On the A_α-index of C_4-free graphs with given order or size

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Abstract

For a graph G and a real number $\alpha \in [0,1]$, Nikiforov (2017) proposed the A_α-matrix for G, which is defined as $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$, where $A(G)$ and $D(G)$ are the adjacency matrix and the degree diagonal matrix of G, respectively. The largest eigenvalue of $A_\alpha(G)$ is called the A_α-index of G. Let $\mathcal{F}$ be a set of graphs, we say a graph G is $\mathcal{F}$-free if it does not contain a member in $\mathcal{F}$ as a subgraph. In 2010, Nikiforov conjectured that for n large enough, the $\{C_{2k+1}, C_{2k+2}\}$-free graph of maximum spectral radius is $S_{n,k}$, the join of a clique on k vertices with an independent set of $n-k$ vertices and that the C_{2k+2}-free graph of maximum spectral radius is $S_{n,k}^{+}$, the graph obtained from $S_{n,k}$ by adding one edge. Cioabă, Desai and Tait (2022) used a novel method to solve this two-part conjecture. We also note that the well-known Mantel's theorem, which claims that every graph of order n with size $m > \lfloor n/4 \rfloor$ contains a triangle. Recently, Zhai and Shu (2022) obtained a spectral version of Mantel's theorem. In this paper, on the one hand, with the aid of Cioabă-Desai-Tait's novel method, we identify the graphs with the first two largest A_α-indices among the n-vertex C_4-free graphs for $0 < \alpha < 1$ and $n \geqslant \frac{9}{\alpha^6}$. On the other hand, with the help of Zhai-Shu's eigenvector method, we identify the C_4-free graphs (other than the star) of size m with no isolated vertex having the largest A_α-index for $\frac{1}{2} \leqslant \alpha < 1$ and $m \geqslant 3$. Our results improve some known ones of Tian, Chen, Cui (2021), Guo, Zhang (2022), Feng, Wei (2022) and Li, Qin (2021).

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1 Introduction

Let $\mathcal{F}$ be a set of graphs and let G be a graph. We say that G is *$\mathcal{F}$-free* if it does not contain any graph in $\mathcal{F}$ as a subgraph. In particular, if $\mathcal{F} = \{F\}$, we also say that G is

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F-free. As usual, let P_n, C_n and K_n be the path, the cycle and the complete graph on n vertices, respectively. And let $K_{a,b}$ be the complete bipartite graph with the sizes of partite sets being a and b, respectively.

In 2013, Füredi and Simonovits [7] posed the following problem:

Problem 1 (Füredi-Simonovits type problem)**.** Assume $\mathbb{U}$ is a family of graphs and G is in $\mathbb{U}$. For a specific pair of parameters (τ, υ) on G, our aim is to maximize the second parameter υ under the condition that G is $\mathcal{F}$-free and its first parameter τ is given.

For a simple graph $G = (V(G), E(G))$, we use $n := |V(G)|$ and $m := |E(G)|$ to denote the *order* and the *size* of G, respectively. With no confusion, we also use the *size* to denote the cardinality of a set.

If the pair of parameters in Problem 1 are the order and size of a graph, i.e., $(\tau, \upsilon) = (n, m)$, then the Füredi-Simonovits type problem is just the classical Turán type problem: Determine the maximum number of edges, $\mathrm{ex}(n, \mathcal{F})$, of an n-vertex $\mathcal{F}$-free graph. The value $\mathrm{ex}(n, \mathcal{F})$ is called the *Turán number* of $\mathcal{F}$. The research for the Turán number attracts much attention, and it has become to be one of the most attractive fundamental problems in extremal graph theory (see [7, 24] for surveys). Up till now, the exact value of $\mathrm{ex}(n, C_{2k})$ is still unknown, even for $k = 2$.

Let G be a graph of order n. We say that two vertices u and v in G are *adjacent* (or *neighbours*) if they are joined by an edge and we write it as $u \sim v$. Then the *adjacency matrix* of G is defined as an $n \times n$ $(0, 1)$-matrix $A(G) = (a_{ij})$ with $a_{ij} = 1$ if and only if $v_i \sim v_j$. The *degree* $d_G(u)$ of a vertex u (in a graph G) is the number of edges incident with it. Then the *degree diagonal matrix* of G is defined as an $n \times n$ diagonal matrix $D(G) = \mathrm{diag}(d_G(v_1), \ldots, d_G(v_n))$. In 2017, Nikiforov [25] proposed the A_α-*matrix* of G, which is a convex combination of $D(G)$ and $A(G)$, i.e.,

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G), \ \ \alpha \in [0,\, 1].$$

It is obvious that $A_0(G) = A(G)$, $A_{\frac{1}{2}}(G) = \frac{1}{2}Q(G)$ and $A_1(G) = D(G)$, where $Q(G) = D(G) + A(G)$ is the *signless Laplacian matrix* of G.

Note that $A_\alpha(G)$ is real symmetric, its *eigenvalues* are real. The largest eigenvalue of $A_\alpha(G)$ is called the A_α-*index* of G, denoted by $\lambda_\alpha(G)$ as usual. The A_0-index (resp. twice of $A_{\frac{1}{2}}$-index) of G is usually referred to as the *index* (resp. Q-*index*) of G, denoted by $\rho(G)$ (resp. $q(G)$). If G is connected and $\alpha \neq 1$, then the matrix $A_\alpha(G)$ is non-negative and irreducible. From Perron-Frobenius theorem, for $\alpha \in [0, 1)$, there exists a unique (up to multiples) positive eigenvector of $A_\alpha(G)$ corresponding to $\lambda_\alpha(G)$, we call this vector the *Perron vector* of $A_\alpha(G)$.

In Problem 1, if one lets $(\tau, \upsilon) = (n, \rho(G))$, i.e., the pair of parameters are the order and the index on $\mathbb{U}$, then it becomes to be the spectral Turán type problem (also known as Brualdi-Solheid-Turán type problem, see [3]): What is the maximum index of an $\mathcal{F}$-free graph with order n? Over the past decade, much attention has been paid to the Brualdi-Solheid-Turán type problem. For more details, one may see [4, 12, 23, 29, 31, 32, 33, 35] and a survey [15].

Let G and H be two disjoint graphs. The *union* of G and H is denoted by $G \cup H$. The *join* of G and H, denoted by $G \vee H$, is the graph obtained from $G \cup H$ by joining each vertex of G to each vertex of H. Then for odd $n \geqslant 3$, define $F_n = K_1 \vee \frac{n-1}{2} K_2$; for even $n \geqslant 4$, define $F_n = K_1 \vee (\frac{n-2}{2} K_2 \cup K_1)$. Nikiforov [22] solved the spectral Turán type problem for C_4.

Theorem 2 ([22])**.** *Let G be a graph of order n with $\rho(G) = \rho$. If G is C_4-free, then $\rho^2 - \rho - (n-1) \leqslant 0$. Equality holds if and only if n is odd and $G \cong F_n$.*

When the order of G is even, Zhai and Wang [37] extended the above result as follows.

Theorem 3 ([37])**.** *Let G be a graph of even order n with $\rho(G) = \rho$. If G is C_4-free, then $\rho^3 - \rho^2 - (n-1)\rho + 1 \leqslant 0$. Equality holds if and only if $G \cong F_n$.*

In Problem 1, if one lets $(\tau, \upsilon) = (m, \rho(G))$, i.e., the pair of parameters are the size and the index on $\mathbb{U}$, then it becomes to be another spectral Turán type problem (also known as Brualdi-Hoffman-Turán type problem, see [2]): What is the maximum index of an $\mathcal{F}$-free graph with size m? Nosal [27] solved this spectral Turán type problem for triangle. Nikiforov [19, 20] solved this spectral Turán type problem for K_{r+1}. Over the past three years, much attention has been focused on this spectral Turán type problem. For more details, one may see [5, 16, 17, 18, 28, 34].

Note that Nikiforov [22] solved Brualdi-Hoffman-Turán type problem for C_4, which is described as follows.

Theorem 4 ([22])**.** *Let G be a graph of size $m \geqslant 10$ with no isolated vertex. If G is C_4-free, then $\rho(G) \leqslant \rho(K_{1,m})$. Equality holds if and only if $G \cong K_{1,m}$.*

Let $K_{1,m-1} + e$ be the graph obtained from $K_{1,m-1}$ by adding an edge within its independent set. Following Theorem 4, Zhai and Shu [36] considered the spectral Turán type problem for C_4 in non-bipartite graphs and obtained the following result.

