Let n and m be two positive integers with $n - 1 \leq m \leq 2n - 3$.*

- (1). *If $\alpha \in (\frac{1}{2}, 1)$ or $\alpha = \frac{1}{2}$ and $m \neq n + 2$, then $S_{n,m}$ is the unique graph that maximizes the A_α -spectral radius in $\mathcal{H}_{n,m}$.*
- (2). *If $\alpha = \frac{1}{2}$ and $m = n + 2$, then $S_{n,n+2}$ and $L_{n,n+2}$ are the two precisely connected graphs that maximize the $A_{\frac{1}{2}}$ -spectral radius in $\mathcal{H}_{n,n+2}$ (the definition of $L_{n,m}$ is given in Section 2).*

On the other hand, the problem of determining the maximal A_α -spectral radius in $\mathcal{G}_{n,m}$ has attracted much attention. When $\alpha = 0$ (respectively $\alpha = 1/2$), the maximal A_α -spectral radius problem becomes the well-known maximal spectral radius problem (respectively, the maximal Q -spectral radius problem). Whereas the maximal spectral radius problem over the class $\mathcal{G}_{n,m}$ has been studied by Brualdi and Hoffman [4], Friedland [15] and has been completely solved [24]. The maximal Q -spectral radius in $\mathcal{G}_{n,m}$ has also been investigated by Chang and Tam [8], Anđelić et. al. [1], etc. The maximal A_α -spectral radius problem over the class $\mathcal{G}_{n,m}$ has been treated by Chang and Tam [9], Chen and Huang [10], Li and Qin [17], etc. Recently, Li and Tam et al [19] proposed the following problem for $m = 2n - 2$.

Problem 1.4. [8] For given two positive integers $n \geq 4$ and $m = 2n - 2$, characterize graphs that maximize $A_{1/2}$ -spectral radius of graphs in $\mathcal{G}_{n,m}$.

Motivated by the above problems, we have investigated the A_α -spectral radius of a simple connected graph of order n with size m . The main results can be stated as follows.

Theorem 1.5. Let $n \geq 4$ and $m = 2n - 2$. If G' is any graph having the maximum $A_{1/2}$ -spectral radius of graphs in $\mathcal{G}_{n,m}$ which consists of all graphs of order n with size m , then $G' \cong K_5 \cup K_1$ for $n = 6$, and $G' \cong S_{n,2n-2}$ for $n \neq 6$.

Theorem 1.5 fully resolves the problem proposed by Chang and Tam [8].

Theorem 1.6. Let r, n and m be three positive integers satisfying $r \geq 3$, $n > \frac{30r-63+5\sqrt{32r^2-136r+137}}{2}$ and $n - 1 \leq m \leq rn - \frac{r(r+1)}{2}$.

- (1). If $\alpha \in (\frac{1}{2}, 1)$, or $\alpha = \frac{1}{2}$ and $m \neq (r-1)n - \frac{r(r-1)}{2} + 3$, then $S_{n,m}$ is the only extremal graph that maximizes the A_α -spectral radius in $\mathcal{H}_{n,m}$.
- (2). If $\alpha = \frac{1}{2}$ and $m = (r-1)n - \frac{r(r-1)}{2} + 3$, then $S_{n,m}$ and $\tilde{S}_{n,m}$ are the two extremal graphs that maximize the $A_{\frac{1}{2}}$ -spectral radius in $\mathcal{H}_{n,m}$ (the definition of $\tilde{S}_{n,m}$ is given in Section 2).

The rest of this paper is organized as follows. In Section 2, we introduce some definitions and some known results which are useful in this paper. In Section 3, several new graph transformations of A_α -spectral radius are proposed which will be interesting on their own. In Section 4, based on these transformations, the proofs of Theorems 1.5 and 1.6 are presented.

2 Preliminaries

In this section, we introduce some notations and some known results which will be used later. Let H_1 and H_2 be two disjoint graphs. Denote by $H_1 \cup H_2$ the sum of H_1 and H_2 , where $V(H_1 \cup H_2) = V(H_1) \cup V(H_2)$, $E(H_1 \cup H_2) = E(H_1) \cup E(H_2)$. Denote by $H_1 \vee H_2$ the product of H_1 and H_2 , obtained by adding all edges between H_1 and H_2 , i.e. $V(H_1 \vee H_2) = V(H_1) \cup V(H_2)$, the edges set of $H_1 \vee H_2$ consisting of $E(H_1) \cup E(H_2)$ and $\{uv\}$ for each $u \in V(H_1)$ and $v \in V(H_2)$. Moreover, denote by K_n the complete graph of order n , $K_{1,n-1}$ the star of order n , $\bar{K}_n$ (or nK_1) the graph consisting n isolated vertices. In particular, $K_{1,0}$ has only one isolated vertex.

For two positive integers n, m with $n - 1 \leq m$, let k be the largest integer such that $m \geq \sum_{i=1}^k (n - i)$ and $a = m - \sum_{i=1}^k (n - i)$. The graph $S_{n,m}$ of order n with size m is defined to be

$$S_{n,m} = K_k \vee \left(K_{1,a} \cup (n - a - k - 1)K_1 \right),$$

which is called quasi-star graph. Clearly, if $m = n - 1$, then $S_{n,m}$ is the star $K_{1,n-1}$; if $m = n(n-1)/2$, then $S_{n,m}$ is the complete graph K_n . In addition, if $m = kn - \frac{k(k+1)}{2} + 3$, then $a = 3$ and the graph $\tilde{S}_{n,m}$ of order n with size m is defined to be

$$\tilde{S}_{n,m} = K_k \vee \left(K_3 \cup (n - k - 3)K_1 \right).$$

On the other hand, let $\bar{k}$ be the largest integer such that $m - n + 1 \geq \sum_{i=1}^{\bar{k}-1} i$ and $\bar{a} = m - n + 1 - \sum_{i=1}^{\bar{k}-1} i$. The graph $L_{n,m}$ of order n with size m is defined to be

$$L_{n,m} = \begin{cases} (K_{\bar{k}} \cup (n - \bar{k} - 1)K_1) \vee K_1, & \text{for } \bar{a} = 0; \\ (K_{\bar{a}} \vee (K_{\bar{k}-\bar{a}} \cup K_1) \cup (n - \bar{k} - 2)K_1) \vee K_1, & \text{for } \bar{a} > 0. \end{cases}$$

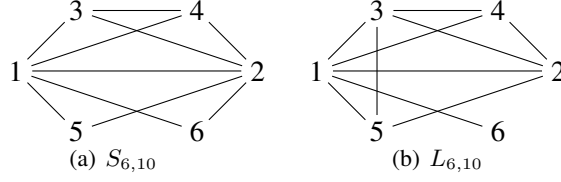


Figure 1: $S_{n,m}$ and $L_{n,m}$ with $n = 6$, $m = 10$

For example, if $n = 6$ and $m = 10$, then $S_{6,10}$ and $L_{6,10}$ are depicted in Figure 1, where $k = 2$, $a = 1$; $\bar{k} = 3$, $\bar{a} = 2$.

A simple graph $G = (V, E)$ is called a threshold graph if G has no induced subgraph of the forms $2K_2$, C_4 , P_4 . Clearly, $S_{n,m}$ and $L_{n,m}$ are threshold graphs. Threshold graphs have a beautiful structure and possess many important mathematical properties such as being the extreme cases of certain graph properties (see [23]). For more information on threshold graphs, the reader may refer to the monograph [20]. We state the following characterizations of threshold graphs which are useful in this paper.

Lemma 2.1. [23] *Let $G = (V, E)$ be a simple graph with degree sequence $(d_1, d_2, \dots, d_n)$. The following statements are equivalent:*

- (1). G is a threshold graph.
- (2). G can be constructed from the one-vertex graph by repeatedly adding an isolated vertex or a universal (or dominating) vertex (a vertex adjacent to every other vertex).
- (3). Every three distinct vertices i, j, k of G satisfy: if $d_i \geq d_j$ and jk is an edge, then ik is an edge.

Lemma 2.2. [16] *Any threshold graph is uniquely determined by its degree sequence.*

Let $D = (d_1, d_2, \dots, d_n)$ be a non-increasing positive integral sequence. The Ferrers matrix (or Ferrers diagram; see e.g. [20, p62]) of D is an $n \times n$ matrix F of $\circ$'s, $\bullet$'s and, $+$'s such that (i). All the diagonal entries and no others are $+$; (ii). For each i , $i \in [n]$, the number of $\bullet$'s contained in the i th row is d_i ; (iii). The signals $\bullet$'s in each row are to the left. Moreover, the Ferrers matrix $F(G)$ of a graph G is defined to be the Ferrers matrix of the degree sequence $D(G)$ of G . If G is a threshold graph, it is easy to see that the adjacency matrix of G is obtained from the Ferrers matrix of G by replacing symbols $\circ$ and $+$ with 0, and replacing the symbol $\bullet$ with 1. So the Ferrers matrix of a threshold graph is symmetric. For example, the Ferrers matrix of a threshold graph $S_{6,9}$ is symmetric (see Figure 2), the Ferrers matrix of a non-threshold graph $G_{6,9}$ (see Figure 3) is asymmetric. Brualdi and Hoffman in [4] defined a class of matrices in studying the spectral radius of graphs of order n with size m .



Figure 2: The Ferrers matrix of a threshold graph is symmetric



Figure 3: The Ferrers matrix of a non-threshold graph $G_{6,9}$ is asymmetrical

Definition 2.3. [4] Let $A = (a_{ij})_{n \times n}$ be a $(0, 1)$ matrix, and $\text{tr}(A) = 0$. A is said to be stepwise if it has the following property:

If $h > k$ and $a_{hk} = 1$, then $a_{ij} = 1$ for all $j < i \leq h$ and $j \leq k$.

It is easy to see that the following lemma holds.

