The $A_\alpha$ spectral radius of $k$-connected graphs with given diameter

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Abstract

Let $G$ be a graph with adjacency matrix $A(G)$ and degree diagonal matrix $D(G)$. In 2017, Nikiforov defined the matrix $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$ for any real $\alpha \in [0,1]$. The largest eigenvalue of $A_\alpha(G)$ is called the $A_\alpha$ spectral radius or the $A_\alpha$-index of $G$.

Let $G^d_{n,k}$ be the set of $k$-connected graphs with order $n$ and diameter $d$. In this paper, we determine the graphs with maximum $A_\alpha$ spectral radius among all graphs in $G^d_{n,k}$ for any $\alpha \in [0,1)$, where $k \geq 2$ and $d \geq 2$. We generalize the results of adjacency matrix in [P. Huang, W.C. Shiu, P.K. Sun, Linear Algebra Appl., 2016, Theorem 3.6] and the results of signless Laplacian matrix in [P. Huang, J.X. Li, W.C. Shiu, Linear Algebra Appl., 2021, Theorem 3.4].

Key Words: $A_\alpha$ spectral radius; $k$-connected; diameter

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1 Introduction

All graphs considered here are simple. Let $G$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The order of $G$ is $n$ and the size of $G$ is $m$, where $n = |V(G)|$ and $m = |E(G)|$. The neighbor set of a vertex $v$ in $G$ is denoted by $N_G(v)$, the degree of the vertex $v$ in $G$ is denoted by $d_G(v)$, where $d_G(v) = |N_G(v)|$. The minimum degree and the maximum degree of $G$ are denoted by $\delta(G)$ and $\Delta(G)$, respectively. The distance $d_G(u,v)$ between two distinct vertices $u,v$ of a connected graph $G$ is the length of the shortest path connecting them. The diameter $d$ of $G$ is the maximum distance among
all distinct vertices pairs of $G$. For a subset $W \subseteq V(G)$, let $G[W]$ be the subgraph induced by $W$ and $G-W = G[V(G) \setminus W]$. A graph is $k$-connected if $G-W$ is connected for any subset $W \subseteq V(G)$ with $|W| < k$. The sequential join $G_1 \vee \cdots \vee G_k$ of graphs $G_1, \ldots, G_k$, is the graph formed by taking one copy of each graph and adding additional edges from each vertex of $G_i$ to all vertices of $G_{i+1}$, for $i = 1, 2, \ldots, k-1$. A path and a complete graph of order $n$ are denoted by $P_n$ and $K_n$, respectively. Unless otherwise stated, we use the standard notations and terminologies in [2, 23].

The Laplacian matrix of a graph $G$ is the largest eigenvalue of $M$, where $M$ is a corresponding graph matrix defined in a prescribed way, such as adjacency matrix, (signless) Laplacian matrix and others. The adjacency matrix of a graph $G$ with order $n$ is an $n \times n$ 0-1 matrix, denoted by $A(G) = [a_{ij}]_{n \times n}$, where $a_{ij} = 1$ if $v_i v_j \in E(G)$, and $a_{ij} = 0$ otherwise. The degree diagonal matrix of $G$ is $D(G) = \text{diag}(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$. The Laplacian matrix of a graph $G$ is $L(G) = D(G) - A(G)$, and the signless Laplacian matrix of $G$ is $Q(G) = D(G) + A(G)$. In 2017, Nikiforov [19] defined the $A_\alpha$ matrix of a graph $G$ as $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$ for any real $\alpha \in [0, 1]$, which can underpin a unified theory of $A(G)$ and $Q(G)$. The $A_\alpha$ spectral radius of a graph $G$ is denoted as $\lambda_\alpha(G)$. Based on the well-known Perron-Frobenius theorem, there exists a positive eigenvector $X = (x_1, x_2, \ldots, x_n)^T$ corresponding to $\lambda_\alpha(G)$, also called the Perron vector of $G$. For a vertex $v \in V(G)$, the eigenequation of $A_\alpha(G)$ corresponding to $v$ is written as

$$
\lambda_\alpha(G)x_v = \alpha d_G(v)x_v + (1 - \alpha) \sum_{uv \in E(G)} x_u.
$$

Moreover, we have

$$
X^T A_\alpha X = \alpha \sum_{u \in V(G)} d_G(u)x_u^2 + 2(1 - \alpha) \sum_{uv \in E(G)} x_u x_v.
$$

By Rayleigh Quotient, we have

$$
\lambda_\alpha(G) = \sup_{\|X\| \neq 0} \frac{X^T A_\alpha(G) X}{X^T X}.
$$

The Brualdi-Solheid problem, which was first presented in 1986 by Brualdi and Solheid in article [31], is a well-known question about finding a tight bound for the spectral radius in a set of graphs and characterizing the extremal graphs. Many recent results on this problem for various kinds of graphs and their adjacency spectral radius have been obtained, we refer to articles [11, 17, 21, 29], some monographs [22, 23] and the references therein. The results of the Brualdi-Solheid problem about the signless Laplacian spectral radius and $A_\alpha$ spectral radius, we refer to articles [10, 11, 15, 18, 28] and [1, 4, 7, 8, 12, 16, 21, 30], respectively. Further, other results for the $A_\alpha$ spectral radius of digraph can be referred to [17, 25, 26] and the references therein. Recently, the spectral extremal problem of adjacency matrix and $A_\alpha$ matrix has also attracted lots of attention, some results can be found in articles [3, 6] and the references therein.

Let $G^d_{n,k}$ be the set of $k$-connected graphs of order $n$ with given diameter $d$. Huang, Shiu, Sun [13] and Huang, Li, Shiu [13] solved the Brualdi-Solheid problem in $G^d_{n,k}$ for adjacency spectral radius and signless Laplacian spectral radius, respectively. Their conclusions are as follows.
Theorem 1.1 ([13, 14]). For $k \geq 2$ and $d \geq 2$, the graph $K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$ attains the maximum (signless Laplacian) spectral radius in $\mathcal{G}^d_{n,k}$, where $n_i = k$ for $i \in \{1, 2, \ldots, d-1\} \setminus \{\lfloor \frac{d}{2} \rfloor\}$, and $n_{\lfloor \frac{d}{2} \rfloor} \geq 2k$.

Furthermore, Huang, Li and Shiu [13] believed that the results of Theorem 1.1 also hold for $A_\alpha$ spectral radius in $\mathcal{G}^d_{n,k}$ with $\alpha \in [0, 1)$. For $d = 1$, it is obvious that $K_n$ is the unique graph with the maximum $A_\alpha$ spectral radius. For $k = 1$ and $d \geq 2$, Xue et al. [27] characterized that $K_{n-d}(\lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil)$ is the unique graph with the maximum $A_\alpha$ spectral radius, where $K_{n-d}(\lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil)$ is the graph obtained from $K_{n-d}$ by connecting its all vertices to an end vertex of $P_{\lfloor \frac{d}{2} \rfloor}$ and an end vertex of $P_{\lceil \frac{d}{2} \rceil}$. In this paper, we confirm Huang, Li and Shiu’s conjecture for all $d \geq 2$ and $k \geq 2$. Our conclusion is as follows.

Theorem 1.2. For $k \geq 2$ and $d \geq 2$, the graph $G = K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$ attains the maximum $A_\alpha$ spectral radius in $\mathcal{G}^d_{n,k}$, where $n_i = k$ for each $i \in \{1, 2, \ldots, d-1\} \setminus \{\lfloor \frac{d}{2} \rfloor\}$, $n_{\lfloor \frac{d}{2} \rfloor} \geq 2k$. Further, $\frac{1}{2}(\alpha(n_{\lfloor \frac{d}{2} \rfloor} + 2k) + \sqrt{\alpha^2(n_{\lfloor \frac{d}{2} \rfloor} + 2k + 1)^2 + 4(n_{\lfloor \frac{d}{2} \rfloor} + 2k)(1-2\alpha)}) < \lambda_\alpha(G) < n_{\lfloor \frac{d}{2} \rfloor} + 2k - 1.$

The rest of this paper is structured as follows. We provide several useful Lemmas in Section 2 and present our proof of Theorem 1.2 in Section 3.

2 Preliminaries

In this section, we present some preliminary results, which will be used in Section 3.

A graph is called diameter critical if its diameter decreases with any addition of an edge. The structure of a diameter critical $k$-connected graph was characterized by Ore [20] in 1968.

Lemma 2.1 ([20]). Let $G$ be a graph in $\mathcal{G}^d_{n,k}$. If $G$ is a diameter critical graph, then $G \cong K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$, where $n_i \geq k$ for each $i = 1, 2, \ldots, d-1$.

