




# Sharp upper bounds of $A_\alpha$ -spectral radius of cacti with given pendant vertices

Shaohui Wang<sup>1</sup> , Chunxiang Wang<sup>\*2</sup> , Jia-Bao Liu<sup>3</sup> 

<sup>1</sup>Department of Mathematics, Louisiana College, Pineville, LA 71359, USA

<sup>2</sup>School of Mathematics and Statistics, Central China Normal University, Wuhan, 430079, P.R. China

<sup>3</sup>School of Mathematics and Physics, Anhui Jianzhu University, Hefei, 230601, P.R. China

## Abstract

For  $\alpha \in [0, 1]$ , let  $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$  be  $A_\alpha$ -matrix, where  $A(G)$  is the adjacent matrix and  $D(G)$  is the diagonal matrix of the degrees of a graph  $G$ . Clearly,  $A_0(G)$  is the adjacent matrix and  $2A_{\frac{1}{2}}$  is the signless Laplacian matrix. A connected graph is a cactus graph if any two cycles of  $G$  have at most one common vertex. We first propose the result for subdivision graphs, and determine the cacti maximizing  $A_\alpha$ -spectral radius subject to fixed pendant vertices. In addition, the corresponding extremal graphs are provided. As consequences, we determine the graph with the  $A_\alpha$ -spectral radius among all the cacti with  $n$  vertices; we also characterize the  $n$ -vertex cacti with a perfect matching having the largest  $A_\alpha$ -spectral radius.

**Mathematics Subject Classification (2020).** 05C50, 15A48

**Keywords.** adjacent matrix, trees, cacti, bounds

## 1. Introduction

Throughout this paper, we consider finite simple connected graph  $G$  with vertex set  $V(G)$  and edge set  $E(G)$ . The order of a graph is the number of vertices  $|V(G)| = n$  and the size is the number of edges  $|E(G)|$ . Let  $v \in V(G)$  be a vertex of  $G$ ,  $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$  be the neighborhood of  $v$ , and  $d_G(v)$  (or briefly  $d_v$ ) be the degree of  $v$  with  $d_G(v) = |N(v)|$ . If  $e$  is an edge of  $G$  and  $G - e$  contains at least two components, then  $e$  is a cut edge of  $G$ . If  $P_k = v_1 v_2 \cdots v_k$  is a subgraph of  $G$  such that  $v_1$  is a cut vertex of degree at least 3,  $d(v_k) = 1$  and  $d(v_i) = 2$  for  $i \in [2, k - 1]$ , then  $P_k$  is called a pendant path in  $G$ . For other undefined notations and terminologies, refer to [2].

It's known that  $A(G)$  is the adjacency matrix and  $D(G)$  is the diagonal matrix of the degrees of  $G$ . The signless Laplacian matrix of  $G$  is  $Q(G) = D(G) + A(G)$ . For  $\alpha \in [0, 1]$ , the  $A_\alpha$ -matrix

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$$

is given by Nikiforov [15]. Clearly,  $A_0(G)$  is the adjacent matrix and  $2A_{\frac{1}{2}}$  is the signless Laplacian matrix of  $G$ , respectively.

\*Corresponding Author.

Email addresses: shaohuiwang@yahoo.com (S. Wang), wcxiang@mail.ccnu.edu.cn (C. Wang), liujiabaoad@163.com (J.-B. Liu)

Received: 31.01.2019; Accepted: 20.04.2020

The studies of the (adjacency, signless Laplacian) spectral radius are interesting and meaningful [7, 10–12, 19–23]. As examples, the spectral radius of trees are proposed by Lovász and J. Pelikán [14]. Feng et al. [10] studied the minimal Laplacian spectral radius of trees with given matching number. Chen [4] found the properties of spectra of graphs and their line graphs. Cvetković [8] explored the signless Laplacian spectra of graphs and a spectral theory in graphs. The bounds of signless Laplacian spectral radius and its hamiltonicity are studied by Zhou [24]. Lin and Zhou [13] obtained graphs with at most one signless Laplacian eigenvalue larger than three. In addition to the successful considerations of these spectral radius,  $A_\alpha$ -spectral radius is provided as a general version of adjacency and signless Laplacian radius, and this area would be challenging. For the  $A_\alpha$ -spectral radius, Nikiforov et al. [15, 16] introduced some properties of this spectral radius and provided the upper bounds on trees.

It is known that a tree is a noncyclic graph. If some vertices in a tree are replaced by cycles, then this graph has some cycles. The trees are extended as the definition that a cactus graph is a connected graph such that any two cycles have at most one common vertex. Denoted by  $\mathcal{C}_n^k$  the set of all cacti with  $n$  vertices and  $k$  pendant vertices.

The cactus graphs have attracted many interests among the mathematical literature including algebra and graph theory. For instance, the properties of cacti with  $n$  vertices [3] are explored by Borovićanin and Petrović. Chen and Zhou [5] investigated some upper bounds of the signless Laplacian spectral radius of cactus graphs. The signless Laplacian spectral radius of cacti with given matching number are obtained by Shen et al. [17]. Some results for spectral radius on cacti with  $k$  pendant vertices are studied Wu et al. [18]. Ye et al. [22] gave the maximal adjacency or signless Laplacian spectral radius of graphs subject to fixed connectivity.

