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DOMINATION NUMBER AND (SIGNLESS LAPLACIAN) SPECTRAL RADIUS OF CACTUS GRAPHS*

YAQI CUI†, YUANYUAN CHEN‡, DAN LI†, AND YUE ZHANG§

Abstract. A cactus graph is a connected graph whose block is either an edge or a cycle. A vertex set $S \subseteq V(G)$ is said to a dominating set of a graph G if every vertex in $V(G) \setminus S$ is adjacent to a vertex in S. There are several results on the (signless Laplacian) spectral radius and domination number in graph theory. In this paper, we determine the unique graph with the maximum adjacency spectral radius and signless Laplacian spectral radius among all cactus graphs with fixed domination number.

Key words. Cactus; Domination number, (Signless Laplacian), Spectral radius.

AMS subject classifications. 05C50.

1. Introduction. All graphs in this paper are simple and undirected. Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, the neighborhood of v is the set $N_G(v) = \{u \in V(G)|uv \in E(G)\}$. The degree of $v \in V(G)$, denoted by $d_G(v)$ (or $d(v)$ for short), is defined as the number of neighbors of v in G, i.e., $d_G(v)$=$|N_G(v)|$. The adjacency matrix $A(G) = (a_{ij})$ of G is defined as an $n \times n$ $(0,1)$–matrix with $a_{ij} = 1$ if and only if $v_iv_j \in E(G)$. The signless Laplacian matrix of G is defined as $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees of G. The largest eigenvalue of $A(G)$ (resp. $Q(G)$), denoted by $\rho(G)$ (resp. $q(G)$), is called the adjacency (resp. signless Laplacian) spectral radius of G. A vertex $v \in V(G)$ is called a cut vertex if moving v from G increases the number of components. A block of G is a maximal connected subgraph of G without any cut vertex. A cactus is a connected graph in which its blocks are either edges or cycles and any two blocks have at most one common vertex.

Recently, the research of spectral radius of cactus graphs has attracted much attention. In [16], Xue, Liu and Liu determined the maximum spectral radius of cactus graphs with fixed independence number. A unique graph whose spectral radius is maximal among all cactus graphs was determined by Borovićanin and Petrović [1]. Hou and Li [8] considered the spectral radius of cactus graphs with given matching number. Huang, Deng and Simić obtained the maximum spectral radius of all cactuses on $2m$ vertices, k cycles, and with perfect matchings in [7]. At the same time, the research of the signless Laplacian spectral of cactus graphs also has some conclusions. For example, the signless Laplacian spread of cacti was studied by Lin and Guo [12]. In [9], Li and Zhang determined the graph with the largest signless Laplacian index among all the cacti with n vertices and the cacti with a perfect matching, respectively. Shen and You et al. [13] characterized the unique graph with the maximal signless Laplacian spectral radius in the cactus graph.

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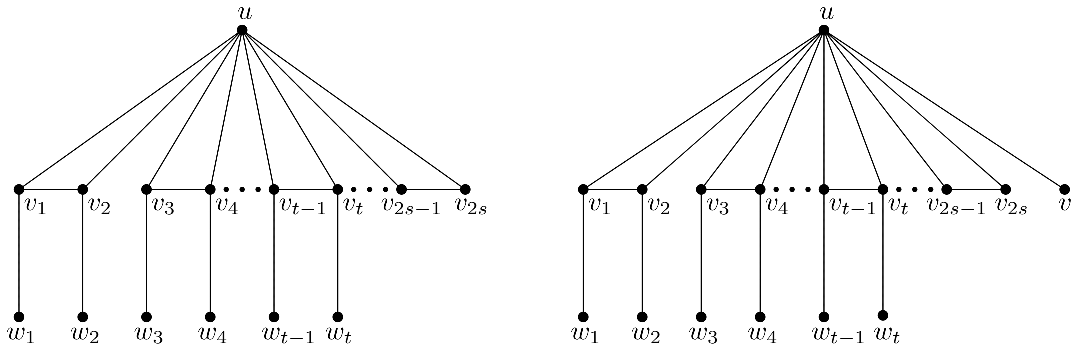
†College of Mathematics and System Science, Xinjiang University, Urumqi, Xinjiang 830017, China (cuiyq_0129@163.com, ldxjedu@163.com). Supported by National Natural Science Foundation of China (No. 12401468), Natural Science Foundation of Xinjiang Uygur Autonomous Region (No. 2023D01C165).

‡College of Mathematics and System Science, Xinjiang University, Urumqi, Xinjiang 830017, China (chenyy_de@sina.com).

§Xinjiang Normal University Department Graduates, Xinjiang Normal University, Urumqi, Xinjiang 830017, China (12300813lz@sina.com).



$C_{s,t}$ $C^e_{s,t}$

FIGURE 1. *Graphs* $C_{s,t}$ *and* $C^e_{s,t}$.

A vertex set $S \subseteq V(G)$ is said to a dominating set of a graph G if every vertex in $V(G) \setminus S$ is adjacent to a vertex in S. The domination number of G, denoted by $\gamma(G)$, is the minimum cardinality of a dominating set, i.e., $\gamma(G) = \min_{S \subseteq V(G)}\{|S|\}$. A dominating set of G of minimum cardinality is called a $\gamma(G)$-set. Domination number is widely and profoundly used in mathematical problems such as coverage and location determination, and there are several results on the (signless Laplacian) spectral radius and domination number in graph theory. In [2], Chen and He studied the spectral radii of tree with given domination number. In [3], Fan and Tan researched the least eigenvalue of signless Laplacian of non-bipartite graph with given domination number. There are also some conclusions about domination number in graphs, one can see [5, 6, 11, 14, 15].

