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ΝΟΤΕ



On the Signless Laplacian Spectral Radius of Cacti

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- This paper is dedicated to prof. Nenad trinajstić on the occasion of his 80^{th} birthday

Abstract: A cactus is a connected graph in which any two cycles have at most one vertex in common. We determine the unique graphs with maximum signless Laplacian spectral radius in the class of cacti with given number of cycles (cut edges, respectively) as well as in the class of cacti with perfect matchings and given number of cycles.

Keywords: signless Laplacian spectral radius, graph, cactus, cycle, perfect matching, cut edge.

INTRODUCTION

A LL graphs in this paper are simple. Let G be a graph on n vertices with vertex set V(G) and edge set E(G). Let A(G) be the adjacency matrix of G. The matrix Q(G) = D(G) + A(G) is called the signless Laplacian matrix of G, where D(G) is a diagonal matrix of (vertex) degrees of G. It is well known that Q(G) is a semi-definite matrix and thus its eigenvalues are all nonnegative. The signless Laplacian spectral radius of G is the largest eigenvalue of Q(G), denoted by q(G). For more matrices associated to a graph, see the book of Janežič *et al.*^[1]

If G is connected, then Q(G) is irreducible and by the Perron-Frobenius theorem, q(G) has multiplicity one and there exists a unique positive unit eigenvector corresponding to q(G), which is the Perron vector of Q(G). The study of the signless Laplacian spectral radius of graphs has received much attention.^[2–10]

A cactus is a connected graph in which every edge appears in at most one cycle, see, *e.g.* Ref. [11]. Note that trees and unicyclic graphs are cacti. The (adjacency) spectral radius and least eigenvalue of a cactus have been studied to some extent,^[12–15] and the distance spectral radius of a cactus was also studied.^[16] Li and Zhang^[7] determined the unique graphs with maximum signless Laplacian spectral radius in the class of cacti with given numbers of vertices and pendant vertices, and in the class of cacti with perfect matching and given number of vertices, respectively. For $0 \le k \le [(n - 1)/2]$, let $\mathbb{C}(n,k)$ be the class of all cacti on *n* vertices with *k* cycles.

For $0 \le k \le n-3$, let $\mathbb{F}(n,k)$ be the class of all caction n vertices with k cut edges.

For $0 \le k \le n - 1$, let $\mathbb{G}(n,k)$ be the class of all caction 2n vertices with perfect matchings and k cycles.

In this paper, we determine the unique cacti with maximum signless Laplacian spectral radius in $\mathbb{C}(n,k)$ for $0 \le k \le [(n-1)/2]$, $\mathbb{F}(n,k)$ for $0 \le k \le n-3$, and $\mathbb{G}(n,k)$ for $0 \le k \le n-1$, respectively.

The spectral radius was, long ago, put forward as a measure of molecular branching,^[17] while the Laplacian spectral radius was used for describing the shape and folding of DNA molecules.^[18] It is well known that the Laplacian and signless Laplacian spectra of bipartite graphs coincide. Thus, chemically interesting cases for signless Laplacian spectral radius are the fullerenes, fluoranthenes and other non-alternant conjugated species.

PRELIMINARIES

Let *G* be a connected graph with $V(G) = \{v_1,...,v_n\}$. The Perron vector of Q(G) is the column vector $\mathbf{x} = (x_{v_1},...,x_{v_n})^T$, which can be considered as a function defined on V(G) which maps vertex v_i to x_{v_n} for i = 1, 2,..., n.

For an edge subset *F* of a graph *G*, G - F denotes the graph obtained from *G* by deleting the edges in *F*, while for



an edge subset F' of the complement of G, G + F' denotes the graph obtained from G by adding the edges from F'.

Denote by C_n , P_n and S_n the cycle, the path and the star on n vertices, respectively.

For a graph G with $u \in V(G)$, $N_G(u)$ denotes the set of neighbors of u in G, and the degree of u in G is $d_G(u) = |N_G(u)|$.

The following two lemmas were proved in Refs. [19] and [20], respectively.

