# On the index of quasi-tree graphs with perfect matchings*

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**Abstract:** A connected graph $G = (V(G), E(G))$ is called a quasi-tree graph if there exists a vertex $u_0 \in V(G)$ such that $G - u_0$ is a tree. Set $\mathscr{P}(2k) := \{G : G$ is a quasi-tree graph on $2k$ vertices with perfect matching$\}$, and $\mathscr{P}(2k, d_0) := \{G : G \in \mathscr{P}(2k)$, and there is a vertex $u_0 \in V(G)$ such that $G - u_0$ is a tree with $d_G(u_0) = d_0\}$. In this paper, the maximal indices of all graphs in the sets $\mathscr{P}(2k)$, $\mathscr{P}(2k, d_0)$ are determined, respectively. The corresponding extremal graphs are also characterized.

*Keywords*: Quasi-tree graph; Index; Perfect matching

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## 1. Introduction

All graphs considered in this paper are finite, undirected and simple. Let $G = (V(G), E(G))$ be a graph with $n$ vertices and let $A(G)$ be its adjacency matrix. Since $A(G)$ is symmetric, its eigenvalues are real. Hence, they can be arranged as $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ and call them the eigenvalues of $G$. The *characteristic polynomial* of $G$ is just $\det(\lambda I - A(G))$, and is denoted by $\phi(G; \lambda)$. The largest eigenvalue $\lambda_1(G)$ is called the *index* of $G$, denoted by $\rho(G)$. If $G$ is connected, then $A(G)$ is irreducible and by the

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Perron-Frobenius theory of non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho(G)$. We shall refer to such an eigenvector as the *Perron vector* of $G$.

Two edges of a graph $G$ are said to be *independent* if they are not adjacent in $G$. The vertex $v$ in $G$ is *M-saturated* if $v$ is incident with an edge in $M$; otherwise, $v$ is *M-unsaturated*. We call $M$ a *perfect matching* of $G$ if each vertex of $G$ is $M$-saturated. Graphs with perfect matchings always have an even number of vertices. A connected graph $G = (V(G), E(G))$ is called a *quasi-tree graph*, if there exists a vertex $u_0 \in V(G)$ such that $G - u_0$ is a tree. The concept of quasi-tree graph was first introduced in [21, 22]. Set $\mathscr{P}(2k) := \{G : G$ is a quasi-tree graph on $2k$ vertices with a perfect matching$\}$, and $\mathscr{P}(2k, d_0) := \{G : G \in \mathscr{P}(2k)$, and there is a vertex $u_0 \in V(G)$ such that $G - u_0$ is a tree with $d_G(u_0) = d_0\}$.

The investigation of the index of graphs is an important topic in the theory of graph spectra. The Ref. [5] is a wonderful survey which includes a large number of references on this topic. The recent developments on this topic also involve the research concerning graphs with maximal or minimal index of a given class of graphs (see [1, 7, 8, 10, 12, 13, 14, 15, 20, 23, 26, 27]) which are motivated by the problem proposed by Brualdi and Solheid [1]: Given a set of graphs $\mathcal{G}$, find an upper bound for the index of graphs in $\mathcal{G}$ and characterize the graphs in which the maximal index is attained. On the other hand, one may hope to study the structure properties of graphs by its spectral properties. It is hard to see the structure of a graph in certain class of graphs each of which contains a perfect matching. If one pays attention to the graph with maximal index in certain class of graphs each of which contains a perfect matching, one finds that the corresponding graph has a special structure; see, for example, [2, 3, 9, 28]. Motivated by these facts and problems, we study the index of quasi-tree graphs each containing a perfect matching in this paper.

In fact, quasi-tree graph attracts more and more researchers' attention (e.g., see [11, 18, 19, 24, 29]). In particular, Liu and Lu [21] determined the $n$-vertex quasi-tree with maximal index; Xu and Meng characterized the unique quasi-tree graph with maximum Laplacian spread among all quasi-tree graphs; Geng and Li [11] identified the unique quasi-tree graph with maximal index among all quasi-tree graphs each with $k$ pendants. In this article, we determine the maximal indices of all graphs in the set $\mathscr{P}(2k)$, $\mathscr{P}(2k, d_0)$, respectively. The corresponding extremal graphs are also characterized.

## 2. Preliminaries

For $v \in V(G)$, we use $N_G(v)$ to denote the *neighbors* of $v$ and set $d_G(v) = |N_G(v)|$. For a subgraph $H$ of $G$, let $N_H(v) = N_G(v) \cap V(H)$ and $d_H(v) = |N_H(v)|$ for $v \in V(G)$. A *pendant vertex* of a graph is a vertex of degree 1.We will use $G - x$ or $G - xy$ to denote the graph that arises from $G$ by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from $G$ by adding an edge $xy \notin E(G)$, where $x, y \in V(G)$. A *pendant path* of $G$ is a walk $v_0v_1 \dots v_s (s \geq 1)$ such that the vertices $v_0, v_1, \dots, v_s$ are distinct, $d_G(v_0) > 2, d_G(v_s) = 1$, and $d_G(v_i) = 2$, whenever $0 < i < s$. When we say a pendant path $P = v_0v_1 \dots v_s$ is *attached* to a vertex $u$, we actually mean identifying $v_0$ with $u$. For two vertices $u, v \in V(G), u \neq v$, the *distance* between $u$ and $v$, which would be noted by $d_G(u, v)$, is the number of edges in a shortest path joining $u$ and $v$.