Following that, we present several results on the $A_\alpha$ spectral radius. In this paper, the vertices $u$ and $v$ of $G$ are said to be equivalent, if there exists an automorphism $p: G \rightarrow G$ such that $p(u) = v$.

Lemma 2.2 ([19]). Let $G \cong K_n$. Then $\lambda_\alpha(G) = n - 1$.

Lemma 2.3 ([19]). Let $G$ be a connected graph and $G_0$ be a proper subgraph of $G$. Then $\lambda_\alpha(G_0) < \lambda_\alpha(G)$ for $\alpha \in [0, 1)$.

Lemma 2.4 ([19]). Let $G$ be a connected graph. Let $u$ and $v$ be two equivalent vertices in $G$. If $X$ is the positive eigenvector of $A_\alpha(G)$ corresponding to $\lambda_\alpha(G)$, then $x_u = x_v$ for $\alpha \in [0, 1]$.

Lemma 2.5 ([19]). Let $G$ be a graph with maximum degree $\Delta(G) = \Delta$. If $\alpha \in [0, 1)$, then

$$\lambda_\alpha(G) \geq \frac{1}{2}\left(\alpha(\Delta + 1) + \sqrt{\alpha^2(\Delta + 1)^2 + 4\Delta(1-2\alpha)} \right).$$

If $G$ is connected, then equality holds if and only if $G \cong K_{1,\Delta}$. In particular,

$$\lambda_\alpha(G) \geq \begin{cases} 
\alpha(\Delta + 1), & \text{if } \alpha \in [0, \frac{1}{2}], \\
\alpha \Delta + \frac{(1-\alpha)^2}{\alpha}, & \text{if } \alpha \in [\frac{1}{2}, 1).
\end{cases}$$
Lemma 2.6. (19) Let $G$ be a graph. If $\alpha \in [0,1]$, then
\[
\frac{2|E(G)|}{|V(G)|} \leq \lambda_\alpha(G) \leq \max_{uw \in E(G)} \{ad_G(u) + (1 - \alpha)d_G(v)\}.
\]
The first equality holds if and only if $G$ is regular.

Lemma 2.7 (27). Let $G$ be a connected graph and $X(G) = (x_1, x_2, \ldots, x_n)^T$ be a positive eigenvector of $A_\alpha(G)$ corresponding to $\lambda_\alpha(G)$. For two distinct vertices $u, v$ of $G$, suppose $Y \subseteq N_G(u) \setminus (N_G(v) \cup \{v\})$. Let $G' = G - \{uw : w \in Y\} + \{vw : w \in Y\}$. If $Y \neq \emptyset$ and $x_v \geq x_u$, then $\lambda_\alpha(G') > \lambda_\alpha(G)$ for $\alpha \in [0,1)$.

In order to prove our main results, we generalize Lemma 2.7, our conclusion is shown in Lemma 2.8. In addition, we characterize the $A_\alpha$ spectral radius about the sequential join $K_{n_1} \lor K_{n_2} \lor K_{n_3}$ of three complete graphs $K_{n_1}$, $K_{n_2}$, and $K_{n_3}$, the results are shown in Lemma 2.9.

Lemma 2.8. Let $G$ be a connected graph and $X(G) = (x_1, x_2, \ldots, x_n)^T$ be a positive eigenvector of $A_\alpha(G)$ corresponding to $\lambda_\alpha(G)$. Let $U$ and $V$ be two disjoint subsets of $V(G)$ that satisfy $|U| = |V| = k$. For each pair of vertices $u_1, u_2 \in U$ (resp. $v_1, v_2 \in V$) are equivalent in $G$, then $x_{u_1} = x_{u_2}$ (resp. $x_{v_1} = x_{v_2}$). Suppose $W = N_G(U) \setminus \{N_G(V) \cup V\}$. Let $G'$ be a graph from $G$ by deleting all edges between $U$ and $W$ and adding all edges between $V$ and $W$. If $x_{v_1} \geq x_{u_1}$, then $\lambda_\alpha(G') > \lambda_\alpha(G)$.

Proof. By Equations (2) and (3), we have
\[
\lambda_\alpha(G') - \lambda_\alpha(G) \geq X(G')^T(A_\alpha(G') - A_\alpha(G))X(G)
\geq 2(1 - \alpha)k \sum_{w \in W} x_w(x_{v_1} - x_{u_1}) + \alpha|W|k(x_{v_1}^2 - x_{u_1}^2) \geq 0.
\]

By a similar argument as the proof of Lemma 2.2 in [27], we can deduce that $\lambda_\alpha(G') > \lambda_\alpha(G)$. These complete the proof. \hfill \Box

Lemma 2.9. Let $G = K_{n_1} \lor K_{n_2} \lor K_{n_3}$. Then $\lambda_\alpha(G)$ is the largest root of $f(x) = 0$, where
\[
f(x) = x^3 + [3 - (\alpha + 1)(n_1 + n_3) - (2\alpha + 1)n_2]x^2 + [n_2\alpha^2(n_1 + n_2 + n_3) + \alpha(n_1 + 2n_2 + n_3)(n_1 + n_2 + n_3 - 2) + 3 - 2(n_1 + n_2 + n_3) + n_1n_3]\alpha^2(n_1n_2(1 - n_1 - 2n_2) + n_2n_3(1 - n_3 + 2n_2) + n_2^2(1 - n_2)) + \alpha((1 - n_3)n_1^2 + (3n_2 + 3n_3 - 4n_2n_3 - n_3^2 - 1)n_1 + (2n_2 + n_3)(n_2 + n_3 - 1)) + n_1n_3(n_2 + 1) + 1 - (n_1 + n - 2 + n_3)].
\]

In particular, we have the following two results.

(i) If $n_1 = n_3$, then $\lambda_\alpha(G) = \frac{1}{2}[(n_1 + n_2 - 2) + \alpha(2n_1 + n_2) + g(x)]$, where
\[
g(x) = \sqrt{(2n_1 + n_2)^2\alpha^2 - 2(2n_1^2 + 5n_1n_2 + n_2^2)\alpha + n_1^2 + 6n_1n_2 + n_2^2}.
\]

(ii) If $n_1 = n_2 = n_3 = k$ ($k \in \mathbb{Z}^+$), then $\lambda_\alpha(G) = \frac{3\alpha + 2 + \sqrt{9\alpha^2 - 16\alpha + 8}}{2}k - 1$. 

4
Proof. Note that all vertices in $V(K_{n_1})$, all vertices in $V(K_{n_2})$ and all vertices in $V(K_{n_3})$ are equivalent, respectively. Let $X(G) = (x_1, \ldots, x_1, x_2, \ldots, x_2, x_3, \ldots, x_3)^T$ be the Perron vector corresponding to $\lambda_\alpha(G)$, where $x_i = x_{v_i} = x_{v'_i} = \ldots = x_{v'_{n_i}}$ for each $i = 1, 2, 3$. By Equation (4), we have

\[
\begin{align*}
[\lambda_\alpha(G) - \alpha(n_1 + n_2 - 1) - (1 - \alpha)(n_1 - 1)]x_1 - (1 - \alpha)n_2x_2 &= 0, \\
-\alpha n_1 x_1 + [\lambda_\alpha(G) - \alpha(n_1 + n_2 + n_3 - 1) - (1 - \alpha)(n_2 - 1)]x_2 - (1 - \alpha)n_3x_3 &= 0, \\
-\alpha n_2 x_2 + [\lambda_\alpha(G) - \alpha(n_2 + n_3 - 1) - (1 - \alpha)(n_3 - 1)]x_3 &= 0.
\end{align*}
\]

Let $f(x)$ be the determinant of the coefficient matrix of the Equation (4). Notice that $X(G) \neq 0$, by using the theory of solving homogeneous linear equations, then $\lambda_\alpha(G)$ is the largest root of $f(x) = 0$, where

\[
f(x) = x^3 + [3 - (\alpha + 1)(n_1 + n_3) - (2\alpha + 1)n_2]x^2 + [(\alpha^2n_2 - 2)(n_1 + n_2 + n_3) + \alpha n_1(n_1 + 3n_2 + 2n_3 - 2)]x + [\alpha n_2(2n_2 + 3n_3 - 4) + \alpha n_3(n_3 - 2) + n_1n_3 + 3]x + (\alpha - \alpha n_3 - \alpha^2n_2)n_i^2 + [-2\alpha^2n_2^2 + (3\alpha + n_3 - 4\alpha n_3 + \alpha^2)n_1]n_i + [(n_3 - 1)(\alpha - an_3 + 1)n_1 - (\alpha n_2 + \alpha n_3 - 1)(\alpha n_2 - 1)(n_2 + n_3 - 1)].
\]