Lemma 2.1. Let G be a connected graph with $u, v \in V(G)$. Suppose that $w_1, ..., w_s \in N_G(v) \setminus (N_G(u) \cup \{u\})$, where $s \ge 1$. Let $\mathbf{x} = (x_1, ..., x_n)^>$ be the Perron vector of Q(G), and $G' = G - \{vw_i: i = 1, ..., s\} + \{uw_i: i = 1, ..., s\}$. If $x_u \ge x_v$, then q(G') > q(G).

Lemma 2.2. Let *G* be a connected graph and e = uv a non-pendant edge of *G*. Suppose that $N_G(u) \cap N_G(v) = \emptyset$. Let *G'* be the graph obtained from $G - \{uv\}$ by identifying *u* and *v* into *u*, and adding a new pendant edge at *u*. Then, q(G') > q(G).

The following lemma follows from the Perron-Frobenius theorem, see, *e.g.*, Ref. [5].

Lemma 2.3. Let H be a proper subgraph of a connected graph G. Then, q(G) > q(H).

For $n \ge 3$, $k \ge 0$, and $0 \le p \le (n - 2k - 1)/2$, let $G_{n,k,p}$ be an *n*-vertex graph obtained by identifying a vertex of each of *k* triangles, a vertex of each of *t* paths P_2 , and a terminal vertex of each of *p* paths P_3 , where t = n - 2k - 2p - 1, see Figure 1.

Lemma 2.4. For $n \ge 3$, $k \ge 0$, and $0 \le p \le (n - 2k - 1)/2$, $q(G_{n,k,p})$ is the largest root of the equation f(x) = 0, where f(x) $= x^5 - (n - p + 6)x^4 + (6n - 6p + 10)x^3 - (10n + 4k - 9p + 3)x^2 + (3n + 12k)x - 4k$. In particular, $q(G_{n,k,0})$ is the largest root of the equation $x^3 - (n + 3)x^2 + 3nx - 4k = 0$, and for odd n,

$$q(G_{n,(n-1)/2,0}) = \frac{n+2+\sqrt{n^2-4n+12}}{2}$$

Proof. The characteristic polynomial of $Q(G_{n,k,p})$ was given in the proof of Lemma 4 in Ref. [8], from which the first part follows.

Let $g(x) = x^3 - (n + 3)x^2 + 3nx - 4k$. If p = 0, then it is easy to see that $f(x) = (x^2 - 3x + 1)g(x)$, which, together with the fact that $q(G_{n,k,0}) \ge q(P_3) = 3$, implies that $q(G_{n,k,0})$ is the largest root of the equation g(x) = 0.

If p = 0, k = (n - 1)/2, then $f(x) = (x^2 - 3x + 1)(x - 1)[x^2 - (n + 2)x + 2n - 2]$, and thus

$$q(G_{n,(n-1)/2,0}) = \frac{n+2+\sqrt{n^2-4n+12}}{2} .$$

For a cactus G with at least one cycle, the deletion of all edges of G on cycles results in a forest. A nontrivial



Figure 1. Graph G_{n,k,p}.

connected component of such a forest containing a unique vertex v on some cycle is said to be a branch of G at v. If G is a tree, we also call it a branch at one of its vertices.

SIGNLESS LAPLACIAN SPECTRAL RADIUS OF GRAPHS IN $\mathbb{C}(n,k)$

Let $G_{n,k} = G_{n,k,0}$. Note that $G_{n,0} = S_n$.

Theorem 3.1. Let $G \in \mathbb{C}(n,k)$, where $0 \le k \le [(n - 1)/2]$ and $n \ge 3$. Then, $q(G) \le q(G_{n,k})$ with equality if and only if $G \cong G_{n,k}$, where $q(G_{n,k})$ is the largest root of the equation $x^3 - (n + 3)x^2 + 3nx - 4k = 0$.

Proof. By Lemma 2.4, $q(G_{n,k})$ is the largest root of the equation $x^3 - (n + 3)x^2 + 3nx - 4k = 0$. Let *G* be a graph in $\mathbb{C}(n,k)$ with maximum signless Laplacian spectral radius. We need only to show that $G \cong G_{n,k}$.

Let **x** be the Perron vector of Q(G).