**Lemma 2.1** ([27]). *Let $G$ be a connected graph and $\rho(G)$ be the spectral radius of $A(G)$. Let u,v be two vertices of $G$. Suppose that $v_1, v_2, \dots, v_s \in N_G(v) \setminus N_G(u)$ $(1 \leq s \leq d_G(v))$ and $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ is the Perron vector of $A(G)$, where $x_i$ corresponds to $v_i (1 \leq i \leq n)$. Let $G^*$ be the graph obtained from $G$ by deleting the edges $vv_i$ and inserting the edges $uv_i$ $(1 \leq i \leq s)$. If $x_u \geq x_v$, then $\rho(G) < \rho(G^*)$.*

**Lemma 2.2.** *Let $G_1$ and $G_2$ be two graphs.*

(i) ([17]) *If $G_2$ is a proper spanning subgraph of $G_1$ and $G_1$ is a connected graph. Then $\phi(G_2; \lambda) > \phi(G_1; \lambda)$ for $\lambda \geq \rho(G_1)$;*
(ii) ([4, 6]) *If $\phi(G_2; \lambda) > \phi(G_1; \lambda)$ for $\lambda \geq \rho(G_2)$, then $\rho(G_1) > \rho(G_2)$;*
(iii) ([16]) *If $G_2$ is a proper subgraph of $G_1$ and $G_1$ is a connected graph, then $\rho(G_2) < \rho(G_1)$.*

**Lemma 2.3** ([4, 25]). (i) *Let $u$ be a vertex of $G$, and let $\mathscr{C}(u)$ be the set of all cycles containing $u$. Then*

$$\begin{aligned}\phi(G;\lambda) &= \lambda\phi(G-u;\lambda) - \sum_{v\in N(u)} \phi(G-v-u;\lambda) \\ &\quad -2\sum_{Z\in\mathscr{C}(u)} \phi(G-V(Z);\lambda). \qquad (2.1)\end{aligned}$$

*In particular, if $u$ is a pendant vertex of a graph $G$ and $vu \in E(G)$, then*

$$\phi(G;\lambda) = \lambda\phi(G-u;\lambda) - \sum \phi(G-v-u;\lambda).$$

(ii) *Let $uv$ be an edge of $G$ and $\mathscr{C}_{uv}$ be the set of all cycles containing $uv$. Then*

$$\begin{aligned}\phi(G;\lambda) &= \phi(G-uv;\lambda) - \sum_{v\in N(u)} \phi(G-v-u;\lambda) \\ &\quad -2\sum_{Z\in\mathscr{C}_{uv}} \phi(G-V(Z);\lambda). \qquad (2.2)\end{aligned}$$

*We assume that $\phi(G;\lambda) = 1$ if $G$ is the empty graph (i.e. with no vertices).*

**Lemma 2.4** ([4, 25]). *If $G_1, G_2, \ldots, G_t$ are the components of a graph $G$, then we have*

$$\phi(G;\lambda) = \phi(G_1;\lambda)\phi(G_2;\lambda)\ldots\phi(G_t;\lambda) = \prod_{i=1}^{t} \phi(G_i;\lambda).$$

## 3. Maximal index of graphs in $\mathscr{P}(2k)$

In this section, we shall determine the maximal index of graphs in $\mathscr{P}(2k)$ ($k \geq 2$).

- Let $S_1^*$ be the tree of order $2k-1$ obtained from a star $K_{1,k-1}$ by adding a new pendant edge at each pendant vertex of $K_{1,k-1}$ (as depicted in Fig. 1), the center of $K_{1,k-1}$ is also called the center of $S_1^*$. Let $B_{2k}^1$ be the graph obtained from $S_1^*$ and an isolated vertex $u_0$ by adding $2k-1$ edges joining $u_0$ to each vertex of $S_1^*$.

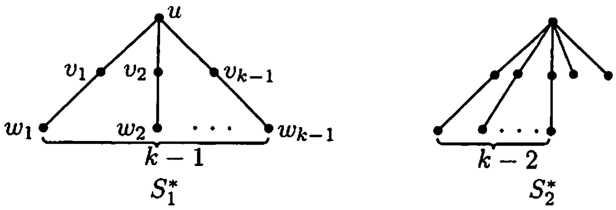


Figure 1: Graph $S_1^*$ and $S_2^*$.

- Let $S_2^*$ be the tree of order $2k-1$ obtained from a star $K_{1,k}$ by adding a new pendant edge at each of $k-2$ pendant vertices of $K_{1,k}$ respectively (as depicted in Fig. 1), the center of $K_{1,k}$ is also called the center of $S_2^*$. Let $B_{2k}^2$ be the graph obtained from $S_2^*$ and an isolated vertex $u_0$ by adding $2k-1$ edges joining $u_0$ to each vertex of $S_2^*$.


Figure 2: Graph $B_6^1$ and $B_6^2$ for $k=3$.

For example, $B_6^1, B_6^2$ are shown in Fig. 2. Note that $B_{2k}^1, B_{2k}^2 \in \mathscr{P}(2k)$ for $k \geq 2$.

**Lemma 3.1.** *$\rho(B_{2k}^1) < \rho(B_{2k}^2)$ for $k \geq 3$.*

*Proof.* Denote the center of $S_1^*$ by $u$, $N_{S_1^*}(u) = \{v_1, v_2, \ldots, v_{k-1}\}$, and $N_{S_1^*}(v_1) \setminus \{u\} = \{w_1\}$ (see Fig. 1). If $x_u \geq x_{v_1}$, since $B_{2k}^1 - w_1v_1 + w_1u \cong B_{2k}^2$, we have $\rho(B_{2k}^2) > \rho(B_{2k}^1)$ by Lemma 2.1; If $x_u < x_{v_1}$, since $B_{2k}^1 - \{uv_2, \ldots, uv_{k-1}\} + \{v_1v_2, \ldots, v_1v_{k-1}\} \cong B_{2k}^2$, we have $\rho(B_{2k}^2) > \rho(B_{2k}^1)$ by Lemma 2.1. This completes the proof.

**Theorem 3.2.** *Let $G \in \mathscr{P}(2k)(k \geq 2)$. Then $\rho(G) \leq \rho(B_{2k}^2)$ and the equality holds if and only if $G \cong B_{2k}^2$.*

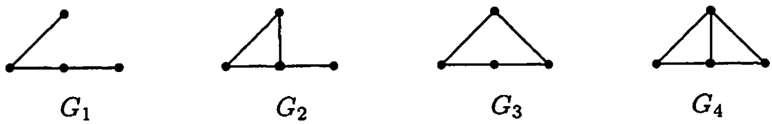


Figure 3: Graphs $G_1, G_2, G_3$ and $G_4$.