(i) If $n_1 = n_3$, then the vertices in $V(K_{n_1}) \cup V(K_{n_3})$ are equivalent in $G$, that is $x_1 = x_3$. similarly we have

\[
\begin{align*}
[\lambda_\alpha(G) - \alpha(n_1 + n_2 - 1) - (1 - \alpha)(n_1 - 1)]x_1 - (1 - \alpha)n_2x_2 &= 0, \\
-\alpha n_1 x_1 + [\lambda_\alpha(G) - \alpha(2n_1 + n_2 - 1) - (1 - \alpha)(n_2 - 1)]x_2 &= 0.
\end{align*}
\]

Similarly, according to the theory of solving homogeneous linear equations, by direct calculation, we have $\lambda_\alpha(G) = \frac{1}{2}[(n_1 + n_2 - 2) + \alpha(2n_1 + n_2) + g(x)]$, where

\[
g(x) = \sqrt{(2n_1 + n_2)^2\alpha^2 - 2(2n_1^2 + 5n_1n_2 + n_2^2)\alpha + n_1^2 + 6n_1n_2 + n_2^2}.
\]

(ii) If $n_1 = n_2 = n_3 = k$ ($k \in \mathbb{Z}^+$), by direct calculation, then

\[
\lambda_\alpha(G) = \frac{1}{2}[(n_1 + n_2 - 2) + \alpha(2n_1 + n_2) + \\
\sqrt{(2n_1 + n_2)^2\alpha^2 - 2(2n_1^2 + 5n_1n_2 + n_2^2)\alpha + n_1^2 + 6n_1n_2 + n_2^2}] \\
= 3\alpha + 2 + \sqrt{9\alpha^2 - 16\alpha + 8}k - 1.
\]

These complete the proof. \qed

Lemma 2.10. Let $G = K_{n_1} \lor K_{n_2} \lor K_{n_3} \lor K_{n_1}$. Then $\lambda_\alpha(G) = \frac{1}{2}[(\alpha(n_1 + n_2) + n_1 + 2n_2 - 2) + \alpha(2n_1 + n_2) + g(x)]$, where $g(x) = \sqrt{(\alpha - 1)^2n_1^2 + 2\alpha(\alpha - 1)n_1n_2 + (\alpha - 2)^2n_2^2}$. In particular, if $n_1 = n_2 = k$ ($k \in \mathbb{Z}^+$), then $\lambda_\alpha(G) = \frac{(2\alpha + 3 + \sqrt{4\alpha^2 - 8\alpha + 5})}{2}k - 1$. 

5
Proof. Note that all vertices in \(V(K_{n_1})\) and all vertices in \(V(K_{n_2})\) are equivalent, respectively. Let \(X(G)\) be the Perron vector corresponding to \(\lambda_\alpha(G)\). By symmetry, we have

\[
X(G) = (x_1, x_1, x_2, x_2, \ldots, x_2, x_1, \ldots, x_1)^T.
\]

By using Equation (1), we have

\[
\begin{align*}
\{ & \lambda_\alpha(G) - \alpha(n_1 + n_2 - 1) - (1 - \alpha)(n_1 - 1)]x_1 - (1 - \alpha)n_2x_2 = 0, \\
& -(1 - \alpha)n_1x_1 + [\lambda_\alpha(G) - \alpha(n_1 + 2n_2 - 1) - (1 - \alpha)(2n_2 - 1)]x_2 = 0.
\end{align*}
\]

Similar to the proof of Lemma 2.9 by direct calculation, our results can be obtained easily.

3 Proof of Theorem 1.2

Let \(G\) be the graph with the maximum \(A_\alpha\) spectral radius among all graphs in \(G^d_{n,k}\). We call the graph \(G\) is maximal in \(G^d_{n,k}\).

According to Lemmas 2.1 and 2.3, the maximal graph \(G\) must be diameter critical. Since adding edges increases the \(A_\alpha\) spectral radius. We have \(G \cong K_{n_0} \lor \cdots \lor K_{n_d}\), where \(n_0 = n_1 = 1\) and \(n_i \geq k\) for each \(i = 1, 2, \ldots, d - 1\), as shown in Figure 1. The vertices sets of the subgraph \(K_{n_i}\) in \(G\) are simply denoted as \(V_i\) for each \(i = 0, 1, \ldots, d\). Therefore, \(\{V_0, V_1, \ldots, V_d\}\) is a partition of \(V(G)\).

![Figure 1: The graph \(G = K_{n_0} \lor \cdots \lor K_{n_d}\) with the subgraph \(H\).](image)

Note that any two distinct vertices in \(V_1\) (resp. \(V_2, \ldots, V_{d-1}\)) are equivalent. Let \(X(G)\) be the Perron vector corresponding to \(\lambda_\alpha(G)\). Then we have \(X(G) = (x_0, x_1, \ldots, x_1, \ldots, x_{d-1}, x_{d-1}, x_d)^T\).

![Figure 2: The graph \(G = K_{n_0} \lor \cdots \lor K_{n_d}\) with the subgraph \(H\).](image)
Let \( H \cong K_{d-1} \cup K_d \) be a subgraph of \( G \) with vertex set \( V(H) \). Let 
\[ Z = V(G) \setminus V(H) = \cup_{i=0}^{d} Z_i, \]
where \( Z_i \subset V_i, i = 0, 1, \ldots, d \), as shown in Figure 2.
Thus \( \{V_0(H), V_1(H), \ldots, V_d(H)\} \) is a partition of \( V(H) \), where \( V_0(H) = V_0, V_d(H) = V_d, \)
\( V_i(H) \subset V_i \subset V(G) \) and \( |V_i(H)| = k \) for each \( i = 1, 2, \ldots, d-1 \).
Similarly, \( \{Z_0, Z_1, \ldots, Z_d\} \) is a partition of \( Z \). It is possible that \( Z_i = \emptyset \) for some \( i \in [0, d] \), for instance \( Z_0 = Z_d = \emptyset \).

Let \( G_1 \) be the set of all graphs of order \( n \), in which each graph is isomorphic to \( K_{n_0} \cup \cdots \cup K_{n_d} \), where \( n_0 = n_d = 1 \), and there exists only one \( j \in \{1, 2, \ldots, d-1\} \) such that \( n_j \geq k \) and \( n_i = k \) for each \( i \in \{2, \ldots, d-1\} \setminus \{j\} \). Obviously, \( H \in G_1 \subseteq G_{n,k}^d \).

Next, we keep the notations defined in the preceding section unless otherwise stated and prove several Lemmas.

**Lemma 3.1.** Let \( G \) be a maximal graph in \( G_{n,k}^d \). If \( d \geq 2 \) and \( k \geq 1 \), then \( G \in G_1 \).

**Proof.** For \( d = 2 \) and \( k \geq 1 \), it is obvious that \( G \in G_1 \). Next we consider \( d \geq 3 \) and \( k \geq 2 \).

By contradiction, we suppose \( G \notin G_1 \), then there exists at least two \( j_1, \ldots, j_s \in \{1, 2, \ldots, d-1\} \) such that \( Z_{j_1}, \ldots, Z_{j_s} \neq \emptyset \) (\( s \geq 2 \)) and \( Z_i = \emptyset \) for each \( i \in \{1, 2, \ldots, d-1\} \setminus \{j_1, \ldots, j_s\} \), which also implies that \( |Z| \geq 2 \).

For \( d = 3 \) and \( k \geq 2 \), if \( G \notin G_1 \), then \( Z_1 \neq \emptyset \) and \( Z_2 \neq \emptyset \). Let \( G' \) be a graph obtained from \( G \) by deleting all edges between \( Z_1 \) and \( V_0 \) and adding all edges between \( Z_i \) and \( V_d \). Without loss of generality, we assume \( x_d \geq x_0 \). Since \( |V_0| = |V_d| = 1 \), by using Lemma 2.7, we have \( \lambda_\alpha(G') > \lambda_\alpha(G) \). Note that \( G' \in G_1 \subseteq G_{n,k}^d \), which contradicts the assumption that \( G \) is the maximal graph in \( G_{n,k}^d \). Thus \( G \in G_1 \).