Motivated by the above results, in this paper, we generalize the results of  $A_\alpha$ -spectra from the trees to the cacti subject to fixed pendant vertices. For  $\alpha \in [0, 1]$ , we first propose the result for subdivision graphs, and determine the cacti maximizing  $A_\alpha$ -spectral radius subject to fixed pendant vertices. In addition, the corresponding extremal graphs are determined. As consequences, we determine the graph with the  $A_\alpha$ -spectral radius among all the cacti with  $n$  vertices; we also characterize the  $n$ -vertex cacti with a perfect matching having the largest  $A_\alpha$ -spectral radius.

## 2. Preliminary

In this section, we provide some important concepts and lemmas that will be used in the main proofs.

If  $G$  is a graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ , then the  $A_\alpha$ -matrix  $A_\alpha(G)$  of  $G$  has the  $(i, j)$ -entry of  $A_\alpha(G)$  is  $1 - \alpha$  if  $v_i v_j \in E(G)$ ;  $\alpha d(v_i)$  if  $i = j$ , and otherwise 0. For  $\alpha \in [0, 1]$ , let  $\lambda_1(A_\alpha(G)) \geq \lambda_2(A_\alpha(G)) \geq \dots \geq \lambda_n(A_\alpha(G))$  be the eigenvalues of  $A_\alpha(G)$ . The  $A_\alpha$ -spectral radius of  $G$  is considered as the maximal eigenvalue  $\rho(G) := \lambda_1(A_\alpha(G))$ . Let  $X = (x_{v_1}, x_{v_2}, \dots, x_{v_n})^T$  be a real vector of  $\rho(G)$ . By  $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$ , we have the quadratic formula of  $X^T A_\alpha(G) X$  can be expressed that

$$X^T A_\alpha(G) X = \alpha \sum_{v_i \in V(G)} x_{v_i}^2 d_{v_i} + 2(1 - \alpha) \sum_{v_i v_j \in E(G)} x_{v_i} x_{v_j}.$$

Because  $A_\alpha(G)$  is a real symmetric matrix, and by Rayleigh principle, we have the formula  $\rho(G) = \max_{X \neq 0} \frac{X^T A_\alpha(G) X}{X^T X}$ . Furthermore, if  $X$  is a unit eigenvector of  $A_\alpha(G)$  corresponding to  $\rho(G)$ , then we have the formula  $\rho(G) = X^T A_\alpha(G) X$ .

As we know that once  $X$  is an eigenvector of  $\rho(G)$  for a connected graph  $G$ ,  $X$  should be unique and positive. The corresponding eigenequations for  $A_\alpha(G)$  is rewritten as

$$\rho(G)x_{v_i} = \alpha d_{v_i}x_{v_i} + (1 - \alpha) \sum_{v_i v_j \in E(G)} x_{v_j}. \quad (2.1)$$

As  $A_1(G) = D(G)$ , we study the  $A_\alpha$ -matrix for  $\alpha \in [0, 1)$  below. Based on the definition of  $A_\alpha$ -spectral radius, we have

**Lemma 2.1** ([16, 21]). Denote by  $A_\alpha(G)$  the  $A_\alpha$ -matrix of a connected graph  $G$  with  $\alpha \in [0, 1)$ ,  $v, w \in V(G)$ ,  $u \in S \subset V(G)$  such that  $S \subset N(v) \setminus (N(w) \cup \{w\})$ . Let  $H$  be a graph with vertex set  $V(G)$  and edge set  $E(G) \setminus \{uv, u \in S\} \cup \{uw, u \in S\}$ , and  $X$  a unit eigenvector to  $\rho(A_\alpha(G))$ . If  $x_w \geq x_v$  and  $|S| \neq 0$ , then  $\rho(H) \geq \rho(G)$ .

**Lemma 2.2** ([22]). Let  $A_\alpha(G)$  the  $A_\alpha$ -matrix of a connected graph  $G$  with  $\alpha \in [0, 1)$ ,  $s, t, u, v \in V(G)$ ,  $st, uv \in E(G)$ ,  $sv, tu \notin E(G)$ . Let  $H$  be a graph with vertex set  $V(G)$  and edge set  $E(G) \setminus \{uv, st\} \cup \{sv, ut\}$ , and  $X$  a unit eigenvector to  $\rho(A_\alpha(G))$ . If  $(x_s - x_u)(x_v - x_t) \geq 0$ , then  $\rho(H) \geq \rho(G)$ .

If  $G$  is a connected graph, then  $A_\alpha(G)$  is a nonnegative irreducible symmetric matrix. By the results of [1, 6, 15], if we add some edges to a connected graph, then  $A_\alpha$ -spectral radius will increase and the following lemma is straightforward.

**Lemma 2.3.** If  $H$  is a proper subgraph of a connected graph  $G$ , and  $\rho$  is the  $A_\alpha$ -spectral radius, then  $\rho(H) < \rho(G)$ .

Let  $P_t = v_0 v_1 v_2 \cdots v_t$  be a subgraph of  $G$ . If  $v_0$  is a cut vertex of degree at least 3,  $d(v_t) = 1$  and  $d(v_j) = 2$  with  $j \in [1, t - 1]$ , then  $P_t$  is called a pendant path in  $G$ . The following lemma is useful below.