Suppose that $k \ge 1$ and there is a cycle of length at least 4. Let $v_1 \dots v_r v_1$ be such a cycle with length $r \ge 4$. Without loss of generality assume that $x_{v1} \ge x_{v2}$. Let $G' = G - \{v_2v_3\} + \{v_1v_3\}$. Obviously, $G' \in \mathbb{C}(n,k)$. By Lemma 2.1, we have $q(G^0) > q(G)$, a contradiction. Thus, if $k \ge 1$, then all cycles of *G* are triangles. If n = 3, then k = 1 and thus the result follows. So let $n \ge 4$.

Claim 1. If $k \ge 2$, then any two triangles of *G* have one common vertex.

Suppose that there are two disjoint triangles T_1 and T_2 in G. Then, there exists a unique shortest path $v_1 \dots v_s$ joining them, where $s \ge 2$, $v_1 \in V(T_1)$, $v_s \in V(T_2)$. If s > 2, then $v_i \notin V(T_1) \cup V(T_2)$ for $2 \le i \le s - 1$. Since G is a cactus, any path joining T_1 and T_2 starts from v_1 and ends in v_s . We may assume that $x_{v1} \ge x_{vs}$. Let w_1 and w_2 the neighbors of v_s in T_2 . Let $G' = G - \{v_s w_1, v_s w_2\} + \{v_1 w_1, v_1 w_2\}$. Obviously, $G' \in \mathbb{C}(n, k)$. By Lemma 2.1, we have q(G') > q(G), a contradiction. This proves Claim 1.

Claim 2. If $k \ge 3$, then any three triangles of *G* have exactly one common vertex.

Suppose that there are three triangles T_1 , T_2 and T_3 in G such that they have no common vertex. By Claim 1, the common vertices of T_1 and T_2 , T_2 and T_3 , and T_1 and T_3 induce



another triangle having a common edge with T_1 , a contradiction. Thus, Claim 2 follows.

By Claims 1 and 2, we have: if $k \ge 2$, then all triangles of *G* have exactly one common vertex, which we denote by v_0 . If k = 1, choose v_0 such that x_{v_0} is maximum among vertices with degree at least 3 on the unique triangle, and if k = 0, choose v_0 to be a non-pendant vertex.

Claim 3. For $k \ge 1$, there is no branch of *G* at a vertex different from v_0 .

Suppose that there is a branch *T* at vertex *v* on some triangle *L* of *G* with $v \neq v_0$. Let $G' = G - \{vw : w \in N_T(v)\} + \{v_0w : w \in N_T(v)\}$ for $x_{v_0} \ge x_v$, and $G' = G - \{v_0w : w \in N_G(v_0) \setminus V(L)\} + \{vw : w \in N_G(v_0) \setminus V(L)\}$ for $x_{v_0} < x_v$. In either case, $G' \in \mathbb{C}(n,k)$, and by Lemma 2.1, we have q(G') > q(G), a contradiction. Thus, Claim 3 follows.

If there is a branch *T* of *G* at v_0 (possibly k = 0 and G = T), then *T* is a star with center v_0 . Otherwise, suppose that there is a path $v_0v_1...v_s$ in *T*, where $s \ge 2$. Let *G* be the graph obtained from *G* by deleting the edge v_0v_1 , identifying v_0 and v_1 into v_0 , and adding a new pendant edge to v_0 . Obviously, $G' \in \mathbb{C}(n,k)$. By Lemma 2.2, q(G) < q(G'), a contradiction. Now by Claims 1–3, $G \cong G_{n,k}$.

Let *G* be a cactus on $n \ge 3$ vertices. Let *k* be the number of cycles of *G*, where $0 \le k \le [(n-1)/2]$. By Theorem 3.1 and Lemma 2.3, $q(G) \le q(G_{n,k}) \le q(G_{n,[(n-1)/2]})$ with equalities if and only if $G \cong G_{n,k}$ and k = [(n-1)/2], *i.e.*, $G \cong G_{n,[(n-1)/2]}$. Thus, $q(G) \le q(G_{n,[(n-1)/2]})$ with equality if and only if $G \cong G_{n,k}$. By Theorem 3.1, we have $q(G_{n,[(n-1)/2]}) = (n+2+\sqrt{n^2-4n+12})/2$ for odd *n*, and $q(G_{n,[(n-1)/2]})$ is the largest root of the equation $x^3 - (n+3)x^2 + 3nx - 2n + 4 = 0$ for even *n*.