The union of two graphs G_1 and G_2 is denoted by $G_1 \cup G_2$, which is a graph such that vertex set $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$, and the join of two graphs G_1 and G_2 is written as $G_1 \vee G_2$, which is a graph such that vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$. It is obvious that the cactus graph is $(K_2 \vee 2K_1)$-free and $K_{2,3}$-free. Let $v \in V(G)$, if $d_G(v) = 1$, then we call v is a pendant vertex of G. A pendant edge is an edge that is incident to a pendant vertex. Let $C_{s,t}$ be a connected graph obtained from the $K_1 \vee sK_2$ by attaching t pendant edges to vertices of the sK_2 such that for any $v \in V(sK_2)$, $d_{C_{s,t}}(v) \le 3$, where $s \ge \frac{t}{2}$. Let $C^e_{s,t}$ be a connected graph obtained from the $K_1 \vee (K_1 \cup sK_2)$ by attaching t pendant edges to vertices of the sK_2 such that for any $v \in V(sK_2)$, $d_{C^e_{s,t}}(v) \le 3$, where $s \ge \frac{t}{2}$ (see Fig. 1).

In this paper, we pay attention to the relation between the (signless Laplacian) spectral radius and the domination number of a cactus. In order to give the main results for $\rho(G)$ and $q(G)$ simultaneously, we introduce the matrix $A_a(G) = aD(G) + A(G)$ and denote by $\rho_a(G)$ the largest eigenvalue of $A_a(G)$, where $a \in \{0, 1\}$. Clearly, $A_0(G) = A(G)$ (resp. $A_1(G) = Q(G)$) and $\rho_0(G) = \rho(G)$ (resp. $\rho_1(G) = q(G)$). Let $\mathcal{G}_n$ be the set of cactus graphs on $n\,(\ge 24)$ vertices. For integers $n(\ge 24)$, γ, let $\mathcal{G}_n^{\gamma}$ and $\mathcal{G}_n^{\le \gamma}$ be the set of all cactus graphs on n vertices with domination number γ and with domination number at most γ, respectively. The main results are shown as below.

THEOREM 1.1. *Let* $G \in \mathcal{G}_n^{\le \gamma}$, *where* $n \ge 24$. *Then we have*

$$\rho_a(G) \le \begin{cases} \rho_a(C_{\frac{n-\gamma}{2}, \gamma-1}), & \text{when } n-\gamma \equiv 0 \ (mod\ 2); \\ \rho_a(C^e_{\frac{n-\gamma-1}{2}, \gamma-1}), & \text{when } n-\gamma \equiv 1 \ (mod\ 2), \end{cases}$$

with equality if and only if $G \cong C_{\frac{n-\gamma}{2},\gamma-1}$ *or* $G \cong C^e_{\frac{n-\gamma-1}{2},\gamma-1}$. *In particular, when* $n = 2\gamma$, *we have* $n-\gamma \equiv 1 \pmod 2$.

Note that $\gamma(C_{\frac{n-\gamma}{2},\gamma-1}) = \gamma$. Thus, if $n-\gamma \equiv 0 \pmod 2$, then $C_{\frac{n-\gamma}{2},\gamma-1}$ is also the unique cactus graph in $\mathcal{G}_n^\gamma$ which has the maximum largest eigenvalue of $A_a(G)$. Similarly, $C^e_{\frac{n-\gamma-1}{2},\gamma-1}$ is the unique cactus graph in $\mathcal{G}_n^\gamma$ which has the maximum largest eigenvalue of $A_a(G)$ if $n-\gamma \equiv 1 \pmod 2$. Then we get the following result immediately.

Theorem 1.2. *Let* $G \in \mathcal{G}_n^\gamma$, *where* $n \geq 24$. *Then we have*

$$\rho_a(G) \leq \begin{cases} \rho_a(C_{\frac{n-\gamma}{2},\gamma-1}), & \text{when } n-\gamma \equiv 0 \pmod 2; \\ \rho_a(C^e_{\frac{n-\gamma-1}{2},\gamma-1}), & \text{when } n-\gamma \equiv 1 \pmod 2, \end{cases}$$

with equality if and only if $G \cong C_{\frac{n-\gamma}{2},\gamma-1}$ *or* $G \cong C^e_{\frac{n-\gamma-1}{2},\gamma-1}$. *In particular, when* $n = 2\gamma$, *we have* $n-\gamma \equiv 1 \pmod 2$.

2. Preliminaries.

By the Perron–Frobenius Theorem, there is a unique positive unit eigenvector $\boldsymbol{x} = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$ of $A_a(G)$ corresponding to $\rho_a(G)$, which is called the A_a-Perron vector of G. Such a unit eigenvector is also called a principal eigenvector of G. We denote by x_{v_i} the entry of $\boldsymbol{x}$ corresponding to the vertex v_i. By $\rho_a(G)\boldsymbol{x} = A_a(G)\boldsymbol{x}$, we know the eigenequations for $A_a(G)$ can be written as

$$\rho_a x_{v_i} = a d_G(v_i) x_{v_i} + \sum_{v_i \sim v_j} x_{v_j}, \quad i = 1, 2, \ldots, n. \tag{2.1}$$

The following lemma shows an edge transformation that increases the spectral radius. This result was proved for $A(G)$ and $Q(G)$ in [10, 17], and we can be easily extended to the general matrix $A_a(G)$ for $a \in \{0, 1\}$.

