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# On the signless Laplacian index of cacti with a given number of pendant vertices ☆

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ABSTRACT

A connected graph $G$ is a cactus if any two of its cycles have at most one common vertex. In this article, we determine graphs with the largest signless Laplacian index among all the cacti with $n$ vertices and $k$ pendant vertices. As a consequence, we determine the graph with the largest signless Laplacian index among all the cacti with $n$ vertices; we also characterize the $n$-vertex cacti with a perfect matching having the largest signless Laplacian index.



## 1. Introduction

Spectral graph theory [1,2,4,6,7] studies properties of graphs using the spectrum of related matrices. We consider only simple graphs (i.e., finite, undirected graphs without loops or multiple edges). Let $G = (V_G, E_G)$ be a simple graph on $n$ vertices and $m$ edges (so $n = |V_G|$ is its order, and $m = |E_G|$ is its size). The most studied matrix associated with $G$ appears to be *adjacency matrix* $A = (a_{ij})$ where $a_{ij} = 1$ if $v_i$ and $v_j$ of the graph $G$ are adjacent and 0 otherwise. Another well studied matrix is the *Laplacian*, defined by $L = D - A$ where $D$ is the diagonal matrix with degrees of the vertices on the main diagonal (see [1,12,22]). The matrix $Q = D + A$ is called the *signless Laplacian* matrix of $G$ (see [8]) and has attracted the attention of many researchers. Computer investigations of graphs with up

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to 11 vertices [11] suggest that the spectrum of $D+A$ performs better than the spectrum of $A$ or $D-A$ in distinguishing non-isomorphic graphs.

If $N$ is the vertex-edge incidence matrix of $G$ then

$$NN^T = D + A, \qquad N^T N = A(\hat{L}(G)) + 2I,$$

where $A(\hat{L}(G))$ is the adjacency matrix of the line graph $\hat{L}(G)$. In particular, $D+A$ is positive semi-definite. It is also easy to see that the matrix $Q = D + A$ is real symmetric, the eigenvalues of $Q$ can be arranged as $q_1(Q) \geqslant q_2(Q) \geqslant \cdots \geqslant q_n(Q) \geqslant 0$, where $q_1(Q)$ is the signless Laplacian index of graph $G$. If in addition $G$ is connected, there exists a unique (up to multiples) and (entrywise) positive eigenvector, say $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$, corresponding to this index. It will be convenient to associate a labelling of vertices of $G$ (with respect to $\mathbf{x}$) in which $x_v$ is a label of $v$. The *signless Laplacian characteristic polynomial* of $G$, equal to $\det(xI - Q)$, is denoted by $\psi(G, x)$ (or, for short, by $\psi(G)$).

Recently there is a lot of work on the signless Laplacian eigenvalues, especially the signless Laplacian index of a graph. The papers [8–10] give a survey on this work. Several bounds for the signless Laplacian index can be found in [11–14], and the relations between this index and graph parameters are discussed in [13–21,24–28]. The least signless Laplacian eigenvalues is also studied; see e.g., [5,13]. Other work can be found in [23] for the $Q$-spread.

In [29], Zhu proposed the following problem concerning the signless Laplacian index: Given a set of graphs $\mathscr{G}$, find an upper bound for the signless Laplacian index and characterize the graphs in which the maximal signless Laplacian index is attained. The problem proposed by Zhu in [29] is actually the signless Laplacian version of the classical Brualdi-Solheid problem for the adjacency matrix; see [3]. In this paper, we study the same question for $\mathscr{C}_{n,k}$, a set of polycyclic graphs (called cacti) in which any two of its cycles have at most one common vertex and each cactus is connected containing $k$ pendant vertices.

In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to [2]. Denote by $C_n$ and $P_n$ the cycle and the path with $n$ vertices, respectively. $G - v$, $G - uv$ denote the graph obtained from $G$ by deleting a vertex $v \in V_G$, or an edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex, or edge, is deleted). Similarly, $G + uv$ is a graph that arises from $G$ by adding an edge $uv \notin E_G$, where $u, v \in V_G$. For $uv \in E(G)$, let $G_{uv}$ be the graph obtained from $G$ by subdividing the edge $uv$, that is, by replacing $uv$ with edges $uw$ and $wv$, where $w$ is an additional vertex. For $v \in V_G$, $d(v)$ denotes the degree of vertex $v$ and $N(v)$ denotes the set of all neighbors of vertex $v \in V_G$. An *internal path* is a path or a cycle, in which the initial and terminal vertices have degree at least three and the internal vertices have degree two.

## 2. Preliminaries

In order to complete the proof of our main results we need the following lemmas.

**Lemma 2.1** [19]. *Let $u$ and $v$ be two distinct vertices of a connected graph $G$. Suppose that $w_1, w_2, \ldots, w_s (s \geqslant 1)$ are neighbors of $v$ but not $u$ and they are all different from $u$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the Perron vector of $Q(G)$, and let $H$ be obtained from $G$ by deleting the edges $vw_i$ and adding the edges $uw_i$ for $i = 1, 2, \ldots, s$. If $x_v \leqslant x_u$, then $q_1(G) < q_1(H)$.*

From the Perron–Frobenius Theorem of non-negative matrices, we have the following lemma.