Next we consider \( d \geq 4 \) and \( k \geq 2 \). Let \( x_0 \geq x_b \geq x_c \) be three largest values in the set \( \{x_i| i = 0, 1, \ldots, d\} \) of the graph \( G \), where \( a, b \) and \( c \) are pairwise distinct. Next we consider the following two cases:

**Case 1.** \( 0 \) or \( d \notin \{a, b, c\} \).

For any a vertex \( v \in Z \), let \( V_{a,v}(H), V_{b,v}(H), V_{c,v}(H) \in V(H) \) be three elements of the vertex partition set of \( V(H) \), whose vertices are adjacent to \( v \). It is possible that \( \{a_v, b_v, c_v\} \cap \{a, b, c\} \neq \emptyset \). Because \( \min \{x_a, x_b, x_c\} \geq x_0 \), without loss of generality, we assume \( x_a \geq x_{a_v}, x_b \geq x_{b_v} \) and \( x_c \geq x_{c_v} \).

**Step 1.** Let \( G_{1,1} \) be a graph obtained from \( G \) by deleting all edges between \( v \) and \( V_{a,v}(H), V_{b,v}(H), V_{c,v}(H) \), respectively, and adding all edges between \( v \) and \( V_a(H), V_b(H), V_c(H) \), respectively.

For \( v \notin Z_1 \) or \( Z_{d-1} \), the graph \( G \) and the graph \( G_{1,1} \) \((v \notin Z_1 \) or \( Z_{d-1}\)) is shown in Figure 3 (a), (b), respectively. In Figure 3 (c), we denote the edge-shifting operation from the graph \( G \) to the graph \( G_{1,1} \) \((v \notin Z_1 \) or \( Z_{d-1}\)) as \( G \rightarrow G_{1,1} \).

In Figures 3, we take Figure 3 (c) as an example, we just show the edge-shifting operations between the corresponding two graphs.

If \( v \notin Z_1 \) or \( Z_{d-1} \), by using Equations (2) and (3), then
\[
\lambda_\alpha(G_{1,1}) - \lambda_\alpha(G) \\
\geq X(G)^T [A_\alpha(G_{1,1}) - A_\alpha(G)] X(G) \\
= 2k(1 - \alpha)x_v(x_a + x_b + x_c - x_{a_v} - x_{b_v} - x_{c_v}) +
\]
\[
\alpha k(x_a^2 + x_b^2 + x_c^2 - x_{aw}^2 - x_{bw}^2 - x_{cw}^2) \geq 0.
\]

If \( v \in Z_1 \) or \( Z_{d-1} \), by symmetry, we can suppose \( v \in Z_1 \). By using Equations (2) and (3), then we have

\[
\lambda_\alpha(G_{1,1}) - \lambda_\alpha(G) \\
\geq X(G)^T[A_\alpha(G_{1,1}) - A_\alpha(G)]X(G) \\
= 2k(1-\alpha)x_v(x_a + x_b + x_c - x_0 - x_1 - x_2) + \alpha k(x_a^2 + x_b^2 + x_c^2 - x_0^2 - x_1^2 - x_2^2) + \\
2(k-1)((1-\alpha)x_vx_0 + \frac{\alpha}{2}x_0^2 + \frac{\alpha}{2}x_v^2) \geq 0.
\]

Therefore, \( \lambda_\alpha(G_{1,1}) > \lambda_\alpha(G) \).

---

Figure 3: \( G \rightarrow G_{1,1} \) (\( v \notin Z_1 \) or \( Z_{d-1} \)).

Step 2. Let \( w \) be a vertex of \( G \) and \( w \in Z \setminus \{v\} \).

If \( w \notin Z_1 \) or \( Z_{d-1} \), let \( V_{aw}(H), V_{bw}(H), V_{cw}(H) \in V(H) \) be three elements of the vertex partition set of \( V(H) \), whose vertices are adjacent to \( w \). According to our assumption, \( \min\{x_a, x_b, x_c\} \geq \max\{x_{aw}, x_{bw}, x_{cw}\} \), thus without loss of generality, we assume \( x_a \geq x_{aw}, x_b \geq x_{bw}, x_c \geq x_{cw} \). Next we do the same operation as Step 1, and obtain a graph \( G_{1,2} \) from \( G_{1,1} \) by deleting all edges between \( w \) and \( V_{aw}(H), V_{bw}(H), V_{cw}(H) \), respectively, and adding all edges between \( w \) and \( V_a(H), V_b(H), V_c(H) \), respectively. Then

\[
\lambda_\alpha(G_{1,2}) - \lambda_\alpha(G)
\]
Step 3. Let $G$ be a clique. Then $G$ is still a diameter critical graph, and prove that our conclusions hold, we do the final step. If $w \notin Z_{d-1}$, by symmetry, we suppose $w \in Z_1$. By using Equations (2) and (3), then we have

$$\lambda_\alpha(G_{1,2}) - \lambda_\alpha(G) = \lambda_\alpha(G_{1,2}) - \lambda_\alpha(G_{1,1}) + \lambda_\alpha(G_{1,1}) - \lambda_\alpha(G) \geq X(G_{1,2})^T A_\alpha(G_{1,2}) X(G_{1,2}) - X(G)^T A_\alpha(G) X(G) \geq X(G)^T [A_\alpha(G_{1,2}) - A_\alpha(G)] X(G)
\geq 2k(1 - \alpha)x_w (x_a + x_b + x_c - x_{aw} - x_{bw} - x_{cw}) + \alpha k(x_a^2 + x_b^2 + x_c^2 - x_{aw}^2 - x_{bw}^2 - x_{cw}^2) + 2(1 - \alpha)x_w x_0 + \frac{\alpha}{2} x_0^2 + \frac{\alpha}{2} x_w^2 \geq 0.$$ 

Repeat this step until all of the vertices in $Z$ have been chosen. Thus in the final graph, denoted by $G_2$, all vertices in $Z$ are adjacent to $V_a(H)$, $V_b(H)$ and $V_c(H)$, and $\lambda_\alpha(G_2) > \lambda_\alpha(G)$.

In order to ensure that the maximal graph $G$ after the edge-shifting operation is still a diameter critical graph, and prove that our conclusions hold, we do the Step 3.

Step 3. Let $G_{2,1}$ be the graph obtained from $G_2$ by adding some edges so that $G_{2,1}[Z]$ is a clique. Then $\lambda_\alpha(G_{2,1}) > \lambda_\alpha(G_2) \geq \lambda_\alpha(G)$.

If $G[V_a(H) \cup V_b(H) \cup V_c(H)] = K_k \vee K_k \vee K_k$, then our results hold. Next we consider the following two cases.

![Figure 4: $G_{2,1} \rightarrow G_{2,2}$.](image)

Case 1.1. $G[V_a(H) \cup V_b(H) \cup V_c(H)] = (K_k \vee K_k) \cup K_k$.

Let $G_{2,2}$ be the graph obtained from $G_{2,1}$ by deleting all edges between $V_b(H)$ and $V_{b+1}(H)$, all edges between $V_c(H)$ and $V_{c+1}(H)$, and adding all edges between $V_b(H)$ and $V_c(H)$, all edges between $V_{b+1}(H)$ and $V_{c+1}(H)$, as shown in Figure 4.
If $c + 1 \neq d$, then

$$\lambda_{\alpha}(G_{2,2}) - \lambda_{\alpha}(G_{2,1}) \geq 2(1 - \alpha)k^2(x_b - x_{b+1})(x_c - x_{b+1}) \geq 0.$$ 

If $c + 1 = d$, then

$$\lambda_{\alpha}(G_{2,2}) - \lambda_{\alpha}(G_{2,1}) \geq 2(1 - \alpha)k^2(x_b - x_{c+1})(x_c - x_{b+1}) + 2(1 - \alpha)k(k - 1)(x_{c+1}x_c - x_{b+1}x_{c+1}) + \alpha k(k - 1)(x_{c}^2 - x_{b+1}^2) \geq 0.$$ 

Then $\lambda_{\alpha}(G_{2,2}) > \lambda_{\alpha}(G_{2,1}) > \lambda_{\alpha}(G) > \lambda_{\alpha}(G)$, and $G_{2,2} \in G_1 \subset \mathcal{G}^d_{n,k}$. This contradicts that $G \notin G_1$ is the maximal graph in $\mathcal{G}^d_{n,k}$. Thus the maximal graph $G \in G_1 \subset \mathcal{G}^d_{n,k}$.

![Diagram](image)

Figure 5: $G_{2,1} \rightarrow G_{2,3}$.

Case 1.2. $G[V_a(H) \cup V_b(H) \cup V_c(H)] = K_k \cup K_k \cup K_k$.