Lemma 2.1 ([10], [17]). *Let* u, v *be two vertices of the connected graph* G. *Suppose that* $v_1, v_2, \ldots, v_s$ $(1 \leq s \leq d_v)$ *are some vertices of* $N_G(v) \setminus N_G(u)$ *and* $\boldsymbol{x} = (x_1, x_2, \ldots x_n)^T$ *is the Perron vector of* $A_a(G)$, *where* $a \in \{0, 1\}$ *and* x_i *corresponds to the vertex* v_i $(1 \leq i \leq n)$. *Let* G^* *be the graph obtained from* G *by deleting the edges* $\{vv_i\}$ *and adding the edges* $\{uv_i\}$ $(1 \leq i \leq s)$. *If* $x_u \geq x_v$, *then* $\rho_a(G) < \rho_a(G^*)$.

Lemma 2.2 ([5]). *If* G *is a connected graph and* C *is an arbitrary cycle in* G, *then there is an edge* e *of* C *such that* $\gamma(G - e) = \gamma(G)$.

By the well-known Perron–Frobenius theorem, we can easily deduce the following result.

Lemma 2.3 ([4]). *Let* $a \geq 0$. *If* H *is a spanning subgraph of a connected graph* G, *then*

$$\rho_a(H) \leq \rho_a(G),$$

with equality if and only if $H \cong G$.

Lemma 2.4. *Let* $C_{s,t}$ *and* $C^e_{s,t}$ *be two graphs depicted in* Fig.1. *If* $s \geq 3$, $t \geq 2$, *then we have*

(i) $\rho_a(C_{s,t}) < \rho_a(C_{s+1,t-2})$;
(ii) $\rho_a(C^e_{s,t}) < \rho_a(C^e_{s+1,t-2})$.

Proof. (i). Let $\boldsymbol{x} = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$ be a principal eigenvector of $C_{s,t}$ corresponding to $\rho_a(C_{s,t})$. For simplicity, let $\rho_a = \rho_a(C_{s,t})$. Note that every cycle block in $C_{s,t}$ is a triangle, then we can partition the vertex set of $C_{s,t}$ as $V(C_{s,t}) = \{u\} \cup \{v_1, v_2, \ldots, v_{2s}\} \cup \{w_1, w_2, \ldots, w_t\}$ such that $uv_iv_{i+1}u$ is a triangle for $1 \le i \le 2s-1$, where i is odd and v_jw_j is a pendant edge for $1 \le j \le t$. According to the symmetry of $C_{s,t}$, we know that $x_{w_1} = \cdots = x_{w_t}$ and $x_{v_1} = \cdots = x_{v_t}$, where $t \ge 2$. Since $s \ge 3$, $K_1 \vee 3K_2$ is a subgraph of $C_{s,t}$, it follows from Lemma 2.3 that $\rho_a \ge \rho_a(K_1 \vee 3K_2)$. By simple calculation, we have

$$\rho_a \ge \rho_a(K_1 \vee 3K_2) = \frac{8a + 1 + \sqrt{16a^2 - 8a + 25}}{2}.$$

From equation (2.1), we have

$$\begin{cases} \rho_a x_{v_1} = 3a x_{v_1} + x_u + x_{v_2} + x_{w_1}, \\ \rho_a x_{w_1} = a x_{w_1} + x_{v_1}. \end{cases}$$

Then we obtain that

$$\begin{aligned} x_u &= \frac{\rho_a^2 - (4a+1)\rho_a + 3a^2 + a - 1}{\rho_a - a} x_{v_1} \\ &> \frac{3a\sqrt{16a^2 - 8a + 25} - 7a + 6a^2 + 10}{8a + \sqrt{16a^2 - 8a + 25} + 1} x_{v_1} \\ &> x_{v_1}. \end{aligned}$$

This implies that $x_u > x_{v_1} (= x_{v_2})$. Consider a new cactus graph $G = C_{s,t} - \{v_1w_1, v_2w_2\} + \{uw_1, uw_2\}$. Then by Lemma 2.1, we have $\rho_a(C_{s,t}) < \rho_a(G)$. Note that $C_{s+1,t-2} = G + \{w_1w_2\}$. Then we have $\rho_a(C_{s,t}) < \rho_a(G) < \rho_a(C_{s+1,t-2})$ by Lemma 2.3.

(ii). Similarly, one can show that $\rho_a(C^e_{s,t}) < \rho_a(C^e_{s+1,t-2})$. ∎

3. Proof of the Theorem 1.1. We first introduce some notions that will be used in the proof of Theorem 1.1. If a block has exactly one cut vertex, we say that the block is an end block of G. An internal block is a block which has at least two cut vertices. The block degree of v, denoted by $d^b(v)$, is the number of blocks containing the vertex v. For $u, v \in V(G)$, the distance u and v in G is the length of a shortest path connecting them, denoted by $dist(u,v)$, and $N_G(u) = \{v \in V(G) | dist(v,u) = 1\}$, $N^2_G(u) = \{v \in V(G) | dist(v,u) = 2\}$. For a set $U \subseteq V(G)$, we use $G[U]$ to denote the subgraph of G induced by U.

Proof. Suppose that G is a cactus graph in $\mathcal{G}_n^{\le\gamma}$ with the maximum spectral radius. Let S be a minimum domination set in G, that is, $|S| = \gamma(G)$. Note that $C_{\frac{n-\gamma}{2},\gamma-1}$ is a cactus graph on n vertices with domination number γ. Since $n \ge 24$, we have $\frac{n-\gamma}{2} \ge \frac{n}{4} \ge 6$, which implies that $K_1 \vee 6K_2$ is a subgraph of $C_{\frac{n-\gamma}{2},\gamma-1}$. By Lemma 2.3, we have

$$\rho_a(G) \ge \rho_a\left(C_{\frac{n-\gamma}{2},\gamma-1}\right) \ge \rho_a(K_1 \vee 6K_2) = 7a + \frac{1}{2} + \frac{\sqrt{100a^2 - 20a + 49}}{2}.$$

Similarly, we also have

$$\rho_a(G) \ge \rho_a\left(C^e_{\frac{n-\gamma-1}{2},\gamma-1}\right) \ge \rho_a(K_1 \vee 6K_2) = 7a + \frac{1}{2} + \frac{\sqrt{100a^2 - 20a + 49}}{2}.$$

In particular, $\rho = \rho_0(G) \geq 4$ and $q = \rho_1(G) \geq 13.1789$.