SIGNLESS LAPLACIAN SPECTRAL RADIUS OF GRAPHS IN $\mathbb{F}(n,k)$

In view of the proofs of Lemmas 2.6 and 2.7 in Ref. [7], we deduce the following two lemmas.

Lemma 4.1. Let Y be a connected graph with $u_0 \in V(Y)$. For $m \ge 5$, let G_1 be the graph obtained by identifying u_0 and a vertex of C_m , G_2 be the graph obtained by identifying u_0 and a vertex of each of (m - 1)/2 triangles for odd m, and G_3 be the graph obtained by identifying u_0 , a vertex of each of (m - 4)/2 triangles, and a vertex of one quadrangle for even m, see Figure 2. Then, $q(G_1) < q(G_2)$ if m is odd, and $q(G_1) < q(G_3)$ if m is even.

Lemma 4.2. Let Y be a connected graph with $u_0 \in V$ (Y). Let G_4 be the graph obtained by identifying u_0 and a vertex of each of two quadrangles, and G_5 be the graph obtained by identifying u_0 and a vertex of each of three triangles, see Figure 3. Then, $q(G_4) < q(G_5)$.

For $1 \le r \le n/2 - 1$, let $G_{n,r}^{'}$ be *n*-vertex graph obtained by identifying a vertex of each of r - 1 triangles, a

vertex of a quadrangle, and a vertex of each of n - 2r - 2 paths P_2 , see Figure 4.

Lemma 4.3. For $n \ge 4$ and $1 \le r \le n/2 - 1$, $q(G_{n,r})$ is the largest root of the equation f(x) = 0, where $f(x) = x^5 - (n+6)x^4 + (7n+7)x^3 - (14n+4r-10)x^2 + (6n+16r-16)x - 8r + 8$.



Figure 2. Graphs G_1 , G_2 , and G_3 .



Figure 3. Graphs G_4 , and G_5 .



Figure 4. Graph G'n,r.



Proof. Let t = n - 2r - 2. Label the vertices of $G_{n,r}$ as $v_0, u_1, ..., u_{r-1}, u_1, ..., u_{r-1}, v_1, v_2, v, w_1, ..., w_t$, see Figure 4.

Let $Q = Q(G'_{n,r})$, $q = q(G'_{n,r})$ and **x** be the Perron vector of Q. By Lemma 2.3, $q \ge q(C_4) = 4$.

Since $(q-2) x_{u_i} = x_{v_0} + x_{u_i}$ and $(q-2) x_{u_i} = x_{v_0} + x_{u_i}$ for $1 \le i \le r-1$, we have $x_{u_i} = x_{u_i}$ for $1 \le i \le r-1$ and thus $x_{u_1} = \dots = x_{u_{r-1}} = x_{u_{r-1}} = \dots = x_{u_{r-1}}$. Since $(q-1) x_{w_i} = x_{v_0}$ for $1 \le i \le t$, we have $x_{w_1} = x_{v_1}$. Thus,

$$\begin{aligned} x_{v_0} - (q-3)x_{u_1} &= 0\\ x_{v_0} - (q-2)x_{v_1} + x_v &= 0\\ 2x_{v_1} - (q-2)x_v &= 0\\ x_{v_0} - (q-1)x_{w_1} &= 0\\ (q-2r-t)x_{v_0} - (2r-2)x_{u_1} - 2x_{v_1} - tx_{w_1} &= 0 \end{aligned}$$

Since **x** \neq **0**, we have $(x_{v_0}, x_{v_1}, x_{v_1}, x_v, x_{w_1})^T \neq 0$, and thus det(*D*) = 0, where

	(1	3 – q	0	0	0)
D -	1	0	2 – q	1	0
	0	0	2	2 – q	0
<i>D</i> =	1	0	0	0	1 - q
	q – 2r – t	2 – <i>r</i>	- 2	0	-t
					J

By a direct calculation, we have det(D) = f(q).

Now it follows that *q* is the largest root of the equation f(x) = 0.

Theorem 4.1. Let $G \in \mathbb{F}(n,k)$, where $0 \le k \le n-3$. (i) If n - k is odd, then $q(G) \le q(G_{n,(n-k-1)/2})$ with equality if and only if $G \cong G_{n,(n-k-1)/2}$, where $q(G_{n,(n-k-1)/2})$ is the largest root of the equation $x^3 - (n+3)x^2 + 3nx - 2n + 2k + 2 = 0$.