Let $G_{2,3}$ be the graph obtained from $G_{2,1}$ by deleting all edges between $V_a(H)$ and $V_{a+1}(H)$, all edges between $V_b(H)$ and $V_{b+1}(H)$, all edges between $V_c(H)$ and $V_{c+1}(H)$, all edges between $V_b(H)$ and $V_{b-1}(H)$, and adding all edges between $V_a(H)$ and $V_b(H)$, all edges between $V_b(H)$ and $V_c(H)$, all edges between $V_{a+1}(H)$ and $V_{b+1}(H)$, all edges between $V_{b-1}(H)$ and $V_{c+1}(H)$, as shown in Figure 5.

If $c + 1 \neq d$, then

$$\lambda_{\alpha}(G_{2,3}) - \lambda_{\alpha}(G_{2,1}) \geq 2(1 - \alpha)k^2[(x_a - x_{b+1})(x_b - x_{a+1}) + (x_b - x_{c+1})(x_c - x_{b-1})] \geq 0.$$ 

If $c + 1 = d$, then

$$\lambda_{\alpha}(G_{2,3}) - \lambda_{\alpha}(G_{2,1}) \geq 2(1 - \alpha)k^2[(x_a - x_{b+1})(x_b - x_{a+1}) + (x_b - x_{c+1})(x_c - x_{b-1})] + 2(1 - \alpha)k(k - 1)(x_{c+1}x_c - x_{b-1}x_{c+1}) + \alpha k(k - 1)(x_{c}^2 - x_{b-1}^2) \geq 0.$$ 

Then $\lambda_{\alpha}(G_{2,3}) > \lambda_{\alpha}(G_{2,1}) > \lambda_{\alpha}(G)$ and $G_{2,3} \in G_1 \subset \mathcal{G}^d_{n,k}$. This contradicts that $G \notin G_1$ is the maximal graph in $\mathcal{G}^d_{n,k}$. Thus the maximal graph $G \in G_1 \subset \mathcal{G}^d_{n,k}$.

Case 2. $0$ or $d \in \{a, b, c\}$.

Since $x_0 = \frac{(1-\alpha)|V_1|}{\lambda_{\alpha}-\alpha|V_1|}x_1$, by using Proposition 36. in [19] and Lemma 2.3, then $\lambda_{\alpha} >$
\(|V_1| + 1\) = \(|V_1|\), that is \(x_0 < x_1\). Because of symmetry, we have \(x_d < x_{d-1}\). Thus, \(\{a, b, c\} = \{0, 1, r\}\) or \(\{r, d-1, d\}\), where \(1 \leq r \leq d-1\). Without loss of generality, we assume \(\{a, b, c\} = \{0, 1, r\}\), where \(2 \leq r \leq d-1\). Next we consider two cases: first, \(Z_1 = Z_{d-1} = \emptyset\), second, \(Z_1 \neq Z_{d-1} \neq \emptyset\). The case of \(Z_1 \neq Z_{d-1} \neq \emptyset\) can be converted to the case that \(Z_1 \neq \emptyset\) and \(Z_d \neq \emptyset\) by using some edge-shifting operations.

**Figure 6:** \(G \rightarrow G_{3,1}\).

**Figure 7:** \(G_{3,1} \rightarrow G_{3,2}\).

**Figure 8:** \(G_{3,2} \rightarrow G_{3,3}\).

Case 2.1. \(Z_1 = Z_{d-1} = \emptyset\).
Let \(x_{a'} \geq x_{b'} \geq x_{c'}\) be the three largest components of \(X(G) \setminus \{x_0, x_d\} = (x_1, x_2, \ldots, x_{d-1})^T\) corresponding to all vertices of \(V_{a'}, V_{b'}, V_{c'}\) (\(a', b'\) and \(c'\) are
pairwise distinct), respectively. We follow all steps as Case 1., then we can obtain the graphs like $G_{1,1}, G_{1,2}, G_{2,1}, G_{2,2}$ or $G_{2,3}$, such that $\lambda_\alpha(G_{2,3}) \lambda_\alpha(G_{2,2})) > \lambda_\alpha(G_{2,1}) > \lambda_\alpha(G_{2})(\lambda_\alpha(G_{1,2}), \lambda_\alpha(G_{1,1})) > \lambda_\alpha(G)$, where $G_{2,3}$ and $G_{2,2}$ are in $G_1 \subseteq G_{d,n,k}$. Then we obtain a same contradiction like Case 1. that $G$ is a maximal graph in $G_{d,n,k}$ and $G \notin G_1$.

**Case 2.2.** $Z_1 \neq Z_{d-1} \neq \emptyset$ and $r \neq d - 1$.

Let $G_{3,1}$ be a graph obtained from $G$ by deleting all edges between $Z_{d-1}$ and $V_d(H), V_{d-1}(H)$, respectively, and adding all edges between $Z_{d-1}$ and $V_0(H), V_1(H)$, respectively, as shown in Figure 9. Then there is no edge between $Z$ and
$V_{d-1}(H) \cup V_d(H)$. By using Lemma 2.8 then $\lambda_\alpha(G_{3,1}) > \lambda_\alpha(G)$. The following discussion also applies to the case that one of $Z_1$, $Z_{d-1}$ is not an empty set.

First, we choose one vertex $w$ from $V_{d-1}(H)$. Let $G_{3,2}$ be a graph obtained from $G$ by deleting all edges between $w$ and $(V_{d-1}(H) \setminus w) \cup V_d(H)$, all edges between $V_{d-2}(H)$ and $V_{d-1}(H) \setminus w$, and adding all edges between $V_{d-1}(H) \setminus w$ and $V_1(H) \cup V_0(H)$, and the edge $V_0V_d$, see Figure 7. By using Lemma 2.8 we have $\lambda_\alpha(G_{3,2}) > \lambda_\alpha(G)$.

Second, let $G_{3,3}$ be a graph obtained from $G_{3,2}$ by adding all edges between $V_{d-1} \setminus w$ and $Z_1$, as shown in Figure 8. By using Lemma 2.3 we have $\lambda_\alpha(G_{3,3}) > \lambda_\alpha(G)$.

Third, if $Z_{d-2} = \emptyset$, then we may follow the proof of Case 1., otherwise, if $Z_{d-2} \neq \emptyset$, let $G_{3,4}$ be a graph obtained from $G_{3,3}$ by deleting all edges between $w$ and $Z_{d-2}$, and adding all edges between $V_0$ and $Z_{d-2}$, as shown in Figure 9. By using Lemma 2.8 we have $\lambda_\alpha(G_{3,4}) > \lambda_\alpha(G)$. Next, we may follow the proof of Case 1. and get a contraction. Thus the maximal graph $G \in \mathcal{G}_1 \subset \mathcal{G}_n^d$.

Case 2.3. $Z_1 \neq Z_{d-1} \neq \emptyset$ and $r = d - 1 \ (\{a, b, c\} = \{0, 1, r\}$.

First, we keep all edges between $Z_1$ and $V_0 \cup V_1(H)$, keep all edges between $Z_{d-1}$ and $V_{d-1}(H)$. Next we delete all edges between $Z_{d-1}$ and $V_d$ and add all edges between $Z_{d-1}$ and $V_0$.

Second, let $x_j$ be the largest component of $X(G) \setminus \{x_0, x_1, x_{d-1}, x_d\}$. Then we repeat the similar operations of Step 1.–Step 3. in Case 1. and obtain a graph $G_{3,5}$ with $\lambda_\alpha(G_{3,5}) > \lambda_\alpha(G)$, as shown in Figure 10. Let $G_{3,6}$ be a graph obtained from $G_{3,5}$ by deleting all edges between $Z_1$ and $V_1(H)$, all edges between $Z_{d-1}$ and $V_d(H)$, and adding all edges between $Z_1$ and $V_{d-1}(H)$, all edges between $Z_{d-1}$ and $V_1(H)$, as shown in Figure 11. Then by using Lemma 2.3 we have $\lambda_\alpha(G_{3,5}) > \lambda_\alpha(G)$. Note that the graph $G_{3,6}$ satisfies $G_{3,6} \in \mathcal{G}_n^d$, and in the graph $G_{3,6}$, one of $Z_1$ and $Z_{d-1}$ is $\neq \emptyset$ and $r \neq d - 1$. It belongs to Case 2.2.

These complete the proof of Lemma 3.1.

![Figure 12: $G(l, d-l)$](image)

**Lemma 3.2.** Let $G = G(l, d-l) = K_{n_0} \cup \cdots \cup K_{n_{l-1}} \cup K_{n_l} \cup K_{n_{l+1}} \cdots \cup K_{n_d}$, where $n_0 = n_d = 1$, $n_l \geq 2k$, $n_i = k$ for each $i \in \{1, 2, \ldots, d-1\} \setminus \{l\}$, as shown in Figure 12.