Lemma 2.4. A connected graph G is threshold graph if and only if there exists a permutation matrix P such that $P^T A(G) P$ is a stepwise matrix.

Hence in the sequel, for a threshold graph G , we always assume that the adjacency matrix of G is a stepwise matrix with degree sequence $d_1 \geq d_2 \geq \dots \geq d_n$. The following Lemma presents some structure properties of graphs having maximum A_α -spectral radius in $\mathcal{H}_{n,m}$.

Lemma 2.5. [19] For given two positive integers n and $m \geq n - 1$, and $0 \leq \alpha < 1$, if a connected graph G maximizes the A_α -spectral radius in $\mathcal{H}_{n,m}$, then G must be a threshold graph.

Lemma 2.6. [19, 25] Let u, v be distinct vertices of a connected graph G and $x = (x_w)_{w \in V(G)}^T$ be the Perron vector of $A_\alpha(G)$ with $\alpha \in [0, 1)$.

- (i). If $N(u) \setminus \{v\} \supset N(v) \setminus \{u\}$, then $x_u > x_v$.
- (ii). If $N(u) \setminus \{v\} = N(v) \setminus \{u\}$, then $x_u = x_v$.

It follows from Lemma 2.6 that we have the following corollary.

Corollary 2.7. Let G be a connected threshold graph with non-increasing degree sequence $(d_1, d_2, \dots, d_n)$ and $(y_1, y_2, \dots, y_n)^T$ be the Perron vector of $A_\alpha(G)$, then

- (i). $y_1 \geq y_2 \geq \dots \geq y_n$.
- (ii). If $d_i = d_j$, then $y_i = y_j$ for $1 \leq i, j \leq n$.

Let M be a real symmetric $n \times n$ matrix, and let $V = \{1, 2, \dots, n\} = [n]$. Given a partition $\Pi : V = V_1 \cup V_2 \dots \cup V_k$, the matrix M can be correspondingly partitioned as

$$\begin{pmatrix} M_{1,1} & M_{1,2} & \cdots & M_{1,k} \\ M_{2,1} & M_{2,2} & \cdots & M_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ M_{k,1} & M_{k,2} & \cdots & M_{k,k} \end{pmatrix}$$

The quotient matrix of M with respect to Π is defined as the $k \times k$ matrix $M_\Pi = (b_{i,j})_{i,j=1}^k$ where $b_{i,j}$ is the average value of all row sums of $M_{i,j}$. The partition Π is called equitable if each block $M_{i,j}$ of M has constant row sum $b_{i,j}$. We also say that the quotient matrix M_Π is equitable if Π is an equitable partition of M . The relationship between eigenvalues of M and M_Π may be stated as follows.

Lemma 2.8. [3] Let M be a real symmetric matrix and $\lambda(M)$ be its largest eigenvalue. If M_Π be an equitable quotient matrix of M , then the eigenvalues of M_Π are also eigenvalues of M . Furthermore, if M is nonnegative and irreducible, then $\lambda(M) = \lambda(M_\Pi)$.

In order to obtain our results, we also present some properties of the signless Laplacian spectral radius $q(G)$ of the signless Laplacian matrix $Q(G) = D(G) + A(G)$ of a simple graph G .

Lemma 2.9. [13, 14] If $G \in \mathcal{H}_{n,m}$, then

$$q(G) = \max_{v \in V(G)} \{d_v + \frac{1}{d_v} \sum_{w \in N(v)} d_w\} \leq \frac{2m}{n-1} + n - 2.$$

Moreover, $q(G) = \frac{2m}{n-1} + n - 2$ if and only if G is isomorphic to either S_n or K_n .

Lemma 2.10. If $n \geq 4$, then $q(S_{n,2n-2}) \geq n + 1.6$ and $q(S_{n,2n-1}) \geq n + 1.75$.

Proof. Let $\Pi = \{\{v_1, v_2\}, \{v_3, v_4\}, \{v_5, \dots, v_n\}\}$. Then $Q(S_{n,2n-2})_\Pi$ is an equitable quotient matrix of $Q(S_{n,2n-2})$. Hence

$$Q(S_{n,2n-2})_\Pi = \begin{pmatrix} n & 2 & n-4 \\ 2 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix}$$

Let $f(x) = \det(xI_3 - Q(S_{n,2n-2})_\Pi) = x^3 + (-n-6)x^2 + (4n+12)x - 24$. It is easy to see that the largest eigenvalue of $Q(S_{n,2n-2})_\Pi$ is greater than $n+1.6$. By Lemma 2.8, $q(S_{n,2n-2}) \geq n+1.6$.

Let $\Pi = \{\{v_1, v_2\}, \{v_3\}, \{v_4, v_5\}, \{v_6, \dots, v_n\}\}$. Then $Q(S_{n,2n-1})_\Pi$ is an equitable quotient matrix of $Q(S_{n,2n-1})$. Hence

$$Q(S_{n,2n-1})_\Pi = \begin{pmatrix} n & 1 & 2 & n-5 \\ 2 & 4 & 2 & 0 \\ 2 & 1 & 3 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix}$$

Let $g(x) = \det(xI_4 - Q(S_{n,2n-1})_\Pi) = x^4 + (-n-9)x^3 + (7n+28)x^2 + (-10n-64)x + 72$. It is easy to see that $q(S_{n,2n-1}) \geq n + 1.75$ by Lemma 2.8. $\blacksquare$

3 Transformations

In this section, we introduce several transformations and their properties, which will play a key role in the proof of the main results. Denote by $E_{pq} = (e_{ij})_{n \times n}$ the $(0, 1)$ -matrix with $e_{pq} = e_{qp} = 1$, and 0 in the other positions.

Definition 3.1. Let $A(G) = (a_{ij})_{n \times n}$ be the stepwise adjacency matrix of a connected threshold graph G . We say the graph G' is obtained from G by a Transformation $(p, q; h, k)$, if there exist four positive integers p, q, h, k such that the following conditions hold:

- (i). $2 \leq q < k < h < p$.
- (ii). $a_{pq} = 0, a_{pj} = 1$ whenever $j < q$; $a_{iq} = 1$ whenever $q < i < p$.
- (iii). $a_{hk} = 1, a_{hj} = 0$ whenever $j > k$; $a_{ik} = 0$ whenever $i > h$.
- (iv). $G' = G - v_h v_k + v_p v_q$.

Clearly, G' is also a connected threshold graph and $A(G') = A(G) - E_{hk} + E_{pq}$.

Lemma 3.2. Let $A(G) = (a_{ij})_{n \times n}$ be the stepwise adjacency matrix of a connected threshold graph G and the graph G' be obtained from G by a Transformation $(p, q; h, k)$. If $x = (x_1, x_2, \dots, x_n)^T$ and $y = (y_1, y_2, \dots, y_n)^T$ are the Perron vectors corresponding to $\rho_1 = \rho_\alpha(G)$ and $\rho_2 = \rho_\alpha(G')$, respectively, then

$$(\rho_1 - k\alpha)(x_h - x_p) = (k - q + 1)\alpha x_p + (1 - \alpha)(x_q + \dots + x_k), \quad (1)$$

$$(\rho_2 - p\alpha + 1)(y_q - y_k) = (p - h + 1)\alpha y_k + (1 - \alpha)(y_h + \dots + y_p). \quad (2)$$

Proof. By the h -th and p -th equations of $\rho_\alpha(G)x = A_\alpha(G)x$, we have

$$\rho_1 x_h = k\alpha x_h + (1 - \alpha)(x_1 + x_2 + x_3 + \dots + x_k), \quad (3a)$$

$$\rho_1 x_p = (q - 1)\alpha x_p + (1 - \alpha)(x_1 + x_2 + x_3 + \dots + x_{q-1}). \quad (3b)$$

By subtracting (3b) from (3a),

$$\rho_1(x_h - x_p) = k\alpha x_h - (q - 1)\alpha x_p + (1 - \alpha)(x_q + \dots + x_k), \quad (4)$$

which implies

$$(\rho_1 - k\alpha)(x_h - x_p) = (k - q + 1)\alpha x_p + (1 - \alpha)(x_q + \dots + x_k),$$

i.e. (1) holds.

By the q -th and k -th equations of $\rho_\alpha(G')y = A_\alpha(G')y$, we have

$$\rho_2 y_q = p\alpha y_q - y_q + (1 - \alpha)(y_1 + y_2 + y_3 + \dots + y_p), \quad (5a)$$

$$\rho_2 y_k = (h - 1)\alpha y_k - y_k + (1 - \alpha)(y_1 + y_2 + y_3 + \dots + y_{h-1}). \quad (5b)$$

By subtracting (5b) from (5a),

$$\rho_2(y_q - y_k) = p\alpha y_q - (h - 1)\alpha y_k - (y_q - y_k) + (1 - \alpha)(y_h + \dots + y_p), \quad (6)$$

which implies

$$(\rho_2 - p\alpha + 1)(y_q - y_k) = (p - h + 1)\alpha y_k + (1 - \alpha)(y_h + \dots + y_p),$$

i.e. (2) holds. ■

Lemma 3.3. Let G' be a connected threshold graph obtained from a connected threshold graph G with degree sequence $(d_G(v_1), d_G(v_2), \dots, d_G(v_n))$ by a Transformation $(p, q; h, k)$ with $k = q + 1$. If $\alpha \in [1/2, 1)$, then $\rho_\alpha(G') \geq \rho_\alpha(G)$, with equality if and only if $\alpha = 1/2$ and $p = h + 1 = q + 3$.