**Lemma 2.2** [14]. *If $G'$ is a proper subgraph of a connected graph $G$, then $q_1(G') < q_1(G)$.*

**Lemma 2.3** [17]. *Let $G$ be a connected graph and let $uv$ be an edge on an internal path of $G$. Let $G_{uv}$ be obtained from $G$ by subdividing the edge $uv$. Then $q_1(G_{uv}) < q_1(G)$.*

Let $H$ be a connected $(n-m)$-vertex graph with $u_0 \in V_H$ having $k$ pendants if $u_0$ is a pendant and $k-1$ pendants otherwise. Set $G_1$ (resp. $G_2$) be an $n$-vertex graph obtained from $H$ by attaching $P_{m+1}$

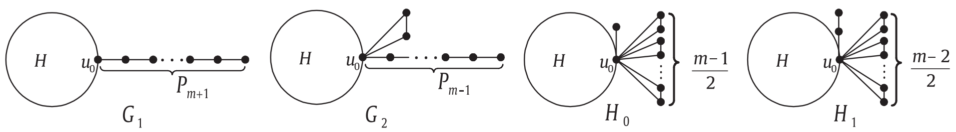


**Fig. 1**. Graphs $G_1$, $G_2$, $H_0$ and $H_1$.

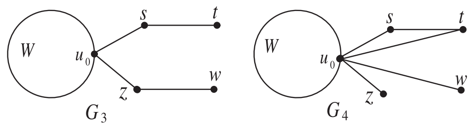


**Fig. 2**. Graphs $G_3$ and $G_4$.

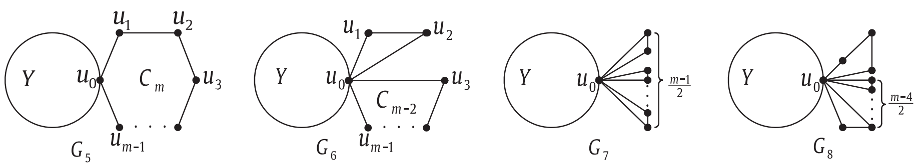


**Fig. 3**. Graphs $G_5$, $G_6$, $G_7$ and $G_8$.

(resp. $P_{m-1}$ and $C_3$) to $u_0$ (see Fig. 1); $H_0$ (resp. $H_1$) be an $n$-vertex graph obtained from $H$ by attaching $\frac{m-1}{2}$ $C_3$'s and a $P_2$ (resp. $\frac{m-2}{2}$ $C_3$'s and a $P_3$) to $u_0$ when $m$ is odd (resp. even), where $m \geqslant 3$. Graphs $H_0$ and $H_1$ are depicted in Fig. 1.

**Lemma 2.4.** *Let $G_1$, $G_2$, $H_0$ and $H_1$ be graphs as shown in Fig. 1. Then*

(i) $q_1(G_1) < q_1(G_2)$;
(ii) $q_1(G_1) < q_1(H_0)$ *or* $q_1(G_1) < q_1(H_1)$.

**Proof.** (i) Let $P_{m+1} = u_0u_1 \ldots u_m (m \geqslant 3)$. Now, consider the Perron vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ of $Q(G_1)$. If $x_{u_0} \geqslant x_{u_2}$, let $G' = G_1 - u_2u_3 + u_0u_3$; otherwise, let $G' = G_1 - \{u_0y | y \in N(u_0)\backslash\{u_1\}\} + \{u_2y | y \in N(u_0)\backslash\{u_1\}\}$. By Lemma 2.1, we have $q_1(G_1) < q_1(G')$. It is easy to see that $G_2 = G' + u_0u_2$, then in view of Lemma 2.2, we have $q_1(G') < q_1(G_2)$. So we have $q_1(G_1) < q_1(G_2)$.

(ii) If $m = 3$ or, 4, it is easy to see that $H_0 \cong G_2$ or, $H_1 \cong G_2$. Then in view of (i), our result holds immediately. If $m \geqslant 5$, by repeatedly applying (i) to $G_2$, then we can finally get a graph $H_0$ when $m$ is odd or, a graph $H_1$ when $m$ is even. Therefore, $q_1(G_1) < q_1(H_0)$ or, $q_1(G_1) < q_1(H_1)$.

This completes the proof. □

Let $W$ be a connected $(n-4)$-vertex graph with $u_0 \in V_W$ having $k-1$ pendants if $u_0$ is a pendant and $k-2$ pendants otherwise. The graph $G_3$ is the graph obtained from $W$ by attaching two paths of length 2 to $u_0$; see Fig. 2. Set $G_4 = G_3 - zw + \{u_0w, u_0t\}$ (see Fig. 2). It is easy to see that $G_3$ (resp. $G_4$) is an $n$-vertex graph with $k$ pendant vertices.

**Lemma 2.5.** *Let $G_3$ and $G_4$ be the graphs as depicted in Fig. 2. Then $q_1(G_3) < q_1(G_4)$.*

**Proof.** Consider the Perron vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ of $G_3$. If $x_{u_0} \geqslant x_z$, then let $G' = G_3 - zw + u_0w$; otherwise, let $G' = G_3 - \{u_0u | u \in N(u_0)\backslash\{z\}\} + \{zu | u \in N(u_0)\backslash\{z\}\}$. Hence, by Lemma 2.1 we get $q_1(G_3) < q_1(G')$. On the other hand, it is straightforward to check that $G_4 = G' + u_0t$ if $x_{u_0} \geqslant x_z$ and $G_4 = G' + zt$ otherwise. Therefore, our result follows by Lemma 2.2.