Theorem 5 ([36])**.** *Let G be a non-bipartite graph of size $m \geqslant 26$ with no isolated vertex. If G is C_4-free, then $\rho(G) \leqslant \rho(K_{1,m-1} + e)$. Equality holds if and only if $G \cong K_{1,m-1} + e$.*

In Problem 1, if one lets $(\tau, \upsilon) = (n, \lambda_\alpha(G))$, i.e., the pair of parameters are the order and the A_α-index on $\mathbb{U}$, then it becomes to be the A_α-spectral Turán type problem posed by Nikiforov [25]:

Problem 6 ([25])**.** Given a graph F, what is the maximum $\lambda_\alpha(G)$ of an F-free graph G of order n?

Nikiforov [25] solved Problem 6 for K_r; the authors of the current paper [13] solved Problem 6 for C_{2k}, where $k \geqslant 3$. The authors of the current paper and Zhang [14] solved Problem 6 for disjoint cycles. Tian, Chen, Cui [30] and Guo, Zhang [10], independently, considered Problem 6 for C_4.

Let $\mathcal{G}(n, C_4)$ denote the set of C_4-free graphs of order n, and let $F_n - e$ be the graph obtained from F_n by deleting the edge e which joins two vertices of degree 2 in F_n.

Theorem 7 ([30, 10])**.** *Let $n \geqslant 4$ and let $\alpha \in [\frac{1}{2}, 1)$. If $G \in \mathcal{G}(n, C_4)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(F_n)$ and equality holds if and only if $G \cong F_n$.*

Motivated by Theorem 7, our first result solves Problem 6 for C_4, which extends the result of Theorem 7.

Theorem 8. *Let $0 < \alpha < 1$ be given, and let $n \geqslant \frac{9}{\alpha^6}$.*

- (i) *If $G \in \mathcal{G}(n, C_4)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(F_n)$ with equality if and only if $G \cong F_n$.*
- (ii) *If $G \in \mathcal{G}(n, C_4) \backslash F_n$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(F_n - e)$ with equality if and only if $G \cong F_n - e$.*

In Problem 1, if one lets $(\tau, \upsilon) = (m, \lambda_\alpha(G))$, i.e., the pair of parameters are the size and the A_α-index on $\mathbb{U}$, then it becomes to be another A_α-spectral Turán type problem:

Problem 9. Given a graph F, what is the maximum $\lambda_\alpha(G)$ of an F-free graph G of size m with no isolated vertex?

In this paper, we consider Problem 9 when $F = C_4$ for $\frac{1}{2} \leqslant \alpha < 1$. Let $\mathcal{H}(m)$ denote the set of graphs of size m with no isolated vertex, and let $\mathcal{H}(m, C_4)$ denote the set of C_4-free graphs of size m with no isolated vertex. Feng, Wei [6] and Li, Qin [11], independently, determined the graphs with maximum A_α-index over $\mathcal{H}(m)$ for $\frac{1}{2} \leqslant \alpha < 1$.

Theorem 10 ([6, 11])**.** *Let $\frac{1}{2} \leqslant \alpha < 1$ be given. If $G \in \mathcal{H}(m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{1,m})$. Equality holds if and only if $G \cong K_{1,m}$, unless $\alpha = \frac{1}{2}$ and $m = 3$, in which case equality holds if and only if $G \cong K_{1,3}$ or $G \cong K_3$.*

Note that both $K_{1,m}$ and K_3 are C_4-free. By Theorem 10, the following result is clear.

Corollary 11. *Let $\frac{1}{2} \leqslant \alpha < 1$ be given. If $G \in \mathcal{H}(m, C_4)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{1,m})$. Equality holds if and only if $G \cong K_{1,m}$, unless $\alpha = \frac{1}{2}$ and $m = 3$, in which case equality holds if and only if $G \cong K_{1,3}$ or $G \cong K_3$.*

Based on Corollary 11, and motivated by Theorem 5, our second main result is given by:

Theorem 12. *Let $\frac{1}{2} \leqslant \alpha < 1$ be given, and let $m \geqslant 3$. If $G \in \mathcal{H}(m, C_4) \backslash K_{1,m}$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{1,m-1} + e)$. Equality holds if and only if $G \cong K_{1,m-1} + e$.*

As $K_{1,m}$ is bipartite, and $K_{1,m-1} + e$ is non-bipartite. From Theorem 12, we can obtain the following corollary immediately.

Corollary 13. *Let $\frac{1}{2} \leqslant \alpha < 1$ be given, and let G be a non-bipartite graph of size $m \geqslant 3$ with no isolated vertex. If G is C_4-free, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{1,m-1} + e)$. Equality holds if and only if $G \cong K_{1,m-1} + e$.*

Outline of our paper. In the remainder of this section, we introduce some necessary notations and terminologies. In Section 2, we give some necessary preliminaries. In Section 3, we progressively refine the structure of our extremal graphs and complete the proof of Theorem 8, finally. The techniques used in the proof of Theorem 8 is originated from Cioabă, Desai and Tait [4]. In Section 4, we complete the proof of Theorem 12, the technique in our proof borrows some ideas from Zhai and Shu [36].

Notations and terminologies. In this paper, we consider only simple and finite graphs. Unless otherwise stated, we follow the traditional notations and terminologies (see, for instance, Bollobás [1], Godsil and Royle [8]). For two disjoint vertex subsets V_1 and V_2 of $V(G)$, denote by $G[V_1]$ a subgraph of G induced on V_1 and $G[V_1, V_2]$ a subgraph of G induced on the edges between V_1 and V_2. Then the number of edges of $G[V_1]$ and $G[V_1, V_2]$ can be abbreviated to $e(V_1)$ and $e(V_1, V_2)$, respectively. The *set of neighbours* of a vertex v (in a graph G) is denoted by $N_G(v)$. The *maximum degree* and *minimum degree* of G are denoted by $\Delta(G)$ and $\delta(G)$, respectively.

2 Preliminaries

Lemma 14 ([21])**.** *Assume that $k \geqslant 1$ and let the vertex set of a graph G be partitioned into two sets U and W. If*

$$2e(U) + e(U, W) > (2k-1)|U| + k|W|,$$

then there exists a path of order $2k+1$ with both ends in U.

Lemma 15 ([25])**.** *Let G be a graph, for $0 \leqslant \alpha \leqslant 1$, one has*

$$\alpha\Delta(G) \leqslant \lambda_\alpha(G) \leqslant \alpha\Delta(G) + (1-\alpha)\rho(G).$$

Lemma 16 ([25])**.** *Let G be a graph, for $\frac{1}{2} \leqslant \alpha < 1$, one has*

$$\lambda_\alpha(G) \geqslant \alpha\Delta(G) + \frac{(1-\alpha)^2}{\alpha}.$$

Lemma 17 ([4])**.** *Let B be a non-negative symmetric matrix, and let $\mathbf{y}$ be a non-negative non-zero vector. If there is a constant $c > 0$ such that $B\mathbf{y} \geqslant c\mathbf{y}$ entrywise, then $\lambda(B) \geqslant c$, where $\lambda(B)$ is the largest eigenvalue of B.*

Lemma 18 ([26])**.** *Let $\alpha \in [0, 1)$ and let G be a connected graph with Perron vector $\mathbf{x}$. Suppose that $u, v \in V(G)$ and $S \subseteq V(G)$ satisfy $u, v \notin S$ and for every $w \in S$, $w \sim u$ and $w \nsim v$. Let H be the graph obtained from G by deleting the edges wu and adding the edges wv for all $w \in S$. If S is nonempty and $\mathbf{x}_v \geqslant \mathbf{x}_u$, then $\lambda_\alpha(H) > \lambda_\alpha(G)$.*

Lemma 19 ([13])**.** *Let G be a connected graph and let $\mathbf{y}$ be a Perron vector of $A_\alpha(G)$. Then, for each $v \in V(G)$, one has*

$$\lambda_\alpha^2(G)\mathbf{y}_v = \alpha d_G(v)\lambda_\alpha(G)\mathbf{y}_v + \alpha(1-\alpha)\sum_{u\sim v} d_G(u)\mathbf{y}_u + (1-\alpha)^2\sum_{w\sim v}\sum_{u\sim w}\mathbf{y}_u. \tag{1}$$

3 Proof of Theorem 8

For $\alpha \in (0,1)$ and $n \geqslant 3$, let G (resp. G') be a graph in $\mathcal{G}(n, C_4)$ (resp. $\mathcal{G}(n, C_4)\backslash F_n$) with maximum A_α-index. (Note that G and G' depend on α and n.) In this section, we are going to progressively refine the structure of our extremal graphs G and G', and complete the proof of Theorem 8, finally.