Let $X(G) = (x_0, x_1, \ldots, x_1, \ldots, x_{d-1}, \ldots, x_{d-1}, x_d)^T$ be the Perron vector of the graph $G$.
corresponding to $\lambda_\alpha(G)$, where $x_i = x_{v_i^1} = x_{v_i^2} = \ldots = x_{v_i^{l_i}}$ for each $i = 1, 2, \ldots, d - 1$. If $\alpha \in [0, 1)$, $n_l \geq 2k$, and $l \geq d - l + 1$. Then

(i) $x_{l-1} > \cdots > x_1 > x_0$ and $x_{l+1} > \cdots > x_{d-1} > x_d$.

(ii) $n_l t_l > A t_{l-1}$.

(iii) $x_d > x_0$ and $x_i < x_{d-i}$ for each $i = 1, 2, \ldots, d - l - 1$, where $l \geq d - l + 2$.

Proof. We keep all notations above unless otherwise stated. Let $A_\alpha(G) = \lambda_\alpha$. Since $n_l \geq 2k$, by Lemmas 2.2 and 2.3, then $\lambda_\alpha > \lambda_\alpha(K_k \vee K_{2k}) = 3k - 1$. By Equation (1), we have $\lambda_\alpha x_0 = \alpha k x_0 + (1 - \alpha) k x_1$, then $x_0 = \frac{(1 - \alpha) k x_1 < x_1}$ for any $\alpha \in [0, 1)$.

(i) $x_{l-1} > \cdots > x_1 > x_0$ and $x_{l+1} > \cdots > x_{d-1} > x_d$.

In terms of symmetry, we just consider $i = 0, 1, \ldots, l - 1$. It is similar for $i = l + 1, l + 2, \ldots, d$. Next we are going to consider the following two cases:

Case 1. $l \geq 4$.

By the eigenvalues of $A_\alpha(G)$, we have the following recurrence equations:

$$(1 - \alpha) k x_{i+1} + (2 k \alpha + k - 1 - \lambda_\alpha) x_i + (1 - \alpha) k x_{i-1} = 0, \quad i = 1, 2, \ldots, l - 1.$$  

Let $x_1, x_2, \ldots, x_{l-1}$ be a sequence of numbers satisfying the above recursive formula. Thus its characteristic equation is

$$(1 - \alpha) k t^2 + (2 k \alpha + k - 1 - \lambda_\alpha) t + (1 - \alpha) k = 0.$$  

Notice that $\lambda_\alpha > 3k - 1$, then $(2 k \alpha + k - 1 - \lambda_\alpha)^2 - 4(1 - \alpha)^2 k^2 > 0$, thus Equation (6) has two different real roots $t_1$ and $t_2$ such that

$$t_1 t_2 = 1, \quad t_1 + t_2 = \frac{\lambda_\alpha - 2 k \alpha + 1 - k}{(1 - \alpha) k} > \frac{(3k - 1) - 2 k \alpha + 1 - k}{(1 - \alpha) k} = 2.$$  

It is clear that $t_1 > t_2 > 0$. Since $\lambda_\alpha > 3k - 1$, if $t = 1$, then the Equation (6) is equal to $3k - 1 - \lambda_\alpha < 0$. By Lemmas 2.3 and 2.9(i), for $l \geq d - l + 1 \geq 5$, we have $\lambda_\alpha > \lambda_\alpha(K_k \vee K_{2k} \vee K_k) = \frac{4 \alpha + 3 + \sqrt{16 \alpha^2 - 32 \alpha + 17}}{2} k - 1$, if $t = 2$, then the Equation (6) is equal to $(7 - \alpha) k - 2 - 2 \lambda_\alpha < (4 - 5 \alpha - \sqrt{16 \alpha^2 - 32 \alpha + 17}) k < 0$, that is $t_1 = 2 > 2$. Therefore, we have $t_1 > 2, 1 > t_2 > 0$. By the theory of linear recurrence equation about the sequence, there exist $A$ and $B$ such that $x_i = A t_{i-1}^2 + B t_{i-1}^{l-1}, \quad i = 2, 3, \ldots, l - 2$. The boundary conditions are as follows:

$$\begin{cases}
  x_1 = A + B, \\
  x_2 = A t_1 + B t_2, \\
  \lambda_\alpha x_2 = 2 \alpha k x_1 + (1 - \alpha)(x_0 + (k - 1)x_1 + k x_2).
\end{cases}$$

Then

$$\begin{cases}
  A = \frac{[\lambda_\alpha - (1 + \alpha) k + (1 - \alpha)(1 - t_2 k)] x_1 - (1 - \alpha) x_0}{(1 - \alpha)(t_1 - t_2) k}, \\
  B = \frac{[\lambda_\alpha - (1 + \alpha) k + (1 - \alpha)(1 - t_1 k)] x_1 + (1 - \alpha) x_0}{(1 - \alpha)(t_1 - t_2) k}.
\end{cases}$$

That is,

$$x_i = \frac{(t_i^{l-1} - t_i^{l-1}) ([\lambda_\alpha - (1 + \alpha) k] x_1 + (1 - \alpha)(x_1 - x_0)] - k(1 - \alpha)(t_i^{l-2} - t_i^{l-2}) x_1}{(1 - \alpha)(t_1 - t_2) k}.$$
Thus
\[
\frac{x_i}{x_{i-1}} = \frac{(t_{i-1}^1 - t_{i-2}^1)[(\lambda - (1 + \alpha)k)x_1 + (1 - \alpha)(x_1 - x_0)] - k(1 - \alpha)(t_{i-2}^1 - t_{i-2}^2)x_1}{(t_{i-1}^2 - t_{i-2}^2)[(\lambda - (1 + \alpha)k)x_1 + (1 - \alpha)(x_1 - x_0)] - k(1 - \alpha)(t_{i-3}^1 - t_{i-3}^2)x_1},
\]
where \(i = 2, \ldots, l - 1\).

Since \(t_1 t_2 = 1\), \(t_1 > 2\) and \(1 > t_2 > 0\) for any \(\alpha \in [0, 1]\), then \(t_{i-1}^1 - t_{i-2}^1 = t_1(t_{i-2}^1 - t_{i-2}^2) > t_1(t_{i-2}^1 - t_{i-2}^2) > 2(t_{i-2}^1 - t_{i-2}^2) > 0\).

By using Lemma 2.9(i), we have \(\lambda > \frac{4\alpha + 3 + \sqrt{16\alpha^2 - 32\alpha + 17}}{2}k - 1\). Then for \(k \geq 2\), then we have \(\lambda_{\alpha} - (1 + \alpha)k - k > \frac{2\alpha - 1 + \sqrt{16\alpha^2 - 32\alpha + 17}}{2}k - 1 > 0.93k - 1 > 0\). Thus \(\lambda_{\alpha} - (1 + \alpha)k > k > (1 - \alpha)k\), for any \(\alpha \in (0, 1)\).

Let \(h_1(t_1, t_2) = (t_{i-1}^1 - t_{i-2}^1)[(\lambda - (1 + \alpha)k)x_1 + (1 - \alpha)(x_1 - x_0)] - k(1 - \alpha)(t_{i-2}^1 - t_{i-2}^2)x_1\), and \(h_2(t_1, t_2) = (t_{i-2}^1 - t_{i-2}^2)[(\lambda - (1 + \alpha)k)x_1 + (1 - \alpha)(x_1 - x_0)] - k(1 - \alpha)(t_{i-3}^1 - t_{i-3}^2)x_1\).

Notice that \(x_1 > x_0\), then we have
\[
\begin{align*}
&h_1(t_1, t_2) - h_2(t_1, t_2) = [(t_{i-1}^1 - t_{i-2}^1) - (t_{i-2}^1 - t_{i-2}^2)](\lambda - (1 + \alpha)k)x_1 \\
&+ [(t_{i-3}^1 - t_{i-3}^2) - (t_{i-2}^1 - t_{i-2}^2)](1 - \alpha)kx_1 \\
&+ [(t_{i-1}^1 - t_{i-2}^1) - (t_{i-2}^1 - t_{i-2}^2)](1 - \alpha)(x_1 - x_0) \\
&> [(t_{i-1}^1 - t_{i-2}^1) - (t_{i-2}^1 - t_{i-2}^2)](\lambda - (1 + \alpha)k)x_1 \\
&+ [(t_{i-3}^1 - t_{i-3}^2) - (t_{i-2}^1 - t_{i-2}^2)](1 - \alpha)kx_1 \\
&> (t_{i-1}^1 - t_{i-2}^1) - 2(t_{i-2}^1 - t_{i-2}^2) + (t_{i-3}^1 - t_{i-3}^2)(1 - \alpha)kx_1 \\
&> (t_{i-3}^1 - t_{i-2}^2)(1 - \alpha)kx_1 > 0.
\end{align*}
\]

Thus we have \(x_i > x_{i-1}\), for each \(i = 2, \ldots, l - 1\) when \(l \geq 4\). By symmetry, we have \(x_j > x_{j+1}\), for each \(l + 1 \leq j \leq d - 2\) where \(d - l \geq 4\).