Proof. Denote $t = p + q - h - k = p - h - 1 \geq 0$, $\rho_1 = \rho_\alpha(G)$, $\rho_2 = \rho_\alpha(G')$. Let $x = (x_1, x_2, \dots, x_n)^T$ and $y = (y_1, y_2, \dots, y_n)^T$ be the Perron vectors of G and G' , respectively. By Corollary 2.7, we have $x_1 \geq x_2 \geq \dots \geq x_n > 0$ and $y_1 \geq y_2 \geq \dots \geq y_n > 0$. By $k = q + 1$, we have $d_{G'}(v_h) = d_{G'}(v_{h+1}) = \dots = d_{G'}(v_p)$. Furthermore, by $d_{G'}(v_h) = d_{G'}(v_{h+1}) = \dots = d_{G'}(v_p)$ and (ii) in Corollary 2.7,

$$y_h = y_{h+1} = \dots = y_p. \quad (7)$$

By the definition of Transformation $(p, q; h, k)$, $2 \leq q < k < h < p$, which implies that $y_k \geq y_h$. Hence by $\alpha \in [1/2, 1)$, we have

$$\alpha y_k + (1 - \alpha)y_h \geq \alpha y_h + (1 - \alpha)y_k, \quad (8)$$

with equality if and only if $\alpha = \frac{1}{2}$ or $h = k + 1$. Similarly by $x_q \geq x_p$, we have

$$\alpha x_q + (1 - \alpha)x_p \geq \alpha x_p + (1 - \alpha)x_q, \quad (9)$$

with equality if and only if $\alpha = \frac{1}{2}$. On the one hand, by (2) in Lemma 3.2 and $y_h = y_{h+1} = \dots = y_p$,

$$(\rho_2 - p\alpha + 1)(y_q - y_k) = (p - h + 1)\alpha y_k + (1 - \alpha)(y_h + \dots + y_p) = (p - h + 1)(\alpha y_k + (1 - \alpha)y_h). \quad (10)$$

On the other hand, by (1) in Lemma 3.2 and $x_q \geq x_{q+1} \geq \dots \geq x_k$,

$$(\rho_1 - k\alpha)(x_h - x_p) = (k - q + 1)\alpha x_p + (1 - \alpha)(x_q + \dots + x_k) \leq (k - q + 1)(\alpha x_p + (1 - \alpha)x_q). \quad (11)$$

In addition,

$$x^T A_\alpha(G)y = \alpha \sum_{v_i v_j \in E(G)} (x_i y_i + x_j y_j) + (1 - \alpha) \sum_{v_i v_j \in E(G)} (x_i y_j + x_j y_i). \quad (12)$$

Hence, by $x_q \geq x_k$ and by (7)-(12),

$$\begin{aligned} & x^T(\rho_2 - \rho_1)y \\ &= x^T(A_\alpha(G') - A_\alpha(G))y \\ &= \alpha(x_p y_p + x_q y_q - x_h y_h - x_k y_k) + (1 - \alpha)(x_p y_q + x_q y_p - x_h y_k - x_k y_h) \\ &= (x_q - x_k)(\alpha y_k + (1 - \alpha)y_h) + (y_q - y_k)(\alpha x_q + (1 - \alpha)x_p) \\ &\quad + (y_p - y_h)(\alpha x_p + (1 - \alpha)x_q) + (x_p - x_h)(\alpha y_h + (1 - \alpha)y_k) \\ &\geq (y_q - y_k)(\alpha x_q + (1 - \alpha)x_p) + (x_p - x_h)(\alpha y_h + (1 - \alpha)y_k) \\ &\geq (\alpha x_q + (1 - \alpha)x_p)(\alpha y_k + (1 - \alpha)y_h) \frac{p-h+1}{\rho_2-p\alpha+1} \\ &\quad - (\alpha y_h + (1 - \alpha)y_k)(\alpha x_p + (1 - \alpha)x_q) \frac{k-q+1}{\rho_1-k\alpha} \\ &\geq (\alpha x_q + (1 - \alpha)x_p)(\alpha y_k + (1 - \alpha)y_h) \left[\frac{p-h+1}{\rho_2-p\alpha+1} - \frac{k-q+1}{\rho_1-k\alpha} \right] \\ &= (\alpha x_q + (1 - \alpha)x_p)(\alpha y_k + (1 - \alpha)y_h) \frac{(p-h+1)(\rho_1-k\alpha) - (k-q+1)(\rho_2-p\alpha+1)}{(\rho_2-p\alpha+1)(\rho_1-k\alpha)} \\ &= (\alpha x_q + (1 - \alpha)x_p)(\alpha y_k + (1 - \alpha)y_h) \frac{(k-q+1)(\rho_1-\rho_2) + (k-q+1)(p\alpha-1-k\alpha) + t(\rho_1-k\alpha)}{(\rho_2-p\alpha+1)(\rho_1-k\alpha)}. \end{aligned} \quad (13)$$

Hence, (13) yields

$$\begin{aligned} & (\rho_2 - \rho_1)(x^T y \frac{(\rho_2-p\alpha+1)(\rho_1-k\alpha)}{(\alpha x_q + (1-\alpha)x_p)(\alpha y_k + (1-\alpha)y_h)} + k - q + 1) \\ &\geq (k - q + 1)(p\alpha - 1 - k\alpha) + t(\rho_1 - k\alpha) \\ &\geq 0. \end{aligned} \quad (14)$$

It follows that $\rho_2 \geq \rho_1$.

Moreover, $\rho_2 = \rho_1$ holds if and only if $x_q = x_k$, $t = 0$, $p\alpha - 1 - k\alpha = 0$ and $\alpha = \frac{1}{2}$, therefore, $p = k + 2 = h + 1 = q + 3$ and $\alpha = \frac{1}{2}$. $\blacksquare$

Lemma 3.4. Let G' be the graph obtained from a connected threshold graph G by a Transformation $(p, q; h, k)$ with $k = q + 2$. If $\alpha \in [1/2, 1)$ and $p > h + 1$, then $\rho_\alpha(G') > \rho_\alpha(G)$.

Proof. Let $d_G(v_1) \geq d_G(v_2) \geq \dots \geq d_G(v_n)$ be the degree sequence of a connected threshold graph G . Clearly $p > d_G(v_{q+1}) + 1 \geq h$. Denote by $p_1 = d_G(v_{q+1}) + 1$. We consider the following two cases:

Case 1: $d_G(v_{q+1}) < p - 2$.

Clearly $d_G(v_{q+1}) \geq h - 1$ and $p \geq d_G(v_{q+1}) + 3$. Let G_1 be the graph obtained from G by a Transformation $(p_1 + 1, q + 1; h, q + 2)$. Hence, G' can be obtained from G_1 by a Transformation $(p, q; p_1 + 1, q + 1)$. By Lemma 3.3, $\rho_\alpha(G') \geq \rho_\alpha(G_1)$ and $\rho_\alpha(G_1) \geq \rho_\alpha(G)$. Furthermore, by

Lemma 3.3, $\rho_\alpha(G') = \rho_\alpha(G)$ implies $p_1 + 1 = q + 4$ and $p_1 + 1 = q + 2$, which is a contradiction. Therefore, $\rho_\alpha(G') > \rho_\alpha(G)$.

Case 2: $d_G(v_{q+1}) = p - 2$.

Clearly $d_G(v_q) = p - 2$, $d_G(v_{q+1}) = p - 2$ and $p \geq h + 2$. Let G_1 be the graph from G by a Transformation $(p, q; p - 1, q + 1)$. Hence, G_1 is a connected threshold graph in $\mathcal{H}_{n,m}$. By Lemma 3.3, $\rho_\alpha(G_1) \geq \rho_\alpha(G)$. Then it is easy to see that G' is the graph also obtained from G_1 by a Transformation $(p - 1, q + 1; h, q + 2)$. Hence by Lemma 3.3, $\rho_\alpha(G') \geq \rho_\alpha(G_1) \geq \rho_\alpha(G)$. Furthermore, by Lemma 3.3, $\rho_\alpha(G') = \rho_\alpha(G)$ implies $p = q + 3$ and $p - 1 = q + 4$, which is a contradiction. Therefore, $\rho_\alpha(G') > \rho_\alpha(G)$. ■

In order to prove the main results, we also introduce the other two general transformations:

Definition 3.5. Let $A(G) = (a_{ij})_{n \times n}$ be the stepwise adjacency matrix of a connected threshold graph G . We say the graph G' is obtained from G by a Transformation $(p, q; h, k; l + 1, 1)$, if there exist four positive integers p, q, h, k and one nonnegative integer l such that the following conditions holds:

- (i). $q < k \leq k + l < h < p - l$.
- (ii). $a_{iq} = 0$, $a_{ij} = 1$ whenever for all integers $p - 1 \leq i \leq p$, $j < q$; $a_{iq} = 1$ whenever $i < p - l$.
- (iii). $a_{hi} = 1$, $a_{hj} = 0$, $a_{h+1,i} = 0$ whenever for all integers $k \leq i \leq k + l$, $j > k + l$.
- (iv).

$$G' = G - \sum_{j=0}^l v_h v_{k+j} + \sum_{j=0}^l v_{p-j} v_q.$$

Clearly, G' is also a connected threshold graph and

$$A(G') = A(G) - \sum_{j=0}^l E_{h,k+j} + \sum_{j=0}^l E_{p-j,q}.$$

Remark 1. If $l = 0$, then the Transformation $(p, q; h, k; l + 1, 1)$ is actually the Transformation $(p, q; h, k)$.

Remark 2. Let G be a connected threshold graph with the non-increasing degree sequence $(d_1, \dots, d_n)$. If G' is obtained from G by a Transformation $(p, q; h, k; l + 1, 1)$, then the non-increasing degree sequence $d' = (d'_1, \dots, d'_n)$ of G' is the same as the degree sequence of G except $d'_q = p - 1$, $d'_h = k - 1$, $d'_k = \dots = d'_{k+l} = h - 2$ and $d'_p = \dots = d'_{p-l} = q$.

For example, there is a concrete transformation from $L_{7,12}$ to $S_{7,12}$ with respect to $(7, 2; 5, 3; 2, 1)$ which is depicted in Figure 4.