This completes the proof. □

Let $Y$ be a connected $(n-m+1)$-vertex graph with $u_0 \in V_Y$ having $k+1$ pendants if $u_0$ is a pendant and $k$ pendants otherwise. Let $G_5$ (resp. $G_6$) be an $n$-vertex graph obtained from $Y$ by attaching $C_m$

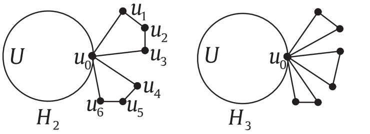


**Fig. 4**. Graphs $H_2$ and $H_3$.

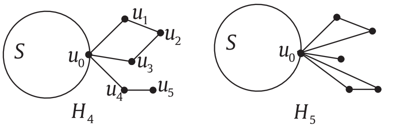


**Fig. 5**. Graphs $H_4$ and $H_5$.

(resp. $C_{m-2}$ and $C_3$) to $u_0$ (see Fig. 3); $G_7$ (resp. $G_8$) be an $n$-vertex graph obtained from $Y$ by attaching $\frac{m-1}{2}$ $C_3$'s (resp. $\frac{m-4}{2}$ $C_3$'s and a $C_4$) to $u_0$ when $m$ is odd (resp. even), where $m \geqslant 5$. Graphs $G_7$ and $G_8$ are depicted in Fig. 3.

**Lemma 2.6.** *Let $G_5$, $G_6$, $G_7$ and $G_8$ be the graphs defined as above (see Fig. 3). Then*

(i) $q_1(G_5) < q_1(G_6)$;
(ii) $q_1(G_5) < q_1(G_7)$ *or,* $q_1(G_5) < q_1(G_8)$.

**Proof.** (i) Let $C_m = u_0u_1 \dots u_{m-1}u_0$ $(m \geqslant 5)$. Now, we consider the Perron vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ of $G_5$. If $x_{u_0} \geqslant x_{u_3}$, then let $G' = G_5 - u_2u_3 + u_0u_2$; otherwise, let $G' = G_5 - \{u_0y|y \in N(u_0)\backslash\{u_{m-1}\}\} + \{u_3y|y \in N(u_0)\backslash\{u_{m-1}\}\}$. By Lemma 2.1, we get $q_1(G_5) < q_1(G')$. Note that $G_6 = G' + u_0u_3$, hence by Lemma 2.2 we have $q_1(G') < q_1(G_6)$, i.e., $q_1(G_5) < q_1(G_6)$.

(ii) If $m = 5, 6$, then in view of (i) we know that our result holds. If $m \geqslant 7$, by repeatedly applying (i) to $G_5$, we can finally get graph $G_7$ when $m$ is odd or, get graph $G_8$ when $m$ is even. So, $q_1(G_5) < q_1(G_7)$ or $q_1(G_5) < q_1(G_8)$.

This completes the proof. □

**Lemma 2.7.** *Let $H_2$ and $H_3$ be the graphs as depicted in Fig. 4, where $U$ is a connected $(n-6)$-vertex graph with $k$ pendants. Then $q_1(H_2) < q_1(H_3)$.*

**Proof.** Consider the Perron vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ of $H_2$. If $x_{u_0} \geqslant x_{u_6}$, let $H' = H_2 - u_5u_6 + u_0u_5$; otherwise, let $H'' = H_2 - \{u_0y|y \in N(u_0)\backslash\{u_6\}\} + \{u_6y|y \in N(u_0)\backslash\{u_6\}\}$. It is straightforward to check that $H' \cong H''$. By Lemma 2.1, we get $q_1(H_2) < q_1(H')$.

Now consider the Perron vector $\mathbf{y} = (y_1, y_2, \dots, y_n)^T$ of $H'$. If $y_{u_0} \geqslant y_{u_1}$, let $H^* = H' - u_1u_2 + u_0u_2$; otherwise, let $H^{**} = H' - \{u_0y|y \in N(u_0)\backslash\{u_1\}\} + \{u_1y|y \in N(u_0)\backslash\{u_1\}\}$. It is straightforward to check that $H^* \cong H^{**}$. By Lemma 2.1, we get $q_1(H') < q_1(H^*)$. It is easy to see that $H_3 \cong H^* + u_1u_6$. Hence, by Lemma 2.2, we have $q_1(H^*) < q_1(H_3)$. Therefore, $q_1(H_2) < q_1(H_3)$.

This completes the proof. □

**Lemma 2.8.** *Let $H_4$ and $H_5$ be the $n$-vertex graphs as shown in Fig. 5, where $S$ is a connected $(n-5)$-vertex graph with $k-1$ pendants. Then $q_1(H_4) < q_1(H_5)$.*

**Proof.** Consider the Perron vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ of $H_4$. If $x_{u_0} \geqslant x_{u_3}$, let $M' = H_4 - u_2u_3 + u_0u_2$; otherwise, let $M'' = H_4 - \{u_0y|y \in N(u_0)\backslash\{u_3\}\} + \{u_3y|y \in N(u_0)\backslash\{u_3\}\}$. It is straightforward to check that $M' \cong M''$. By Lemma 2.1, we have $q_1(H_4) < q_1(M') = q_1(M'')$.