**Case 2.** \(l = 1, 2, 3\).

It is clear that \(x_{l-1} > \cdots > x_1 > x_0\) holds for \(l = 1\) and \(l = 2\). Next we are going to proof that \(x_{l-1} > \cdots > x_1 > x_0\) holds for \(l = 3\), that is \(x_2 > x_1 > x_0\). By the eigenequations of \(A_\alpha(G)\) corresponding to \(x_0\) and \(x_1\), we have
\[
\begin{align*}
\begin{cases}
(1 - \alpha)\frac{kx_1}{x_0} + (k \alpha - \lambda_\alpha) = 0, \\
(1 - \alpha)\frac{kx_2}{x_1} + [(k + 1)\alpha + k - 1 - \lambda_\alpha] + (1 - \alpha)\frac{x_0}{x_1} = 0.
\end{cases}
\end{align*}
\]
Then we have
\[
\begin{align*}
\frac{x_1}{x_0} = & \frac{\lambda_\alpha - k \alpha}{(1 - \alpha)k}, \\
\frac{x_2}{x_1} = & \frac{\lambda_\alpha + 1 - k - (k + 1)\alpha}{(1 - \alpha)k} - \frac{x_0}{kx_1}.
\end{align*}
\]
Thus \(\frac{x_2}{x_1} = \frac{(\lambda_\alpha + 1 - k - (k + 1)\alpha)(\lambda_\alpha - k \alpha) - (1 - \alpha)k}{(\lambda_\alpha - k \alpha)(1 - \alpha)k}\). Let \(g_1 = (\lambda_\alpha + 1 - k - (k + 1)\alpha)(\lambda_\alpha - k \alpha) - (1 - \alpha)k\), \(g_2 = (\lambda_\alpha - k \alpha)(1 - \alpha)k\). Therefore, in order to prove \(\frac{x_2}{x_1} > 1\), we only need to prove \(g_1 - g_2 > 0\). Let \(g_3 = g_1 - g_2\). By direct calculation, we have
\[
g_3 = g_1 - g_2 = \lambda_\alpha^2 + (1 - k \alpha - 2k - \alpha)\lambda_\alpha - k(1 - 2k \alpha - \alpha).
\]
Note that \( g_3 \) is a function of \( \lambda_\alpha \), so \( g_3 = 0 \) has solutions if and only if \((1-k\alpha-2k-\alpha)^2+4k(1-2k\alpha-\alpha) > 0\). Note that \((1-k\alpha-2k-\alpha)^2+4k(1-2k\alpha-\alpha) = (k+1)^2\alpha^2-(4k^2+2k+2)\alpha+4k^2+1\). By direct calculation, it is easy to prove that \((k+1)^2\alpha^2-(4k^2+2k+2)\alpha+4k^2+1 > 0\) holds for \( \alpha \in [0,1) \) and \( k \geq 2 \).

Thus in order to prove \( g_3 = g_1 - g_2 > 0 \), we need to prove that \( \lambda_\alpha \) is greater than the maximum solution of \( g_3 = 0 \), that is \( \lambda_\alpha > \frac{1}{2}(\alpha+\sqrt{(\alpha-\alpha)^2+2}\alpha(\alpha-1)k+1+1) \). Notice that \( \lambda_\alpha > 3k-1 \), then we need to prove that \( 3k-1 > \frac{1}{2}(\alpha+\sqrt{(\alpha-\alpha)^2+2}\alpha(\alpha-1)k+1+1) \).

By the eigenequation corresponding to \( x \), we have \( g_4 = (12-4\alpha)k^2-(4\alpha+8)k+4\alpha > 0 \). Let \( g_4 = (12-4\alpha)k^2-(4\alpha+8)k+4\alpha \). By direct calculation, we have \((4\alpha+8)^2-16\alpha(12-4\alpha) = 16(5\alpha^2-8\alpha+4) > 0\) holds for each \( \alpha \in [0,1) \). Thus, if \( k \) is greater than the maximum solution of \( g_4 = 0 \), then \( g_4 > 0 \). By direct calculation, we have the maximum solution of \( g_4 = 0 \) is \( \frac{\alpha+\sqrt{(5\alpha^2-8\alpha+4)^2}}{2(3-\alpha)} \in [0.6667,1) \) for each \( \alpha \in [0,1) \). Thus \( g_4 > 0 \) holds for each \( k \geq 2 \) and each \( \alpha \in [0,1) \). Thus \( g_3 = g_1 - g_2 > 0 \). Then \( \frac{\alpha}{x_1} > 1 \).

Thus we have \( x_i > x_{i-1} \), for each \( i = 2, \ldots, l-1 \) when \( 1 \leq l \leq 3 \). By symmetry, we have \( x_j > x_{j+1} \), for each \( l+1 \leq j \leq d-2 \) when \( 1 \leq d-l \leq 3 \).

These complete the proof of (i) in this Lemma 3.2. Next we are going to prove \( n_i x_l > k x_{l-1} \).

(ii) \( n_i x_l > k x_{l-1} \).

By the eigenequation corresponding to \( x_{l-1} \), that is

\[
(1-\alpha)\frac{n_i x_l}{x_{l-1}} + [(n_i + k)\alpha + k - 1 - \lambda_\alpha] + (1 - \alpha)\frac{k x_{l-2}}{x_{l-1}} = 0.
\]

Note that \( k \geq 2 \), \( x_{l-1} > x_{l-2} \) and \( \alpha \in [0,1) \). Then we have

\[
\frac{n_i x_l}{k x_{l-1}} = \frac{1}{k(1-\alpha)}[-(n_i + k)\alpha + k - 1 + \lambda_\alpha] - \frac{x_{l-2}}{x_{l-1}},
\]

\[
> \frac{1}{k(1-\alpha)}[-(n_i + k)\alpha + k - 1 + \lambda_\alpha] - 1,
\]

\[
> \frac{1}{k(1-\alpha)}[-(n_i + k)\alpha + k - 1 + (n_i + k - 1)] - 1 > 1.
\]

Thus we have \( n_i x_l > k x_{l-1} \). These complete the proof of the first and second results (i) and (ii) in this Lemma 3.2.

(iii) \( x_d > x_0 \) and \( x_i < x_{d-i} \) for each \( i = 1, 2, \ldots, d-1 \), where \( l \geq d - l + 2 \).
By the eigenequations of $A_\alpha(G)$, we have

$$
\begin{aligned}
(1-\alpha)\frac{kx_1}{x_0} + (k\alpha - \lambda_\alpha) &= 0, \\
(1-\alpha)\frac{kx_2}{x_1} + [(k+1)\alpha + k - 1 - \lambda_\alpha] + (1-\alpha)\frac{x_2}{x_1} &= 0, \\
(1-\alpha)\frac{kx_3}{x_2} + (2k\alpha + k - 1 - \lambda_\alpha) + (1-\alpha)\frac{kx_1}{x_2} &= 0, \\
&\vdots \\
(1-\alpha)\frac{kx_{d-1}}{x_d} + (2k\alpha + k - 1 - \lambda_\alpha) + (1-\alpha)\frac{kx_{d-3}}{x_{d-2}} &= 0, \\
(1-\alpha)\frac{kx_d}{x_{d-1}} + (2k\alpha + k - 1 - \lambda_\alpha) + (1-\alpha)\frac{kx_{d-2}}{x_{d-1}} &= 0, \\
&\vdots \\
(1-\alpha)\frac{kx_{d-1}}{x_d} + (2k\alpha + k - 1 - \lambda_\alpha) + (1-\alpha)\frac{kx_{d-3}}{x_{d-2}} &= 0, \\
&\vdots
\end{aligned}
$$

Since $l \geq d-l+1$ and $k \geq 2$, then

$$
\frac{kx_{d-1}}{x_d} = \frac{kx_1}{x_0}, \quad \frac{kx_{d-2}}{x_{d-1}} = \frac{kx_2}{x_1}, \ldots, \quad \frac{kx_{l+1}}{x_{l+2}} = \frac{kx_{d-l-1}}{x_d}.
$$

Notice that $n_l \geq 2k$, by the eigenequations corresponding to $x_{d-l-1}, x_{l+1}$, these are

$$
\begin{aligned}
(1-\alpha)\frac{kx_{d-1}}{x_d} + (2k\alpha + k - 1 - \lambda_\alpha) + (1-\alpha)\frac{kx_{d-1}}{x_{d-l-1}} &= 0, \\
(1-\alpha)\frac{n_l}{x_{l+1}} + [(n_l + k)\alpha + k - 1 - \lambda_\alpha] + (1-\alpha)\frac{x_{d-l}}{x_{d-l-1}} &= 0.
\end{aligned}
$$

Thus $\frac{kx_{d-l}}{x_{d-l-1}} > \frac{n_l}{x_{l+1}}$. Since $n_l x_l > k x_{d-l}$, then $x_{d-l-1} < x_{l+1}$, by Equation (7), we have $x_i < x_{d-i}$ and $x_d > x_0$, for each $i = 1, 2, \ldots, d-l-1$.