Let C_l be a cycle with length l in G. Suppose that $v_i \in V(C_l)$. Then we denote by $G(i)$ the component contains the vertex v_i after deleting the edges in C_l. Let $\gamma_G(H)$ be the domination number of H in G, where $H \subseteq G$. Let $\boldsymbol{x} = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$ be a principal eigenvector of G corresponding to $\rho_a(G)$. In order to present the structural properties of the graph G, we obtain six claims in the following.

Claim 1. *All the cycles of G are triangles.*

Proof. Let $C_l = v_1v_2\ldots v_lv_1$ with $l \geq 3$ in G. It suffices to show that $l = 3$. By contradiction, suppose that $l \geq 4$. Without loss of generality, we may assume that $x_{v_1} = max\{x_{v_i}|1 \leq i \leq l\}$. Let $M = (V(C_l) \setminus \{v_1\}) \cap S$. If $M \neq \emptyset$, without loss of generality, suppose that $v_k \in M$. Then let $G' = G - \{v_kv^*|v^* \in N_G(v_k) \setminus V(C_l)\} + \{v_1v^*|v^* \in N_G(v_k) \setminus V(C_l)\}$. By Lemma 1, we have $\rho_a(G') > \rho_a(G)$. Let

$$G_1 = \begin{cases} G' + \{v_1v_i|3 \leq i \leq l-1\} - \{v_iv_{i+1}|3 \leq i \leq l-1\}, & \text{if } M \neq \emptyset; \\ G + \{v_1v_i|3 \leq i \leq l-1\} - \{v_iv_{i+1}|3 \leq i \leq l-1\}, & \text{if } M = \emptyset. \end{cases}$$

Obviously, $G_1 \in \mathcal{G}_n$.

If $v_1 \in S$, then S is also a domination set in G_1. This implies that $\gamma(G_1) \leq |S| = \gamma(G)$.

If $v_1 \notin S$ and $M \neq \emptyset$, let $v_k \in M$, then $(S \setminus \{v_k\}) \cup \{v_1\}$ is the domination set in G_1, we obtain that $\gamma(G_1) \leq |(S \setminus \{v_k\}) \cup \{v_1\}| = |S| = \gamma(G)$.

If $v_1 \notin S$ and $M = \emptyset$, then v_i is controlled by vertex in $V(G(i))$ $(1 \leq i \leq l)$. Note that $\gamma_G(G(i) - v_i) = \gamma_{G_1}(G_1(i) - v_i)$ $(1 \leq i \leq l)$. Thus, S is minimum domination set in G_1, that is, $\gamma(G_1) = |S| = \gamma(G)$.

This leads us to the conclusion that $G_1 \in \mathcal{G}_n^{\leq\gamma}$. Let $\boldsymbol{y} = (y_{v_1}, y_{v_2}, \ldots, y_{v_n})^T$ be a principal eigenvector of G' corresponding to $\rho_a(G')$. Obviously, we get $y_{v_1} = \max\{y_{v_i}|1 \leq i \leq l\}$. If $M \neq \emptyset$. Since $\rho_a(G') = \boldsymbol{y}^T A_a(G')\boldsymbol{y}$ and $\rho_a(G_1) \geq \boldsymbol{y}^T A_a(G_1)\boldsymbol{y}$, it follows that

$$\begin{aligned} \frac{\rho_a(G_1) - \rho_a(G')}{2} &\geq \frac{\boldsymbol{y}^T(A_a(G_1) - A_a(G'))\boldsymbol{y}}{2} \\ &= \sum_{3\leq i\leq l-1} y_{v_1}y_{v_i} - \sum_{3\leq i\leq l-1} y_{v_i}y_{v_{i+1}} + \frac{(l-3)a}{2}y_{v_1}^2 - \frac{a}{2}\sum_{4\leq i\leq l} y_{v_i}^2 \\ &= \sum_{3\leq i\leq l-1} (y_{v_1} - y_{v_{i+1}})y_{v_i} + \frac{a}{2}\sum_{4\leq i\leq l}(y_{v_1} - y_{v_i})^2 \\ &> 0 \ \left(\text{since } y_{v_1} = \max\{y_{v_i}|1 \leq i \leq l\}\right). \end{aligned}$$

Then we have $\rho_a(G_1) > \rho_a(G') > \rho_a(G)$. If $M = \emptyset$, the same can be obtained $\rho_a(G_1) > \rho_a(G)$. Contradicting the maximality of G, the Claim 1 hold. ☐

Claim 2. *Let $v \in V(G)$, if v is contained in edge block, then it is contained in at most one edge block.*

Proof. Suppose to the contrary that v is a vertex in G which belongs to two edge blocks, say B_1, B_2, where $B_1 \cong B_2 = K_2$. Let $V(B_1) = \{v, v_1\}$, $V(B_2) = \{v, v_2\}$, clearly, v_1 and v_2 are nonadjacent in G. Let $G_2 = G + \{v_1v_2\}$, then $G_2 \in \mathcal{G}_n$ and vv_1v_2v is a triangle. According to Lemma 2.2, we can see that $\gamma(G_2 - \{v_1v_2\}) = \gamma(G_2)$, otherwise, remove either edge vv_1 or edge vv_2, the vertex v is contained in an edge block, a contradiction. Since $G_2 - \{v_1v_2\} \cong G$, hence $\gamma(G) = \gamma(G_2)$, that is, $G_2 \in \mathcal{G}_n^{\leq\gamma}$. However, according to Lemma 2.3, we have $\rho_a(G_2) > \rho_a(G)$, a contradiction. ☐

Suppose that u is a vertex in G which has the maximum entry, that is, $x_u = max\{x_v|v \in V(G)\}$, then we have the following claim.