Note that $H_5 \cong M' + u_0u_5$, hence $M'$ is a proper subgraph of $H_5$. By Lemma 2.2, we have $q_1(M') < q_1(H_5)$. Hence, we get $q_1(H_4) < q_1(H_5)$.

This completes the proof. □

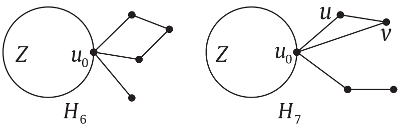


**Fig. 6**. Graphs $H_6$ and $H_7$.

**Lemma 2.9.** *Let $H_6$ and $H_7$ be the n-vertex graphs as shown in Fig. 6, where Z is a connected subgraph with $k-1$ pendants. Then $q_1(H_6) < q_1(H_7)$.*

**Proof.** Note that $H_7$ contains a cycle $C_3 = u_0uvu_0$. Let $N' = (H_7)_{uv}$, i.e., $N'$ is obtained from $H_7$ by subdividing the edge $uv$. It is easy to see that $u_0uvu_0$ is an internal path of $H_7$, hence by Lemma 2.3 we get $q_1(N') < q_1(H_7)$.

Note that $H_6$ is a proper subgraph of $N'$, hence in view of Lemma 2.2, we have $q_1(H_6) < q_1(N')$. Therefore, we obtain that $q_1(H_6) < q_1(H_7)$.

This completes the proof. □

## 3. Main results

We call graph $G$ a *cactus* if $G$ is connected and any two of its cycles intersect in at most one vertex. For a cactus graph $G$, we call it a *bundle* if all cycles of $G$ have exactly one common vertex. Denote by $\mathscr{C}_{n,k}$ the set of all connected cacti on $n$ vertices with $k$ pendant vertices. In the following, we determine the graphs with the largest signless Laplacian indices in the class $\mathscr{C}_{n,k}$.

**Theorem 3.1.** *Let G be a graph in $\mathscr{C}_{n,k}$.*

(i) *If $n-k \equiv 1 \pmod 2$, then $q_1(G) \leqslant q_1(C^1(n,k))$ with equality if and only if $G \cong C^1(n,k)$, where $C^1(n,k)$ is depicted in Fig. 7 and $q_1(C^1(n,k))$ is the largest root of the equation $g(x) = 0$, here*

$$g(x) = x^3 - (k+6)x^2 - (n-4k-12)x + n - k - 7.$$

(ii) *If $n-k \equiv 0 \pmod 2$, then $q_1(G) \leqslant q_1(C^2(n,k))$ with equality if and only if $G \cong C^2(n,k)$, where $C^2(n,k)$ is depicted in Fig. 7 and $q_1(C^2(n,k))$ is the largest root of the equation $h(x) = 0$, here*

$$h(x) = x^5 - (k+9)x^4 - (n-7k-32)x^3 + (4n-14k-54)x^2 - (4n-7k-40)x + n - k - 8.$$

**Proof.** Choose $G \in \mathscr{C}_{n,k}$ such that its signless Laplacian index is as large as possible. Denote the vertex set of $G$ by $V_G = \{v_1, v_2, \ldots, v_n\}$ and the Perron vector of $G$ by $\mathbf{x} = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$, where $x_{v_i}$ corresponds to the vertex $v_i$, $i = 1, 2, \ldots, n$.

We first prove that the graph $G$ is a bundle. In order to do so we will prove the following claims.

**Claim 1.** *Any two cycles of the graph G have one common vertex.*

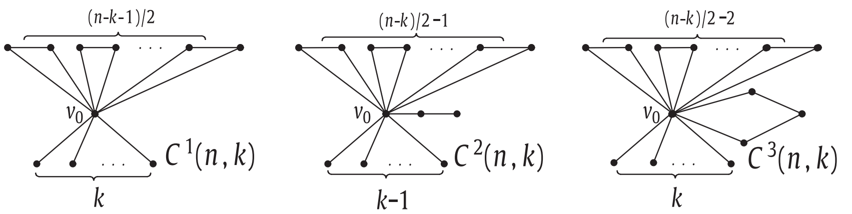


**Fig. 7**. Graphs $C^1(n,k)$, $C^2(n,k)$ and $C^3(n,k)$.

**Proof.** Note that any two cycles of $G$ have no edge in common, hence assume, on the contrary, that there are two disjoint cycles $C^1$ and $C^2$ contained in $G$. Then, we can choose cycles $C^1$ and $C^2$ such that the path $P$ of length $p \geqslant 2$ connects $C^1$ and $C^2$ is the shortest. For convenience, let $V_{C^1} \cap V_P = \{u_1\}$ and $V_{C^2} \cap V_P = \{u_p\}$. We distinguish the following two possible cases to complete the proof of Claim 1.

**Case 1.** The path $P$ (connecting $C^1$ and $C^2$) has no common edge with any other cycle(s) contained in $G$. Without loss of generality, we may assume that $x_{u_1} \geqslant x_{u_p}$. Let $y$ in $V_{C^2}$ be a neighbor of $u_p$, then set $G' := G - \{u_p y\} + \{u_1 y\}$. Thus $G' \in \mathscr{C}_{n,k}$. By Lemma 2.1 we have $q_1(G') > q_1(G)$, a contradiction.