Our first lemma shows both G and G' are connected.

Lemma 20. *If $n \geqslant 5$, then the graphs G and G' are connected.*

Proof. By the Perron-Frobenius theory, adding an edge between two components of a disconnected graph does not create any quadrilaterals and increases the A_α-index strictly. The graph G is connected.

On the other hand, suppose to the contrary that G' is not connected. Let G_1 and G_2 be two components of G' with $\lambda_\alpha(G_2) \leqslant \lambda_\alpha(G_1) = \lambda_\alpha(G')$. Take a vertex $u \in V(G_1)$ with $d_{G_1}(u) = \delta(G_1)$ and an arbitrary vertex $v \in V(G_2)$. Let $G'' = G' + uv$. As $n \geqslant 5$, G'' is C_4-free and $G'' \ncong F_n$, i.e., $G'' \in \mathcal{G}(n, C_4)\backslash F_n$. However, by the Perron-Frobenius theory, $\lambda_\alpha(G'') > \lambda_\alpha(G_1) = \lambda_\alpha(G')$, a contradiction to the choice of G'. □

The following lemma establishes a lower bound and an upper bound on $\lambda_\alpha(G)$ and $\lambda_\alpha(G')$, which will be used frequently in this section.

Lemma 21. *Let $0 < \alpha < 1$ be given. One has*

$$\alpha(n-1) \leqslant \lambda_\alpha(G') \leqslant \lambda_\alpha(G) \leqslant \alpha(n-1) + (1-\alpha)\frac{1+\sqrt{4n-3}}{2}.$$

Proof. Note that $F_n - e \in \mathcal{G}(n, C_4)\backslash F_n$, by the definition of G', one has $\lambda_\alpha(G') \geqslant \lambda_\alpha(F_n - e)$. Then by Lemma 15,

$$\lambda_\alpha(G') \geqslant \lambda_\alpha(F_n - e) \geqslant \alpha\Delta(F_n - e) = \alpha(n-1).$$

According to the definition of G and G', $\lambda_\alpha(G') \leqslant \lambda_\alpha(G)$ is clear.

On the other hand, as G is C_4-free. By Theorem 2 and Lemma 15, one has

$$\lambda_\alpha(G) \leqslant \alpha\Delta(G) + (1-\alpha)\rho(G) \leqslant \alpha(n-1) + (1-\alpha)\frac{1+\sqrt{4n-3}}{2}.$$

This completes the proof. □

In what follows, we fix $0 < \alpha < 1$ and $n \geqslant \frac{9}{\alpha^6}$. In this section, we denote by $\lambda_\alpha := \lambda_\alpha(G)$ and $\lambda'_\alpha := \lambda_\alpha(G')$. Let $\mathbf{x}$ (resp. $\mathbf{y}$) be the Perron vector of $A_\alpha(G)$ (resp. $A_\alpha(G')$) whose maximum entry is equal to 1, and let z (resp. z') be a vertex in G (resp. G') with $\mathbf{x}_z = \mathbf{y}_{z'} = 1$.

Denote by $V := V(G)$, $V' := V(G')$, and let

$$L = \left\{v \in V | \mathbf{x}_v \geqslant \frac{2}{3}\right\}, \quad S = \left\{v \in V | \mathbf{x}_v < \frac{2}{3}\right\};$$

$$L' = \left\{ v \in V' | \mathbf{y}_v \geqslant \frac{2}{3} \right\}, \quad S' = \left\{ v \in V' | \mathbf{y}_v < \frac{2}{3} \right\}.$$

For $v \in V$ and $v' \in V'$, denote by $d(v) := d_G(v)$, $d'(v') := d_{G'}(v')$. And let $N_G^2(v)$ (resp. $N_{G'}^2(v')$) be the set of vertices at distance 2 from $v \in V$ (resp. $v' \in V'$).

As G and G' are both C_4-free, for each $v \in V$ and $v' \in V'$, $G[N_G(v) \cup N_G^2(v)]$ (resp. $G'[N_{G'}(v') \cup N_{G'}^2(v')]$) contains no P_3 with both endpoints in $N_G(v)$ (resp. $N_{G'}(v')$). Then by Lemma 14, one has

$$2e(N_G(v)) + e(N_G(v), N_G^2(v)) \leqslant n - 1 \text{ and } 2e(N_{G'}(v')) + e(N_{G'}(v'), N_{G'}^2(v')) \leqslant n - 1. \tag{2}$$

The next lemma shows the vertices in L (resp. L') have "large" degrees in G (resp. G').

Lemma 22. *For all $v \in L$ and $v' \in L'$, one has $d(v) \geqslant n - \sqrt{n}$ and $d'(v') \geqslant n - \sqrt{n}$.*

Proof. Suppose to the contrary that there is a vertex $v \in L$ such that $d(v) < n - \sqrt{n}$. Applying (1) to v, one has

$$\begin{aligned}
\lambda_\alpha^2 \mathbf{x}_v =& \alpha d(v)\lambda_\alpha \mathbf{x}_v + \alpha(1-\alpha)\sum_{u\sim v} d(u)\mathbf{x}_u + (1-\alpha)^2 \sum_{w\sim v}\sum_{u\sim w} \mathbf{x}_u \\
\leqslant& \alpha d(v)\lambda_\alpha \mathbf{x}_v + \alpha(1-\alpha)[d(v) + 2e(N_G(v)) + e(N_G(v), N_G^2(v))] \\
&+ (1-\alpha)^2[d(v) + 2e(N_G(v)) + e(N_G(v), N_G^2(v))] \\
\leqslant& \alpha d(v)\lambda_\alpha \mathbf{x}_v + (1-\alpha)(d(v) + n - 1). \qquad \text{(by (2))}
\end{aligned}$$

That is

$$\lambda_\alpha(\lambda_\alpha - \alpha d(v))\mathbf{x}_v \leqslant (1-\alpha)(d(v) + n - 1) < (1-\alpha)(2n - \sqrt{n} - 1). \tag{3}$$

On the other hand, as $d(v) < n - \sqrt{n}$. By Lemma 15 and the definition of L, one has

$$\lambda_\alpha(\lambda_\alpha - \alpha d(v))\mathbf{x}_v > \alpha(n-1)[\alpha(n-1) - \alpha(n - \sqrt{n})] \cdot \frac{2}{3} = \frac{2}{3}\alpha^2(n-1)(\sqrt{n} - 1).$$

Together with (3), one has

$$\frac{2}{3}\alpha^2(n-1)(\sqrt{n}-1) < (1-\alpha)(2n - \sqrt{n} - 1).$$

This is equivalent to

$$\frac{2}{3}\alpha^2(\sqrt{n})^3 - \left(\frac{2}{3}\alpha^2 + 2 - 2\alpha\right)(\sqrt{n})^2 - \left(\frac{2}{3}\alpha^2 - 1 + \alpha\right)\sqrt{n} + \frac{2}{3}\alpha^2 + 1 - \alpha < 0. \tag{4}$$

Note that $n \geqslant \frac{9}{\alpha^6}$. By (4), one has

$$\left(\frac{2}{\alpha} - \frac{2}{3}\alpha^2 - 2 + 2\alpha\right)(\sqrt{n})^2 - \left(\frac{2}{3}\alpha^2 - 1 + \alpha\right)\sqrt{n} + \frac{2}{3}\alpha^2 + 1 - \alpha < 0. \tag{5}$$

Since $\frac{2}{\alpha} - \frac{2}{3}\alpha^2 - 2 + 2\alpha \geqslant 4 - \frac{2}{3}\alpha^2 - 2 > 1$, $n \geqslant \frac{9}{\alpha^6}$, it can be deduced from (5) that

$$\left(\frac{3}{\alpha^3} - \frac{2}{3}\alpha^2 + 1 - \alpha\right)\sqrt{n} + \frac{2}{3}\alpha^2 + 1 - \alpha < 0,$$

a contradiction. Therefore, for all $v \in L$, one has $d(v) \geqslant n - \sqrt{n}$.