**Lemma 2.4.** Let  $G \in \mathcal{C}_n^k$ . If  $\rho(G)$  is maximal, then all pendant paths share a common vertex.

**Proof.** Assume that  $G$  is a cactus graph with  $k$  pendant vertices and contains at least two pendant paths  $P_t = v_0 v_1 \cdots v_t$  and  $P_s = u_0 u_1 \cdots u_s$ . Note that  $d(u_0), d(v_0) \geq 3$ . Without loss of generality, let  $x_{v_0} \geq x_{u_0}$ . Suppose that  $u_0$  is a vertex in a cycle and this cycle contains at least one edge of the shortest path  $P[u_0, v_0]$  between  $u_0$  and  $v_0$ . Set  $G_1$  to be a new graph with vertex set  $V(G)$  and edge set  $E(G) \setminus \{u_0 v, v \in N\} \cup \{v_0 v, v \in N\}$  with  $N = N(u_0) \setminus \{w_1, w_2\}$ , where  $w_1$  is in  $P[u_0, v_0]$ , and  $v_0, w_1, w_2$  are in the same cycle; if  $u_0$  is not in any cycle, then let  $G_2$  be a new graph with vertex set  $V(G)$  and edge set  $E(G) - \{u_0 v, v \in N\} \cup \{v_0 v, v \in N\}$  with  $N = N(u_0) \setminus \{w_1, w_2\}$ , where  $w_1$  is in the shortest path between  $v_0$  and  $u_0$ , and  $w_2$  is another neighbor of  $u_0$ .

Note that both  $G_1$  and  $G_2$  are cacti with  $k$  pendant vertices. By Lemma 2.1, we have  $\rho(G_1) \geq \rho(G)$  and  $\rho(G_2) \geq \rho(G)$ . We can continue this process and move all pendant paths to a common vertex such that  $\rho(G)$  is increasing. Then this lemma is proved.  $\square$

**Lemma 2.5.** Let  $G \in \mathcal{C}_n^k$ . If  $\rho(G)$  is maximal, then the length of any pendant path is at most 2, and there is at most one pendant path of the length 2.

**Proof.** First we prove the length of any pendant path is at most 2. We prove it by a contradiction. Assume there are have a pendent path  $P$ ,  $P = v_0 v_1 \cdots v_m$ ,  $m \geq 3$ . Let  $G_1$  be a new graph with vertex set  $V(G)$  and  $E(G) + v_1 v_{m-1}$ , then  $G_1$  is a cactus with  $k$  pendent vertices and  $\rho(G_1) > \rho(G)$  (by Lemma 2.3). Then there exists a contradicted graph. Thus, if  $\rho(G)$  is maximal, then the length of any pendant path is at most 2. Next we prove there is at most one pendant path of length 2. Suppose there are  $r$ , ( $r > 1$ ) pendent path of the length 2. Without loss of generality  $P_i = v_0 v_{i1} v_{i2}$ ; ( $i = 1, 2, \cdots, r$ ). Let  $G_2$  be a new graph with vertex set  $V(G)$  and  $E(G) \cup \{v_{11} v_{21}, v_{31} v_{41}, \cdots, v_{2[\frac{r}{2}] - 1} v_{2[\frac{r}{2}] 1}\}$ ,

then  $G_2$  is a cactus with  $k$  pendent vertices and  $\rho(G_2) > \rho(G)$  (by Lemma 2.3). Then there exists a contradicted graph. Thus, if  $\rho(G)$  is maximal, there is at most one pendant path of the length 2. This completes the proof.  $\square$

**Lemma 2.6.** Let  $G \in \mathcal{C}_n^k$ . If  $\rho(G)$  is maximal, then there does not exist an internal path such that it is built by cut edges.

*Proof.* We prove it by a contradiction. Note that  $d(v_0), d(v_t) \geq 3$ . Let  $P_t = v_0v_1 \cdots v_t$  be an internal path of  $G$  such that every edge of  $P_t$  is an cut edge. If  $t \geq 2$ , then let  $G_1 = G + v_0v_t$ . Then  $G_1$  is a cactus with  $k$  pendant vertices and  $G$  is a proper subgraph of  $G_1$ . By Lemma 2.3, we have  $\rho(G_1) > \rho(G)$ , which is a contradiction. Next we consider  $t = 1$ . Without loss of generality, let  $x_0 \geq x_1$  and  $w \in N(v_1) \setminus \{v_0, v'_1\}$  such that  $v'_1$  is a neighbor except for  $v_0$ . Denote a new graph  $G_2$  with vertex set  $V(G_2) = V(G)$  and edge set  $E(G_2) = E(G) \setminus \{v_1w, w \in N(v_1) \setminus \{v_0, v'_1\}\} \cup \{v_0w, w \in N(v_1) \setminus \{v_0, v'_1\}\}$ . Then  $G_2$  is a cactus with  $k$  pendant vertices and  $\rho(G_2) \geq \rho(G)$  (by Lemma 2.1). These are contradictions and this lemma is proved.  $\square$