(ii) If n - k is even, then $q(G) \le q(G'_{n,(n-k-2)/2})$ with equality if and only if $G \cong G'_{n,(n-k-2)/2}$, where $q(G'_{n,(n-k-2)/2})$ is the largest root of the equation $x^5 - (n+6)x^4 + (7n+7)x^3 - (16n-2k-14)x^2 + (14n-8k-32)x - 4n + 4k + 16 = 0.$

Proof. By Lemmas 2.4 and 4.3, if n - k is odd, then $q(G_{n,(n-k-2)/2})$ is the largest root of the equation $x^3 - (n + 3)x^2 + 3nx - 2n + 2k + 2 = 0$, and if n - k is even, then $q(G'_{n,(n-k-1)/2})$ is the largest root of the equation $x^5 - (n + 6)x^4 + (7n + 7)x^3 - (16n - 2k - 14)x^2 + (14n - 8k - 32)x - 4n + 4k + 16 = 0$. Let *G* be a graph in F(n,k) with maximum signless Laplacian spectral radius. We only need to show that is odd and is even.

The result is trivial for n = 3 and for n = 4 with k = 0. Suppose $n \ge 4$ and $(n,k) \ne (4,0)$. By Lemma 2.3 and the fact that $q(C_s) = 4$ for $s \ge 3$, we have $G \not\cong C_n$.

Since $k \le n - 3$, *G* contains at least one cycle. By similar arguments as in Claims 1 and 2 in the proof of Theorem 3.1, if there are at least two cycles, then all cycles of *G* have exactly one common vertex, denoted by v_0 . If there is exactly one cycle in *G*, then choose v_0 such that the corresponding entry of the Perron vector of Q(G) is maximum among vertices with degree at least 3 on the unique cycle. By similar arguments as in Claim 3 in the proof of Theorem 3.1, there is no branch of *G* at a vertex different from v_0 . If there is a branch *T* of *G* at v_0 , then by Lemma 2.2, *T* is a star with center v_0 .

If *G* contains a cycle of length at least 5, then by Lemma 4.1, we may have a graph $G' \in \mathbb{F}(n,k)$ (of the form G_2 or G_3) such that q(G) < q(G'), a contradiction. Thus, any cycle of *G* has length 3 or 4. If *G* contains two quadrangles, then by Lemma 4.2, we may have a graph $G' \in \mathbb{F}(n,k)$ (of the form G_5) such that q(G) < q(G'), a contradiction. Thus, *G* has at most one quadrangle. Thus, $G \cong G_{n,(n-k-1)/2}$ if n - kis odd and $G \cong G'_{n,(n-k-2)/2}$ if n - k is even.

SIGNLESS LAPLACIAN SPECTRAL RADIUS OF GRAPHS IN $\mathbb{G}(n,k)$

For a graph *G*, let $\Delta_1(G)$ be the maximum degree of *G*. If $d_G(u) = \Delta_1(G)$, where $u \in V(G)$, then let $\Delta_2(G) = \max\{d_G(v) : v \in V(G) \setminus \{u\}\}$.

The following lemma is a particular case of Theorem 4.2 in Ref. [21].

Lemma 5.1. Let G be a graph on at least two vertices with $\Delta_i = \Delta_i(G)$ for i = 1, 2. Then,

$$q(G) \leq \frac{\Delta_1 + 2\Delta_2 - 1 + \sqrt{(\Delta_1 - 2\Delta_2 - 1)^2 + 8(\Delta_1 - \Delta_2)}}{2}$$





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The following lemma was given in Page 23 of Ref. [2] in plain text.

Lemma 5.2. Let G be a connected graph on $n \ge 4$ vertices. Then, $q(G) \ge \Delta_1(G) + 1$ with equality if and only if G is the star S_n .

For $n \ge 2$, $k \ge 0$, $0 \le i \le k$, and $n - k - i - 1 \ge 0$, let $H_{n,k,i}$ be the graph obtained from $G_{2n-2i,k,n-k-i-1}$ by attaching a pendant edge at each vertex with degree two of *i* triangles, see Figure 5.