By a similar discussion as above, we can show $d'(v') \geqslant n - \sqrt{n}$ for all $v' \in L'$. This completes the proof. □

Lemma 23. *Both L and L' contain exactly one vertex.*

Proof. By the choice of z and the definition of L, we know that $z \in L$, i.e., $L \neq \emptyset$. Suppose to the contrary that L contains two or more vertices. Take $v \in L$ with $v \neq z$. Then by Lemma 22, one has $d(v) \geqslant n - \sqrt{n}$ and $d(z) \geqslant n - \sqrt{n}$. And so $d(v) + d(z) \geqslant 2(n - \sqrt{n}) \geqslant n + 2$ (as $n \geqslant \frac{9}{\alpha^6}$). This implies $|N_G(v) \cap N_G(z)| = |N_G(v)| + |N_G(z)| - |N_G(v) \cup N_G(z)| \geqslant 2$, i.e., there are at least two vertices being adjacent to both v and z. Then G contains a quadrilateral, a contradiction. Therefore, L contains exactly one vertex.

By a similar discussion as above, we can show L' contains exactly one vertex. This completes the proof. □

By Lemma 23, we know that $L = \{z\}$, $L' = \{z'\}$. Let $N = N_G(z)$, $N' = N_{G'}(z')$, and let $R = V \backslash (N \cup \{z\})$, $R' = V' \backslash (N' \cup \{z'\})$. By Lemma 22, we know that $|N| \geqslant n - \sqrt{n}$, $|N'| \geqslant n - \sqrt{n}$. And so $|R| \leqslant \sqrt{n} - 1$, $|R'| \leqslant \sqrt{n} - 1$.

3.1 Proof of Theorem 8 (i)

In order to complete the proof of Theorem 8 (i), we need the following two lemmas.

Lemma 24. *For all $v \in V$, it holds that $\mathbf{x}_v \geqslant \frac{1-\alpha}{\lambda_\alpha - \alpha}$.*

Proof. If $v = z$, then $\mathbf{x}_v = 1 \geqslant \frac{1-\alpha}{\lambda_\alpha - \alpha}$. In what follows, we only need consider $v \in V \backslash \{z\} = N \cup R$.

If $v \in N$, then $z \sim v$. By $A_\alpha(G)\mathbf{x} = \lambda_\alpha \mathbf{x}$, one has

$$\lambda_\alpha \mathbf{x}_v = \alpha d(v)\mathbf{x}_v + (1-\alpha)\sum_{u \sim v} \mathbf{x}_u \geqslant \alpha \mathbf{x}_v + (1-\alpha)\mathbf{x}_z = \alpha \mathbf{x}_v + 1 - \alpha.$$

And so $\mathbf{x}_v \geqslant \frac{1-\alpha}{\lambda_\alpha - \alpha}$.

The remainder of our proof is to consider $v \in R$. If $R = \emptyset$, then we complete the proof of this lemma. If $R \neq \emptyset$, then for all $v \in R$, v is not adjacent to z and is adjacent to at most one vertex in N. Now, $A_\alpha(G)\mathbf{x} = \lambda_\alpha \mathbf{x}$ gives

$$\lambda_\alpha \mathbf{x}_v = \alpha d(v)\mathbf{x}_v + (1-\alpha)\sum_{u \sim v} \mathbf{x}_u \leqslant \alpha |R| \mathbf{x}_v + \frac{2}{3}(1-\alpha)|R|.$$

And so $\mathbf{x}_v \leqslant \frac{2(1-\alpha)|R|}{3(\lambda_\alpha - \alpha|R|)}$.

Suppose to the contrary that there is a vertex $v \in R$ such that $\mathbf{x}_v < \frac{1-\alpha}{\lambda_\alpha - \alpha}$. Construct a new graph $G^* = G - \{vu | u \in N_G(v)\} + vz$. Clearly, G^* is C_4-free. On the other hand, as $\mathbf{x}$ is the Perron vector of G, by the Courant-Fischer theorem (see [9, Section 2.6]), one has

$$\begin{aligned}\lambda_\alpha(G^*) - \lambda_\alpha \geqslant & \frac{\mathbf{x}^T(A_\alpha(G^*) - A_\alpha(G))\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \\ = & \frac{[\alpha\mathbf{x}_z^2 + 2(1-\alpha)\mathbf{x}_z\mathbf{x}_v + \alpha\mathbf{x}_v^2] - \sum_{u\sim v}[\alpha\mathbf{x}_u^2 + 2(1-\alpha)\mathbf{x}_u\mathbf{x}_v + \alpha\mathbf{x}_v^2]}{\mathbf{x}^T\mathbf{x}} \\ = & \frac{[\alpha + (1-\alpha)\mathbf{x}_v] - \sum_{u\sim v}[\alpha\mathbf{x}_u + (1-\alpha)\mathbf{x}_v]\mathbf{x}_u}{\mathbf{x}^T\mathbf{x}} \\ & + \frac{\mathbf{x}_v[\alpha\mathbf{x}_v + 1 - \alpha - \sum_{u\sim v}(\alpha\mathbf{x}_v + (1-\alpha)\mathbf{x}_u)]}{\mathbf{x}^T\mathbf{x}}. \end{aligned} \tag{6}$$

As $\mathbf{x}_v < \frac{1-\alpha}{\lambda_\alpha - \alpha}$, one has $\sum_{u\sim v}(\alpha\mathbf{x}_v + (1-\alpha)\mathbf{x}_u) = \lambda_\alpha\mathbf{x}_v = (\lambda_\alpha - \alpha)\mathbf{x}_v + \alpha\mathbf{x}_v < 1 - \alpha + \alpha\mathbf{x}_v$. Together with (6), one has

$$\lambda_\alpha(G^*) - \lambda_\alpha > \frac{[\alpha + (1-\alpha)\mathbf{x}_v] - \sum_{u\sim v}[\alpha\mathbf{x}_u + (1-\alpha)\mathbf{x}_v]\mathbf{x}_u}{\mathbf{x}^T\mathbf{x}}. \tag{7}$$

Note that $\mathbf{x}_u < \frac{2}{3}$ if $u \in N$, and $\mathbf{x}_u \leqslant \frac{2(1-\alpha)|R|}{3(\lambda_\alpha - \alpha|R|)}$ if $u \in R$. Together with (7) and the facts v is not adjacent to z, and is adjacent to at most one vertex in N, at most $|R| - 1$ vertices in R, we obtain

$$\begin{aligned}[\lambda_\alpha(G^*) - \lambda_\alpha]\mathbf{x}^T\mathbf{x} > & [\alpha + (1-\alpha)\mathbf{x}_v] - \sum_{u\sim v, u\in N}[\alpha\mathbf{x}_u + (1-\alpha)\mathbf{x}_v]\mathbf{x}_u \\ & - \sum_{u\sim v, u\in R}[\alpha\mathbf{x}_u + (1-\alpha)\mathbf{x}_v]\mathbf{x}_u \\ > & [\alpha + (1-\alpha)\mathbf{x}_v] - \frac{2}{9}[2\alpha + 3(1-\alpha)\mathbf{x}_v] \\ & - (|R| - 1)\frac{2(1-\alpha)|R|}{3(\lambda_\alpha - \alpha|R|)}\left[\frac{2(1-\alpha)|R|}{3(\lambda_\alpha - \alpha|R|)}\alpha + (1-\alpha)\mathbf{x}_v\right] \\ = & \alpha\left[\frac{5}{9} - \frac{4(1-\alpha)^2|R|^2(|R|-1)}{9(\lambda_\alpha - \alpha|R|)^2}\right] \\ & + (1-\alpha)\left[\frac{1}{3} - \frac{2(1-\alpha)|R|(|R|-1)}{3(\lambda_\alpha - \alpha|R|)}\right]\mathbf{x}_v \\ > & \alpha\left[\frac{5}{9} - \frac{4(1-\alpha)^2|R|^2(|R|-1)}{9(\lambda_\alpha - \alpha|R|)^2}\right] - \frac{2(1-\alpha)^2|R|(|R|-1)}{3(\lambda_\alpha - \alpha|R|)}\mathbf{x}_v \\ \geqslant & \frac{5}{9}\alpha - \frac{4(1-\alpha)^2|R|^2(|R|-1)}{9(\lambda_\alpha - \alpha|R|)^2} \qquad \left(\text{by } \mathbf{x}_v \leqslant \tfrac{2(1-\alpha)|R|}{3(\lambda_\alpha - \alpha|R|)}\right) \\ > & \frac{5}{9}\alpha - \frac{4(1-\alpha)^2|R|^3}{9(\lambda_\alpha - \alpha|R|)^2}. \end{aligned}$$