These complete the proof of this Lemma 3.2.

In the following, we use all the notations in Lemma 3.2 unless otherwise stated.

**Lemma 3.3.** Let $G = G(l, d-l)$ be a maximal graph in $G_{n,k}^d$. Suppose $l \geq d-l+2$, then $x_{d-i+1} < x_i, \quad i = 1, 2, \ldots, d-l-1$.

**Proof.** By Lemma 3.2, we have $x_0 < x_d$, so $x_{d-i} \neq x_i, \quad i = 1, 2, \ldots, d-l-1$. Recall that $Z = Z_l = \{V_l \setminus V(K_k)\}$. Let $G'$ be a graph obtained from the maximal graph $G$ by deleting all edges between $Z$ and $V_{l+1}$ and adding all edges between $Z$ and $V_{l-2}$. If $x_l-2 \geq x_{l+1}$, then by Lemma 2.8, we have $\lambda_\alpha(G') > \lambda_\alpha(G)$. Thus this contradicts that $G$ is the maximal graph in $G_{n,k}^d$. Thus $x_{l-2} < x_{l+1}$. Similarly, we have $x_{l-1} > x_{l+2}$. Next we prove $x_d < x_1$.

Suppose $x_d > x_1$. We select one vertex $w$ of $V_1$. Since $n_0 = n_d = 1$, then we denote the two vertices in $V_0, V_d$ as $u, v$, respectively. Let $G''$ be a graph obtained from $G$ by deleting
all edges between $V_1 \setminus \{w\}$ and $w$, all edges between $V_1 \setminus \{w\}$ and $V_2$, edge $wu$, and adding edge $vu$, all edges between $V_1 \setminus \{w\}$ and $V_{d-1}$, all edges between $V_1 \setminus \{w\}$ and $v$. Obviously, $G'' \in G^d_{n,k}$. Then

$$0 > \lambda_\alpha(G'') - \lambda_\alpha(G) > (1 - \alpha)[(k-1)x_1(x_{d-1} - x_2) + (k-1)x_1(x_d - x_1) + x_0(x_d - x_1)]$$

$$+ \alpha[(k-1)(x^2_{d-1} - x^2_2) + k(x^2_d - x^2_1)]$$

$$> (1 - \alpha)k(k-1)x_1(x_{d-1} - x_2) + \alpha(k-1)(x^2_{d-1} - x^2_2).$$

Thus if $x_d > x_1$, then $x_{d-1} < x_2$ holds.

Next we obtain the graph $G''$ by using a different edge-shifting operation. Let $G''$ be the graph obtained from $G$ by deleting all edges between $V_{d-2}$ and $V_{d-1}$, all edges between $V_2$ and $V_3$ and adding all edges between $V_{d-2}$ and $V_2$, all edges between $V_{d-1}$ and $V_3$. Then we have

$$0 > \lambda_\alpha(G'') - \lambda_\alpha(G) > (1 - \alpha)k^2(x_{d-2} - x_3)(x_2 - x_{d-1}).$$

Thus if $x_d > x_1$ and $x_{d-1} < x_2$, then $x_{d-2} < x_3$ holds. Through gradual recursion, let $G''$ be the graph obtained from $G$ by deleting all edges between $V_j$ and $V_{j+1}$, all edges between $V_{d-j}$ and $V_{d-j+1}$ and adding all edges between $V_j$ and $V_{d-j}$, all edges between $V_{j+1}$ and $V_{d-j+1}$, for $j = 2, \ldots, l - 2$. Thus we have if $x_d > x_1$, then $x_{d-1} < x_2$, $x_{d-2} < x_3$, $x_{l-1} < x_{d-l} < x_{d-l+1} < \ldots < x_{l-2}$. There is a contradiction that $x_{l-2} < x_{l+1}$ in the maximal graph $G$. Thus $x_d < x_1$.

Assume $x_{d-i+1} < x_i$ for $i = 1, 2, \ldots, d - l - 2$, and we now prove $x_{d-i} < x_{i+1}$. Let $G''$ be a graph obtained from $G$ by deleting all edges between $V_i$ and $V_{i+1}$, all edges between $V_{d-i}$ and $V_{d-i+1}$ and adding all edges between $V_i$ and $V_{d-i}$, all edges between $V_{i+1}$ and $V_{d-i+1}$. Then

$$0 > \lambda_\alpha(G'') - \lambda_\alpha(G) > (1 - \alpha)k^2(x_{d-i} - x_{i+1})(x_i - x_{d-i+1}).$$

Since $x_i > x_{d-i+1}$, we have $x_{d-i} < x_{i+1}$, for each $i = 1, 2, \ldots, d - l - 2$. These complete the proof. 

Now we have all the ingredients to present our proof of Theorem 1.2.

**Proof of Theorem 1.2.** In this proof, we use the notations in Lemma 3.2 unless otherwise stated. Let $G^* = G(l, d-l) = K_{n_0} \lor \cdots \lor K_{n_{l-1}} \lor K_{n_l} \lor K_{n_{l+1}} \lor \cdots \lor K_{n_d}$, where $n_0 = n_d = 1$, $n_l \geq 2k$, $n_i = k$, $i \in \{1, 2, \ldots, d - 1\} \setminus \{l\}$, as shown in Figure 12. By Lemma 3.1, the result hold when $d = 2$ or 3. Thus we only consider the case $d \geq 4$ in the following.

In order to prove a contradiction, we suppose $l \geq d - l + 2$. Let $G''$ be a graph obtained from $G^*$ by deleting all the edges between $V_i$ and $V_{i+1}$ and the edges between $V_{d-l+1}$ and $V_{d-l+2}$, then adding all the edges between $V_{i+1}$ and $V_{d-l+2}$ and the edges between $V_i$ and $V_{d-l+1}$. Evidently, $G'' = G(l-1, d-l+1) \in G^d_{n,k}$. Note that $n_{i+1} x_i > k x_{l-1} > k x_{d-l+2}$ by Lemma 3.2 and $x_{l+1} > x_{l-2} > x_{l-1} > x_{d-l+1}$. Then from Equation 2 we have

$$\lambda_\alpha(G'') - \lambda_\alpha(G^*) \geq (1 - \alpha)[-n_l n_{d-l+1} x_l x_{l+1} - n_{d-l+1} n_{d-l+2} x_{d-l+1} x_{d-l+2} + n_{l+1} n_d x_{l+1} x_{d-l+2} + n_{l+1} n_{d-l+1} x_{l+1} x_{d-l+1}]$$

$$+ \alpha[(n_l - n_{d-l+1}) x^2_{d-l+1} + (n_{l+1} - n_{d-l+1}) x^2_{d-l+2} + (n_l - n_{d-l+2}) x^2_{l+1}].$$

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\[
\geq (1 - \alpha)(n_{d-l+1}x_{d-l+1} - n_{l+1}x_{l+1})(n_lx_l - n_{d-l+2}x_{d-l+2}) + \\
\alpha(2k + 1 - 2k)x_{d-l+1}^2 \geq 0.
\]

Thus \(\lambda_\alpha(G'') > \lambda_\alpha(G^*)\), which contradicts the fact that \(G^*\) is the maximal graph in \(G_{n,k}^k\). Thus we have \(l \leq d - l + 1\).

Notice that \(\Delta(G^*) = (n_\lfloor d \rfloor + 2k - 1)\), by Lemmas 2.5 and 2.6, our conclusion can be obtained directly. These complete the proof.

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