Lemma 3.6. Let G' be the graph obtained from a connected threshold graph G by a Transformation $(p, q; h, k; l + 1, 1)$. If $\alpha \in [1/2, 1)$ and $k = q + 1$, then $\rho_\alpha(G') \geq \rho_\alpha(G)$, with equality if and only if $\alpha = 1/2$, $l = 0$ and $p = h + 1 = q + 3$.

Proof. Let $\rho_1 = \rho_\alpha(G)$ and $\rho_2 = \rho_\alpha(G')$. By Definition 3.5 and $k = q + 1$, we have $d_{G'}(v_h) = d_{G'}(v_p)$. By Corollary 2.7, we have $x_1 \geq x_2 \geq \dots \geq x_n > 0$ and $y_1 \geq y_2 \geq \dots \geq y_n > 0$. By $d_G(v_k) = d_G(v_{k+1}) = \dots = d_G(v_{k+l})$, we have $x_k = x_{k+1} = \dots = x_{k+l}$. By $d_G(v_{p-l}) = d_G(v_{p-l+1}) = \dots = d_G(v_p)$, we have $x_p = x_{p-1} = \dots = x_{p-l}$. Moreover, $d_{G'}(v_k) = d_{G'}(v_{k+1}) = \dots = d_{G'}(v_{k+l})$ implies that $y_k = y_{k+1} = \dots = y_{k+l}$. $d_{G'}(v_p) = d_{G'}(v_{p-1}) = \dots = d_{G'}(v_h)$ implies that $y_p = y_{p-1} = \dots = y_h$.

		1	2	3	4	5	6	7		1	2	3	4	5	6	7
			q	k							q	k				
1		+	•	•	•	•	•	•		+	•	•	•	•	•	•
2		•	+	•	•	•	○	○		•	+	•	•	•	•	•
3		•	•	+	•	•	○	○		•	•	+	•	○	○	○
4		•	•	•	+	•	○	○		•	•	•	+	○	○	○
5	h	•	•			+	○	○		•	•			+	○	○
6	p-1	•		○	○	○	+	○		•		○	○	○	+	○
7	p	•		○	○	○	○	+		•		○	○	○	○	+

Figure 4: Transformation $(7, 2; 5, 3; 2, 1)$ from $L_{7,12}$ to $S_{7,12}$

Hence, by (12),

$$\begin{aligned}
& x^T(\rho_2 - \rho_1)y \\
&= x^T(A_\alpha(G') - A_\alpha(G))y \\
&= \sum_{j=0}^l [\alpha(x_{p-j}y_{p-j} + x_qy_q - x_hy_h - x_{k+j}y_{k+j}) \\
&\quad + (1-\alpha)(x_{p-j}y_q + x_qy_{p-j} - x_hy_{k+j} - x_{k+j}y_h)] \\
&= (l+1)[\alpha(x_py_p + x_qy_q - x_hy_h - x_ky_k) + (1-\alpha)(x_py_q + x_qy_p - x_hy_k - x_ky_h)] \\
&= (l+1)[(x_q - x_k)(\alpha y_k + (1-\alpha)y_h) + (y_q - y_k)(\alpha x_q + (1-\alpha)x_p) \\
&\quad + (y_p - y_h)(\alpha x_p + (1-\alpha)x_q) + (x_p - x_h)(\alpha y_h + (1-\alpha)y_k)] \\
&\geq (l+1)[(y_q - y_k)(\alpha x_q + (1-\alpha)x_p) + (x_p - x_h)(\alpha y_h + (1-\alpha)y_k)] \\
&\geq (l+1)[\frac{p-h+1}{\rho_2-\alpha p+1}(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p) \\
&\quad - \frac{k+l-q+1}{\rho_1-\alpha(k+l)}(\alpha x_p + (1-\alpha)x_q)(\alpha y_h + (1-\alpha)y_k)] \\
&\geq (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)(\frac{p-h+1}{\rho_2-\alpha p+1} - \frac{k+l-q+1}{\rho_1-\alpha(k+l)}) \\
&= (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p) \frac{(p-h+1)(\rho_1-\alpha(k+l)) - (k+l-q+1)(\rho_2-\alpha p+1)}{(\rho_2-\alpha p+1)(\rho_1-\alpha(k+l))} \\
&= (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p) \\
&\quad \times \frac{(k+l-q+1)(\rho_1-\rho_2) + (k+l-q+1)(\alpha(p-k-l)-1) + (p+q-h-k-l)(\rho_1-\alpha(k+l))}{(\rho_2-\alpha p+1)(\rho_1-\alpha(k+l))}.
\end{aligned} \tag{15}$$

Hence by (15), we have

$$\begin{aligned}
& (\rho_2 - \rho_1)[x^T y \frac{(\rho_2 - \alpha p + 1)(\rho_1 - \alpha(k+l))}{(l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)} + k + l - q + 1] \\
&\geq (k + l - q + 1)(\alpha(p - k - l) - 1) + (p + q - h - k - l)(\rho_1 - \alpha(k+l)) \\
&\geq 0,
\end{aligned}$$

which implies $\rho_2 \geq \rho_1$.

Further, $\rho_2 = \rho_1$ holds if and only if $x_q = x_k$, $p + q - h - k - l = 0$, $\alpha(p - k - l) - 1 = 0$ and $\alpha = \frac{1}{2}$, therefore, $l = 0$, $p = k + 2 = h + 1 = q + 3$ and $\alpha = \frac{1}{2}$. $\blacksquare$

We also need the following transformation.

Definition 3.7. Let $A(G) = (a_{ij})_{n \times n}$ be the stepwise adjacency matrix of a connected threshold graph G . We say the graph G' is obtained from G by a Transformation $(p, q; h, k; 1, l + 1)$, if there exist four positive integers p, q, h, k and one nonnegative integer l such that the following conditions holds:

- (i). $2 \leq q - l \leq q < k < h - l \leq h < p$.

- (ii). $a_{ps} = 0$, $a_{pj} = 1$ whenever $j < q - l$ and $a_{is} = 1$ whenever $s < i < p$, for all integers $q - l \leq s \leq q$.
 (iii). $a_{sk} = 1$, $a_{sj} = 0$ whenever $j > k$ and $a_{ik} = 0$ whenever $i > h$, for all integers $h - l \leq s \leq h$.
 (iv).

$$G' = G - \sum_{j=0}^l v_{h-j}v_k + \sum_{j=0}^l v_p v_{q-j}.$$

Clearly, G' is also a connected threshold graph and

$$A(G') = A(G) - \sum_{j=0}^l E_{h-j,k} + \sum_{j=0}^l E_{p,q-j}.$$

For example, $S_{9,23}$ is the graph obtained from $G_{9,23}$ by a Transformation $(9, 3; 8, 4; 1, 2)$, which is depicted in Figure 5.

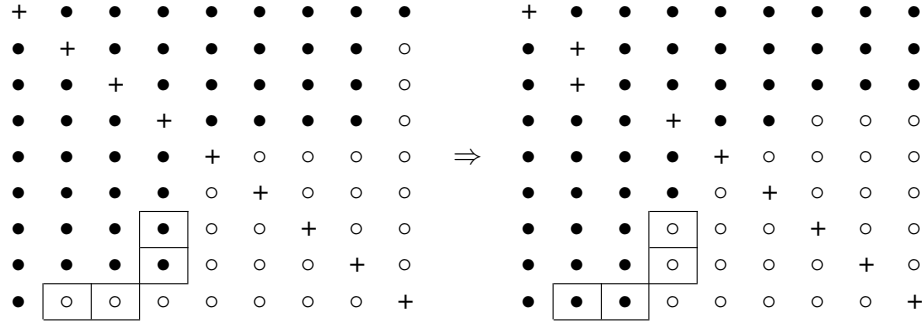


Figure 5: Transformation $(9, 3; 8, 4; 1, 2)$ from $G_{9,23}$ to $S_{9,23}$

Lemma 3.8. *Let G' be obtained by a Transformation $(p, q; h, k; 1, l+1)$ from a connected threshold graph G . If $\alpha \in [1/2, 1)$ and $k = q + 1$, then $\rho_\alpha(G') \geq \rho_\alpha(G)$, with equality if and only if $\alpha = 1/2$, $l = 0$, and $p = h + 1 = q + 3$.*

Proof. Let $\rho_1 = \rho_\alpha(G)$, $\rho_2 = \rho_\alpha(G')$. By Definition 3.7 and $k = q + 1$, $d_{G'}(v_h) = d_{G'}(v_p)$. By Corollary 2.7, $x_1 \geq x_2 \geq \dots \geq x_n > 0$ and $y_1 \geq y_2 \geq \dots \geq y_n > 0$. By $d_G(v_{q-l}) = d_G(v_{q-l+1}) = \dots = d_G(v_q)$, $x_q = x_{q-1} = \dots = x_{q-l}$. By $d_G(v_{h-l}) = d_G(v_{h-l+1}) = \dots = d_G(v_h)$, $x_h = x_{h-1} = \dots = x_{h-l}$. Moreover, $d_{G'}(v_{q-l}) = d_{G'}(v_{q-l+1}) = \dots = d_{G'}(v_q)$ implies that $y_{q-l} = y_{q-l+1} = \dots = y_q$. $d_{G'}(v_p) = d_{G'}(v_{p-1}) = \dots = d_{G'}(v_{h-l})$ implies that