As $|R| \leqslant \sqrt{n}-1$ and $\lambda_\alpha \geqslant \alpha(n-1)$ (see Lemma 21), one has

$$[\lambda_\alpha(G^*)-\lambda_\alpha]\mathbf{x}^T\mathbf{x} > \frac{5}{9}\alpha - \frac{4(1-\alpha)^2(\sqrt{n}-1)^3}{9[\alpha(n-1)-\alpha(\sqrt{n}-1)]^2} \geqslant \frac{5}{9}\alpha - \frac{4(1-\alpha)^2}{9\alpha^2\sqrt{n}} > 0$$

for $n \geqslant \frac{9}{\alpha^6}$. Therefore, $\lambda_\alpha(G^*) > \lambda_\alpha$, a contradiction to the choice of G. This completes the proof. □

Lemma 25. *$R = \emptyset$, and so $d(z) = n-1$.*

Proof. Suppose to the contrary that $R \neq \emptyset$. For all $v \in R$, by Lemma 24, one has $\mathbf{x}_v \geqslant \frac{1-\alpha}{\lambda_\alpha - \alpha}$. As v is not adjacent to z, and is adjacent to at most one vertex in N. According to $A_\alpha(G)\mathbf{x} = \lambda_\alpha \mathbf{x}$, one has

$$\begin{aligned}
\lambda_\alpha \mathbf{x}_v =& \alpha d(v)\mathbf{x}_v + (1-\alpha)\sum_{u\sim v}\mathbf{x}_u \\
=& \alpha d(v)\mathbf{x}_v + (1-\alpha)\left(\sum_{u\sim v,\, u\in N}\mathbf{x}_u + \sum_{u\sim v,\, u\in R}\mathbf{x}_u\right) \\
\leqslant& \alpha(1+d_{G[R]}(v))\mathbf{x}_v + (1-\alpha)\left(\frac{2}{3} + \sum_{u\sim v, u\in R}\mathbf{x}_u\right) \\
=& \alpha\mathbf{x}_v + \frac{2}{3}(1-\alpha) + \left[\alpha d_{G[R]}(v)\mathbf{x}_v + (1-\alpha)\sum_{u\sim v, u\in R}\mathbf{x}_u\right] \\
=& \alpha\mathbf{x}_v + \frac{2}{3}(1-\alpha) + (A_\alpha(G[R])\mathbf{w})_v
\end{aligned}$$

for all vertices $v \in R$, where $\mathbf{w}$ is the restriction of the vector $\mathbf{x}$ to the set R. Then

$$\frac{(A_\alpha(G[R])\mathbf{w})_v}{(\lambda_\alpha-\alpha)\mathbf{x}_v} \geqslant 1 - \frac{2(1-\alpha)}{3(\lambda_\alpha-\alpha)\mathbf{x}_v} \geqslant 1 - \frac{2}{3} = \frac{1}{3}$$

for all vertices $v \in R$. And so $(A_\alpha(G[R])\mathbf{w})_v \geqslant \frac{1}{3}(\lambda_\alpha-\alpha)\mathbf{x}_v = \frac{1}{3}(\lambda_\alpha-\alpha)\mathbf{w}_v$ for all vertices $v \in R$, i.e., $A_\alpha(G[R])\mathbf{w} \geqslant \frac{1}{3}(\lambda_\alpha-\alpha)\mathbf{w}$ entrywise. Then by Lemma 17, one has $\lambda_\alpha(G[R]) \geqslant \frac{1}{3}(\lambda_\alpha-\alpha)$. And so by Lemma 21, one has $\lambda_\alpha(G[R]) \geqslant \frac{1}{3}(n-2)\alpha$.

On the other hand, as $G[R]$ is C_4-free and $|R| < \sqrt{n}$, by Lemma 21, one has

$$\lambda_\alpha(G[R]) \leqslant \alpha(|R|-1) + (1-\alpha)\frac{1+\sqrt{4|R|-3}}{2} < \alpha(\sqrt{n}-1) + (1-\alpha)\frac{1+\sqrt{4\sqrt{n}-3}}{2}.$$

And so

$$\frac{1}{3}(n-2)\alpha < \alpha(\sqrt{n}-1) + (1-\alpha)\frac{1+\sqrt{4\sqrt{n}-3}}{2} < \alpha(\sqrt{n}-1) + (1-\alpha)\frac{1+2\sqrt[4]{n}}{2},$$

i.e.,

$$\frac{\alpha}{3}n - \alpha\sqrt{n} - (1-\alpha)\sqrt[4]{n} + \frac{5\alpha}{6} - \frac{1}{2} < 0. \tag{8}$$

Note that $n \geqslant \frac{9}{\alpha^6}$, by (8), one has

$$\left(\frac{1}{\alpha^2} - \alpha\right)\sqrt{n} - (1-\alpha)\sqrt[4]{n} + \frac{5\alpha}{6} - \frac{1}{2} < 0.$$

Together with $n \geqslant \frac{9}{\alpha^6} > 1$ and $\alpha < 1$, one has

$$0 > \left(\frac{1}{\alpha^2} - \alpha - 1 + \alpha\right)\sqrt[4]{n} + \frac{5\alpha}{6} - \frac{1}{2} > \frac{1}{\alpha^2} - 1 + \frac{5\alpha}{6} - \frac{1}{2} \geqslant 2\sqrt{\frac{5}{6\alpha}} - \frac{3}{2} > 0,$$

a contradiction.

Therefore, $R = \emptyset$, and so $d(z) = n-1$. □

Proof of Theorem 8(i). It follows from Lemma 25 that $d(z) = n-1$. As G is C_4-free, $G[N_G(z)]$ is P_3-free. And so $G \subseteq F_n$. By the Perron-Frobenius theory, one has $\lambda_\alpha(G) \leqslant \lambda_\alpha(F_n)$, with equality if and only if $G \cong F_n$. This completes the proof of Theorem 8 (i). □

3.2 Proof of Theorem 8(ii)

In order to complete the proof of Theorem 8(ii), we need the following two lemmas.

Lemma 26. *If $|R'| \geqslant 2$, then for all $v \in V'$, it holds that $\mathbf{y}_v \geqslant \frac{1-\alpha}{\lambda'_\alpha - \alpha}$.*

Proof. If $v = z'$, then $\mathbf{y}_v = 1 \geqslant \frac{1-\alpha}{\lambda'_\alpha - \alpha}$. In what follows, we only need consider $v \in V' \backslash \{z'\} = N' \cup R'$.

If $v \in N'$, then $z' \sim v$. By $A_\alpha(G')\mathbf{y} = \lambda'_\alpha \mathbf{y}$, one has

$$\lambda'_\alpha \mathbf{y}_v = \alpha d'(v)\mathbf{y}_v + (1-\alpha)\sum_{u\sim v} \mathbf{y}_u \geqslant \alpha \mathbf{y}_v + (1-\alpha)\mathbf{y}_{z'} = \alpha \mathbf{y}_v + 1 - \alpha.$$

And so $\mathbf{y}_v \geqslant \frac{1-\alpha}{\lambda'_\alpha - \alpha}$.

The remainder of our proof is to consider $v \in R'$. Suppose to the contrary that there is a vertex $v \in R'$ such that $\mathbf{y}_v < \frac{1-\alpha}{\lambda'_\alpha - \alpha}$. Construct a new graph $G^* = G' - \{vu | u \in N_{G'}(v)\} + vz'$. Clearly, G^* is C_4-free. And as $|R'| \geqslant 2$, the graph G^* is not isomorphic to F_n, i.e., $G^* \in \mathcal{G}(n, C_4) \backslash F_n$. On the other hand, a similar discussion as the proof of Lemma 24 shows $\lambda_\alpha(G^*) \geqslant \lambda'_\alpha$, a contradiction to the choice of G'. This completes the proof. □

Lemma 27. $|R'| \leqslant 1$*, and so* $d'(z') \geqslant n-2$.