**Lemma 2.7.** Let  $G \in \mathcal{C}_n^k$ . If  $\rho(G)$  is maximal, then all cycles share a common vertex.

*Proof.* Suppose that there are two cut vertices  $v_0, v_1$  in  $G$  such that not all cycles contain them. If there are only two cycles, then it is proved by Lemma 2.6: there does not exist an internal path such that it is built by cut edges. If there are more 3 cycles, then choose such  $v_0$  and  $v_1$  having the longest distance. Then  $d(v_0), d(v_1) \geq 4$ . Without loss of generality, let  $x_{v_0} \geq x_{v_1}$  and  $w \in N(v_1) \setminus \{v_0\}$ . Denote a new graph  $G_1$  with vertex set  $V(G_1) = V(G)$  and edge set  $E(G_1) = E(G) \setminus \{v_1w, w \in N(v_1) \setminus \{v_l, v'_l\}\} \cup \{v_0w, w \in N(v_1) \setminus \{v_l, v'_l\}\}$ , where  $v_l, v'_l$  are neighbors of  $v_1$  and on a same cycle. Then  $G_2$  is a cactus with  $k$  pendant vertices and  $\rho(G_1) \geq \rho(G)$  (by Lemma 2.1). We can continue this method to increase  $\rho(G)$  until there exist a unique cut vertex sharing with all cycles. So, the result is proved.  $\square$

**Lemma 2.8.** Let  $G \in \mathcal{C}_n^k$ . If  $\rho(G)$  is maximal, then the length of any cycle is at most 4, and there is at most one cycle of length 4.

*Proof.* Let  $C_t = v_1v_2 \cdots v_tv_1$  be a cycle of length  $t$  in  $G$  and  $v_1$  is a cut vertex. If  $x_{v_1} \geq x_{v_3}$ , we build a new graph  $G_1$  such that  $V(G_1) = V(G)$  and  $E(G_1) = E(G) \setminus \{v_3v_4\} \cup \{v_1v_4\}$ . Then  $\rho(G) \leq \rho(G_1)$  (by Lemma 2.1). In addition,  $G_1$  is a subgraph of  $G_2 = G_1 \cup \{v_1v_3\}$ , which yields that  $\rho(G_1) < \rho(G_2)$  (by Lemma 2.3). If  $x_{v_1} \leq x_{v_3}$ , then we set up a graph  $G_3$  such that  $V(G_3) = V(G)$  and  $E(G_3) = E(G) \setminus \{v_tv_1\} \cup \{v_tv_3\}$ . We have  $\rho(G) \leq \rho(G_3)$  (by Lemma 2.1).  $G_4$  is a graph by connecting  $v_1$  and  $v_3$  from  $G_3$ . So,  $G_3$  is a subgraph of  $G_4$ . By Lemma 2.3, we have  $\rho(G_4) > \rho(G_3)$ . Thus, if  $G$  contains a cycle of length at least 5, then there exists a contradicted graph.

Next we show that there is at most one cycle of length 4. Suppose that there at least two 4-cycles  $C_1$  and  $C_2$  in  $G$ . By Lemma 2.7, these two cycles share a common cut vertex. Let  $C_1 = v_0v_1v_2v_3v_0$  and  $C_2 = v_0u_1u_2u_3v_0$ . If  $x_{v_0} \geq \min\{x_{v_1}, x_{v_3}\}$  and  $x_{v_0} \geq \min\{x_{u_1}, x_{u_3}\}$ , say  $x_{v_0} \geq x_{v_1}, x_{v_0} \geq x_{u_1}$ , then we set a new graph  $H_1$  such that  $V(H_1) = V(G)$  and  $E(H_1) = E(G) \setminus \{v_2v_1, u_2u_1\} \cup \{v_2v_0, u_2v_0\}$ . By Lemma 2.1, we have  $\rho(G) \leq \rho(H_1)$ . Let  $H_2$  be a graph from  $H_1$  by connecting  $u_1v_1$ . Since  $H_2$  is a proper subgraph of  $H_1$ , then  $\rho(H_1) < \rho(H_2)$ . This is a contradiction to the assumption that  $\rho(G)$  is maximal.

If  $x_{v_0} \leq \min\{x_{v_1}, x_{v_3}\}$  and  $x_{v_0} \leq \min\{x_{u_1}, x_{u_3}\}$ , say  $x_{v_0} \leq x_{v_1}, x_{v_0} \leq x_{u_1}$ , then we set new graphs  $H_3$  with vertex set  $V(H_3) = V(G)$  and  $E(H_3) = E(G) \setminus \{v_3v_0, u_3u_0\} \cup \{v_3v_1, u_3u_1\}$ ,  $H_4$  from  $H_3$  by connecting  $v_1u_1$ . By Lemmas 2.1,2.3, we have  $\rho(G) < \rho(H_3) < \rho(H_4)$ . We can use Lemma 2.7 to find a graph in  $\mathcal{C}_n^k$  with only one common vertex among cycles. This is a contradiction to the choice of  $G$ .