*Proof.* When $k = 2$, $\mathscr{P}(4) = \{G_1, G_2, G_3, G_4\}$ as shown in Fig. 3. It's routine to check that $B_{2k}^2$ has the maximal index among all the graphs in $\mathscr{P}(2k)$. When $k \geq 3$, choose $G \in \mathscr{P}(2k)$ such that $\rho(G)$ is as large as possible. Let $\mathbf{x} = (x_1, x_2, \ldots, x_{2k})^T$ be the Perron vector of $A(G)$, where $x_i$ corresponds to the vertex $u_i$ for $1 \leq i \leq 2k$ (By $x_v$, we mean the coordinate of $\mathbf{x}$ corresponding to the vertex $v$ ). Assume that $G' := G - u_0$ is a tree. Choose a vertex $u_1 \in V(G')$ such that $d_{G'}(u_1)$ is as large as possible. Let $M$ be a perfect matching of $G$. First, we establish the following sequence of facts.

**Fact 1.** *For each vertex $v \in V(G'), vu_0 \in E(G)$.*

*Proof.* Suppose to the contrary that there exists one vertex $u_i \in V(G')$ such that $u_0u_i \notin E(G)$. Then $G + u_0u_i \in \mathscr{P}(2k)$, and $\rho(G + u_0u_i) > \rho(G)$ by Lemma 2.2 (iii), hence we get a contradiction. □

**Fact 2.** *For each vertex $v \in V(G')\backslash\{u_1\}$, one has $d_{G'}(v) \leq 2$.*

*Proof.* Suppose to the contrary that there exists $u_i \in V(G')\backslash\{u_1\}$ such that $d_{G'}(u_i) \geq 3$. Denote $N_{G'}(u_i) = \{z_0, z_1, z_2, \ldots, z_t,\}$ and $N_{G'}(u_1) = \{w_0, w_1, w_2, \ldots, w_s\}$. By the choice of $u_1$ and $u_i$, $s \geq t \geq 2$. Since $G'$ is a tree, there is an unique path $P_m$ connecting $u_1$ and $u_i$ in $G'$. Assume that $z_0$, $w_0$ belongs to $P_m$ (possibly $z_0 = u_1$ or $w_0 = u_i$ ). Note that $|M \cap \{u_1w_1, u_1w_2, \ldots, u_1w_s\}| \leq 1$, and $|M \cap \{u_iz_1, u_iz_2, \ldots, u_iz_t\}| \leq 1$. Without loss of generality, assume $u_1w_2, \ldots, u_1w_s, u_iz_2, \ldots, u_iz_t \notin M$. Let

$$G^* = \begin{cases} G - \{u_iz_2, \ldots, u_iz_t\} + \{u_1z_2, \ldots, u_1z_t\}, & \text{if } x_1 \geq x_i; \\ G - \{u_1w_2, \ldots, u_1w_s\} + \{u_iw_2, \ldots, u_iw_s\}, & \text{if } x_1 < x_i. \end{cases}$$

Then $G^* \in \mathscr{P}(2k)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. □

By Fact 2, $G'$ is a tree with some pendant paths attached to $u_1$.

**Fact 3.** $d_{G'}(u_1) \geq 3$.

*Proof.* Suppose to the contrary that $d_{G'}(u_1) < 3$. For the choice of $u_1$, $d_{G'}(u_1) \geq 2$, hence we have $d_{G'}(u_1) = 2$. Thus, $G'$ is a path with order $2k-1$. Let $G' = v_1v_2\dots v_{2k-1}$, then $d_{G'}(v_i) = 2$ for all $2 \leq i \leq 2k-2$. By Fact 1, $u_0$ is adjacent with $v_i$ for all $1 \leq i \leq 2k-1$. Hence, set $v_k = u_1$. Note that $|M \cap \{v_{k-1}v_k, v_kv_{k+1}\}| \leq 1$. Without loss of generality, assume $v_kv_{k+1} \notin M$. If $k = 3$, then $G \cong B_{2k}^1$. By Lemma 3.1, $\rho(G) < \rho(B_{2k}^2)$, a contradiction; If $k \geq 4$, there exists at least one edge, say $v_mv_{m+1}$, satisfying $v_mv_{m+1} \notin M$ and $m \leq k-2$. Let

$$G^* = \begin{cases} G - v_mv_{m+1} + v_mv_k, & \text{if } x_{v_k} \geq x_{v_{m+1}}; \\ G - v_{k+1}v_k + v_{k+1}v_{m+1}, & \text{if } x_{v_k} < x_{v_{m+1}}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. ❑

Denote the paths attached to $u_1$ in $G'$ by $P_{l_1}, P_{l_2}, \dots, P_{l_s} (s \geq 3)$.

**Fact 4.** *Each pendant path attached to $u_1$ in $G'$ has length no more than 2, that is to say, $l_i \leq 3$ for $1 \leq i \leq s$.*

*Proof.* On the contrary, suppose that, $P_{l_j} := u_1u_2\dots u_{l_j}$ is such a path of length $l_j - 1 \geq 3$. Then there exists at least one edge $e \in E(P_{l_j})$ satisfying : $e \notin M$, and $e$ is different from $u_1u_2$. Assume $u_mu_{m+1}$ is the first such edge. Denote $N(u_1) = \{u_0, w_1, w_2, w_3 \dots, w_s\}$, where $w_2 = u_2$. Note that $|M \cap \{u_1w_1, u_1w_2, \dots, u_1w_s\}| \leq 1$. Without loss of generality, assume $u_1w_1 \notin M$. Let

$$G^* = \begin{cases} G - u_mu_{m+1} + u_1u_{m+1}, & \text{if } x_1 \geq x_m; \\ G - w_1u_1 + w_1u_m, & \text{if } x_1 < x_m. \end{cases}$$

Then $G^* \in \mathscr{P}(2k)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. ❑

Denote $Q = \{v \in V(G') | d_{G'}(v) = 1, u_1v \in E(G)\}$. Note that $G$ has a perfect matching. Hence, by Fact 4, $|Q| = 0$, or $|Q| = 2$.

If $|Q| = 0$, then $G \cong B_{2k}^1$. Thus, $\rho(G) = \rho(B_{2k}^1) < \rho(B_{2k}^2)$ by Lemma 3.1; If $|Q| = 2$, then $G \cong B_{2k}^2$ and the result holds immediately.