**Case 2.** The path $P$ (connecting $C^1$ and $C^2$) has common edge(s) with some other cycle, say $C^3$, contained in $G$. Note that, by the selection of $C^1$ and $C^2$, it suffices to consider that $u_1$ is just the common vertex of $C^3$ and $C^1$, whereas $u_p$ is the only common vertex of $C^3$ and $C^2$. Without loss of generality, we may assume that $x_{u_1} \geqslant x_{u_p}$. Note that there exist two neighbors in $V_{C^2}$, say $y_1$ and $y_2$, of $u_p$. Set $G'' := G - \{u_p y_1, u_p y_2\} + \{u_0 y_1, u_0 y_2\}$. It is easy to see that $G'' \in \mathscr{C}_{n,k}$. By Lemma 2.1 we have $q_1(G'') > q_1(G)$, a contradiction.

This completes the proof of Claim 1. □

**Claim 2.** *Any three cycles contained in $G$ have exactly one common vertex.*

**Proof.** It is the direct consequence of Claim 1. In fact, assume that in $G$ there exist three cycles, say $C^1$, $C^2$ and $C^3$, such that they have no vertex in common. By Claim 1, we have in $G$ that $V_{C^1} \cap V_{C^2} \neq \emptyset$, $V_{C^1} \cap V_{C^3} \neq \emptyset$ and $V_{C^2} \cap V_{C^3} \neq \emptyset$. Hence, it is easy to check that there exist two cycles in $G$ that have common edge(s), a contradiction to the assumption of $G$. □

By Claims 1 and 2, we know that all of the cycles contained in $G$ have exactly one common vertex, say $u_0$, i.e., $G$ is a bundle. By Claims 1 and 2 we also know that the graph in $\mathscr{C}_{n,k}$ having the largest signless Laplacian index is a bundle with some pendant trees attached.

Next we are to show that if $G$ contains a pendant tree $T$, then $T$ is attached to the vertex $u_0$ of $G$.

**Claim 3.** *Any tree $T$ of graph $G$ is attached to the common vertex $u_0$ of all cycles of the bundle.*

**Proof.** Assume, to the contrary, that there exists a tree $T$ attached to a vertex $u$ on a cycle $C$ of $G$ with $u \neq u_0$. Let $y_1, y_2, \ldots, y_t$ be all of the neighbors of vertex $u$ in $T$.

If $x_{u_0} \geqslant x_u$, let $G' = G - \{uy_1, uy_2, \ldots, uy_t\} + \{u_0 y_1, u_0 y_2, \ldots, u_0 y_t\}$; otherwise, let $G'' = G - \{u_0 y | y \in N(u_0) \backslash V_C\} + \{uy | y \in N(v_0) \backslash V_C\}$. It is straightforward to check that $G' \cong G''$ and $G' \in \mathscr{C}_{n,k}$. By Lemma 2.1, we have $q_1(G') > q_1(G)$, a contradiction. □

We further prove the following claim.

**Claim 4.** *Let $T$ be the tree attached to the common vertex $u_0$ of all the cycles contained in $G$, then for any $u \in V_T \backslash \{u_0\}$ we have $d(u) \leqslant 2$.*

**Proof.** In the opposite case, there exists a vertex $u$ in $V_T \backslash \{u_0\}$ such that $d(u) \geqslant 3$. Let $N_u$ denote the set of all neighbors of $u$ in $T$ such that $d(u_0, v) = d(u_0, u) + 1$ for each $v \in N_u$. For convenience, let $v_0$ be in $N_u$.

If $x_{u_0} \geqslant x_u$, then let $G' = G - \{uv | v \in N_u \backslash \{v_0\}\} + \{u_0 v | v \in N_u \backslash \{v_0\}\}$; If $x_{u_0} < x_u$, choose a neighbor in some cycle, say $y$, of $u_0$ and set $G'' = G - \{u_0 y\} + \{uy\}$. It is straightforward to check that $G', G'' \in \mathscr{C}_{n,k}$. By Lemma 2.1, we have $q_1(G') > q_1(G)$ and $q_1(G'') > q_1(G)$, a contradiction. □

Now we come back to complete the proof of Theorem 3.1. By Claim 4, Lemmas 2.4 and 2.5, we conclude that there exists at most one vertex, say $u$, of degree 2 in the attached tree such that $u$ is the neighbor of vertex $u_0$. By Lemmas 2.6 and 2.7, the lengths of all cycles in $G$ are 3 or 4, and at most one of them is of length 4. By Lemma 2.8, $G$ cannot contain both a cycle of length 4 and a vertex $u$ ($\neq u_0$) of degree 2 in the attached tree. Hence, if $n-k \equiv 1 \pmod 2$, then $G \cong C^1(n,k)$ (see Fig. 7); if $n-k \equiv 0$

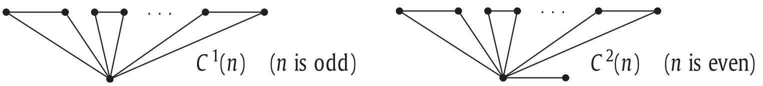


**Fig. 8**. Graphs $C^1(n)$ and $C^2(n)$.

(mod 2), then $G \cong C^2(n,k)$ or, $C^3(n,k)$, where $C^2(n,k)$ and $C^3(n,k)$ are depicted in Fig. 7. And by Lemma 2.9, we know that $q_1(C^2(n,k) > q_1(C^3(n,k))$. So, $G \cong C^2(n,k)$ when $n-k \equiv 0 \pmod 2$.