$y_p = y_{p-1} = \dots = y_{h-l}$. By (12) and similar to Lemma 3.3, we have

$$\begin{aligned}
& x^T(\rho_2 - \rho_1)y \\
&= x^T(A_\alpha(G') - A_\alpha(G))y \\
&= \sum_{j=0}^l [\alpha(x_{q-j}y_{q-j} + x_p y_p - x_k y_k - x_{h-j}y_{h-j}) \\
&\quad + (1-\alpha)(x_{q-j}y_p + x_p y_{q-j} - x_k y_{h-j} - x_{h-j}y_k)] \\
&= (l+1)[\alpha(x_p y_p + x_q y_q - x_h y_h - x_k y_k) + (1-\alpha)(x_p y_q + x_q y_p - x_h y_k - x_k y_h)] \\
&= (l+1)[(\alpha(x_q - x_k)(\alpha y_k + (1-\alpha)y_h) + (y_q - y_k)(\alpha x_q + (1-\alpha)x_p) \\
&\quad + (y_p - y_h)(\alpha x_p + (1-\alpha)x_q) + (x_p - x_h)(\alpha y_h + (1-\alpha)y_k))] \\
&\geq (l+1)[(y_q - y_k)(\alpha x_q + (1-\alpha)x_p) + (x_p - x_h)(\alpha y_h + (1-\alpha)y_k)] \\
&\geq (l+1)\left[\frac{p-h+l+1}{\rho_2-\alpha p+1}(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p) \right. \\
&\quad \left. - \frac{k-q+l+1}{\rho_1-\alpha k}(\alpha x_p + (1-\alpha)x_q)(\alpha y_h + (1-\alpha)y_k)\right] \\
&\geq (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)\left(\frac{p-h+l+1}{\rho_2-\alpha p+1} - \frac{k+l-q+1}{\rho_1-\alpha k}\right) \\
&= (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)\frac{(p-h+l+1)(\rho_1-\alpha k) - (k+l-q+1)(\rho_2-\alpha p+1)}{(\rho_2-\alpha p+1)(\rho_1-\alpha k)} \\
&= (l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p) \\
&\quad \times \frac{(k+l-q+1)(\rho_1-\rho_2) + (k+l-q+1)(\alpha p - \alpha k - 1) + (p+q-h-k)(\rho_1-\alpha k)}{(\rho_2-\alpha p+1)(\rho_1-\alpha k)}.
\end{aligned} \tag{16}$$

Multiply both sides by $\frac{(\rho_2-\alpha p+1)(\rho_1-\alpha k)}{(l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)}$, (16) can be rearranged to the following form:

$$\begin{aligned}
& (\rho_2 - \rho_1)\left(\frac{x^T y(\rho_2-\alpha p+1)(\rho_1-\alpha k)}{(l+1)(\alpha y_k + (1-\alpha)y_h)(\alpha x_q + (1-\alpha)x_p)} + k + l - q + 1\right) \\
&\geq (k + l - q + 1)(\alpha p - \alpha k - 1) + (p + q - h - k)(\rho_1 - \alpha k) \\
&\geq 0.
\end{aligned} \tag{17}$$

Further, $\rho_2 = \rho_1$ holds if and only if $x_q = x_k$, $p + q - h - k = 0$, $\alpha(p - k) - 1 = 0$ and $\alpha = \frac{1}{2}$, therefore, $l = 0$, $p = k + 2 = h + 1 = q + 3$ and $\alpha = \frac{1}{2}$. $\blacksquare$

4 Proof of Theorems 1.5 and 1.6

In this section, we first prove the following theorem, which extends the main results of Li et.al [19] for $n - 1 \leq m \leq 2n - 3$ and Chang and Tam [7] for $n - 1 \leq m \leq 2n - 3$ and $\alpha = 1/2$.

Theorem 4.1. *Let $n - 1 \leq m \leq 2n - 2$.*

- (i). *If $\alpha \in (\frac{1}{2}, 1)$ or $m \neq n + 2$ and $\alpha = \frac{1}{2}$, then $S_{n,m}$ is the only extremal graph that maximizes the A_α -spectral radius in $\mathcal{H}_{n,m}$.*
- (ii). *If $m = n + 2$ and $\alpha = \frac{1}{2}$, then $S_{n,n+2}$ and $\tilde{S}_{n,n+2}$ are all extremal graphs that maximize the $A_{\frac{1}{2}}$ -spectral radius in $\mathcal{H}_{n,n+2}$.*

Proof. Note that $\rho_\alpha(\tilde{S}_{n,n+2}) = \rho_\alpha(S_{n,n+2})$. It is sufficient to prove that if $G' \neq S_{n,m}$ is a graph which has the maximum A_α -spectral radius in $\mathcal{H}_{n,m}$ then $m = n + 2$, $\alpha = 1/2$ and $G' = \tilde{S}_{n,m}$.

If $n \leq 5$, it is easy to see that the assertion holds. So we assume that $n \geq 6$. By Lemma 2.5, we assume that $G' \neq S_{n,m}$ is a connected threshold graph with degree sequence $d_{G'}(v_1) \geq d_{G'}(v_2) \geq \dots \geq d_{G'}(v_n)$. Since there is only one threshold graph $S_{n,m}$ in $\mathcal{H}_{n,m}$ for $n - 1 \leq m \leq n + 1$, we have $m \geq n + 2$. Further, since $G' \neq S_{n,m}$ is a threshold graph, it is easy to see that $d_{G'}(v_1) = n - 1$, $n - 2 \geq d_{G'}(v_2) \geq d_{G'}(v_3) \geq 3$ and $d(v_n) = 1$. Let $\delta_1 = |\{i : d_{G'}(v_i) = 1\}|$ and $\delta_2 = |\{i : d_{G'}(v_i) = 2, i > 2\}|$. Let s be the largest positive number such that $d_{G'}(v_{s+2}) \geq 3$ and $d_{G'}(v_{s+3}) \leq 2$. Denote by $\theta = d_{G'}(v_{s+2}) - 2 > 0$. Then the number $e(G')$ of G' is at

least $(n-1) + (n-\delta_1-2) + \theta + (\theta-1) + \dots + 1 = 2n-3-\delta_1 + \theta(\theta+1)/2$. Hence $2n-3-\delta_1 + \theta(\theta+1)/2 \leq 2n-2$, which implies that $\delta_1 \geq \theta(\theta+1)/2 - 1$. So $\delta_1 \geq \theta$. Let G_1 be obtained from G' by a Transformation $(n-\delta_1+\theta, 2; n-\delta_1-\delta_2, 3; \theta, 1)$ of Definition 3.5. By Lemma 3.6, $\rho_\alpha(G_1) \geq \rho_\alpha(G')$. On the other hand, by the definition of G' and $G_1 \in \mathcal{H}_{n,m}$, $\rho_\alpha(G_1) \leq \rho_\alpha(G')$. Hence $\rho_\alpha(G_1) = \rho_\alpha(G')$. Hence by Lemma 3.6 again, we have $\alpha = \frac{1}{2}$, $\theta-1=0$, $n-\delta_1+\theta=2+3$, $n-\delta_1-\delta_2=4$, which implies $\delta_2=0$ and $\theta=1$, Hence $m=n+2$. Furthermore, it is easy to see that $G' = \tilde{S}_{n,n+2}$. So we finish our proof. ■

Now we are ready to present **Proof of Theorem 1.5**.

Proof. It is easy to see that assertion holds for $n \leq 16$ with the help of Python programming. So we assume that $n > 16$. Let G' be any graph which maximizes the spectral signless radius of all graphs of order n with size $m = 2n-2$. Then G' is a threshold graph. Suppose that G' is disconnected. Note that any threshold graph has at most one non-trivial component. So we assume that $G' = G^* \cup \bar{K}_s$, where G^* is a connected threshold graph of order n^* with size $m^* = 2n-2$. Then by $n^*(n^*-1)/2 \geq m^* = 2n-2$, we have $\frac{1+\sqrt{16n-15}}{2} \leq n^* \leq n-1$ and $q(G') = q(G^*)$. By Lemma 2.9,

$$q(G^*) \leq \frac{2(2n-2)}{n^*-1} + n^* - 2.$$

Let $f(x) = \frac{4n-4}{x} + x - 1$ for $x \in [\frac{-1+\sqrt{16n-15}}{2}, n-2]$. By $f''(x) > 0$, we have $f(x) \leq \max\{f(\frac{-1+\sqrt{16n-15}}{2}), f(n-2)\}$. Hence by $\frac{-1+\sqrt{16n-15}}{2} \leq n^*-1 \leq n-2$, we have

$$q(G^*) \leq \max\{\sqrt{16n-15} - 1, n + \frac{4}{n-2}\} < n + 1.6 \leq q(S_{n,2n-2}),$$

which is a contradiction. Hence G' must be a connected graph. Therefore, by Theorem 4.1, $G' = S_{n,2n-2}$. ■

In order to prove Theorem 1.6, we firstly prove the following key theorem.

Theorem 4.2. *Let $r \geq 3$, n and m be three positive number with $n > \frac{30r-63+5\sqrt{32r^2-136r+137}}{2}$ and $(r-1)n - \frac{r(r-1)}{2} < m \leq rn - \frac{r(r+1)}{2}$.*

(i). *If $\alpha \in (\frac{1}{2}, 1)$ or $\alpha = \frac{1}{2}$ and $m \neq (r-1)n - \frac{r(r-1)}{2} + 3$, then $S_{n,m}$ is the unique extremal graph that maximizes the A_α -spectral radius in $\mathcal{H}_{n,m}$.*

(ii). *If $\alpha = \frac{1}{2}$ and $m = (r-1)n - \frac{r(r-1)}{2} + 3$, then $S_{n,m}$ and $\tilde{S}_{n,m}$ are the only two extremal graphs that maximize the $A_{\frac{1}{2}}$ -spectral radius in $\mathcal{H}_{n,m}$.*

Proof. Note that $\rho_\alpha(S_{n,m}) = \rho_\alpha(\tilde{S}_{n,m})$ for $m = (r-1)n - \frac{r(r-1)}{2} + 3$. Hence it is sufficient to prove that if $G' \neq S_{n,m}$ is any graph which has the maximal A_α -spectral radius of $\mathcal{H}_{n,m}$, then $\alpha = \frac{1}{2}$, $m = (r-1)n - \frac{r(r-1)}{2} + 3$ and $G' = \tilde{S}_{n,m}$.