Claim 3. *$u \in S$.*

Proof. If u is contained in end block, then $d_G(u) > 2$ due to $x_u = max\{x_v|v \in V(G)\}$, and thus $u \in S$, as required. If u is not contained in end block, then u only belongs to internal blocks. Without loss of generality, we may assume that B_3 is a internal block such that $uu_1 \in E(B_3)$ and $u \notin S$. Let B_4 be the block which contained u_1 different from B_3. Without loss of generality, set $u_1 \in S$, $N_1 = N_G(u_1) \setminus N_{B_3}(u_1)$. Let $G_3 = G - \{u_1u^*|u^* \in N_1\} + \{uu^*|u^* \in N_1\} \in \mathcal{G}_n$, then $(S \setminus \{u_1\}) \cup \{u\}$ is the domination set in G_3, this implies that

$$\gamma(G_3) \leq |(S \setminus \{u_1\}) \cup \{u\}| = |S| = \gamma(G),$$

that is $G_3 \in \mathcal{G}_n^{\leq\gamma}$. Note that $x_u > x_{u_1}$, we have $\rho_a(G_3) > \rho_a(G)$ by Lemma 2.1, a contradiction. □

Claim 4. *Let $v \in V(G)$, then $dist(u, v) \leq 2$.*

Proof. Suppose that v is a vertex with $dist(u, v) = \max\{dist(u, w)|w \in V(G)\} = d$. We assume to the contrary that $d \geq 3$. Let $P = vv_1v_2 \dots v_{d-1}u$ be a shortest path from v to u, then vv_1 is contained in end block.

Case 1. *v_1v_2 is an edge block.*

Let $N_2 = N_G(v_1) \setminus \{v_2\}$, $G_4 = G - \{v_1u^*|u^* \in N_2\} + \{uu^*|u^* \in N_2\} \in \mathcal{G}_n$. Note that $v_1 \in S$ due to vv_1 is contained in end block, and $u \in S$ by Claim 3. Thus, we have S is the domination set in G_4. This implies that $\gamma(G_4) \leq |S| = \gamma(G)$, that is, $G_4 \in \mathcal{G}_n^{\leq\gamma}$. Since $x_u > x_{v_1}$, it follows from Lemma 2.1 that $\rho_a(G_4) > \rho_a(G)$, a contradiction.

Case 2. *v_1v_2 is contained in triangle.*

Let B_5 be a triangle with $V(B_5) = \{v_1, v_2, w_1\}$.

Subcase 1. *w_1 is only contained in the block B_5.*

Let $N_3 = N_G(v_1) \setminus \{w_1, v_2\}$, $G_5 = G - \{v_1u^*|u^* \in N_3\} + \{uu^*|u^* \in N_3\} \in \mathcal{G}_n$. Note that $v_1 \in S$ due to vv_1 is contained in end block, and $u \in S$ by Claim 3. Thus, we have S is the domination set in G_5. This implies that $\gamma(G_5) \leq |S| = \gamma(G)$, that is, $G_5 \in \mathcal{G}_n^{\leq\gamma}$. Note that $x_u > x_{v_1}$, by Lemma 2.1, we obtain that $\rho_a(G_5) > \rho_a(G)$, a contradiction.

Subcase 2. *There are at least two blocks containing the vertex w_1.*

Suppose that B_6 is a block (other than B_5) which contains w_1, then B_6 is an end block (otherwise, P is not the shortest path). Let $N_4 = N_G(w_1) \setminus \{v_1, v_2\}$. Consider the cactus graph $G_6 = G - \{v_1u_1^*, w_1u_2^*|u_1^* \in N_3, u_2^* \in N_4\} + \{uu_1^*, uu_2^*|u_1^* \in N_3, u_2^* \in N_4\}$. Note that $\{v_1, w_1\} \in S$ due to vv_1 is contained in end block and B_6 is end block, and $u \in S$ by Claim 3. Thus, we have S is the domination set in G_6, this implies that $\gamma(G_6) \leq |S| = \gamma(G)$, that is, $G_6 \in \mathcal{G}_n^{\leq\gamma}$. Since $x_u > x_{v_1}$ and $x_u > x_{w_1}$, we have $\rho_a(G_6) > \rho_a(G)$ by Lemma 2.1, a contradiction. □

Claim 5. *Let $v \in N_G(u)$, then $d^b(v) \leq 2$.*

Proof. Suppose that $d^b(v) \geq 3$. Let u and v belong to a block, say B_7. We assume that B_8 and B_9 are two blocks different from B_7, which contain v.

Case 1. *B_7 is a triangle.*

If v contained in edge block, then at most one of B_8 and B_9 is an edge block by Claim 2. The following two cases are discussed.

