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Zhen Lin

China University of Mining and Technology, lnlinzhen@163.com

Shu-Guang Guo

Yancheng Teachers University, ychgsg@163.com

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ORDERING CACTI WITH SIGNLESS LAPLACIAN SPREAD*

ZHEN LIN[†] AND SHU-GUANG GUO[‡]

Abstract. A cactus is a connected graph in which any two cycles have at most one vertex in common. The signless Laplacian spread of a graph is defined as the difference between the largest eigenvalue and the smallest eigenvalue of the associated signless Laplacian matrix. In this paper, all cacti of order n with signless Laplacian spread greater than or equal to $n - \frac{1}{2}$ are determined.

Key words. Cactus, Signless Laplacian spread, Upper bound.

AMS subject classifications. 05C50.

1. Introduction. Let G be a simple undirected graph with vertex set $V(G) = \{v_0, v_1, \dots, v_{n-1}\}$ and edge set $E(G)$. For a graph G , $A(G)$ is its adjacency matrix and $D(G)$ is the diagonal matrix of its degrees. The matrix $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix of G . As usual, we shall index the eigenvalues of $Q(G)$ in nonincreasing order, denote them as $q_1(G) \geq q_2(G) \geq \dots \geq q_{n-1}(G) \geq q_n(G) \geq 0$, where $q_1(G)$ is called the signless Laplacian spectral radius of G .

The spread $s(M)$ of an $n \times n$ complex matrix M is $s(M) = \max_{i,j} |\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of M . There are several results concerning the spread of a matrix, see for example [5, 12] and the references therein. Motivated by the definition of adjacency and Laplacian spreads of a graph G , Liu and Liu [8] defined the signless Laplacian spread of a graph G as $S_Q(G) = q_1(G) - q_n(G)$, and determined the unique unicyclic graph with maximum signless Laplacian spread among the class of connected unicyclic graphs of order n . Oliveira et al. [13] proved that $2 \leq S_Q(G) \leq 2n - 4$ for any graph on $n \geq 5$ vertices and characterized the equality cases in both bounds. Further, they proved that $S_Q(G) < 2n - 4$ for any connected graph G with $n \geq 5$, and conjectured that there is no connected graph G with $n \geq 5$ vertices such that $\sqrt{4n^2 - 20n + 33} < S_Q(G) < 2n - 4$. Fan and Fallat [4] proved a conjecture on minimal signless Laplacian spread proposed by Cvetković, Rowlinson and Simić in [2]. Maden et al. [11] established some lower and upper bounds for $S_Q(G)$ in terms of clique and independence numbers. Sun and Wang [15] determined the bicyclic graphs with the largest or the second largest signless Laplacian spread among the class of connected bicyclic graphs of order n . You [17] determined the unique graph with minimum signless Laplacian spread among the class of unicyclic graphs with n vertices.

A cactus is a connected graph in which any two cycles have at most one vertex in common. Let \mathcal{C}_n denote the set of cacti with n vertices. For $G \in \mathcal{C}_n$, G contains c cycles if and only if $|E(G)| = n - 1 + c$. The cactus has been an interesting topic in mathematical literature and has been studied extensively. For related results, one may refer to [7, 14] and the references therein. Moreover, researches show that the cactus plays an important role in theoretical chemistry, and much work has been done to study the extremal graph

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[†]School of Mathematics, China University of Mining and Technology, Xuzhou, 221116, Jiangsu, P.R. China (lnlinzhen@163.com).

[‡]School of Mathematics and Statistics, Yancheng Teachers University, Yancheng, 224002, Jiangsu, P.R. China (ychgsg@163.com).

according to various chemical indices, we refer the reader to [9, 16] and the references therein.