Lemma 5.3. For $n \ge 3$, $k \ge 1$, $1 \le i \le k$ and $n - k - i - 1 \ge 0$, we have $q(H_{n,k,i}) < q(G(H_{n,k,i-1}))$.

Proof. By Lemma 5.1,

$$\begin{aligned} q(H_{n,k,i}) &\leq \\ \frac{(n+k-1)+6-1+\sqrt{(n+k-i-6-1)^2+8(n+k-1-3)}}{2} &= \\ \frac{(n+k-1)+5+\sqrt{(n+k-i-7)^2+8(n+k-1-3)}}{2}. \end{aligned}$$

By Lemma 5.2, $q(H_{n,k,i-1}) > n + k - i + 2$. If $n + k - i \ge 6$, then $q(H_{n,k,i}) \le n + k - i + 2$, and thus $q(H_{n,k,i}) < q(G(H_{n,k,i-1}))$.

Suppose that n + k - i < 6. Since $k \ge i$ and $n \ge 3$, we have n = 3, 4, 5. Since $k + i \le n - 1$ and $k \ge 1$, we have k = 1, 2. Thus, (n,k,i) = (3,1,1), (4,1,1), (4,2,1), (5,1,1), (5,2,2). By a direct calculation, we have

$q(H_{3,1,1}) = 5.2361$	<	$5.3839 = q(H_{3,1,0}),$
$q(H_{4,1,1}) = 5.7711$	<	$6.2860 = q(H_{4,1,0}),$
$q(H_{4,2,1}) = 6.5741$	<	$7.2871 = q(H_{4,2,0}),$
$q(H_{5,1,1}) = 6.5051$	<	$7.2261 = q(H_{5,1,0}),$
$q(H_{5,2,2}) = 6.7359$	<	$7.4133 = q(H_{5,2,1}).$

Thus, the results follows.

Let $H_{n,k} = H_{n,k,0}$.

Theorem 5.1. Let $G \in \mathbb{G}(n,k)$, where $n \ge 2$ and $0 \le k \le n - 1$. Then, $q(G) \le q(H_{n,k})$ with equality if and only if $G \cong H_{n,k}$, where $q(H_{n,k})$ is the largest root of the equation $x^5 - (n + k + 7)x^4 + (6n + 6k + 16)x^3 - (11n + 13k + 12)x^2 + (6n + 12k)x - 4k = 0$.

Proof. By Lemma 2.4, $q(H_{n,k})$ is the largest root of the equation $x^5 - (n + k + 7)x^4 + (6n + 6k + 16)x^3 - (11n + 13k + 12)x^2 + (6n + 12k)x - 4k = 0$. Let *G* be a graph in $\mathbb{C}(n,k)$ with maximum signless Laplacian spectral radius. We only need to show that $G \cong H_{n,k}$.

Let **x** be the Perron vector of Q(G) and M be a fixed perfect matching of G.

Suppose that $k \ge 1$ and there is a cycle $C = v_1 ... v_p v_1$ of length $p \ge 4$. Without loss of generality assume that $x_{v1} =$ min $\{x_v : v \in V(C)\}$. Obviously, one of v_1v_2 and v_1v_p , say v_1v_2 is not in M. Let $G' = G - \{v_1v_2\} + \{v_pv_2\}$. Then, M is still a perfect matching of G', and $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, q(G') > q(G), a contradiction. Thus, if $k \ge 1$, then all cycles of G are triangles. **Claim 1.** If $k \ge 2$, then any two triangles of *G* have a common vertex.