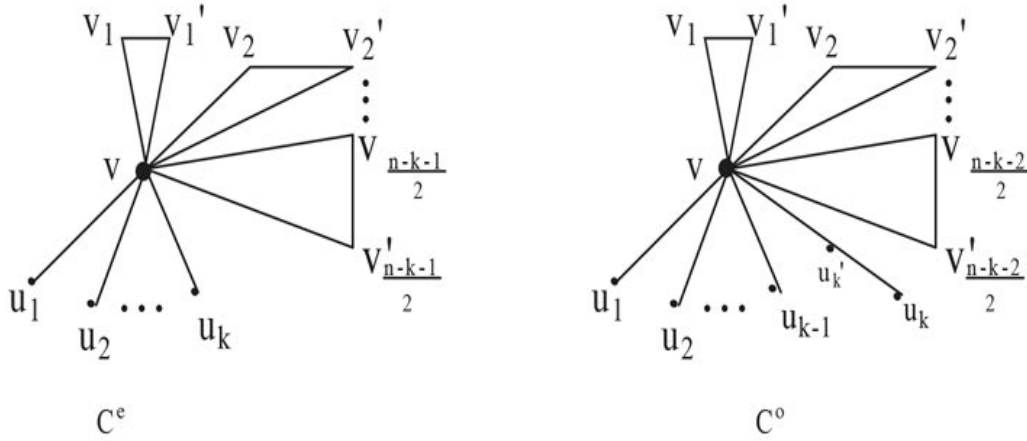
Lastly, without loss of generality, we consider the case of  $\max\{x_{u_1}, x_{u_3}\} \leq x_{v_0} \leq \min\{x_{v_1}, x_{v_3}\}$ , say  $x_{u_1} \leq x_{v_0}$  and  $x_{v_0} \leq x_{v_1}$ . Let  $H_5$  be a graph with  $V(H_5) = V(G)$

and  $E(H_5) = E(G) \setminus \{u_2u_1, v_3v_0\} \cup \{u_2v_0, v_3v_1\}$ . By Lemma 2.1,  $\rho(G) \leq \rho(H_5)$ . We build a new graph  $H_6$  by adding  $v_1u_1$ . Then  $H_5$  is a proper subgraph of  $H_6$  and  $\rho(H_5) < \rho(H_6)$ . We can use Lemma 2.7 to find a graph in  $\mathcal{C}_n^k$  with only one common vertex among cycles. This is a contradiction to the choice of  $G$ . So, this lemma is true.  $\square$

### 3. Main results

In this section, we determine the cacti maximizing  $A_\alpha$ -spectral radius subject to fixed pendant vertices. In addition, we find the graph with the  $A_\alpha$ -spectral radius among all the cacti with  $n$  vertices, and we also characterize the  $n$ -vertex cacti with a perfect matching having the largest  $A_\alpha$ -spectral radius.

Since  $\mathcal{C}_n^k$  is the set of all cacti with  $n > 0$  vertices and  $k > 0$  pendant vertices, then let  $C^e$  be a cactus graph in  $\mathcal{C}_n^k$  such that  $n - k - 1$  is even and all cycles (if any) have length 3, that is,  $C^e$  contains  $\frac{n-k-1}{2}$  cycles  $vv_1v_1'v, vv_2v_2'v, \dots, vv_{\frac{n-k-1}{2}}v_{\frac{n-k-1}{2}}'v$  and  $k$  pendant edges (if any)  $vu_1, vu_2, \dots, vu_k$ . Similarly, let  $C^o$  be a cactus graph in  $\mathcal{C}_n^k$  such that  $n - k - 1$  is odd and all cycles (if any) have length 3, that is  $C^o$  contains  $\frac{n-k-2}{2}$  cycles  $vv_1v_1'v, vv_2v_2'v, \dots, vv_{\frac{n-k-2}{2}}v_{\frac{n-k-2}{2}}'v$ ,  $k - 1$  pendant edges (if any)  $vu_1, vu_2, \dots, vu_{k-1}$  and 1 pendant path  $vu_k' u_k$ .



**Figure 1.**  $C^e$ :  $n - k - 1$  is even, contains  $\frac{n-k-1}{2}$  cycles and  $k$  pendant edges (if any);  $C^o$ :  $n - k - 1$  is odd, contains  $\frac{n-k-2}{2}$  cycles,  $k - 1$  pendant edges (if any) and 1 pendant path.

**Theorem 3.1.** (i) If  $n - k$  is odd and  $G$  is a graph with the maximum  $A_\alpha$ -spectral radius in  $\mathcal{C}_n^k$ , then  $G \cong C^e$ ;  
 (ii) If  $n - k$  is even and  $G$  is a graph with the maximum  $A_\alpha$ -spectral radius in  $\mathcal{C}_n^k$ , then  $G \cong C^o$ .

**Proof.** Choose a cactus graph  $G \in \mathcal{C}_n^k$  such that  $\rho(G)$  is maximal. Assume  $V(G) = \{v_0, v_2, \dots, v_{n-1}\}$ . By Lemma 2.4, we have all pendant paths share a common vertex. By Lemma 2.5 implies that the length of any pendant path is at most 2 and there is at most one pendant path of length 2. By Lemma 2.6 yields that there does not exist an internal path such that it is built by cut edges. By Lemma 2.8 all cycles share a common vertex. By Lemma 2.8 we have the length of any cycle is at most 4, and there is at most one cycle of length 4. In order to find the main results, we need the following two claims.