Subcase 1. *B_8 and B_9 are triangles.*

We may assume that $V(B_8)=\{v,v_1,v_2\}$ and $V(B_9)=\{v,v_1',v_2'\}$ by Claim 1. Let $G_7=G-\{vv_1,vv_2\}+\{uv_1,uv_2\}\in\mathcal{G}_n$. Note that $v\in S$ due to B_8 and B_9 are end blocks by Claim 4, and $u\in S$ by Claim 3. Thus, S is the domination set in G_7, this implies that $\gamma(G_7)\le|S|=\gamma(G)$, that is, $G_7\in\mathcal{G}_n^{\le\gamma}$. Since $x_u>x_v$, by Lemma 2.1, we obtain that $\rho_a(G_7)>\rho_a(G)$, a contradiction.

Subcase 2. *B_8 is edge block and B_9 is triangle.*

A similar argument as above, one can also find a cactus graph in $\mathcal{G}_n^{\le\gamma}$ whose spectral radius is greater than $\rho_a(G)$, a contradiction.

Case 2. *B_7 is an edge block.*

Then B_8, B_9 are triangles that contain v by Claim 2, the proof is similar to Subcase 1. □

Claim 6. *Let $w\in N_G^2(u)$, then w is a pendant vertex.*

Proof. Suppose to the contrary that w is not a pendant vertex, where $w\in N_G^2(u)$. Note that G is $(K_2\vee 2K_1)$-free, we have any vertex of $N_G^2(u)$ has at most one neighbor in $N_G^2(u)$ by Claim 1. Therefore, $G[N_G^2(u)]$ is the union of the vertices and independent edges. We can assume that $G[N_G^2(u)]\cong bK_1\cup cK_2$. Let $N_G(u)=\{v_1,\ldots,v_{|N_G(u)|}\}$, $N_G^2(u)=\{w_1,\ldots,w_{|N_G^2(u)|}\}$.

Case 1. *$c=1$.*

Without loss of generality, set $E(K_2)=w_1w_2$. By the definition of cactus, Claims 1 and 4, we have $N_G(w_1)\setminus\{w_2\}=N_G(w_2)\setminus\{w_1\}=\{v_1\}$. Then $v_1w_1w_2v_1$ is triangle.

Subcase 1. *u is contained in edge block.*

Let B_{10} be the edge block contain u. If $V(B_{10})=\{u,v_1\}$, then we consider the graph $G_8=G-\{w_1w_2\}+\{uw_1\}\in\mathcal{G}_n$. Note that $v_1\in S$ due to $v_1w_1w_2v_1$ is an end block by Claim 4, and $u\in S$ by Claim 3. Thus, S is the domination set in G_8, this implies that $\gamma(G_8)\le|S|=\gamma(G)$, that is, $G_8\in\mathcal{G}_n^{\le\gamma}$. Since $x_u>x_{w_2}$, by Lemma 2.1, we have $\rho_a(G_8)>\rho_a(G)$, a contradiction. If $V(B_{10})\neq\{u,v_1\}$, without loss of generality, let $V(B_{10})=\{u,v_3\}$. Consider the graph $G_9=G-\{w_1w_2,v_1w_2\}+\{v_3w_2,uw_2\}\in\mathcal{G}_n$. Note that $v_1\in S$ due to triangle $v_1w_1w_2v_1$ is an end block by Claim 4, and $u\in S$ by Claim 3. Therefore, S is the domination set in G_9, this implies that $\gamma(G_9)\le|S|=\gamma(G)$, that is, $G_9\in\mathcal{G}_n^{\le\gamma}$. Since $x_{v_3}\ge x_{w_1}$ and $x_u>x_{v_1}$, it follows from Lemma 2.1 that $\rho_a(G_9)>\rho_a(G)$, a contradiction.

Subcase 2. *u is not contained in edge block.*

Let $G_{10}=G-\{v_1w_2,w_1w_2\}+uw_2\in\mathcal{G}_n$. Note that $v_1\in S$ due to triangle $v_1w_1w_2v_1$ is an end block by Claim 4, and $u\in S$ by Claim 3. Thus, S is the domination set in G_{10}, this implies that $\gamma(G_{10})\le|S|=\gamma(G)$, that is $G_{10}\in\mathcal{G}_n^{\le\gamma}$. In the following, we will show $\rho_a(G_{10})>\rho_a(G)$. By symmetry of G, we can see that $x_{w_1}=x_{w_2}$. We divide the proof for $a=0$ and $a=1$.

Subcase 2.1. *$a=0$.*

Then $A_a(G)=A_0(G)=A(G)$ and $\rho_a(G)=\rho_0(G)=\rho(G)$. Let $\rho(G)=\rho$, $\rho(G_{10})=\rho'$. By equation (2.1), we obtain that

$$\begin{cases} \rho x_{v_1} = x_u + x_{v_2} + x_{w_1} + x_{w_2}, \\ \rho x_{w_1} = x_{v_1} + x_{w_2}, \\ \rho x_{v_2} = x_u + x_{v_1} + x_{w_3}, \\ \rho x_{w_3} = x_{v_2}. \end{cases}$$

Set $x_u = r > 0$. Solving the above equations, we obtain that

$$\begin{cases} x_{v_1} = \dfrac{\rho^2 + \rho - 1}{\rho^3 - 4\rho - 2} r, \\ x_{w_1} = x_{w_2} = \dfrac{\rho^2 + \rho - 1}{(\rho - 1)(\rho^3 - 4\rho - 2)} r. \end{cases}$$

Since $\rho = \boldsymbol{x}^T A(G)\boldsymbol{x}$ and $\rho' \geq \boldsymbol{x}^T A(G_{10})\boldsymbol{x}$, it follows that

$$\begin{aligned} \frac{\rho' - \rho}{2} &\geq \frac{\boldsymbol{x}^T (A(G_{10}) - A(G))\boldsymbol{x}}{2} \\ &= x_u x_{w_2} - x_{v_1} x_{w_2} - x_{w_1} x_{w_2} \\ &= (x_u - x_{v_1} - x_{w_1}) x_{w_2} \\ &= \frac{\rho^6 - \rho^5 - 8\rho^4 + 10\rho^2 - \rho - 2}{(\rho^4 - \rho^3 - 4\rho^2 + 2\rho + 2)^2} r^2 \\ &> 0 \quad (\text{since } \rho \geq 4 \text{ and } r > 0). \end{aligned}$$

It follows that $\rho' > \rho$, that is, $\rho(G_{10}) > \rho(G)$, a contradiction.