Proof. Suppose to the contrary that $|R'| \geqslant 2$. Then by Lemma 26, for all $v \in R'$, one has $\mathbf{y}_v \geqslant \frac{1-\alpha}{\lambda'_\alpha - \alpha}$. A similar discussion as the proof of Lemma 25 shows $\frac{1}{3}(n-2)\alpha < \alpha(\sqrt{n} - 1) + (1-\alpha)\frac{1+\sqrt{4\sqrt{n}-3}}{2}$, a contradiction to $n \geqslant \frac{9}{\alpha^6}$.

Therefore, $|R'| \leqslant 1$, and so $d'(z') \geqslant n-2$. □

Proof of Theorem 8(ii). It follows from Lemma 27 that $d'(z') \geqslant n-2$. If $d'(z') = n-2$, then let v be the unique non-neighbour of z' (in G'). As G' is C_4-free, $G'[N_{G'}(z')]$ is P_3-free, and v is adjacent to at most one vertex in $N_{G'}(z')$. The graph G' is a subgraph of G^* or G^{**}, where G^* (resp. G^{**}) is obtained from F_{n-1} by adding a vertex v and an edge vu, where u is a vertex of F_{n-1} with degree 2 (resp. 1). (Note that G^{**} does exist only when n is odd.) By the Perron-Frobenius theory, one has $\lambda_\alpha(G') \leqslant \lambda_\alpha(G^*)$ or $\lambda_\alpha(G') \leqslant \lambda_\alpha(G^{**})$, with equality if and only if $G' \cong G^*$ or $G' \cong G^{**}$.

If $d'(z') = n-1$, then as G' is C_4-free, $G'[N_{G'}(z')]$ is P_3-free. Together with $G' \ncong F_n$, we know that G' is a subgraph of $F_n - e$. By the Perron-Frobenius theory, one has $\lambda_\alpha(G') \leqslant \lambda_\alpha(F_n - e)$, with equality if and only if $G' \cong F_n - e$.

As all of G^*, G^{**} and $F_n - e$ are contained in $\mathcal{G}(n, C_4)\backslash F_n$, the extremal graph G' is isomorphic to one member in $\{G^*, G^{**}, F_n - e\}$. In order to complete the proof of this theorem, we consider the following two cases.

Case 1. n is odd. If G' is isomorphic to G^* or G^{**}. Then $F_n - e = G' - vu + vz'$. Note that $\mathbf{y}_{z'} = 1 > \frac{2}{3} > \mathbf{y}_u$. By Lemma 18, we know that $\lambda_\alpha(F_n - e) > \lambda'_\alpha$, a contradiction to the choice of G'.

Case 2. n is even. In this case, G^{**} does not exist. If G' is isomorphic to G^*, then $F_n - e = G' - uv - u_1u_2 + z'v$, where u_1 and u_2 are two vertices in $N_{G'}(z')\backslash\{u\}$ with $u_1 \sim u_2$. As $\mathbf{y}$ is the Perron vector of G', by the Courant-Fischer theorem (see [9, Section 2.6]), one has

$$\begin{aligned}\lambda_\alpha(F_n - e) - \lambda'_\alpha \geqslant & \frac{1}{\mathbf{y}^T\mathbf{y}}[\mathbf{y}^T(A_\alpha(F_n - e) - A_\alpha(G'))\mathbf{y}] \\ = & \frac{1}{\mathbf{y}^T\mathbf{y}}[\alpha\mathbf{y}_{z'}^2 + 2(1-\alpha)\mathbf{y}_v\mathbf{y}_{z'} + \alpha\mathbf{y}_v^2 - \alpha\mathbf{y}_u^2 - 2(1-\alpha)\mathbf{y}_v\mathbf{y}_u - \alpha\mathbf{y}_v^2 \\ & - \alpha\mathbf{y}_{u_1}^2 - 2(1-\alpha)\mathbf{y}_{u_1}\mathbf{y}_{u_2} - \alpha\mathbf{y}_{u_2}^2]. \qquad (9)\end{aligned}$$

Note that $\mathbf{y}_{z'} = 1$, and by the symmetry of G', we know that $\mathbf{y}_{u_1} = \mathbf{y}_{u_2}$ (see [25, Proposition 16]). Together with (9), one has

$$[\lambda_\alpha(F_n - e) - \lambda'_\alpha]\mathbf{y}^T\mathbf{y} \geqslant \alpha + 2(1-\alpha)\mathbf{y}_v - \alpha\mathbf{y}_u^2 - 2(1-\alpha)\mathbf{y}_v\mathbf{y}_u - 2\mathbf{y}_{u_1}^2 > \alpha - \alpha\mathbf{y}_u^2 - 2\mathbf{y}_{u_1}^2. \quad (10)$$

Let u' be a vertex in $N_{G'}(z')$ with $u' \sim u$. As $\mathbf{y}_{z'} = 1$ and $\mathbf{y}_w < \frac{2}{3}$ for all $w \in V(G')\backslash\{z'\}$. By $A_\alpha(G')\mathbf{y} = \lambda'_\alpha\mathbf{y}$, one has

$$\lambda'_\alpha\mathbf{y}_u = 3\alpha\mathbf{y}_u + (1-\alpha)(\mathbf{y}_{z'} + \mathbf{y}_{u'} + \mathbf{y}_v) \Rightarrow \mathbf{y}_u < \frac{7(1-\alpha)}{3(\lambda'_\alpha - 3\alpha)} \leqslant \frac{7(1-\alpha)}{3(n-4)\alpha} \leqslant \frac{7(1-\alpha)\alpha}{15}$$

and

$$\lambda'_\alpha\mathbf{y}_{u_1} = 2\alpha\mathbf{y}_{u_1} + (1-\alpha)(\mathbf{y}_{z'} + \mathbf{y}_{u_1}) \Rightarrow \mathbf{y}_{u_1} < \frac{5(1-\alpha)}{3(\lambda'_\alpha - 2\alpha)} \leqslant \frac{5(1-\alpha)}{3(n-3)\alpha} \leqslant \frac{5(1-\alpha)\alpha}{18}.$$

Together with (10), we obtain

$$[\lambda_\alpha(F_n - e) - \lambda'_\alpha]\mathbf{y}^T\mathbf{y} > \alpha - \alpha\frac{49(1-\alpha)^2\alpha^2}{225} - \frac{25(1-\alpha)^2\alpha^2}{162} > \alpha(1 - \frac{49}{225} - \frac{25}{162}) > 0,$$

i.e., $\lambda_\alpha(F_n - e) > \lambda'_\alpha$, a contradiction to the choice of G'.

Therefore, $G' \cong F_n - e$. This completes the proof. □

4 Proof of Theorem 12

For $\alpha \in [\frac{1}{2}, 1)$ and $m \geqslant 3$, let H be a graph in $\mathcal{H}(m, C_4)\backslash K_{1,m}$ with maximum A_α-index (Note that H depends on α and m). In this section, we are going to complete the proof of Theorem 12.

Our first lemma shows H is connected.

Lemma 28. *The graph H is connected.*

Proof. Suppose to the contrary that H is not connected. Let $H_1, H_2, \ldots, H_s$ be all components of H with $\lambda_\alpha(H_1) = \lambda_\alpha(H)$. Take $u_i \in H_i$ for $i = 1, 2, \ldots, s$ with $d_{H_1}(u_1) = \delta(H_1)$. Let H^* be the graph obtained from $H_1, H_2, \ldots, H_s$ by identifying $u_1, u_2, \ldots, u_s$. Clearly, $H^* \in \mathcal{H}(m, C_4)$. Furthermore, as $K_{1,m-1} + e \in \mathcal{H}(m, C_4)\backslash K_{1,m}$, by the choice of H, we know that $\lambda_\alpha(H_1) = \lambda_\alpha(H) \geqslant \lambda_\alpha(K_{1,m-1} + e) \geqslant 2$. Then $H_1 \ncong K_2$, and so $H^* \ncong K_{1,m}$. Now, we have $H^* \in \mathcal{H}(m, C_4)\backslash K_{1,m}$. However, H^* contains H_1 as a proper subgraph. By the Perron-Frobenius theory, $\lambda_\alpha(H^*) > \lambda_\alpha(H_1) = \lambda_\alpha(H)$, a contradiction to the choice of H. Therefore, H is connected. $\square$

In the remainder of our paper, fix $\frac{1}{2} \leqslant \alpha < 1$ and $m \geqslant 3$. Denote by $\lambda_\alpha := \lambda_\alpha(H)$. Let $\mathbf{x}$ be the Perron vector of $A_\alpha(H)$ whose maximum entry is equal to 1, and let z be a vertex in H with $\mathbf{x}_z = 1$. For convenience, denote by $V := V(H)$ and $d(v) := d_H(v)$ for $v \in V$. Furthermore, let $N := N_H(z)$ and $W := V\backslash(N \cup \{z\})$.