Suppose that there are two disjoint triangles T_1 and T_2 in G. Then, there exists a unique shortest path $v_1 \dots v_s$ joining them, where $s \ge 2$, $v_1 \in V(T_1)$, $v_s \in V(T_2)$. If s > 2, then $v_i \notin V(T_1) \cup V(T_2)$ for $2 \le i \le s - 1$. Note that any path joining T_1 and T_2 starts from v_1 and ends in v_s . We may assume that $x_{vs} \ge x_{v1}$. Let $T_1 = uv_1w$. Suppose that $uv_1 \in M$. Then, $uw \notin M$ and that $ww' \in M$ for some vertex $w' \in N_G(w) \setminus \{u, v_1\}$. If $x_{v1} \ge x_{wv}$, let $G' = G - \{wy : y \in N_G(w) \setminus \{u, v_1\}\} + \{v_1y : y \in N_G(w) \setminus \{u, v_1\}\}$. Obviously, $M' = M - \{uv_1, ww'\} + \{uw, v_1w'\}$ is a perfect matching of G'. Otherwise, let $G' = G - \{v_1y : y \in N_G(v_1) \setminus \{u, w\}\} + \{wy : y \in N_G(v_1) \setminus \{u, w\}\}$. Obviously, M is still a perfect matching of G'. In either case, $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, q(G') > q(G), a contradiction. Thus, $uv_1 \notin M$. Similarly, $wv_1 \notin M$. Let $G' = G - \{uv_1, wv_1\} + \{uv_s, wv_s\}$. Obviously, $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, q(G') > q(G), a contradiction. Thus, $uv_1 \notin M$. Similarly, $wv_1 \notin M$. Let $G' = G - \{uv_1, wv_1\} + \{uv_s, wv_s\}$. Obviously, $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, q(G') > q(G), a contradiction.

By the same argument as in Theorem 3.1, we have **Claim 2.** If $k \ge 3$, then any three triangles of *G* have exactly one common vertex.

By Claims 1 and 2, we have: if $k \ge 2$, then all the triangles of *G* have exactly one common vertex, denoted by v_0 . If k = 1, choose v_0 such that x_{v_0} is maximum among vertices with degree at least 3 on the unique triangle, and if k = 0, choose v_0 such that x_{v_0} is maximum among vertices of *G*.

Claim 3. If $k \ge 1$ and there is a branch *T* at vertex *v* on some cycle of *G*, then *T* is a tree consisting of pendant paths of length 2 and possibly one of length 1 at *v*. If k = 0, then *G* is a tree consisting of pendant paths of length 2 and possibly one of length 1 at v_0 .

Let *u* be a vertex furthest from *v* in *T* (possibly k = 0, $v = v_0$, and G = T). Suppose that the distance between *v* and *u* in *T* is at least 3. Since *G* has perfect matchings, *u* is a pendant vertex adjacent to a vertex *u*' of degree 2. Let *w* be the neighbor of *u*' different from *u*. Obviously, $w \neq v$. Let *G*' $= G - \{wu'\} + \{vu'\}$ if $x_v \ge x_w$ and $G' = G - \{vv'\} + \{wv'\}$ otherwise, where *v*' is a neighbor of *v* on some cycle such that $vv' \notin M$. Obviously, *M* is still a perfect matching of *G*', and $G' \in \mathbb{G}(n,k)$. By Lemma 2.1, q(G') > q(G), a contradiction. Thus, any vertex in *T* is reachable from *v* by a path of length at most 2. Now Claim 3 follows from the fact that *G* has perfect matchings.

Claim 4. For $k \ge 1$ and a triangle $C = v_0 u u_1$ in G, if there is a pendant edge at u_1 , there is a pendant edge at u_1 .

The claim is trivial for k = 1. Suppose that $k \ge 2$, uv is a pendant edge, and there is no pendant edge at u_1 . Then, $uv, v_0u_1 \in M$. If $x_{v_0} \ge x_u$, let $G' = G - \{uv\} + \{v_0v\}$. Obviously, $M' = M - \{uv, v_0u_1\} + \{uu_1, v_0v\}$ is a perfect matching of G'. Otherwise, let $G' = G - \{v_0y : y \in N_G(v_0) \setminus \{u, u_1\}\} + \{uy : y \in N_G(v_0) \setminus \{u, u_1\}\}$. Obviously, M is still a perfect matching of G'. In either case, $G' \in \mathbb{G}(n, k)$. By Lemma 2.1, q(G') > q(G), a contradiction. Thus, Claim 4 follows.



Claim 5. For $k \ge 1$, there is no pendant path of length 2 in *G* at a vertex different from v_0 .