SUBCASE 2.2. $a = 1$.

Then $A_a(G) = A_1(G) = Q(G)$ and $\rho_a(G) = \rho_1(G) = q(G)$. Let $q(G) = q$, $q(G_{10}) = q'$. By equation (2.1), we obtain that

$$\begin{cases} q x_{v_1} = 4x_{v_1} + x_u + x_{v_2} + x_{w_1} + x_{w_2}, \\ q x_{w_1} = 2x_{w_1} + x_{v_1} + x_{w_2}, \\ q x_{v_2} = 3x_{v_2} + x_u + x_{v_1} + x_{w_3}, \\ q x_{w_3} = x_{w_3} + x_{v_2}. \end{cases}$$

Set $x_u = r > 0$. Solving the above equations, we obtain that

$$\begin{cases} x_{v_1} = \dfrac{(q - 3)(q^2 - 3q + 1)}{q^4 - 11q^3 + 39q^2 - 50q + 17} r, \\ x_{w_1} = x_{w_2} = \dfrac{q^2 - 3q + 1}{q^4 - 11q^3 + 39q^2 - 50q + 17} r. \end{cases}$$

Since $q = \boldsymbol{x}^T Q(G)\boldsymbol{x}$ and $q' \geq \boldsymbol{x}^T Q(G_{10})\boldsymbol{x}$, it follows that

$$\begin{aligned} \frac{q' - q}{2} &\geq \frac{\boldsymbol{x}^T (Q(G_{10}) - Q(G))\boldsymbol{x}}{2} \\ &= x_u x_{w_2} - x_{v_1} x_{w_2} - x_{w_1} x_{w_2} + \frac{1}{2}(x_u^2 - x_{v_1}^2 - x_{w_1}^2 - x_{w_2}^2) \end{aligned}$$

$$
\begin{aligned}
&= (x_u - x_{v_1} - 2x_{w_1})x_{w_1} + \frac{1}{2}(x_u^2 - x_{v_1}^2)\\
&= \frac{q^8 - 22q^7 + 200q^6 - 976q^5 + 2759q^4 - 4538q^3 + 4136q^2 - 1856q + 316}{2(q^4 - 11q^3 + 39q^2 - 50q + 17)^2} r^2\\
&> 0 \quad (\text{since } q \geq 13.1789 \text{ and } r > 0).
\end{aligned}
$$

It follows that $q' > q$, that is, $q(G_{10}) > q(G)$, a contradiction.

Case 2. $c \geq 2$.

Without loss of generality, set $E(cK_2) = \{w_1w_2, w_3w_4, \ldots, w_{2c-1}w_{2c}\}$. By the definition of cactus, Claims 1 and 4, we have $N_G(w_1)\backslash\{w_2\} = N_G(w_2)\backslash\{w_1\} = \{v_1\}$ and $N_G(w_3)\backslash\{w_4\} = N_G(w_4)\backslash\{w_3\} = \{v_2\}$. Then $v_1w_1w_2v_1$ and $v_2w_3w_4v_2$ are triangles.

Let $G_{11} = G - \{v_1w_2, w_1w_2, v_2w_4, w_3w_4\} + \{uw_2, uw_4, w_2w_4\} \in \mathcal{G}_n$. Note that $\{v_1, v_2\} \in S$ due to $v_1w_1w_2v_1$ and $v_2w_3w_4v_2$ are end blocks by Claim 4 and $u \in S$ by Claim 3. Thus, S is the domination set in G_{11}, this implies that $\gamma(G_{11}) \leq |S| = \gamma(G)$, that is, $G_{11} \in \mathcal{G}_n^{\leq\gamma}$. In the following, we will show $\rho_a(G_{11}) > \rho_a(G)$. By symmetry of G, one can see that $x_{v_1} = x_{v_2}$, $x_{w_1} = x_{w_2} = x_{w_3} = x_{w_4}$. We divide the proof for $a = 0$ and $a = 1$.

Subcase 1. $a = 0$.

Then $A_a(G) = A_0(G) = A(G)$ and $\rho_a(G) = \rho_0(G) = \rho(G)$. Let $\rho(G) = \rho$, $\rho(G_{11}) = \rho'$. By equation (2.1), we obtain that

$$
\begin{cases}
\rho x_{v_1} = x_u + x_{v_2} + x_{w_1} + x_{w_2},\\
\rho x_{w_1} = x_{v_1} + x_{w_2}.
\end{cases}
$$

Set $x_u = r > 0$. Solving the above equations, we obtain that

$$
\begin{cases}
x_{v_1} = x_{v_2} = \dfrac{\rho - 1}{\rho^2 - 2\rho - 1} r,\\
x_{w_1} = x_{w_2} = x_{w_3} = x_{w_4} = \dfrac{1}{\rho^2 - 2\rho - 1} r.
\end{cases}
$$