As $K_{1,m-1} + e \in \mathcal{H}(m, C_4)\backslash K_{1,m}$. According to the choice of H, and by Lemma 16, we have

$$\lambda_\alpha \geqslant \lambda_\alpha(K_{1,m-1} + e) \geqslant \alpha\Delta(K_{1,m-1} + e) + \frac{(1-\alpha)^2}{\alpha} = \alpha(m-1) + \frac{(1-\alpha)^2}{\alpha}. \tag{11}$$

The following lemma shows the degree of z in H is at least 2.

Lemma 29. *It holds that $d(z) \geqslant 2$.*

Proof. Suppose to the contrary that $d(z) = 1$, let v be the neighbor of z. Then by $A_\alpha(H)\mathbf{x} = \lambda_\alpha \mathbf{x}$, one has

$$\lambda_\alpha \mathbf{x}_z = \alpha \mathbf{x}_z + (1-\alpha)\mathbf{x}_v.$$

And so $\mathbf{x}_v = \frac{\lambda_\alpha - \alpha}{1-\alpha}\mathbf{x}_z > \mathbf{x}_z$, a contradiction. So $d(z) \geqslant 2$. $\square$

Lemma 30. *It holds that*

$$\frac{\lambda_\alpha(\lambda_\alpha - \alpha d(z))}{1-\alpha} \leqslant d(z) + \frac{2(1-\alpha)e(N) + |W|}{\lambda_\alpha - 1 - \alpha} + e(N, W). \tag{12}$$

Proof. Applying (1) to z gives us

$$\lambda_\alpha^2 \mathbf{x}_z = \alpha d(z)\lambda_\alpha \mathbf{x}_z + \alpha(1-\alpha)\sum_{u\sim z} d(u)\mathbf{x}_u + (1-\alpha)^2 \sum_{u\sim z}\sum_{w\sim u} \mathbf{x}_w.$$

Then

$$\begin{aligned}\lambda_\alpha(\lambda_\alpha - \alpha d(z)) =& \alpha(1-\alpha)\sum_{u\sim z}[1+e(\{u\},N)+e(\{u\},W)]\mathbf{x}_u \\ &+(1-\alpha)^2\left(d(z)+\sum_{uw\in E(H[N])}(\mathbf{x}_u+\mathbf{x}_w)+\sum_{u\sim z}\sum_{w\sim u, w\in W}\mathbf{x}_w\right)\\ \leqslant& (1-\alpha)\left(d(z)+\sum_{uw\in E(H[N])}(\mathbf{x}_u+\mathbf{x}_w)+e(N,W)\right). \qquad (13)\end{aligned}$$

For each $uw \in E(H[N])$, as H is C_4-free, the induced subgraph $H[N]$ is P_3-free. And so $N_H(u)\cap N=\{w\}$, $N_H(w)\cap N=\{u\}$. Then by $A_\alpha(H)\mathbf{x}=\lambda_\alpha\mathbf{x}$, we have

$$\lambda_\alpha\mathbf{x}_u=\alpha d(u)\mathbf{x}_u+(1-\alpha)\sum_{v\sim u}\mathbf{x}_v=2\alpha\mathbf{x}_u+(1-\alpha)(\mathbf{x}_z+\mathbf{x}_w)+\sum_{v\sim u, v\in W}[\alpha\mathbf{x}_u+(1-\alpha)\mathbf{x}_v]$$

and

$$\lambda_\alpha\mathbf{x}_w=\alpha d(w)\mathbf{x}_w+(1-\alpha)\sum_{v\sim w}\mathbf{x}_v=2\alpha\mathbf{x}_w+(1-\alpha)(\mathbf{x}_z+\mathbf{x}_u)+\sum_{v\sim w, v\in W}[\alpha\mathbf{x}_w+(1-\alpha)\mathbf{x}_v].$$

Then

$$\begin{aligned}(\lambda_\alpha-1-\alpha)(\mathbf{x}_u+\mathbf{x}_w) =& 2(1-\alpha)\mathbf{x}_z+\sum_{v\sim u, v\in W}[\alpha\mathbf{x}_u+(1-\alpha)\mathbf{x}_v]\\ &+\sum_{v\sim w, v\in W}[\alpha\mathbf{x}_w+(1-\alpha)\mathbf{x}_v]\\ \leqslant& 2(1-\alpha)+e(\{u\},W)+e(\{w\},W).\end{aligned}$$

Now

$$\sum_{uw\in E(H[N])}(\mathbf{x}_u+\mathbf{x}_w)\leqslant\frac{1}{\lambda_\alpha-1-\alpha}\sum_{uw\in E(H[N])}[2(1-\alpha)+e(\{u\},W)+e(\{w\},W)]. \qquad (14)$$

As H is C_4-free, each vertex in W has at most one neighbor in N. Then

$$\sum_{uw\in E(H[N])}[e(\{u\},W)+e(\{w\},W)]\leqslant |W|.$$

Together with (14), one has

$$\sum_{uw\in E(H[N])}(\mathbf{x}_u+\mathbf{x}_w)\leqslant\frac{2(1-\alpha)e(N)+|W|}{\lambda_\alpha-1-\alpha}.$$

Then by (13), we obtain

$$\frac{\lambda_\alpha(\lambda_\alpha-\alpha d(z))}{1-\alpha}\leqslant d(z)+\frac{2(1-\alpha)e(N)+|W|}{\lambda_\alpha-1-\alpha}+e(N,W).$$

This completes the proof. ☐

Proof of Theorem 12. It suffices to show $H \cong K_{1,m-1}+e$. As $H \in \mathcal{H}(m, C_4)\backslash K_{1,m}$, it holds that $\Delta(H) \leqslant m-1$, and so $d(z) \leqslant m-1$.

Next we show the following claim.

Claim 31. *If $W \neq \emptyset$, then for all $v \in W$, one has $d_{H[W]}(v) \geqslant 1$.*

Proof of Claim 31. Suppose to the contrary that $W \neq \emptyset$ and there is a vertex $v \in W$ such that $d_{H[W]}(v)=0$. As H is connected and contains no quadrilateral, there is exactly one vertex, say u, in N such that $u \sim v$. If $|W|=1$ and $e(N)=0$, then $H-v+wu = K_{1,m-1}+e \in \mathcal{H}(m, C_4)\backslash K_{1,m}$, where w is a vertex in $N\backslash\{u\}$.

On the other hand, by $A_\alpha(H)\mathbf{x} = \lambda_\alpha \mathbf{x}$, one has

$$\lambda_\alpha \mathbf{x}_w = \alpha \mathbf{x}_w + (1-\alpha)\mathbf{x}_z \text{ and } \lambda_\alpha \mathbf{x}_v = \alpha \mathbf{x}_v + (1-\alpha)\mathbf{x}_u.$$

Then

$$\mathbf{x}_w = \frac{(1-\alpha)\mathbf{x}_z}{\lambda_\alpha - \alpha} \geqslant \frac{(1-\alpha)\mathbf{x}_u}{\lambda_\alpha-\alpha} = \mathbf{x}_v.$$

And so by Lemma 18, we have

$$\lambda_\alpha < \lambda_\alpha((K_{1,m-1}+e)\cup\{v\}) = \lambda_\alpha(K_{1,m-1}+e),$$

a contradiction to the choice of H.

If $|W| \geqslant 2$ or $e(N) \geqslant 1$. Let $H^* = H - uv + zv$, then $H^* \in \mathcal{H}(m, C_4)\backslash K_{1,m}$. In fact, by the choice of v, we know that zv is a cut edge of H^*. Therefore, $H \in \mathcal{H}(m, C_4)$ gives $H^* \in \mathcal{H}(m, C_4)$. On the other hand, $|W| \geqslant 2$ or $e(N) \geqslant 1$ imply that there is at least one edge in H^* not adjacent to z. Hence, $H^* \ncong K_{1,m}$, i.e., $H^* \in \mathcal{H}(m, C_4)\backslash K_{1,m}$. On the other hand, by the choice of z, we know that $\mathbf{x}_z \geqslant \mathbf{x}_u$, and so by Lemma 18, one has $\lambda_\alpha(H^*) > \lambda_\alpha(H)$, a contradiction to the choice of H.