**Claim 1.** The pendant paths and cycles share a common vertex.

*Proof.* Suppose that all cycles share a vertex  $v$  and all pendant paths share a vertex  $u$ ,  $u, v \in \{v_0, v_1, \dots, v_{n-1}\}$ . Clearly,  $u$  and  $v$  is in a same cycle  $C'$ . Let  $N'(u) = N(u) \setminus V(C')$

and  $N'(v) = N(v) \setminus V(C')$ . If  $x_u \geq x_v$ , then set a new graph  $G_1$  with vertex set  $V(G_1) = V(G) \setminus \{wv, w \in N'(v)\} \cup \{wu, w \in N'(v)\}$ ; Otherwise, if  $x_u \leq x_v$ , let a new graph  $G_2$  with vertex set  $V(G_2) = V(G) \setminus \{wu, w \in N'(u)\} \cup \{wv, w \in N'(u)\}$ . By Lemma 2.1, we have  $\rho(G) \leq \rho(G_1)$  or  $\rho(G) \leq \rho(G_2)$ . A contradiction yields this claim.

**Claim 2.** If there is a pendant path  $P$  with the length at most 2, then there is no cycle of length 4.

*Proof.* Let  $v_0v_1v_2v_3v_0$  be a cycle of length 4 and  $P$  is a pendant path in  $G$ . By lemma 2.5 we know the length of  $P$  is 1 or 2. Next we prove  $x_{v_0} \geq \max\{x_{v_1}, x_{v_2}, x_{v_3}\}$ . Assume  $x_{v_1} > x_{v_0}$ . Let  $S = N(v_0) \setminus \{v_1, v_3\}$ , set a new graph  $H$  with vertex set  $V(G)$ ,  $E(G) \setminus \{wv_0, w \in S\} \cup \{wv_1, w \in S\}$ . Note that  $H$  is a cactus graph with  $k$  pendent vertices. By Lemma 2.1, we have  $\rho(G) < \rho(H)$ . It contradicts that  $\rho(G)$  is maximal, thus,  $x_{v_0} \geq x_{v_1}$ . Similarity, we have  $x_{v_0} \geq x_{v_2}$  and  $x_{v_0} \geq x_{v_3}$ . Thus,  $x_{v_0} \geq \max\{x_{v_1}, x_{v_2}, x_{v_3}\}$ .

**Case 1.**  $|P| = 2$ . Assume  $P = v_0v_4v_5$ .

Let  $H_1$  be a new graph with vertex set  $V(G)$ ,  $E(G) \setminus \{v_2v_3\} \cup \{v_0v_2\}$ . Since  $x_{v_0} \geq x_{v_3}$ , then  $\rho(G) \leq \rho(H_1)$  (by Lemma 2.1). Let  $H_2$  be a new graph with vertex set  $V(G)$ ,  $E(H_1) + v_3v_4$ .  $H_1$  is proper subgraph of  $H_2$ . By Lemma 2.3, we have  $\rho(H_1) < \rho(H_2)$ . Then,  $\rho(G) < \rho(H_2)$ . Note that  $H_2$  is a cactus graph with  $k$  pendent vertices.

**Case 2.**  $|P| = 1$ . Assume  $P = v_0v_6$ .

**Subcase 2.1.**  $x_{v_2} \leq x_{v_6}$ .

Let  $H_3$  be a new graph with vertex set  $V(G)$ ,  $E(G) \setminus \{v_2v_3\} \cup \{v_3v_6\}$ . Note that  $H_3$  is a cactus graph with  $k$  pendent vertices. By Lemma 2.1, we have  $\rho(G) \leq \rho(H_3)$ .

**Subcase 2.2.**  $x_{v_2} > x_{v_6}$ .

Let  $H_4$  be a new graph with vertex set  $V(G)$ ,  $E(G) \setminus \{v_2v_3, v_0v_6\} \cup \{v_0v_2, v_3v_6\}$ . Note that  $H_4$  is a cactus graph with  $k$  pendent vertices. Since  $x_{v_0} \geq x_{v_3}$  and  $x_{v_2} > x_{v_6}$ , then  $(x_{v_2} - x_{v_6})(x_{v_0} - x_{v_3}) \geq 0$ . By Lemma 2.2, we have  $\rho(G) \leq \rho(H_4)$ . Note that  $H_4$  is a cactus graph with  $k$  pendent vertices. It is a contradiction and this claim is proved.

Therefore, if  $n - k$  is odd, then  $\rho(G) \leq \rho(C^e)$ ; if  $n - k$  is even, then  $\rho(G) \leq \rho(C^o)$ . So, this theorem is proved.  $\square$

**Lemma 3.2** ([9]). Given a partition  $\{1, 2, \dots, n\} = \Delta_1 \cup \Delta_2 \cup \dots \cup \Delta_m$  with  $|\Delta_i| = n_i > 0$ ,  $A$  be any matrix partitioned into blocks  $A_{ij}$ , where  $A_{ij}$  is an  $n_i \times n_j$  block. Suppose that the block  $A_{ij}$  has constant row sums  $b_{ij}$ , and let  $B = (b_{ij})$ . Then the spectrum of  $B$  is contained in the spectrum of  $A$  (taking into account the multiplicities of the eigenvalues).

Next we provide all eigenvalues of  $C^e$  and  $C^o$  in the proposition.