This completes the proof. □

## 4. Maximal index of graphs in $\mathscr{P}(2k, d_0)$

For the set $\mathscr{P}(2k, d_0)$ $(k \geq 2)$, if $d_0 = 1$, then $\mathscr{P}(2k, 1)$ is just the set of all $2k$-vertex trees with a perfect matching. The maximal index of all the graphs in the set $\mathscr{P}(2k, 1)$ is determined in [28]. Hence, we consider the case of $d_0 \geq 2$ in what follows.

- Let $S_1^*$ and $S_2^*$ be the graphs defined as section 3. Denote by $u$ the center vertex of $K_{1,k-1}$. $X_i = \{x \in V(S_i^*) | d_{S_i^*}(x, u) = 1, d_{S_i^*}(x) = 2\}$, $Y_i = \{y \in V(S_i^*) | d_{S_i^*}(y, u) = 2, d_{S_i^*}(y) = 1\}$, $Z_i = \{z \in V(S_i^*) | d_{S_i^*}(z, u) = 1, d_{S_i^*}(z) = 1\}, (i = 1, 2)$. Then $|X_1| = |Y_1| = k - 1, |X_2| = |Y_2| = k - 2, |Z_1| = 0, |Z_2| = 2$. Let $Z_2 = \{z_1, z_2\}$.

- Let $C^1_{2k,d_0}$ be the graph obtained from $S_1^*$ and an isolated vertex $u_0$ by adding an edge to join $u_0$ with each of $d_0$ vertices of $S_1^*$: If $2 \leq d_0 \leq k$, $u_0$ is adjacent with $u$ and $d_0 - 1$ vertices in $X_1$; If $k+1 \leq d_0 \leq 2k-1$, $u_0$ is adjacent with $u$, $k - 1$ vertices in $X_1$, and $d_0 - k$ vertices in $Y_1$.

- Let $C^2_{2k,d_0}$ be the graph obtained from $S_2^*$ and an isolated vertex $u_0$ by adding an edge to join $u_0$ with each of $d_0$ vertices of $S_2^*$: If $2 \leq d_0 \leq k$, $u_0$ is adjacent with $u$, $z_1$, and $d_0 - 2$ vertices in $X_2$; If $k + 1 \leq d_0 \leq 2k - 1$, $u_0$ is adjacent with $u, z_1, z_2$, $k - 2$ vertices in $X_2$, and $d_0 - (k + 1)$ vertices in $Y_2$.

$C^1_{6,4}$ $\qquad$ $C^2_{6,4}$

Figure 4: Graphs $C^1_{6,4}$ and $C^2_{6,4}$ for $k = 3, d_0 = 4$.

For example, $C^1_{6,4}, C^2_{6,4}$ are depicted in Fig. 4. It is routine to check that $C^1_{2k,d_0}, C^2_{2k,d_0} \in \mathscr{P}(2k, d_0)$ for $k \geq 2$.

**Lemma 4.1.** *$\rho(C^1_{2k,d_0}) < \rho(C^2_{2k,d_0})$ for all $k \geq 3$ and $2 \leq d_0 \leq 2k - 1$.*

*Proof.* Denote $N_{S_1^*}(u) = \{v_1, v_2, \ldots, v_{k-1}\}$, and $N_{S_1^*}(v_i) \setminus \{u\} = w_i$ for all $1 \leq i \leq 2k-1$. Assume $N_{C^1_{2k,d_0}}(u_0) = \{u, v_1, \ldots, v_{d_0-1}\}$ if $2 \leq d_0 \leq k$ and $N_{C^1_{2k,d_0}}(u_0) = \{u, v_1, \ldots, v_{k-1}, w_1, \ldots, w_{d_0-k}\}$ otherwise.

If $x_u \geq x_{v_1}$, since $C^1_{2k,d_0} - v_1w_1 + uw_1 \cong C^2_{2k,d_0}$, we have $\rho(C^2_{2k,d_0}) > \rho(C^1_{2k,d_0})$ by Lemma 2.1; If $x_u < x_{v_1}$, since $C^1_{2k,d_0} - \{uv_2, \ldots, uv_{k-1}\} + \{v_1v_2, \ldots, v_1v_{k-1}\} \cong C^2_{2k,d_0}$, we have $\rho(C^2_{2k,d_0}) > \rho(C^1_{2k,d_0})$ by Lemma 2.1.

This completes the proof. ❐

**Theorem 4.2.** *Let $G \in \mathscr{P}(2k, d_0)$ $(k \geq 2,\ d_0 \geq 2)$. Then $\rho(G) \leq \rho(C^2_{2k,d_0})$ and the equality holds if and only if $G \cong C^2_{2k,d_0}$.*

*Proof.* If $k = 2$, then $\mathscr{P}(4,2) = \{G_2, G_3\}$, $\mathscr{P}(4,3) = \{G_4\}$, where $G_1, G_2, G_3, G_4$ are depicted in Fig. 3. It's straight-forward to check that $C^2_{2k,d_0}$ has the maximal index among all the graphs in $\mathscr{P}(2k, d_0)$ for $k = 2, d_0 = 2$ (resp. 3). In order to complete the proof, it suffices to consider $k \geq 3$.

Choose $G \in \mathscr{P}(2k, d_0)$ such that $\rho(G)$ is as large as possible, where $k \geq 3$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_{2k})^T$ be the Perron vector of $A(G)$, where $x_i$ corresponds to the vertex $u_i$ for $1 \leq i \leq 2k$ (By $x_v$, we mean the coordinate of $\mathbf{x}$ corresponding to the vertex $v$ ). Assume that $G' := G - u_0$ is a tree. Choose a vertex $u_1 \in V(G')$ such that $d_{G'}(u_1)$ is as large as possible. Let $M$ be a perfect matching of $G$. Similar to the proof of Theorem 3.2, we obtain that $G'$ is a tree with some pendant paths attached to $u_1$. We will first show that $d_{G'}(u_1) \geq 3$.