Suppose that v_0uu_1 is a triangle in G and there is a pendant path uvw at u. Then, $vw \in M$. If $x_{v0} \ge x_u$, let G' = G - $\{uv\} + \{v_0v\}$. Suppose that $x_{v0} < x_u$. Since G has perfect matchings, we have by Claim 4 that any edge on a triangle incident to v_0 is not in M, implying that there is a branch, say T_0 at v_0 . Then, by our choice of v_0 , we have $k \ge 2$, and for any vertex $y \in N_G(v_0) \setminus (\{u, u_1\} \cup V(T_0)), v_0y / \in M$. Let G' = $G - \{v_0y : y \in N_G(v_0) \setminus (\{u, u_1\} \cup V(T_0))\} + \{uy : y \in N_G(v_0) \setminus (\{u, u_1\} \cup V(T_0))\}$. Obviously, M is still a perfect matching of G' and $G' \in \mathbb{G}(n, k)$ whether $x_{v0} \ge x_u$ or not. By Lemma 2.1, we have q(G') > q(G) in either case, a contradiction. Thus, Claim 5 follows.

By Claims 1–5, $G \cong H_{n,k,i}$ for some i with $0 \le i \le k$. If $n = 2, k \ge 1$ the result is trivial. If $n \ge 3, k \ge 1$, then by Lemma 5.3, $G \cong H_{n,k}$.

Note that $\mathbb{G}(n,0)$ is the set of trees of order 2n with perfect matching. Thus, the case k = 0 in Theorem 5.1 has been studied in Ref. [22].

CONCLUSION

In this paper, we investigate the extremal problems for signless Laplacian spectral radius of cacti. We determine the unique graphs with maximum signless Laplacian spectral radius of graphs in the class of cacti with given number of cycles (cut edges, respectively) and in the class of cacti with perfect matchings and given number of cycles. The extremal graphs (except the case for trees) are not bipartite.

REFERENCES

 D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, Graph-Theoretical Matrices in Chemistry, CRC Press, Boca Raton, 2015.

- [2] D. Cvetković, P. Rowlinson, S. K. Simić, Publ. Inst. Math. 2007, 81, 11.
- [3] D. Cvetković, S. K. Simić, *Linear Algebra Appl.* 2010, 432, 2257.
- [4] D. Cvetković, P. Rowlinson, S. K. Simić, Linear Algebra Appl. 2007, 423, 155.
- [5] Y. Z. Fan, D. Yang, *Graphs Combin.* **2009**, *25*, 35.
- [6] P. Hansen, C. Lucas, *Linear Algebra Appl.* 2010, 432, 3319.
- [7] S. Li, M. Zhang, *Linear Algebra Appl.* **2012**, *436*, 4400.
- [8] H. Lin, B. Zhou, *Linear Multilinear Algebra* 2015, *63*, 377.
- C. S. Oliveir, L. S. de Lima, N. M. M. de Abreu, P. Hansen, *Discrete Appl. Math.* 2010, 158, 355.
- [10] B. Zhou, Linear Algebra Appl. 2010, 432, 566.
- [11] B. Zmazek, J. Zerovnik, Croat. Chem. Acta 2013, 76, 137.
- [12] B. Borovićanin, M. Petrović, *Publ. Inst. Math.* 2006, 79 (93), 13.
- [13] Z. Huang, H. Deng, S. K. Simić, Appl. Anal. Discrete Math. 2011, 5, 14.
- [14] M. Petrović, T. Aleksić, V. Simić, *Linear Algebra Appl.* 2011, 435, 2357.
- [15] R. Xing, B. Zhou, *Linear Algebra Appl.* **2013**, *438*, 2256.
- [16] S. S. Bose, M. Nath, S. Paul, *Linear Algebra Appl.* 2012, 437, 2128.
- [17] D. M. Cvetković, I. Gutman, *Croat. Chem. Acta* 1977, 49, 115.
- [18] M. Randić, M. Vračko, M. Novič, in QSPR/QSAR Studies by Molecular Descriptors (Ed.: M.V. Diudea), Nova Science, New York, 2001, pp. 147–211.
- [19] Y. Hong, X.D. Zhang, Discrete Math. 2005, 296, 187.
- [20] S. G. Guo, Discrete Math. 2008, 308, 4608.
- [21] X. Duan, B. Zhou, Linear Algebra Appl. 2013, 439, 2961.
- [22] J. M. Guo, Linear Algebra Appl. 2003, 368, 379.