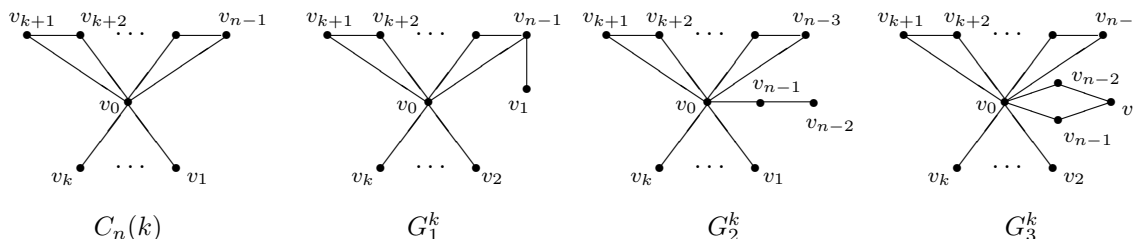


Fig 1.1. Graphs $C_n(k)$, G_1^k , G_2^k , and G_3^k .

Let $n > k \geq 0$ be two integers such that $n - k$ is odd, and $K_{1, n-1}$ denote the star with $V(K_{1, n-1}) = \{v_0, v_1, \dots, v_{n-1}\}$ and $d(v_0) = n - 1$. For $k < n - 1$, let $C_n(k)$ denote the cactus, shown in Fig. 1.1, obtained from $K_{1, n-1}$ by adding the edges $v_{k+1}v_{k+2}, v_{k+3}v_{k+4}, \dots, v_{n-2}v_{n-1}$. For $k = n - 1$, also denote the star $K_{1, n-1}$ by $C_n(n - 1)$. Let

$$g(n) := \frac{16n^3 - 72n^2 + 216n - (8n^2 - 33)\sqrt{4n^2 - 36n + 141}}{432}.$$

It is not difficult to verify that $g(n)$ is a strictly increasing function on n in the interval $(11, +\infty)$. For $n > 11$, noting that $\sqrt{4n^2 - 36n + 141} > 2n - 9$, we have

$$2.2711 \approx g(12) \leq g(n) < \frac{47}{72}n - \frac{11}{16} < n - 1.$$

In this paper, we determine all cacti of order n with signless Laplacian spread greater than or equal to $n - \frac{1}{2}$. The main result of this paper is as follows:

THEOREM 1.1. *Let $n > 11, k_0$ be the smallest integer such that $k_0 \geq g(n)$ and $n - k_0$ is odd, $C_n(k)$ be the cactus shown in Fig. 1.1, and $G \in \mathcal{C}_n \setminus \{C_n(k_0), C_n(k_0 + 2), \dots, C_n(n - 1)\}$. Then*

$$S_Q(G) < n - \frac{1}{2} \leq S_Q(C_n(k_0)) < S_Q(C_n(k_0 + 2)) < \dots < S_Q(C_n(n - 1)).$$

The rest of the paper is organized as follows. In Section 2, we recall some useful notions and lemmas used further. In Section 3, we provide an upper bound on the signless Laplacian spectral radius of a cactus which is the key to the proof of our main result. In Section 4, we give a proof of Theorem 1.1.

2. Preliminaries. For $v \in V(G)$, $N_G(v)$ (or $N(v)$) denotes the neighborhood of v in G , and $d(v) = d_G(v) = |N_G(v)|$ denotes the degree of vertex v in G . We denote by $\Delta = \Delta(G)$ the maximum degree of the vertices of G . Let $G - uv$ denote the graph that arises from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph that arises from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. The signless Laplacian characteristic polynomial of a graph G , is equal to $\det(xI_n - Q(G))$, denoted by $\phi(G, x)$. The double star $S(s, t)$ is the tree obtained by joining the centres of two stars $K_{1, s-1}$ and $K_{1, t-1}$ with an edge. Let I_p be the $p \times p$ identity matrix and $J_{p,q}$ be the $p \times q$ matrix in which every entry is 1, or simply J_p if $p = q$.

DEFINITION 2.1. ([6]) Let M be a matrix of order n , $\sigma(M)$ be the spectrum of M . Let M be a real matrix of order n described in the following block form

$$\begin{pmatrix} M_{11} & \cdots & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \cdots & M_{tt} \end{pmatrix}, \tag{1}$$

where the diagonal blocks M_{ii} are $n_i \times n_i$ matrices for any $i \in \{1, 2, \dots, t\}$ and $n = n_1 + \dots + n_t$. For any $i, j \in \{1, 2, \dots, t\}$, let b_{ij} denote the average row sum of M_{ij} , i.e., b_{ij} is the sum of all entries in M_{ij} divided by the number of rows. Then $B(M) = (b_{ij})$ (simply by B) is called the quotient matrix of M .