Suppose to the contrary that $d_{G'}(u_1) = 2$. Then $G'$ is a path with order $2k-1$. Denote $G' := v_1v_2\ldots, v_{2k-1}$. If $u_0$ is matched with $v_1$ or $v_{2k-1}$, then without loss of generality, assume $u_0v_1 \in M$. Thus, we have $v_{2k-2}v_{2k-1} \in M$, and $v_1v_2 \notin M, v_{2k-3}v_{2k-2} \notin M$. Let

$$G^* = \begin{cases} G - v_1v_2 + v_1v_{2k-3}, & \text{if } x_{v_{2k-3}} \geq x_{v_2}; \\ G - v_{2k-2}v_{2k-3} + v_{2k-2}v_2, & \text{if } x_{v_{2k-3}} < x_{v_2}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Otherwise, we have $u_0v_i \in M$ for some $i \in \{2, 3, \ldots, 2k-2\}$. Moreover, since $G$ has perfect matchings, $3 \leq i \leq 2k-3$. Thus, $v_1v_2 \in M, v_{2k-2}v_{2k-1} \in M$. Hence, we have $v_2v_3 \notin M, v_{2k-3}v_{2k-2} \notin M$ (possibly $v_3 = v_i$ or $v_{2k-3} = v_i$).

In particular, if $k=3$, then $u_0v_3 \in M$. Let

$$G^* = \begin{cases} G - v_1v_2 + v_1v_3, & \text{if } x_{v_2} \leq x_{v_3}; \\ G - v_3v_4 + v_2v_4, & \text{if } x_{v_2} > x_{v_3}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction.

For $k \geq 4$, let

$$G^* = \begin{cases} G - v_2v_3 + v_2v_{2k-3}, & \text{if } x_{v_{2k-3}} \geq x_{v_3}; \\ G - v_{2k-2}v_{2k-3} + v_{2k-2}v_3, & \text{if } x_{v_{2k-3}} < x_{v_3}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Therefore, $d_{G'}(u_1) \geq 3$.

By a similar discussion as in the proof of Fact 4 in Theorem 3.1, we can also get that each pendant path attached to $u_1$ in $G'$ has length no more than 2. Denote $Q = \{v \in V(G') | d_{G'}(v) = 1, u_1v \in E(G)\}$. Note that $G$ has perfect matchings. Hence, $|Q| = 0$, or $|Q| = 2$.

**Case 1.** $|Q| = 0$.

In this case, we denote the paths attached to $u_1$ in $G'$ by $P_{l_1}, P_{l_2}, \ldots, P_{l_{k-1}}$, where $l_i = 2$ for all $1 \leq i \leq k-1$. Denote $P = \{x \in V(G') | d_{G'}(x, u_1) = 1\}$, $R = \{x \in V(G') | d_{G'}(x, u_1) = 2\}$, and let $P_{l_i} \cap P = \{v_i\}$, $P_{l_i} \cap R = \{w_i\}$. Then we have $N_{G'}(u_1) = \{v_1, v_2, \ldots, v_{k-1}\}$. We establish the following sequence of facts.

**Fact 1.** $u_0u_1 \in E(G)$.

*Proof.* Suppose to the contrary that $u_0u_1 \notin E(G)$. Since $d_0 \geq 2$, there exists $u_2 \in V(G') \setminus \{u_1\}$ such that $u_0u_2 \in E(G)$ and $u_0u_2 \notin M$. Then $d_{G'}(u_2, u_1) = 1$ or 2.

First we consider $d_{G'}(u_2, u_1) = 1$. Without loss of generality, set $u_2 = v_1$. Let

$$G^* = \begin{cases} G - u_0v_1 + u_0u_1, & \text{if } x_1 \geq x_{v_1}; \\ G - \{u_1v_2, \ldots, u_1v_{k-1}\} + \{v_1v_2, \ldots, v_1v_{k-1}\}, & \text{if } x_1 < x_{v_1}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Therefore, $u_0u_1 \in E(G)$.

Now we consider $d_{G'}(u_2, u_1) = 2$. Without loss of generality, we may assume $u_2 = w_1$. It is routine to check that $u_0v_i \notin M$ for all $i \in$

$\{1, 2, \ldots, k-1\}$; Otherwise, $w_i$ is not matched in $G$, a contradiction. Note that, by our assumption, $u_0w_1$ is not in $M$. Hence, there exists some $w_j \in \{w_2, w_3, \ldots, w_k\}$ such that $u_0w_j$ is in $M$. By the maximality of $\rho(G)$, we have that $u_0v_j$ is in $E(G)$ and $u_0v_j$ is not in $M$. Hence, $d_{G'}(u_j, u_1) = 1$. By the former discussion, our result holds immediately. Therefore, $u_0u_1 \in E(G)$ holds in this subcase.

This completes the proof of Fact 1.

**Fact 2.** If $w_iu_0 \in E(G)$, then $v_iu_0 \in E(G)$ $(1 \le i \le k-1)$.

*Proof.* Suppose to the contrary that there exists $i_0$, such that $w_{i_0}u_0 \in E(G)$, whereas $v_{i_0}u_0 \notin E(G)$. Let

$$G^* = \begin{cases} G - u_0w_{i_0} + u_0v_{i_0}, & \text{if } x_{v_{i_0}} \ge x_{w_{i_0}}; \\ G - u_1v_{i_0} + u_1w_{i_0}, & \text{if } x_{v_{i_0}} < x_{w_{i_0}}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. □

**Fact 3.** If there exists $i \in \{1, 2, \ldots, k-1\}$ such that $w_iu_0 \in E(G)$, then for any $j \in \{1, 2, \ldots, k-1\}$, we have $v_ju_0 \in E(G)$.

*Proof.* Suppose to the contrary that there exists $j$ such that $v_ju_0 \notin E(G)$. Hence, by Fact 2, we have $u_0v_i \in E(G)$ and $w_ju_0 \notin E(G)$. Obviously, $i \neq j$. Denote $G^* = G - u_0w_i + u_0v_j$, we will show that $\rho(G) < \rho(G^*)$.