This completes the proof of the claim. $\square$

Now we come back to show our result. By Claim 31, one has $e(W) = \frac{\sum_{v\in W} d_{H[W]}(v)}{2} \geqslant \frac{|W|}{2}$. Together with (12), one has

$$\begin{aligned}\frac{\lambda_\alpha(\lambda_\alpha - \alpha d(z))}{1-\alpha} \leqslant & d(z) + \frac{2(1-\alpha)e(N)+2e(W)}{\lambda_\alpha - 1 - \alpha} + e(N,W) \\ =& m + \left[\frac{2(1-\alpha)}{\lambda_\alpha-1-\alpha} - 1\right] e(N) + \left[\frac{2}{\lambda_\alpha - 1-\alpha} - 1\right] e(W). \qquad (15)\end{aligned}$$

In order to complete the proof of this theorem, it suffices to show $d(z)=m-1$ and $W=\emptyset$.

If $d(z) \leqslant m-3$, then by Lemma 29, one has $m \geqslant d(z)+3 \geqslant 5$. On the other hand, by (11),

$$\frac{\lambda_\alpha(\lambda_\alpha - \alpha d(z))}{1-\alpha} \geqslant \frac{1}{1-\alpha}\left[\alpha(m-1) + \frac{(1-\alpha)^2}{\alpha}\right]\left[2\alpha + \frac{(1-\alpha)^2}{\alpha}\right]$$

$$
\begin{aligned}
=&\frac{2\alpha^2(m-1)}{1-\alpha}+(1-\alpha)(m+1)+\frac{(1-\alpha)^3}{\alpha^2}\\
\geqslant&2\alpha(m-1)+(1-\alpha)(m+1)+\frac{(1-\alpha)^3}{\alpha^2} \qquad\qquad (\text{by } \alpha\geqslant \tfrac{1}{2})\\
>&(1+\alpha)m+1-3\alpha. \qquad\qquad (16)
\end{aligned}
$$

If $W=\emptyset$, then $e(N)=m-d(z)\geqslant 3$. As H is C_4-free, the induced subgraph $H[N]$ is P_3-free. And so $d(z)\geqslant 6$, then $m\geqslant 9$.

On the other hand, together with (11), (15) and (16), one has

$$
\alpha m+1-3\alpha<\left[\frac{2(1-\alpha)}{\lambda_\alpha-1-\alpha}-1\right]e(N)<\left[\frac{2(1-\alpha)}{\alpha(m-2)-1}-1\right](m-d(z)).
$$

Then $\frac{2(1-\alpha)}{\alpha(m-2)-1}-1>0$. As $d(z)\geqslant 6$, it holds that $\alpha(m-2)<\left[\frac{2(1-\alpha)}{\alpha(m-2)-1}-1\right](m-6)$. And so $\alpha<\frac{2(1-\alpha)}{\alpha(m-2)-1}-1$, by a direct calculation, this induces a contradiction to $m\geqslant 9$.

If $W\neq\emptyset$, then together with (15) and (16), one has

$$
\begin{aligned}
\alpha m+1-3\alpha&<\left[\frac{2(1-\alpha)}{\lambda_\alpha-1-\alpha}-1\right]e(N)+\left[\frac{2}{\lambda_\alpha-1-\alpha}-1\right]e(W)\\
&\leqslant\left[\frac{2}{\lambda_\alpha-1-\alpha}-1\right][e(W)+e(N)]. \qquad (17)
\end{aligned}
$$

Then $\frac{2}{\lambda_\alpha-1-\alpha}-1>0$.

As $W\neq\emptyset$ and H is connected (see Lemma 28), one has $e(N,W)\geqslant 1$. If $e(N,W)=1$, then as $e(W)\geqslant 1$ (by Claim 31), the graph $H^*=H-uv+zv\in\mathcal{H}(m,C_4)\backslash K_{1,m}$, where $uv\in H[N,W]$ with $u\in N$ and $v\in W$. However, as $\mathbf{x}_z\geqslant\mathbf{x}_u$, by Lemma 18, it holds that $\lambda_\alpha(H^*)>\lambda_\alpha(H)$, a contradiction to the choice of H. Therefore, $e(N,W)\geqslant 2$.

By Lemma 29, we know that $d(z)\geqslant 2$, and so $d(z)+e(N,W)\geqslant 4$. Then $e(W)+e(N)=m-d(z)-e(N,W)\leqslant m-4$. On the other hand, as $\alpha\geqslant\frac{1}{2}$, by (11), one has $\lambda_\alpha-1-\alpha>\alpha(m-2)-1\geqslant\frac{m-4}{2}$. Together with (17), we have

$$
\alpha(m-3)+1<(\frac{4}{m-4}-1)(m-4)=8-m,
$$

and so $m<\frac{7+3\alpha}{1+\alpha}<6$, i.e., $m\leqslant 5$.

In the case $m=5$, one has $d(z)=m-3=2$, $e(N,W)=2$ and $e(W)=1$. Then $H\cong C_5$, and so $\lambda_\alpha=2<4\alpha+\frac{(1-\alpha)^2}{\alpha}$, a contradiction to (11); or by Lemma 18, we can construct a graph $H^*\in\mathcal{H}(5,C_4)\backslash K_{1,5}$ such that $\lambda_\alpha(H^*)>\lambda_\alpha$, which is a contradiction to the choice of H.

If $d(z)=m-2$, then we claim $W=\emptyset$. Otherwise, as H is connected, it holds that $e(N,W)\geqslant 1$. Also by Claim 31, $e(W)\geqslant 1$. And so $e(N,W)=e(W)=1$. Say $uv\in E(H[N,W])$ with $u\in N$ and $v\in W$. Then uv is a cut edge of H. Let $H^*=H-uv+zv$, then $H^*\in\mathcal{H}(m,C_4)\backslash K_{1,m}$. On the other hand, as $\mathbf{x}_z\geqslant\mathbf{x}_u$, by Lemma 18, one has $\lambda_\alpha(H^*)>\lambda_\alpha$, a contradiction to the choice of H.

Therefore, $e(N) = m - d(z) = 2$. As H is C_4-free, the induced subgraph $H[N]$ is P_3-free. Then $e(N) = 2$ implies $d(z) \geqslant 4$, and so $m \geqslant 6$. By (11) and (15), we have

$$\frac{1}{1-\alpha}\left[\alpha(m-1) + \frac{(1-\alpha)^2}{\alpha}\right]\left[\alpha + \frac{(1-\alpha)^2}{\alpha}\right] \leqslant \frac{\lambda_\alpha(\lambda_\alpha - \alpha d(z))}{1-\alpha}$$
$$< m + \frac{4(1-\alpha)}{\alpha(m-2) + \frac{(1-\alpha)^2}{\alpha} - 1} - 2. \quad (18)$$

As $\alpha \geqslant \frac{1}{2}$, i.e., $\alpha \geqslant 1-\alpha$. And when $m \geqslant 6$, the function $g_2(\alpha) := \alpha(m-2) + \frac{(1-\alpha)^2}{\alpha} - 1 = \alpha(m-1) + \frac{1}{\alpha} - 3$ is increasing on $\alpha \in [\frac{1}{2}, 1)$. It holds that $\alpha(m-2) + \frac{(1-\alpha)^2}{\alpha} - 1 \geqslant \frac{m-3}{2}$. Together with (18), one has

$$\alpha(m-1) + m(1-\alpha) + \frac{(1-\alpha)^3}{\alpha^2} < m - 2 + \frac{8(1-\alpha)}{m-3}.$$

And so $2 - \alpha < \frac{8(1-\alpha)}{m-3}$, i.e., $m < \frac{8(1-\alpha)}{2-\alpha} + 3 \leqslant \frac{17}{3}$. This induces a contradiction to $m \geqslant 6$.

If $d(z) = m-1$, then $W = \emptyset$. Otherwise, as H is connected, it holds that $e(N, W) \geqslant 1$. Also by Claim 31, $e(W) \geqslant 1$. And so $d(z) = m - e(N, W) - e(W) \leqslant m-2$, a contradiction. This implies $e(N) = m - d(z) = 1$, and so $H \cong K_{m-1} + e$, as desired. □

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