**Proposition 3.3.** Let  $\alpha \in [0, 1)$ . The following statements hold. (i) The maximum eigenvalues of  $A_\alpha(C^e)$  satisfy the equation:  $f(\rho) = (\alpha - \rho)^3 + (n\alpha - 2\alpha + 1)(\alpha - \rho)^2 + [(1 - n)\alpha^2 + (3n - 4)\alpha + 1 - n](\alpha - \rho) - k(1 - \alpha)^2 = 0$ . (ii) The maximum eigenvalues of  $A_\alpha(C^o)$  satisfy the equation:  $g(\rho) = (n\alpha - 2\alpha - \rho)(\alpha - \rho)(\alpha - \rho + 1)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (k - 1)(1 - \alpha)^2(\alpha - \rho + 1)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (n - k - 2)(1 - \alpha)^2(\alpha - \rho)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (1 - \alpha)^2(\alpha - \rho)^2(\alpha - \rho + 1) = 0$ .

**Proof.** Since the matrix  $A_\alpha = \alpha D + (1 - \alpha)A$ , where  $D$  has on the diagonal the vector  $(n - 1, 2, 1)$  and  $A$  consists of the following three row-vectors, in the order:  $(0, n - k - 1, k)$ ;  $(1, 1, 0)$ ;  $(1, 0, 0)$ . By Lemma 3.2, thus, the eigenvector  $x$  of  $\rho(A_\alpha(C^e))$  ( $C^e$ , see Figure 1) is a constant value  $\beta_2$  on the vertex set  $\{v_1, v'_1, v_2, v'_2, \dots, v_{\frac{n-k-1}{2}}, v'_{\frac{n-k-1}{2}}\}$ , and constant value  $\beta_3$  on the vertex set  $\{u_1, u_2, \dots, u_k\}$ . Defining  $x(v) =: \beta_1$ ,  $\rho(C^e) =: \rho$ , also by (1), we get  $(\rho - (n - 1)\alpha)\beta_1 = (1 - \alpha)((n - k - 1)\beta_2 + k\beta_3)$ ,  $(\rho - 2\alpha)\beta_2 = (1 - \alpha)(\beta_1 + \beta_2)$  and  $(\rho - \alpha)\beta_3 = (1 - \alpha)\beta_1$ .

Then we get:

$$f(\rho) = (\alpha - \rho)^3 + (n\alpha - 2\alpha + 1)(\alpha - \rho)^2 + [(1 - n)\alpha^2 + (3n - 4)\alpha + 1 - n](\alpha - \rho) - k(1 - \alpha)^2 = 0.$$

Next we consider  $A_\alpha(C^o)$  ( $C^o$ , see Figure 1), since the matrix  $A_\alpha = \alpha D + (1 - \alpha)A$ , where  $D$  has on the diagonal the vector  $(n - 2, 2, 1, 2, 1)$  and  $A$  consists of the following five row-vectors, in the order:  $(0, n - k - 2, k - 1, 1, 0)$ ;  $(1, 1, 0, 0, 0)$ ;  $(1, 0, 0, 0, 0)$ ;  $(1, 0, 0, 0, 1)$ ;  $(0, 0, 0, 1, 0)$ . By Lemma 3.2, thus, the eigenvector  $x$  of  $\rho(A_\alpha(C^o))$  is a constant value  $\beta_2$  on the vertex set  $\{v_1, v'_1, \dots, v_{\frac{n-k-2}{2}}, v'_{\frac{n-k-2}{2}}\}$ , and constant value  $\beta_3$  on the vertex set  $\{u_1, u_2, \dots, u_{k-1}\}$ . Defining  $x(v) =: \beta_1$ , and  $x(u'_k) =: \beta_4$ , and  $x(u_k) =: \beta_5$ .  $\rho(C^e) =: \rho$ , also by (1), similarly as above the computation of  $A_\alpha(C^e)$ , we obtain:

$$g(\rho) = (n\alpha - 2\alpha - \rho)(\alpha - \rho)(\alpha - \rho + 1)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (k - 1)(1 - \alpha)^2(\alpha - \rho + 1)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (n - k - 2)(1 - \alpha)^2(\alpha - \rho)(\rho^2 - 3\alpha\rho + \alpha^2 + 2\alpha - 1) - (1 - \alpha)^2(\alpha - \rho)^2(\alpha - \rho + 1) = 0.$$

Thus, our proof is finished.  $\square$

Denote by  $\mathcal{C}_n^*$  be the set of all cacti with  $n$  vertices. Let  $C_n^{*1}$  be a cactus graph in  $\mathcal{C}_n^*$  such that  $n$  is odd and  $C_n^{*1}$  contains  $\frac{n-1}{2}$  cycles of length 3 (if any). Let  $C_n^{*2}$  be a cactus graph in  $\mathcal{C}_n^*$  such that  $n$  is even and  $C_n^{*2}$  contains  $\frac{n-2}{2}$  cycles of length 3 (if any) and one pendant edge.

**Theorem 3.4.** (i) If  $n$  is odd and  $G$  is a graph with the maximum  $A_\alpha$ -spectral radius in  $\mathcal{C}_n^*$ , then  $G \cong C_n^{*1}$ ;  
(ii) If  $n$  is even and  $G$  is a graph with the maximum  $A_\alpha$ -spectral radius in  $\mathcal{C}_n^*$ , then  $G \cong C_n^{*2}$ .