By direct computing (based on (2.2)) we have

$$\begin{aligned} \phi(G^*; \lambda) &= \phi(G^* - u_0v_j; \lambda) - \phi(G^* - u_0 - v_j; \lambda) \\ &\quad -2 \sum_{Z \in \mathscr{C}_{u_0v_j}} \phi(G^* - V(Z); \lambda), \\ \phi(G; \lambda) &= \phi(G - u_0w_i; \lambda) - \phi(G - u_0 - w_i; \lambda) \\ &\quad -2 \sum_{Z \in \mathscr{C}_{u_0w_i}} \phi(G - V(Z); \lambda). \end{aligned}$$

Note that $G^* - u_0v_j = G - u_0w_i$, $G^* - u_0 - v_j$ is a subgraph of $G - u_0 - w_i$. Hence $\phi(G^* - u_0v_j; \lambda) = \phi(G - u_0w_i; \lambda)$, and $\phi(G^* - u_0 - v_j; \lambda) \ge \phi(G - u_0 - w_i; \lambda)$ for all $\lambda \ge \rho(G - u_0 - w_i)$

Note that $u_0$ is adjacent with $d_0 - 3$ vertices in $V(G^*) \setminus \{v_i, v_j, u_1\}$, among which $k_1$ vertices are in $P$, and $k_2$ vertices are in $R$, where $k_1 + k_2 =$

$d_0 - 3, k_1, k_2 \le k - 3$. The cycles passing through edge $u_0v_j$ in $G^*$ are as follows:

- Only one $C_3 = u_0v_ju_1u_0$ satisfying $G^* - \{u_0, v_j, u_1\} = (k-2)K_2 \cup K_1$.
- $k_1+1$ cycles of length 4 (including $u_0v_ju_1v_iu_0$) satisfying $G^* - V(Z) = (k-3)K_2 \cup 2K_1$.
- $k_2$ cycles of length 5 satisfying $G^* - V(Z) = (k-3)K_2 \cup K_1$.

Hence,

$$\begin{aligned}\sum_{Z \in \mathscr{C}_{u_0v_j}} \phi(G^* - V(Z); \lambda) =&(\lambda^2 - 1)^{k-2}\lambda + (1 + k_1)(\lambda^2 - 1)^{k-3}\lambda^2 \\ &+ k_2(\lambda^2 - 1)^{k-3}\lambda \\ =&(\lambda^2 - 1)^{k-3}[\lambda^3 + (k_1 + 1)\lambda^2 + (k_2 - 1)\lambda]. \end{aligned} \tag{4.1}$$

Similarly, $u_0$ is adjacent with $d_0-3$ vertices in $V(G)\backslash\{w_i, v_i, u_1\}$, among which $k_1$ vertices are in $P$, and $k_2$ vertices are in $R$. The cycles passing through edge $u_0w_i$ in $G$ are as follows:

- Only one $C_3 = u_0w_iv_iu_0$ satisfying $G - \{u_0, w_i, v_i\}$ is a tree in which $k - 2$ pendant paths of length 2 are attached to a vertex. By an elementary calculation we have $\phi(G-\{u_0, w_i, u_1\}; \lambda) = (\lambda^2-1)^{k-2}\lambda - (k - 2)(\lambda^2 - 1)^{k-3}\lambda$.
- Only one $C_4 = u_0w_iv_iu_1u_0$ satisfying $G - \{u_0, w_i, v_i, u_1\} = (k-2)K_2$.
- $k_1$ cycles of length 5 satisfying $G - V(Z) = (k - 3)K_2 \cup K_1$.
- $k_2$ cycles of length 6 satisfying $G - V(Z) = (k - 3)K_2$.

Hence,

$$\sum_{Z \in \mathscr{C}_{u_0w_i}} \phi(G - V(Z); \lambda) = (\lambda^2 - 1)^{k-3}[\lambda^3 + \lambda^2 - (k - 1 - k_1)\lambda + k_2 - 1]. \tag{4.2}$$

In view of (4.1) and (4.2), we get

$$\begin{aligned}&\sum_{Z \in \mathscr{C}_{u_0v_j}} \phi(G^* - V(Z); \lambda) - \sum_{Z \in \mathscr{C}(u_0w_i)} \phi(G - V(Z); \lambda) \\ &= (\lambda^2 - 1)^{k-3}[k_1\lambda^2 + (k + k_2 - k_1 - 2)\lambda - k_2 + 1].\end{aligned}$$

Let

$$f(\lambda) = k_1\lambda^2 + (k + k_2 - k_1 - 2)\lambda - k_2 + 1.$$

Note that $f'(\lambda) = 2k_1\lambda + k + k_2 - k_1 - 2 \geq 2k_1 + k + k_2 - k_1 - 2 = k + k_1 + k_2 - 2 > 0$ for $\lambda \geq 1$. Together with $f(1) = k - 1 > 0$, hence $f(\lambda) > 0$ for all $\lambda \geq 1$. Therefore we get

$$\sum_{Z \in \mathscr{C}_{u_0 v_j}} \phi(G^* - V(Z); \lambda) \geq \sum_{Z \in \mathscr{C}_{u_0 w_i}} \phi(G - V(Z); \lambda)$$

for $\lambda \geq 1$. Thus, $\phi(G^*; \lambda) < \phi(G; \lambda)$ for $\lambda \geq \rho(G)(> \rho(G - u_0 - w_i) > 1)$. In view of Lemma 2.2(ii), we have $\rho(G) < \rho(G^*)$, a contradiction.

By Facts 1-4, we get $G \cong C^1_{2k,d_0}$. In view of Lemma 4.1, we have $\rho(G) = \rho(C^1_{2k,d_0}) < \rho(C^2_{2k,d_0})$ in this case.

**Case 2.** $|Q| = 2$.

In this case, let $Q = \{q_1, q_2\}$, and assume $u_0q_1 \in M, u_1q_2 \in M$. Denote the paths attached to $u_1$ in $G'$ by $P_{l_1}, P_{l_2}, \ldots, P_{l_k}$, where $P_{l_{k-1}} = u_1q_1, P_{l_k} = u_1q_2$, and $l_i = 2$ for all $1 \leq i \leq k-2$. Denote $P = \{x \in V(G') | d_{G'}(x, u_1) = 1\}$, $R = \{x \in V(G') | d_{G'}(x, u_1) = 2\}$, and let $P_{l_i} \cap P = \{v_i\}, P_{l_i} \cap R = \{w_i\}$ for all $1 \leq i \leq k-2$. Then we have $N_{G'}(u_1) = \{q_1, q_2, v_1, v_2, \ldots, v_{k-2}\}$. We establish the following sequence of facts.