Let $G' \neq S_{n,m}$ be any graph which has the maximal A_α -spectral radius of $\mathcal{H}_{n,m}$. By Lemma 2.5, we assume that G' is a connected threshold graph with the $n \times n$ stepwise adjacency matrix $A(G') = (a_{ij})_{n \times n}$ and the degree sequence $d_{G'}(v_1) \geq d_{G'}(v_2) \geq \dots \geq d_{G'}(v_n)$. Moreover, denote by

$$\kappa = \kappa(G') = \max\{j : a_{j+1,j} = 1, 1 \leq j \leq n-1\}$$

and

$$\delta_j = \delta_j(G') = |\{i : d_{G'}(v_i) = j, n \geq i > j\}|$$

for $j = 1, \dots, \kappa$. Then we will prove a series of lemmas.

Lemma 4.3. $d_{G'}(v_n) \leq \kappa(G') - 2$, $d_{G'}(v_{r+1}) \geq r + 1$ and $\kappa(G') \geq r + 1$.

Proof. By the definition of $\kappa(G')$, we have $a_{\kappa+2, \kappa+1} = 0$. By $G' \neq S_{n,m}$ being a connected threshold graph, we have $a_{n, \kappa+1} = 0$ which implies that $d_{G'}(v_n) \leq \kappa$. Further, if $d_{G'}(v_n) = \kappa$, then the degree sequence of G' is $(n-1, \dots, n-1, \kappa, \dots, \kappa)$ which implies $G' = K_\kappa \vee (n-\kappa)K_1 = S_{n,m}$, a contradiction. If $d_{G'}(v_n) = \kappa - 1$, then the degree sequence of G' is $(n-1, \dots, n-1, \kappa, \dots, \kappa, \kappa-1, \dots, \kappa-1)$ which implies that $G' = K_{\kappa-1} \vee (K_{1, \delta_\kappa} \cup (n-\kappa-\delta_\kappa)K_1) = S_{n,m}$, a contradiction. Hence $d_{G'}(v_n) \leq \kappa(G') - 2$.

Suppose that $d_{G'}(v_{r+1}) \leq r - 1$. Since $A(G') = (a_{ij})$ is a stepwise adjacency matrix of G' with the degree sequence $d_{G'}(v_1) \geq d_{G'}(v_2) \geq \dots \geq d_{G'}(v_n)$, we have $a_{r+1, r} = 0$ and $a_{r, r+1} = a_{r+1, r} = 0$. So $d_{G'}(v_r) \leq r - 1$, which implies $\sum_{j=r}^n d_{G'}(v_j) \leq (r-1)(n-r+1)$. Hence,

$$\begin{aligned} 2m &= \sum_{j=1}^n d_{G'}(v_j) \\ &= \sum_{j=1}^{r-1} d_{G'}(v_j) + \sum_{j=r}^n d_{G'}(v_j) \\ &\leq (n-1)(r-1) + (r-1)(n-r+1) \\ &= 2(r-1)n - (r-1)r. \end{aligned}$$

So $m \leq (r-1)n - \frac{r(r-1)}{2}$, which contradicts to the assumption of m . Hence $d_{G'}(v_{r+1}) \geq r$.

Furthermore, suppose that $d_{G'}(v_{r+1}) = r$. By $r+1 \in \{i : d_{G'}(v_i) = r, i > r\}$, we have $\delta_r > 0$ and $d_{G'}(v_n) \leq \dots \leq d_{G'}(v_{r+2}) \leq r$. In addition, by $m \leq rn - \frac{r(r+1)}{2}$, we have $d_{G'}(v_n) < r$. Let $\varsigma = \max\{j : \delta_j \neq 0, j < r\}$. We consider the following two cases:

Case 1: $\varsigma < r - 1$.

Since $A(G')$ is the stepwise adjacency symmetric matrix, we have $a_{ij} = 0$, for all $i > j > r$. Hence

$$\begin{aligned} (r-1)n - \frac{r(r-1)}{2} &< m \\ &= \sum_{j=1}^n \sum_{i>j} a_{ij} \\ &= \sum_{j=1}^r \sum_{i>j} a_{ij} + \sum_{j=r+1}^n \sum_{i>j} a_{ij} \\ &= \sum_{j=1}^r \sum_{i>j} a_{ij} \\ &= \sum_{j=1}^r \sum_{i=1}^n a_{ij} - \sum_{j=1}^r \sum_{i \leq j} a_{ij} \\ &= \sum_{j=1}^\varsigma \sum_{i=1}^n a_{ij} + \sum_{j=\varsigma+1}^{r-1} \sum_{i=1}^n a_{ij} + \sum_{i=1}^n a_{ir} - \frac{r(r-1)}{2} \\ &\leq \varsigma(n-1) + (r-\varsigma-1)(n-2) + \delta_r + r-1 - \frac{r(r-1)}{2} \\ &= (r-1)n - \frac{r(r-1)}{2} + \delta_r - (r-1) + \varsigma. \end{aligned}$$

So $r - \varsigma - 1 < \delta_r$. Let G_1 be obtained from G' by a Transformation $(n - \sum_{j=1}^\varsigma \delta_j + 1, r - 1; n - \sum_{j=1}^\varsigma \delta_j, r; 1, r - \varsigma - 1)$ of Definition 3.7. By Lemma 3.8, $\rho_\alpha(G_1) \geq \rho_\alpha(G')$. Hence $\rho_\alpha(G_1) = \rho_\alpha(G')$. By Lemma 3.8 again, we have $n - \sum_{j=1}^\varsigma \delta_j = r + 1$, $\alpha = 1/2$, $r = \varsigma + 2$. Hence $m \leq (r-1)n - \frac{r(r-1)}{2}$ which contradicts to the assumption $m > (r-1)n - \frac{r(r-1)}{2}$. It is impossible.

Case 2: $\varsigma = r - 1$.

Since $G' \neq S_{n,m}$, it is easy to see that $d_{G'}(v_n) < r - 1$ (otherwise, $G' = K_{r-1} \vee (K_{1, \delta_r} \cup (n - r - \delta_r)K_1)$, so $G' = S_{n,m}$). Let $\varsigma_1 = \max\{j : \delta_j \neq 0, j < r - 1\}$. Clearly,

$$\begin{aligned} (r-1)n - \frac{r(r-1)}{2} &< m \\ &= \sum_{j=1}^n \sum_{i>j} a_{ij} \\ &= \sum_{j=1}^r \sum_{i=1}^n a_{ij} - \sum_{j=1}^r \sum_{i \leq j} a_{ij} \\ &= \sum_{j=1}^{\varsigma_1} \sum_{i=1}^n a_{ij} + \sum_{j=\varsigma_1+1}^{r-1} \sum_{i=1}^n a_{ij} + \sum_{i=1}^n a_{ir} - \frac{r(r-1)}{2} \\ &\leq \varsigma_1(n-1) + (r-\varsigma_1-1)(n-2) + \delta_r + r-1 - \frac{r(r-1)}{2} \\ &= (r-1)n - \frac{r(r-1)}{2} + \delta_r - (r-1) + \varsigma_1. \end{aligned}$$

Then $r - \varsigma_1 - 1 < \delta_r$. Let G_1 be obtained from G' by a Transformation $(n - \sum_{j=1}^{\varsigma_1} \delta_j + 1, r - 1; n - \sum_{j=1}^{r-1} \delta_j, r; 1, r - \varsigma_1 - 1)$ of Definition 3.7. By $n - \sum_{j=1}^{\varsigma_1} \delta_j + 1 - n + \sum_{j=1}^{r-1} \delta_j = \delta_{r-1} + 1 \geq 2$ and Lemma 3.8, $\rho_\alpha(G_1) > \rho_\alpha(G')$, which is a contradiction to the choice of G' . It is impossible. Hence $d_{G'}(v_{r+1}) \geq r + 1$. Then we have $a_{r+2, r+1} = a_{r+1, r+2} = 1$, so $\kappa \geq r + 1$. This completes the proof. $\blacksquare$

Lemma 4.4. $\delta_j \times \delta_{j+1} \times \delta_{j+2} = 0$, for $j = 1, 2, \dots, \kappa - 2$.

Proof. Suppose there exists an $1 \leq h \leq \kappa - 2$ such that $\delta_h \times \delta_{h+1} \times \delta_{h+2} \neq 0$. Let G_1 be the threshold graph obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + 1, h; n - \sum_{j=1}^{h+1} \delta_j, h + 1; 1, 1)$ of Definition 3.5. Since $n - \sum_{j=1}^h \delta_j + 1 - (n - \sum_{j=1}^{h+1} \delta_j) = \delta_{h+1} + 1 \geq 2$, we have $\rho_\alpha(G_1) > \rho_\alpha(G')$ by Lemma 3.6, which contradicts to the choice of G' . So the assertion holds. $\blacksquare$

Lemma 4.5. Let s be the largest positive number such that $d(v_{r+s}) \geq r + 1$ and $d(v_{r+s+1}) \leq r$ with $\theta = d(v_{r+s}) - r$. Then $\kappa \geq r + 1$, $\delta_\kappa > 0$, $r + s \geq \kappa + 1$ and $s \geq \theta + 1$.

Proof. By the definition of s , $a_{r+s+1, r+s} = 0$. Hence by the definition of κ , we have $a_{\kappa+1, \kappa} = 1$ and $r + s \geq \kappa + 1$.