By direct computing (one may also refer to the Appendix) we have

$$\psi(C^1(n,k)) = (x-1)^{\frac{n+k-3}{2}}(x-3)^{\frac{n-k-3}{2}}[x^3-(k+6)x^2-(n-4k-12)x+n-k-7] \quad (3.1)$$

and

$$\psi(C^2(n,k)) = (x-1)^{\frac{n+k}{2}-3}(x-3)^{\frac{n-k}{2}-2}[x^5-(k+9)x^4-(n-7k-32)x^3 + (4n-14k-54)x^2-(4n-7k-40)x+n-k-8]. \quad (3.2)$$

It is easy to see that $C_3$ is a proper subgraph of $C^1(n,k)$ (resp. $C^2(n,k)$). Note that $q_1(C_3) = 4$, hence $q_1(C^1(n,k)) > 4$ and $q_1(C^2(n,k)) > 4$. Whence, $q_1(C^1(n,k))$ is the largest root of the equation $x^3-(k+6)x^2-(n-4k-12)x+n-k-7=0$ and $q_1(C^2(n,k))$ is the largest root of the equation $x^5-(k+9)x^4-(n-7k-32)x^3+(4n-14k-54)x^2-(4n-7k-40)x+n-k-8=0$.

This completes the proof of Theorem 3.1. □

Denote by $\mathscr{C}_n$ the set of all connected cacti with $n$ vertices. Let $C^1(n)$ and $C^2(n)$ be the bundles with $n$ vertices as depicted in Fig. 8.

**Theorem 3.2.** *Let $G$ be a graph in $\mathscr{C}_n$. Then*

(i) $q_1(G) \leqslant \frac{5+\sqrt{4n-3}}{2}$ *for odd $n$, and the equality holds if and only if $G \cong C^1(n)$, where $C^1(n)$ is depicted in Fig. 8.*
(ii) $q_1(G) \leqslant q_1(C^2(n))$ *for even $n$, and the equality holds if and only if $G \cong C^2(n)$, where $C^2(n)$ is depicted in Fig. 8 and $q_1(C^2(n))$ is the largest root of the equation $x^3-7x^2-(n-16)x+n-8=0$.*

**Proof.** By Lemma 2.2, we get

$$q_1(C^1(n,k+2)) < q_1(C^1(n,k)), \quad q_1(C^2(n,k+2)) < q_1(C^2(n,k))$$

for $k \geqslant 0$. Hence, if $n$ is odd, then $C^1(n,k)$ is a spanning subgraph of $C^1(n)$; if $n$ is even, then $C^2(n,k)$ is a spanning subgraph of $C^2(n)$. By Lemma 2.2 and Theorem 3.1, we get

$$q_1(C^1(n,k)) < q_1(C^1(n,k-2)) < \cdots < q_1(C^1(n,2)) < q_1(C^1(n))$$

and

$$q_1(C^2(n,k)) < q_1(C^2(n,k-2)) < \cdots < q_1(C^2(n,3)) < q_1(C^2(n)).$$

By direct computing, we have

$$\psi(C^1(n),x) = (x-1)^{\frac{n-1}{2}}(x-3)^{\frac{n-3}{2}}(x^2-5x-n+7)$$

and

$$\psi(C^2(n),x) = (x-1)^{\frac{n-2}{2}}(x-3)^{\frac{n-4}{2}}[x^3-7x^2-(n-16)x+n-8].$$

Note that $C_3$ is a proper subgraph of $C^1(n)$ and $C^2(n)$, hence $q_1(C^1(n)) > q_1(C_3) = 4$ and $q_1(C^2(n)) > q_1(C_3) = 4$. Therefore, $q_1(C^1(n)) = \frac{5+\sqrt{4n-3}}{2}$ and $q_1(C^2(n))$ is the largest root of the equation $x^3 - 7x^2 - (n-16)x + n - 8 = 0$.

This completes the proof. □

At last, based on the results obtained as above, we determine the sharp upper bound for the signless Laplacian index of cacti with a perfect matching. Let $\widetilde{\mathscr{C}_{2k}}$ be the set of all $2k$-vertex cacti with a perfect matching.

Based on Theorem 3.2, we get

**Theorem 3.3.** *Let G be a graph in $\widetilde{\mathscr{C}_{2k}}$. Then $q_1(G) \leqslant q_1(C^2(2k))$, and the equality holds if and only if $G \cong C^2(2k)$, where $q_1(C^2(2k))$ is the largest root of the equation $x^3 - 7x^2 - (2k-16)x + 2k - 8 = 0$..*

It is natural to consider the question: Let $\widetilde{\mathscr{C}_n^m}$ be the set of all $n$-vertex cacti with matching number $m$. How to determine the graph in $\widetilde{\mathscr{C}_n^m}$ which attains the maximal signless Laplacian index? Here we pose the following conjecture.