**Fact 1′.** $u_0u_1 \in E(G)$.

*Proof.* Suppose to the contrary that $u_0u_1 \notin E(G)$. Since $d_0 \geq 2$, there exists $u_2 \in V(G')$ such that $u_0u_2 \in E(G)$. Note that $u_0u_2 \notin M$. Hence, $d_{G'}(u_2, u_1) = 1$ or 2. We first consider $d_{G'}(u_2, u_1) = 1$.

If $d_{G'}(u_2) = 2$, then Without loss of generality, set $u_2 = v_1$. Let $G^* = G - u_0v_1 + u_0u_1$, if $x_1 \geq x_{v_1}$ and $G - \{u_1q_1, u_1v_2, \ldots, u_1v_{k-2}\} + \{v_1q_1, v_1v_2, \ldots, v_1v_{k-2}\}$, otherwise.

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Therefore, $u_0u_1 \in E(G)$

If $d_{G'}(u_2) = 1$, then $u_2 = q_2$. Let $G^* = G - u_0q_2 + u_0u_1$, if $x_1 \geq x_{q_2}$ and $G - \{u_1q_1, u_1v_1, u_1v_2, \ldots, u_1v_{k-2}\} + \{q_2q_1, q_2v_1, q_2v_2, \ldots, q_2v_{k-2}\}$ otherwise.

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Therefore, $u_0u_1 \in E(G)$.

Now consider $d_{G'}(u_2, u_1) = 2$. Without loss of generality, we may assume $u_2 = w_1$. Let $G^* = G - u_0w_1 + u_0u_1$, if $x_1 \geq x_{w_1}$ and $G - \{u_1q_1, u_1v_2, \ldots, u_1v_{k-2}\} + \{w_1q_1, w_1v_2, \ldots, w_1v_{k-2}\}$ otherwise.

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. Therefore, $u_0u_1 \in E(G)$. Hence, $u_0u_1 \in E(G)$, as desired. ⌉

**Fact 2′.** *If $q_2u_0 \in E(G)$, then $v_iu_0 \in E(G)$ for $i \in \{1, 2, \ldots, k-2\}$.*

*Proof.* Suppose to the contrary that there exists $i_0$ such that $q_2u_0 \in E(G)$, whereas $v_{i_0}u_0 \notin E(G)$. Let

$$G^* = \begin{cases} G - u_0q_2 + u_0v_{i_0}, & \text{if } x_{v_{i_0}} \geq x_{q_2}; \\ G - w_{i_0}v_{i_0} + w_{i_0}q_2, & \text{if } x_{v_{i_0}} < x_{q_2}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. □

**Fact 3′.** *If $w_iu_0 \in E(G)$, then $v_iu_0 \in E(G)$ $(1 \leq i \leq k-2)$.*

*Proof.* Suppose to the contrary that there exists $i_0$ such that $w_{i_0}u_0 \in E(G)$, whereas $v_{i_0}u_0 \notin E(G)$. Let

$$G^* = \begin{cases} G - u_0w_{i_0} + u_0v_{i_0}, & \text{if } x_{v_{i_0}} \geq x_{w_{i_0}}; \\ G - u_1v_{i_0} + u_1w_{i_0}, & \text{if } x_{v_{i_0}} < x_{w_{i_0}}. \end{cases}$$

Then $G^* \in \mathscr{P}(2k, d_0)$, and by Lemma 2.1, $\rho(G) < \rho(G^*)$, a contradiction. □

**Fact 4′.** *If there exists $i \in \{1, 2, \ldots, k-2\}$ such that $w_iu_0 \in E(G)$, then $q_2u_0 \in E(G)$.*

*Proof.* Suppose to the contrary that $q_2u_0 \notin E(G)$. By Fact 3′, we have $v_iu_0 \in E(G)$. Denote $G^* = G - u_0w_i + u_0q_2$. We will show that $\rho(G) < \rho(G^*)$. Based on (2.2) we have

$$\begin{aligned} \phi(G^*; \lambda) &= \phi(G^* - u_0q_2; \lambda) - \phi(G^* - u_0 - q_2; \lambda) \\ &\quad -2 \sum_{Z \in \mathscr{C}_{u_0q_2}} \phi(G^* - V(Z); \lambda), \\ \phi(G; \lambda) &= \phi(G - u_0w_i; \lambda) - \phi(G - u_0 - w_i; \lambda) \\ &\quad -2 \sum_{Z \in \mathscr{C}_{u_0w_i}} \phi(G - V(Z); \lambda). \end{aligned}$$

Note that $G^* - u_0q_2 = G - u_0w_i$. Hence, $\phi(G^* - u_0q_2; \lambda) = \phi(G - u_0w_i; \lambda)$. On the other hand, by direct computing it is straightforward to check that $\phi(G^* - u_0 - q_2; \lambda) \geq \phi(G - u_0 - w_i; \lambda)$ for $\lambda \geq 1$.

Note that $u_0$ is adjacent to $d_0 - 4$ vertices in $V(G^*) \setminus \{u_1, q_1, q_2, v_i\}$, among which $k_1$ vertices are in $P$, and $k_2$ vertices are in $R$, where $k_1 + k_2 = d_0 - 4, k_1, k_2 \leq k - 3$. The cycles passing through edge $u_0q_2$ in $G^*$ are as follows:

- One $C_3 = u_0q_2u_1u_0$ satisfying $G^* - \{u_0, q_2, u_1\} = (k-2)K_2 \cup K_1$.
- One $C_4 = u_0q_2u_1q_1u_0$ satisfying $G^* - \{u_0, q_2, u_1, q_1\} = (k-2)K_2$.
- $k_1+1$ cycles of length 4 (including $u_0q_2u_1v_iu_0$) satisfying $G^* - V(Z) = (k-3)K_2 \cup 2K_1$.
- $k_2$ cycles of length 5 satisfying $G^* - V(Z) = (k-3)K_2 \cup K_1$.