Suppose that $s \leq \theta$. By the definition of the stepwise adjacency matrix $A(G')$, we have $a_{r+s, r+\theta+1} = 1$ and $a_{r+s, r+\theta+2} = 0$. By the definition of s , we have $a_{r+s+1, r+\theta+1} = 0$. In addition, since $A(G')$ is symmetric, we have $a_{r+\theta+1, r+s} = 1$ and $a_{r+\theta+1, r+s+1} = 0$, which implies that $d_{G'}(v_{r+\theta+1}) = r + s < r + \theta$, it is a contradiction. So the assertion holds. $\blacksquare$

Lemma 4.6. The edge number of the induced subgraph by vertex set $U_2 = \{v_{r+1}, \dots, v_n\}$ is at most $\sum_{j=1}^{r-1} (r - j) \delta_j$.

Proof. Let $U_1 = \{v_1, \dots, v_r\}$ and $U_2 = \{v_{r+1}, \dots, v_n\}$. Denote by $e(U_1, U_2)$ the edge number between vertex sets U_1 and U_2 , and $e(U_2)$ the edge number in vertex set U_2 , respectively. Since $G' \neq S_{n, m}$ is a connected threshold graph with $m > (r - 1)n - \frac{r(r-1)}{2}$, $d(v_{r+1}) \geq r$ and U_1 is a clique of order r by Lemma 4.3. Let $W_j = \{u \in U_2 : d(u) = j\}$ for $j = 1, \dots, r - 1$. By the definition of δ_j , we have $|W_j| = \delta_j$. Further, by G' being a threshold graph, each vertex in W_j is not adjacent to $v_{j+1}, \dots, v_r$ for $j = 1, \dots, r - 1$ and each vertex in $U_2 \setminus \bigcup_{j=1}^{r-1} W_j$ is adjacent to $v_1, \dots, v_r$. Hence

$$e(U_1, U_2) = r(n - r) - \sum_{i=1}^{r-1} (r - i) \delta_i.$$

Furthermore, by $m \leq rn - \frac{r(r+1)}{2}$, we have

$$e(U_1) + e(U_1, U_2) + e(U_2) = \frac{r(r-1)}{2} + r(n - r) - \sum_{i=1}^{r-1} (r - i) \delta_i + e(U_2) = m \leq rn - \frac{r(r+1)}{2},$$

which implies $e(U_2) \leq \sum_{j=1}^{r-1} (r - j) \delta_j$. $\blacksquare$

Lemma 4.7. If there exist two positive integers $1 \leq h \leq \kappa - 4$ and $3 \leq l \leq \kappa - h - 1$ such that $\delta_h > 0$, $\delta_{h+1} > 0$, $\delta_{h+2} = \dots = \delta_{h+l} = 0$, $\delta_{h+l+1} > 0$, which is depicted in Figure 6, then

- (i). $\delta_h \leq l - 1$ and $\delta_{h+1} \leq l - 2$.
- (ii). $\delta_{h+l+1} \leq l - 2$ and $\delta_{h+l+2} \leq l - 1$ if $h + l + 2 \leq \kappa$.
- (iii). $\sum_{j=h}^{h+l} \delta_j \leq 2l - 3$ and $\sum_{j=h+l+1}^{h+l+2} \delta_j \leq 2(l + 1) - 5$ if $h + l + 2 \leq \kappa$.

	l					
	h	h+1	h+2	...	h+l	h+l+1
$n - \sum_{j=1}^{h+1} \delta_j$	1	1	1	...	1	1
$n - \sum_{j=1}^{h+1} \delta_j + 1$	1	1				
$\vdots$	$\vdots$	$\vdots$				
$n - \sum_{j=1}^h \delta_j$	1	1				
$n - \sum_{j=1}^h \delta_j + 1$	1	0				
$\vdots$	$\vdots$	$\vdots$				
$n - \sum_{j=1}^{h-1} \delta_j$	1	0				

Figure 6: $\delta_h \neq 0, \delta_{h+1} \neq 0, \delta_{h+l+1} \neq 0, \delta_{h+2} = \dots = \delta_{h+l} = 0$

Proof. (i). Suppose that $\delta_h \geq l$. Let G_1 be obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + l, h+1; n - \sum_{j=1}^{h+1} \delta_j, h+2; l, 1)$ of Definition 3.5. Clearly $G_1 \in \mathcal{H}_{n,m}$. By Lemma 3.6, $\rho_\alpha(G_1) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence $\delta_h \leq l-1$.

Furthermore, suppose that $\delta_{h+1} \geq l-1$. Let G_2 be the threshold graph of order n with size m obtained from G' by a Transformation $(n - \sum_{j=1}^{h+1} \delta_j + l-1, h+2; n - \sum_{j=1}^{h+1} \delta_j, h+3; l-1, 1)$ of Definition 3.5 and G_3 be the graph obtained from G_2 by a Transformation $(n - \sum_{j=1}^h \delta_j + 1, h+1; n - \sum_{j=1}^{h+1} \delta_j + l-1, h+2; 1, 1)$ of Definition 3.5. By Lemma 3.6, $\rho_\alpha(G_2) \geq \rho_\alpha(G')$ and $\rho_\alpha(G_3) \geq \rho_\alpha(G_2)$. On the other hand, by $G_3 \in \mathcal{H}_{n,m}$, we have $\rho_\alpha(G_3) \leq \rho_\alpha(G')$. Hence $\rho_\alpha(G') = \rho_\alpha(G_2) = \rho_\alpha(G_3)$. By Lemma 3.6 again, we have $n - \sum_{j=1}^{h+1} \delta_j + l-1 = h+5$ and $n - \sum_{j=1}^{h+1} \delta_j + l-1 = h+3$, which is a contradiction. Therefore, $\delta_{h+1} \leq l-2$.

(ii). Suppose that $\delta_{h+l+1} \geq l-1$. Let G_1 be the threshold graph obtained from G' by a Transformation $(n - \sum_{j=1}^{h+1} \delta_j + l, h+l; n - \sum_{j=1}^{h+1} \delta_j, h+l+1; 1, l-1)$ of Definition 3.7. By Lemma 3.8, $\rho_\alpha(G_1) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence $\delta_{h+l+1} \leq l-2$.

Further, assume that $h+l+2 \leq \kappa$. If $\delta_{h+l+2} \geq l$, let G_2 be the graph obtained from G' by a Transformation $(n - \sum_{j=1}^{h+1} \delta_j + 1, h+l+1; n - \sum_{j=1}^{h+l+1} \delta_j, h+l+2; 1, l)$ of Definition 3.7. By Lemma 3.8, $\rho_\alpha(G_2) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence $\delta_{h+l+2} \leq l-1$.

(iii). It is easy to see that (iii) follows from (i) and (ii). ■

Lemma 4.8. *If there exist two positive integers $1 \leq h \leq \kappa-3$ and $2 \leq l \leq \kappa-h-1$ such that $\delta_h > 0, \delta_{h+1} = \delta_{h+2} = \dots = \delta_{h+l} = 0, \delta_{h+l+1} > 0$, then*

(i). $\delta_h \leq l-1$ and $\delta_{h+l+1} \leq l-1$.

(ii). If $h+l+2 \leq \kappa$, then $\delta_{h+l+2} \leq l$.

Proof. (i). Suppose that $\delta_h \geq l$. Let G_1 be obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + l, h+1; n - \sum_{j=1}^h \delta_j, h+2; l, 1)$ of Definition 3.5. By Lemma 3.6 and $l \geq 2 > 1$, $\rho_\alpha(G_1) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence, $\delta_h \leq l-1$.

Suppose that $\delta_{h+l+1} \geq l$. Let G_2 be obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + l, h+1; n - \sum_{j=1}^h \delta_j, h+l+1; 1, l)$ of Definition 3.7. By Lemma 3.8 and $l \geq 2 > 1$, $\rho_\alpha(G_2) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence $\delta_{h+l+1} \leq l-1$. Therefore (i) holds.

(ii). Suppose that $\delta_{h+l+2} \geq l+1$. Let G_2 be the graph obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + 1, h+l+1; n - \sum_{j=1}^{h+l+1} \delta_j, h+l+2; 1, l+1)$ of Definition 3.7. By Lemma 3.8 and $l+1 \geq 3 > 1$, we have $\rho_\alpha(G_2) > \rho_\alpha(G')$, which contradicts to G' having the maximal A_α -spectral radius in $\mathcal{H}_{n,m}$. Hence $\delta_{h+l+2} \leq l$. So (ii) holds. $\blacksquare$

Lemma 4.9. *If there exists one positive integer $1 \leq h \leq \kappa - 2$ such that $\delta_h > 0$, $\delta_{h+1} = 0$ and $\delta_{h+2} > 0$, then $\alpha = \frac{1}{2}$, $h = \kappa - 2$, $\delta_\kappa = 1$ and $n - \sum_{j=1}^{\kappa-2} \delta_j = \kappa + 1$.*

Proof. Let G_1 be the connected threshold graph obtained from G' by a Transformation $(n - \sum_{j=1}^h \delta_j + 1, h+1; n - \sum_{j=1}^h \delta_j, h+2)$ of Definition 3.1. By Lemma 3.3, $\rho_\alpha(G_1) \geq \rho_\alpha(G')$. On the other hand, by the definition of G' , we have $\rho_\alpha(G_1) \leq \rho_\alpha(G')$. Hence $\rho_\alpha(G_1) = \rho_\alpha(G')$. Therefore by Lemma 3.3 again, we have $\alpha = \frac{1}{2}$ and $n - \sum_{j=1}^h \delta_j = h+3$. In addition, by the definition of κ , it is easy to see that $n = \sum_{j=1}^\kappa \delta_j + \kappa$. Hence by $\delta_\kappa \geq 1$,

$$n = \sum_{j=1}^\kappa \delta_j + \kappa = n + \left(\sum_{j=h+1}^\kappa \delta_j - 1 \right) + (\kappa - h - 2) \geq n.$$

Therefore $\kappa - h - 2 = 0$ and $\sum_{j=h+1}^\kappa \delta_j = 1$. So the assertion holds. $\blacksquare$

In order to present more properties of extremal graphs in $\mathcal{H}_{n,m}$, we also need the following symbol. Let $G' \neq S_{n,m}$ be a connected threshold graph with the $n \times n$ stepwise adjacency matrix $A(G') = (a_{ij})$ and the degree sequence $d_{G'}(v_1) \geq d_{G'}(v_2) \geq \dots \geq d_{G'}(v_n)$. Let s be the largest positive number such that $d(v_{r+s}) \geq r+1$ and $d(v_{r+s+1}) \leq r$. Moreover denote by $\theta = d(v_{r+s}) - r$.