**Conjecture 3.4.** *Let G be a graph in $\widetilde{\mathscr{C}_n^m}$. Then*

(i) *if $n = 2m+1$, then $q_1(G) \leqslant \frac{5+\sqrt{4n-3}}{2}$, and the equality holds if and only if $G \cong C^1(n)$, where $C^1(n)$ is depicted in Fig. 8.*
(ii) *if $n \geqslant 2m+2$, then $q_1(G) \leqslant q_1(C^1(n, n-2m+1))$, and the equality holds if and only if $G \cong C^1(n, n-2m+1)$, where $q_1(C^1(n, n-2m+1))$ is the largest root of the equation $x^3 - (n-2m+7)x^2 + (3n-8m+8)x + 2m - 8 = 0$.*

## Appendix

We shall prove Eqs. (3.1) and (3.2) in what follows. In order to obtain our results, we need the following Propositions which are obtained by Hou and the first author of the current paper in [20]. We give their proofs here for the sake of completeness. Assume that $G$ is a graph with $v \in V_G$, let $Q_v(G)$ denote the principal submatrix of $Q(G)$ by deleting the row and column corresponding to the vertex $v$.

**Proposition 1** [20]. *Let $G = G_1u : vG_2$ be the graph obtained from two disjoint graphs $G_1$ and $G_2$ by joining a vertex u of graph $G_1$ to a vertex v of the graph $G_2$ by an edge. Then*

$$\psi(G) = \psi(G_1)\psi(G_2) - \psi(G_1)\psi(Q_v(G_2)) - \psi(G_2)\psi(Q_u(G_1)).$$

**Proof.** Let $Q(G_1^*)$ (resp. $Q(G_2^*)$) be the principal submatrix obtained by deleting the row and column corresponding to vertex $v$ (resp. $u$) from $Q(G_1u : v)$ (resp. $Q(G_2v : u)$), where $G_1u : v$ (resp. $G_2v : u$) is the graph formed from $G_1$ (resp. $G_2$) by joining a new pendant vertex $v$ (resp. $u$) to $u$ (resp. $v$). Without loss of generality, we may assume that

$$Q(G) = \begin{pmatrix} Q(G_1^*) & E_{11} \\ E_{11}^T & Q(G_2^*) \end{pmatrix},$$

where $E_{11}$ is the $|V_{G_1}| \times |V_{G_2}|$ matrix whose only non-zero entry is 1 in position $(1, 1)$.

By Laplace Theorem for determinants, we have

$$\psi(G) = \psi(G_1^*)\psi(G_2^*) - \psi(Q_u(G_1))\psi(Q_v(G_2)). \tag{a.1}$$

Note that $\psi(G_1^*) = \psi(G_1) - \psi(Q_u(G_1))$ and $\psi(G_2^*) = \psi(G_2) - \psi(Q_v(G_2))$, hence in view of (a.1), we have

$$\psi(G) = \psi(G_1)\psi(G_2) - \psi(G_1)\psi(Q_v(G_2)) - \psi(G_2)\psi(Q_u(G_1)),$$

as desired. □

**Proposition 2** [20]**.** *Let G be an n-vertex connected graph consisting of a subgraph H (with at least two vertices) and* $n - |V_H|$ *distinct pendant edges (not in H) attaching to a vertex v in H. Then*

$$\psi(G) = (x-1)^{n-|V_H|}\psi(H) - (n - |V_H|)x(x-1)^{n-|V_H|-1}\psi(Q_v(H)).$$

**Proof.** Let $m = n - |V_H|$. We prove the proposition by induction on $m$.

When $m = 1$, there is one pendant edge (not in $H$) attached to $v$, denoted as $vv_1$. We regard $G$ as a connected sum of an isolated vertex $v_1$ and $H$ at $v$. By Proposition 1, we have

$$\psi(G) = x\psi(H) - \psi(H) - x\psi(Q_v(H)) = (x-1)\psi(H) - x\psi(Q_v(H)).$$

Suppose the result holds for $m-1$. For $n - |V_H| = m \geqslant 2$, let the pendant edges (not in $H$) attached to $v$ be $vv_1, \dots, vv_m$. We regard $G$ as a connected sum of an isolated vertex $v_m$ and $H'$ at $v$, where $H'$ is the graph obtained from $H$ by attaching $m-1$ pendant edges $vv_1, \dots, vv_{m-1}$. Then by Proposition 1, we have

$$\psi(G) = (x-1)\psi(H') - x\psi(Q_v(H')). \tag{a.2}$$

Moreover, by the inductive hypothesis, we have

$$\psi(H') = (x-1)^{m-1}\psi(H) - (m-1)x(x-1)^{m-2}\psi(Q_v(H)). \tag{a.3}$$

On the other hand,

$$\psi(Q_v(H')) = (x-1)^{m-1}\psi(Q_v(H)). \tag{a.4}$$

In view of (a.2)–(a.4), we have

$$\psi(G) = (x-1)^m\psi(H) - mx(x-1)^{m-1}\psi(Q_v(H)),$$

as required. □

**The proof of Eq. (3.1).** By Proposition 2, we have

$$\psi(C^1(n,k)) = (x-1)^k\psi(C^1(n-k)) - kx(x-1)^{k-1}\psi(Q_v(C^1(n-k))), \tag{a.5}$$

where $C^1(n-k)$ is depicted in Fig. 8. In order to complete the proof, it suffices to determine $\psi(C^1(n-k))$ and $\psi(Q_v(C^1(n-k)))$.