By Lemma 2.3(ii) we have

$$\begin{aligned}
&\sum_{Z \in \mathscr{C}_{u_0q_2}} \phi(G^* - V(Z); \lambda) \\
&= (\lambda^2 - 1)^{k-2}\lambda + (\lambda^2 - 1)^{k-2} + (1 + k_1)(\lambda^2 - 1)^{k-3}\lambda^2 + k_2(\lambda^2 - 1)^{k-3}\lambda \\
&= (\lambda^2 - 1)^{k-4}[\lambda^5 + (k_1 + 1)\lambda^4 + (k_2 - 2)\lambda^3 - (k_1 + 2)\lambda^2 - (k_2 - 1)\lambda + 1] \\
&\quad + (\lambda^2 - 1)^{k-3}\lambda^2.
\end{aligned}$$

Similarly, $u_0$ is adjacent with $d_0 - 4$ vertices in $V(G) \setminus \{u_1, q_1, v_i, w_i\}$, among which $k_1$ vertices are in $P$, and $k_2$ vertices are in $R$. The cycles passing through edge $u_0w_i$ in $G$ are as follows:

- Only one $C_3 = u_0w_iv_iu_0$: in this case $G - \{u_0, w_i, v_i\}$ is a tree in which $k-3$ pendant paths of length 2 and 2 pendant edges are attached to a vertex. It's easy to calculate that $\phi(G - \{u_0, w_i, v_i\}; \lambda) = (\lambda^2 - 1)^{k-3}\lambda^3 - (k-3)(\lambda^2 - 1)^{k-4}\lambda^3 - 2(\lambda^2 - 1)^{k-3}\lambda$.
- Only one $C_4 = u_0w_iv_iu_1u_0$ satisfying $G - \{u_0, w_i, v_i, u_1\} = (k-3)K_2 \cup 2K_1$.
- Only one $C_5 = u_0w_iv_iu_1q_1u_0$ satisfying $G - \{u_0, w_i, v_i, u_1, q_1\} = (k-3)K_2 \cup K_1$.

- $k_1$ cycles of length 5 satisfying $G - V(Z) = (k-4)K_2 \cup 3K_1$.
- $k_2$ cycles of length 6 satisfying $G - V(Z) = (k-4)K_2 \cup 2K_1$.

Hence,

$$\begin{aligned}\sum_{Z\in\mathscr{C}_{u_0 w_i}} \phi(G - V(Z);\lambda) =& (\lambda^2-1)^{k-3}\lambda^3 - (k-3)(\lambda^2-1)^{k-4}\lambda^3 \\ & - 2(\lambda^2-1)^{k-3}\lambda + (\lambda^2-1)^{k-3}\lambda^2 + (\lambda^2-1)^{k-3}\lambda \\ & + k_1(\lambda^2-1)^{k-4}\lambda^3 + k_2(\lambda^2-1)^{k-4}\lambda^2 \\ =& (\lambda^2-1)^{k-4}[\lambda^5 - (k-1-k_1)\lambda^3 + k_2\lambda^2 + \lambda] \\ & + (\lambda^2-1)^{k-3}\lambda^2.\end{aligned}$$

Therefore we get

$$\sum_{Z\in\mathscr{C}_{u_0 q_2}} \phi(G^* - V(Z);\lambda) - \sum_{Z\in\mathscr{C}_{u_0 w_i}} \phi(G - V(Z);\lambda) = (\lambda^2-1)^{k-4} f(\lambda), \quad (4.3)$$

where

$$f(\lambda) = (k_1+1)\lambda^4 + (k+k_2-k_1-3)\lambda^3 - (k_1+k_2+2)\lambda^2 - k_2\lambda + 1.$$

Let

$$g(\lambda) := f'(\lambda) = 4(k_1+1)\lambda^3 + 3(k+k_2-k_1-3)\lambda^2 - 2(k_1+k_2+2)\lambda - k_2.$$

Hence, we have

$$\begin{aligned} g'(\lambda) &= 12(k_1+1)\lambda^2 + 6(k+k_2-k_1-3)\lambda - 2(k_1+k_2+2), \\ g''(\lambda) &= 24(k_1+1)\lambda + 6(k+k_2-k_1-3).\end{aligned}$$

On the one hand, $g'(1) = 4k_1 + 4k_2 + 6k - 10 > 0$ and $g''(\lambda) > 0$ for all $\lambda > 1$. Hence, $g'(\lambda) > 0$ for all $\lambda > 1$. It is easy to see that $g(1) = 4(k_1+1) + 3(k+k_2-k_1-3) - 2(k_1+k_2+2) - k_2 = 3k - k_1 - 9 \geq 0$, hence $f'(\lambda) = g(\lambda) > 0$ for all $\lambda > 1$.

On the other hand,

$$\begin{aligned} f(\sqrt{2}) &= (2-2\sqrt{2})k_1 + (\sqrt{2}-2)k_2 + 2\sqrt{2}k + 1 - 6\sqrt{2} \\ &\geq (2-2\sqrt{2})k_1 + (\sqrt{2}-2)k_2 + \sqrt{2}(k_1+3) \\ &\quad + \sqrt{2}(k_2+3) + 1 - 6\sqrt{2} \\ &= (2-\sqrt{2})k_1 + (2\sqrt{2}-2)k_2 + 1 > 0.\end{aligned}$$

Hence, $f(\lambda) > 0$ for all $\lambda \geq \sqrt{2}$. In view of (4.3) we have

$$\sum_{Z \in \mathscr{C}_{u_0 q_2}} \phi(G^* - V(Z); \lambda) - \sum_{Z \in \mathscr{C}_{u_0 w_i}} \phi(G - V(Z); \lambda) > 0$$

for all $\lambda \geq \sqrt{2}$. Thus, $\phi(G^*; \lambda) < \phi(G; \lambda)$ for $\lambda \geq \rho(G)(> \rho(G - u_0 - w_i) > \sqrt{2} > 1)$. By Lemma 2.2(ii), we get $\rho(G) < \rho(G^*)$, a contradiction.

By Facts 1′-4′, we get $G \cong C^2_{2k,d_0}$. Hence, in view of Cases 1 and 2, we obtain that $\rho(G) \leq \rho(C^2_{2k,d_0})$ for $k \geq 3$. The equality holds if and only if $G \cong C^2_{2k,d_0}$.

This completes the proof of Theorem 4.2.

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