Lemma 4.10. *There exists a $1 \leq h \leq \kappa - 2$ such that $\delta_h > 0$, $\delta_{h+1} = 0$ and $\delta_{h+2} > 0$.*

Proof. By Lemma 4.3, we $d_{G'}(v_n) \leq \kappa - 2$. We define a sequence of numbers by recursive methods.

$$n_0 = n, \quad h_0 = d_{G'}(v_{n_0}) \leq \kappa - 2, \quad l_0 = 0;$$

$$n_i = n_{i-1} - \delta_{h_{i-1}} - \delta_{h_{i-1}+1}, \quad h_i = d_{G'}(v_{n_i}) \leq \kappa - 2, \quad l_i = h_i - h_{i-1} - 1 \geq 1,$$

for $i = 1, \dots, t-1$; and

$$n_t = n_{t-1} - \delta_{h_{t-1}} - \delta_{h_{t-1}+1}, \quad h_t = d_{G'}(v_{n_t}) \geq \kappa - 1.$$

Suppose that there does not exist any $1 \leq h \leq \kappa - 2$ such that $\delta_h > 0$, $\delta_{h+1} = 0$ and $\delta_{h+2} > 0$.

Since $d_{G'}(v_n) \leq \kappa - 2$, $h_0 = d_{G'}(v_{n_0}) \leq \kappa - 2$ and $h_t = d_{G'}(v_{n_t}) \geq \kappa - 1$, we have $t \geq 1$ and $h_t \leq \kappa$. Moreover,

$$n_t \leq \kappa + \delta_\kappa + \delta_{\kappa-1}. \quad (18)$$

Further by Lemmas 4.7 and 4.8, we have

$$n_{i-1} - n_i = \sum_{j=h_{i-1}}^{h_i-1} \delta_j \leq 2(h_i - h_{i-1}) - 5, \quad i = 1, \dots, t. \quad (19)$$

Hence by $h_t \geq \kappa - 1$, $h_0 \geq 1$, $t \geq 1$ and (19), we have

$$n_0 - n_t = \sum_{i=1}^t (n_{i-1} - n_i) \leq \sum_{i=1}^t [2(h_i - h_{i-1}) - 5] = 2(h_t - h_0) - 5t \leq 2\kappa - 7. \quad (20)$$

In addition, by $h_t \geq \kappa - 1$, (20) and the definition of h_i , we have

$$\sum_{i=1}^{\kappa-2} \delta_i \leq \sum_{i=1}^{h_t-1} \delta_i = \sum_{i=1}^t (\delta_{h_{i-1}} + \delta_{h_{i-1}+1}) = \sum_{i=1}^t (n_{i-1} - n_i) = n_0 - n_t \leq 2\kappa - 7. \quad (21)$$

In particular, by $h_1 \leq \kappa$, Lemmas 4.7 and 4.8, we have

$$\delta_{h_0} \leq h_1 - h_0 - 1 - 1 \leq \kappa - 3, \quad \delta_{h_0+1} \leq (h_1 - h_0 - 1) - 2 \leq \kappa - 4. \quad (22)$$

By (21), (22) and $\kappa \geq r + 1$, we have

$$\begin{aligned} \sum_{i=1}^{r-1} (r-i)\delta_i &\leq (r-1)\delta_1 + (r-2)\delta_2 + (r-3) \sum_{i=1}^{r-1} \delta_i \\ &= 2\delta_1 + \delta_2 + (r-3) \sum_{i=3}^{r-1} \delta_i \\ &\leq 2\delta_{h_0} + \delta_{h_0+1} + (r-3) \sum_{i=1}^{r-1} \delta_i \\ &\leq 2(\kappa-3) + (\kappa-4) + (r-3) \sum_{i=1}^{\kappa-2} \delta_i \\ &\leq 3\kappa - 10 + (r-3)(2\kappa-7) \\ &= (2r-3)(\kappa-r) + 2r^2 - 10r + 11. \end{aligned}$$

On the other hand, by $r+s \geq \kappa+1$, the edge number of the induced subgraph by U_2 is

$$\begin{aligned} e(U_2) &\geq 1 + 2 + \dots + (\theta-1) + \theta(s-\theta) + 1 + 2 + \dots + [\kappa - (r+\theta)] \\ &= \frac{\theta(\theta-1)}{2} + \theta s - \theta^2 + \frac{(\kappa-r+1-\theta)(\kappa-r-\theta)}{2} \\ &= \frac{(\kappa-r)(\kappa-r+1)}{2} + (r+s-\kappa-1)\theta \\ &\geq \frac{(\kappa-r)(\kappa-r+1)}{2}. \end{aligned}$$

By Lemma 4.6, we have

$$\frac{(\kappa-r)(\kappa-r+1)}{2} \leq e(U_2) \leq (2r-3)(\kappa-r) + 2r^2 - 10r + 11,$$

which implies

$$\kappa - r \leq \frac{4r-7 + \sqrt{32r^2 - 136r + 137}}{2}. \quad (23)$$

In addition, by Lemma 4.7 and 4.8, we have $\delta_\kappa \leq \kappa - 3$ and $\delta_{\kappa-1} \leq \kappa - 4$. Therefore, by (18), (20), (22) and (23),

$$\begin{aligned} n &= (n_0 - n_t) + n_t \\ &\leq 2\kappa - 7 + \kappa + \delta_\kappa + \delta_{\kappa-1} \\ &\leq 5\kappa - 14 \\ &\leq \frac{30r-63 + 5\sqrt{32r^2 - 136r + 137}}{2}, \end{aligned}$$

which contradicts to the condition of n . Hence the assertion holds. ■

Lemma 4.11. $\alpha = \frac{1}{2}$, $m = (r-1)n - \frac{(r-1)r}{2} + 3$ and $G' = \tilde{S}_{n,m}$.

Proof. By Lemma 4.10, there exists a $1 \leq h \leq \kappa - 2$ such that $\delta_h > 0$, $\delta_{h+1} = 0$ and $\delta_{h+2} > 0$. Hence by Lemma 4.9, $\alpha = \frac{1}{2}$, $h = \kappa - 2$, $\delta_{\kappa-2} > 0$, $\delta_{\kappa-1} = 0$ and $\delta_\kappa = 1$. Let G_2 be the connected threshold graph obtained from G' by a Transformation $(\kappa + 2, \kappa - 1; \kappa + 1, \kappa)$ of Definition 3.1. By Lemma 3.3, $\rho_\alpha(G_2) \geq \rho_\alpha(G')$. Note that $G_2 \in \mathcal{H}_{n,m}$, which implies that $\rho_\alpha(G_2) \leq \rho_\alpha(G')$. Hence $\rho_\alpha(G_2) = \rho_\alpha(G')$, i.e., G_2 is a connected threshold graph having the maximal A_α -spectral radius of $\mathcal{H}_{n,m}$ with $(r-1)n - \frac{r(r-1)}{2} < m \leq rn - \frac{r(r+1)}{2}$. Denote by the adjacency stepwise matrix $A(G_2) = (\tilde{a}_{ij})$, $\tilde{\kappa} = \kappa(G_2) = \max\{j : \tilde{a}_{j+1,j} = 1\}$ and $\tilde{\delta}_j = \tilde{\delta}_j(G') = |\{i : d_{G_2}(v_i) = j, i > j\}|$ for $j = 1, \dots, \tilde{\kappa}$. Then $\tilde{\kappa} = \kappa - 1$, $\tilde{\delta}_{\tilde{\kappa}} = 3$ by $\delta_\kappa = 1$.

Suppose that $G_2 \neq S_{n,m}$. Since G_2 is a connected threshold graph having the maximal A_α -spectral radius of $\mathcal{H}_{n,m}$ with $(r-1)n - \frac{r(r-1)}{2} < m \leq rn - \frac{r(r+1)}{2}$, by Lemma 4.10, there exists a $1 \leq \tilde{h} \leq \tilde{\kappa} - 2$ such that $\tilde{\delta}_{\tilde{h}} > 0$, $\tilde{\delta}_{\tilde{h}+1} = 0$ and $\tilde{\delta}_{\tilde{h}+2} > 0$. Hence by Lemma 4.9, $\tilde{\delta}_{\tilde{\kappa}} = 1$. It is impossible. Therefore $G_2 = S_{n,m} = K_{r-1} \vee (K_{1,\hat{a}} \cup (n-r-\hat{a})K_1)$. So $\tilde{\kappa} = r$ and $\hat{a} = \tilde{\delta}_{\tilde{\kappa}} = 3$, which implies $e(G_2) = (r-1)n - \frac{r(r-1)}{2} + 3$. Then $G' = \tilde{S}_{n,m}$ with $m = e(G') = (r-1)n - \frac{r(r-1)}{2} + 3$. Hence we finish the proof of Theorem 4.2. ■

Now we are ready to present **Proof of Theorem 1.6**.

Proof. Notice that the function $f(r) = \frac{30r-63+5\sqrt{32r^2-136r+137}}{2}$ is an increasing function with respect to r . It follows from Theorem 4.2 for $r \geq 3$ and $(r-1)n - \frac{r(r-1)}{2} < m \leq rn - \frac{r(r+1)}{2}$, and Theorem 4.1 for $n-1 < m \leq rn - \frac{r(r+1)}{2}$ that the assertion holds. ■

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