**Proof.** By the proof of Theorem 3.1, we have the sharp upper bounds of  $A_\alpha$ -spectral radius attain at  $C^e$  and  $C^o$ . We can set up a new graph by connecting any two pendant vertices and the original graph is the proper subgraph of this new graph. By Lemma 2.2, we have  $\rho(G)$  is increasing by this operation. Therefore,  $\rho(G) \leq \rho(C^{*1})$  if  $n$  is odd, and  $\rho(G) \leq \rho(C^{*2})$  if  $n$  is even. Since  $C^{*1}$  is the cactus graph  $C^e$  when  $k = 0$ , and  $C^{*2}$  is the cactus graph  $C^o$  when  $k = 1$ . Thus, this theorem is proved.

By Proposition 3.3, and letting  $k = 0, 1$ , we can also obtain their corresponding eigenvalues.  $\square$

Based on the above outcomes, we can determine the sharp upper bound for the  $A_\alpha$ -spectral radius of cacti with a perfect matching. Let  $\mathcal{C}_{2k}^m$  be the set of all  $2k$ -vertex cacti with a perfect matching.

**Theorem 3.5.** If  $G$  is a graph with the maximum  $A_\alpha$ -spectral radius in  $\mathcal{C}_{2k}^m$ , then  $G \cong C_{2k}^{*2}$ .

**Acknowledgment.** The work was partially supported by the National Natural Science Foundation of China under Grants 11771172 and 11571134. We would like to thank for Ting Huang's suggestions and improvements in our paper.

## References

- [1] A. Berman and R.J. Plemmons, *Nonnegative Matrices in the Mathematical Sciences*, SIAM: Philadelphia, PA, USA, 1994.
- [2] B. Bollobás, *Modern Graph Theory*, Springer: New York, NY, USA, 1998.
- [3] B. Borovićanin and M. Petrović, *On the index of cactuses with  $n$  vertices*, Publ. Inst. Math **79** (93), 13-18, 2006.
- [4] Y. Chen, *Properties of spectra of graphs and line graphs*, Appl. Math. J. Chinese Univ. Ser. B **17** (3), 371-376, 2002.
- [5] M. Chen and B. Zhou, *On the Signless Laplacian Spectral Radius of Cacti*, Croat. Chem. Acta **89** (4), 493-498, 2016.
- [6] L. Collatz and U. Sinogowitz, *Spektrcn endlicher Graten*, Abh. Math. Sem. Univ. Hamburg **21**, 63-77, 1957.

- [7] L. Cui, Y.-Z. Fan, *The signless laplacian spectral radius of graphs with given number of cut vertices*, Discuss. Math. Graph Theory **30** (1), 85-93, 2010.
- [8] D. Cvetković, P. Rowlinson and SK. Simić, *Signless Laplacians of finite graphs*, Linear Algebra Appl. **423** (3), 155-171, 2007.
- [9] D. Cvetkovic, P. Rowlinson, S. Simic, *An Introduction to the Theory of Graph Spectra*, Cambridge University Press, 2009.
- [10] L. Feng , Q. Li and X.-D. Zhang, *Minimizing the Laplacian spectral radius of trees with given matching number*, Linear Multilinear Algebra **55**, 199-207, 2007.
- [11] J. Huang and S. Li, *On the Spectral Characterizations of Graphs*, Discuss. Math. Graph Theory **37**, 729-744, 2017.
- [12] S. Li and M. Zhang, *On the signless Laplacian index of cacti with a given number of pendant vertices*, Linear Algebra Appl. **436**, 4400-4411, 2012.
- [13] H. Lin and B. Zhou, *Graphs with at most one signless Laplacian eigenvalue exceeding three*, Linear Multilinear Algebra **63** (3), 377-383, 2015.
- [14] L. Lovász and J. Pelikán, *On the eigenvalues of trees*, Period. Math. Hungar **3**, 175-182, 1973.
- [15] V. Nikiforov, *Merging the A- and Q-spectral theories*, Appl. Anal. Discrete Math. **11**, 81-107, 2017.
- [16] V. Nikiforov, G. Pastén, O. Rojo and R.L. Soto, *On the  $A_\alpha$ -spectra of trees*, Linear Algebra Appl. **520** (3), 286-305, 2017.
- [17] Y. Shen, L. You, M. Zhang and S. Li, *On a conjecture for the signless Laplacian spectral radius of cacti with given matching number*, Linear Multilinear Algebra **65** (4), 457-474, 2017.
- [18] J. Wu, H. Deng and Q. Jiang, *On the spectral radius of cacti with k-pendant vertices*, Linear Multilinear Algebra **58**, 391-398, 2010.
- [19] T. Wu and H. Zhang, *Per-spectral characterizations of some bipartite graphs*, Discuss. Math. Graph Theory **37**, 935-951, 2017.
- [20] R. Xing and B. Zhou, *On the least eigenvalue of cacti with pendant vertices*, Linear Algebra Appl. **438**, 2256-2273, 2013.
- [21] J. Xue, H. Lin, S. Liu and J. Shu, *On the  $A_\alpha$ -spectral radius of a graph*, Linear Algebra Appl. **550**, 105-120, 2018.
- [22] Y. Yan, C.Wang and S.Wang, *The  $A_\alpha$ -spectral radii of trees with specified maximum degree*, submitted.
- [23] A. Yu, M. Lu and F. Tian, *On the spectral radius of graphs*, Linear Algebra Appl. **387**, 41-49, 2004.
- [24] Bo. Zhou, *Signless Laplacian spectral radius and Hamiltonicity*, Linear Algebra Appl **423** (3), 566-570, 2010.