Note that

$$Q(C^1(n-k)) = \begin{pmatrix} n-k-1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 2 & 1 & \cdots & 0 & 0 \\ 1 & 1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 2 & 1 \\ 1 & 0 & 0 & \cdots & 1 & 2 \end{pmatrix},$$

hence

$$\psi(C^1(n-k)) = \begin{vmatrix} x-(n-k-1) & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & x-2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & -1 & x-2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 0 & 0 & 0 & \cdots & x-2 & -1 \\ -1 & 0 & 0 & 0 & \cdots & -1 & x-2 \end{vmatrix}. \tag{a.6}$$

For convenience, let $\psi(C^1(n-k)) = B_{n-k}$. Consider the last two rows of $\psi(C^1(n-k))$ in (a.6), there are just three non-zero sub-determinants:

$$M_1 = \begin{vmatrix} -1 & x-2 \\ -1 & -1 \end{vmatrix} = x-1,\ M_2 = \begin{vmatrix} -1 & -1 \\ -1 & x-2 \end{vmatrix} = -(x-1),\ M_3 = \begin{vmatrix} x-2 & -1 \\ -1 & x-2 \end{vmatrix} = x^2-4x+3.$$

Hence, we obtain $\psi(C^1(n-k)) = M_1A_1 + M_2A_2 + M_3A_3$, where $A_i$ is the cofactor of $M_i,\ i = 1, 2, 3$, i.e.,

$$A_1 = (-1)^{3n-3k-1} \begin{vmatrix} -1 & -1 & \cdots & -1 & -1 & -1 \\ x-2 & -1 & \cdots & 0 & 0 & 0 \\ -1 & x-2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & x-2 & -1 & 0 \\ 0 & 0 & \cdots & -1 & x-2 & 0 \end{vmatrix} = -(x^2-4x+3)^{\frac{n-k-3}{2}},$$

$$A_2 = (-1)^{3n-3k} \begin{vmatrix} -1 & -1 & \cdots & -1 & -1 & -1 \\ x-2 & -1 & \cdots & 0 & 0 & 0 \\ -1 & x-2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & x-2 & -1 & 0 \\ 0 & 0 & \cdots & -1 & x-2 & 0 \end{vmatrix} = (x^2-4x+3)^{\frac{n-k-3}{2}}$$

and $A_3 = B_{n-k-2}$.

Combine with

$$B_3 = \begin{vmatrix} x-2 & -1 & -1 \\ -1 & x-2 & -1 \\ -1 & -1 & x-2 \end{vmatrix} = (x-4)(x-1)^2,$$

we have

$$\psi(C^1(n-k)) = B_{n-k} = (x-1)(x^2-4x+3)^{\frac{n-k-3}{2}}(x^2-5x+7-n+k). \tag{a.7}$$

On the other hand, we have

$$Q_{v_0}(C^1(n-k)) = \begin{pmatrix} 2 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 2 \end{pmatrix}.$$

Therefore,

$$\psi(Q_{v_0}(C^1(n-k))) = \begin{vmatrix} x-2 & -1 & \cdots & 0 & 0 \\ -1 & x-2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & x-2 & -1 \\ 0 & 0 & \cdots & -1 & x-2 \end{vmatrix} = (x^2-4x+3)^{\frac{n-k-1}{2}}. \quad \text{(a.8)}$$

By (a.5), (a.7) and (a.8), our result follows immediately. □

**The proof of Eq. (3.2).** In $C^2(n,k)$ delete the $k-1$ pendent vertices each of which is adjacent to $v_0$ (see Fig. 7), denote the resultant graph by $H$. For convenience, let $u$ be the vertex of degree 2 on the pendent path of $H$. By Proposition 2, we get

$$\psi(C^2(n,k)) = (x-1)^{k-1}\psi(H) - (k-1)x(x-1)^{k-2}\psi(Q_{v_0}(H)). \quad \text{(a.9)}$$

In order to complete the proof, it suffices to determine $\psi(H)$ and $\psi(Q_{v_0}(H))$. In fact, in view of Propositions 1 and 2, we have

$$\begin{aligned} \psi(H) &= \psi(C^1(n-k-1))\psi(P_2) - \psi(C^1(n-k-1))\psi(Q_u(P_2)) - \psi(P_2)\psi(Q_{v_0}(C^1(n-k-1))) \\ &= (x^2-3x+1)\psi(C^1(n-k-1)) - x(x-2)\psi(Q_{v_0}(C^1(n-k-1))) \\ &= (x^2-3x+1)\psi(C^1(n-k-1)) - x(x-2)(x^2-4x+3)^{\frac{n-k-2}{2}} \\ &= (x^2-3x+1)(x-1)(x^2-4x+3)^{\frac{n-k-4}{2}}(x^2-5x+7-n+k+1) \\ &\quad - x(x-2)(x^2-4x+3)^{\frac{n-k-2}{2}} \\ &= [x^4-9x^3-(n-k-29)x^2+(3n-3k-35)x-(n-k-8)](x-3)^{\frac{n-k-4}{2}}(x-1)^{\frac{n-k-2}{2}}. \end{aligned} \quad \text{(a.10)}$$

On the other hand,

$$\psi(Q_{v_0}(H)) = \begin{vmatrix} x-2 & -1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & x-1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & x-2 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & x-2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & x-2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & -1 & x-2 \end{vmatrix} = (x^2-3x+1)(x^2-4x+3)^{\frac{n-k}{2}-1}. \quad \text{(a.11)}$$

In view of (a.9)–(a.11), our result follows immediately. □

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