Since $\rho = \boldsymbol{x}^T A(G)\boldsymbol{x}$ and $\rho' \geq \boldsymbol{x}^T A(G_{11})\boldsymbol{x}$, it follows that

$$
\begin{aligned}
\frac{\rho' - \rho}{2} &\geq \frac{\boldsymbol{x}^T(A(G_{11}) - A(G))\boldsymbol{x}}{2}\\
&= x_u x_{w_2} + x_u x_{w_4} + x_{w_2}x_{w_4} - x_{v_1}x_{w_2} - x_{w_1}x_{w_2} - x_{v_2}x_{w_4} - x_{w_2}x_{w_4}\\
&= (2x_u - x_{w_1} - 2x_{v_1})x_{w_1}\\
&= \frac{2\rho^2 - 6\rho - 1}{(\rho^2 - 2\rho - 1)^2} r^2\\
&> 0 \quad (\text{since } \rho \geq 4 \text{ and } r > 0).
\end{aligned}
$$

It follows that $\rho' > \rho$, that is, $\rho(G_{11}) > \rho(G)$, a contradiction.

Subcase 2. $a = 1$.

Then $A_a(G) = A_1(G) = Q(G)$ and $\rho_a(G) = \rho_1(G) = q(G)$. Let $q(G) = q$, $q(G_{11}) = q'$. By equation (2.1), we obtain that

$$\begin{cases} qx_{v_1} = 4x_{v_1} + x_u + x_{v_2} + x_{w_1} + x_{w_2}, \\ qx_{w_1} = 2x_{w_1} + x_{v_1} + x_{w_2}. \end{cases}$$

Set $x_u = r > 0$. Solving the above equations, we obtain that

$$\begin{cases} x_{v_1} = x_{v_2} = \dfrac{q-3}{q^2-8q+13}r, \\ x_{w_1} = x_{w_2} = x_{w_3} = x_{w_4} = \dfrac{1}{q^2-8q+13}r. \end{cases}$$

Since $q = \boldsymbol{x}^T Q(G)\boldsymbol{x}$ and $q' \geq \boldsymbol{x}^T Q(G_{11})\boldsymbol{x}$, it follows that

$$\begin{aligned} \frac{q'-q}{2} &\geq \frac{\boldsymbol{x}^T(Q(G_{11}) - Q(G))\boldsymbol{x}}{2} \\ &= x_u x_{w_2} + x_u x_{w_4} + x_{w_2}x_{w_4} - x_{v_1}x_{w_2} - x_{w_1}x_{w_2} - x_{v_2}x_{w_4} - x_{w_2}x_{w_4} \\ &\quad + x_u^2 - \frac{1}{2}(x_{w_1}^2 + x_{w_3}^2 + x_{v_1}^2 + x_{v_2}^2) \\ &= 2(x_u - x_{w_1} - x_{v_1})x_{w_1} + x_u^2 - x_{v_1}^2 \\ &= \frac{q^4 - 16q^3 + 91q^2 - 220q + 190}{(q^2-8q+13)^2} r^2 \\ &> 0 \quad (\text{since } q \geq 13.1789 \text{ and } r > 0). \end{aligned}$$

It follows that $q' > q$, that is, $q(G_{11}) > q(G)$, a contradiction. □

By Claims 3, 5 and 6, we know that $S = \{u\} \cup N_G^2(u)$ and $|N_G^2(u)| = \gamma(G) - 1$. Thus, if $n - \gamma(G) \equiv 0 \pmod 2$, we get $G \cong C_{\frac{n-\gamma(G)}{2},\gamma(G)-1}$ by Claims 1-6. Then we assert $\gamma(G) = \gamma$. Otherwise, $\gamma(G) < \gamma$, by Lemma 2.4 (i) we have

$$\rho_a\left(C_{\frac{n-\gamma(G)}{2},\gamma(G)-1}\right) < \rho_a\left(C_{\frac{n-\gamma(G)}{2}+1,\gamma(G)-3}\right).$$

Note that $C_{\frac{n-\gamma(G)}{2}+1,\gamma(G)-3} \in \mathcal{G}_n^{\leq\gamma}$, which contradicts the maximality of G.

Note that $n \geq 2\gamma$. In particular, if $n = 2\gamma$, we have $n - \gamma(G) \equiv 1 \pmod 2$. Otherwise, $G \cong C_{\frac{n-\gamma}{2},\gamma-1}$. However, since $x_u = max\{x_v | v \in V(G)\}$ and $C^e_{\frac{n-\gamma}{2},\gamma-2} = C_{\frac{n-\gamma}{2},\gamma-1} - \{v_{\gamma-1}w_{\gamma-1}\} + \{uw_{\gamma-1}\}$. We obtain that $\rho(C_{\frac{n-\gamma}{2},\gamma-1}) < \rho(C^e_{\frac{n-\gamma}{2},\gamma-2})$ by Lemma 2.1. Obviously, $C^e_{\frac{n-\gamma}{2},\gamma-2} \in \mathcal{G}_n^{\leq\gamma}$, a contradiction.

For the case of $n - \gamma(G) \equiv 1 \pmod 2$, it can be proved in a similar way. Therefore, we have

$$\rho_a(G) \leq \begin{cases} \rho_a(C_{\frac{n-\gamma}{2},\gamma-1}), & \text{when } n-\gamma \equiv 0 \pmod 2; \\ \rho_a(C^e_{\frac{n-\gamma-1}{2},\gamma-1}), & \text{when } n-\gamma \equiv 1 \pmod 2, \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} C_{\frac{n-\gamma}{2},\gamma-1}, & \text{when } n-\gamma \equiv 0 \pmod 2; \\ C^e_{\frac{n-\gamma-1}{2},\gamma-1}, & \text{when } n-\gamma \equiv 1 \pmod 2. \end{cases}$$

We complete the proof. □

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