Now we introduce the following lemmas that will be used in Sections 3 and 4.

LEMMA 2.2. ([18]) Let $M = (m_{ij})_{n \times n}$ be defined as (1), and for any $i, j \in \{1, 2, \dots, t\}$, $M_{ii} = l_i J_{n_i} + p_i I_{n_i}$, $M_{ij} = s_{ij} J_{n_i, n_j}$, for $i \neq j$, where l_i, p_i, s_{ij} are real numbers, $B = B(M)$ be the quotient matrix of M . Then

$$\sigma(M) = \sigma(B) \cup \{p_i^{[n_i-1]} \mid i = 1, 2, \dots, t\},$$

where $p_i^{[n_i-1]}$ means that p_i is an eigenvalue with multiplicity $n_i - 1$.

LEMMA 2.3. ([10]) Suppose that G is a connected graph with $n \geq 3$ vertices. Then,

$$q_1(G) \leq \max\{d(v) + m(v) \mid v \in V(G) \text{ and } d(v) > 1\},$$

equality holds if and only if G is either a regular graph or a semiregular bipartite graph, where $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.

LEMMA 2.4. ([2]) If G is a graph with at least one edge, then $q_1(G) \geq \Delta(G) + 1$, with equality in the connected case if and only if G is a star.

LEMMA 2.5. ([1]) Let G be a simple graph. Then

$$q_1(G) \leq \max\{d(u) + d(v) \mid uv \in E(G)\}.$$

LEMMA 2.6. ([2]) Let G be a graph with order n and $e \in E(G)$. Then

$$q_1(G) \geq q_1(G - e) \geq q_2(G) \geq q_2(G - e) \geq \dots \geq q_n(G) \geq q_n(G - e) \geq 0.$$

LEMMA 2.7. ([3]) Let G be a graph with minimum degree $\delta > 0$. Then $q_n(G) < \delta$.

3. An upper bound on $q_1(G)$ of a cactus G .

THEOREM 3.1. Let $n > 11$, $G \in \mathcal{C}_n$. Then

$$q_1(G) < \max \left\{ 2 + \frac{n-1}{2}, \Delta(G) + \frac{n-1}{\Delta(G)} \right\} + 1.$$

Proof. Let $u \in V(G)$ such that $d(u) > 1$. By Lemma 2.3, we have

$$\begin{aligned} q_1(G) &\leq d(u) + m(u) \\ &\leq d(u) + \frac{d(u) + (n-1-d(u)) + 2 \cdot \frac{d(u)}{2}}{d(u)} \\ &= d(u) + \frac{n-1}{d(u)} + 1 \\ &\leq \max \left\{ 2 + \frac{n-1}{2}, \Delta(G) + \frac{n-1}{\Delta(G)} \right\} + 1. \end{aligned}$$

Next, we will show that the equalities in the above two inequalities cannot hold simultaneously. Otherwise, by the above proof and Lemma 2.3, G is a regular graph or a semiregular bipartite graph. Let c be the number of cycles in G . Then $0 \leq c \leq \frac{n-1}{2}$.

Case 1. If G is a regular graph, then each vertex of G has degree d . Noting that G has $n-1+c$ edges, we have $dn = 2(n-1+c)$. Since $c \leq \frac{n-1}{2}$, it follows that $d = 2$. Namely, G is the cycle C_n . It is well known that $q_1(C_n) = 4$. However, in this case,

$$\max \left\{ 2 + \frac{n-1}{2}, \Delta(G) + \frac{n-1}{\Delta(G)} \right\} + 1 = 3 + \frac{n-1}{2} > 4 = q_1(C_n)$$

for $n \geq 4$. This is a contradiction.

Case 2. If G is a semiregular bipartite graph, let (X, Y) be the two parts of G , $|X| = x$ and $|Y| = y$. Let d_1 and d_2 be the degree of each vertex in X and Y respectively. Then

$$x + y = n, \quad d_1x = d_2y = n - 1 + c. \quad (2)$$

Without loss of generality, we may assume $d_1 > d_2$. It follows that $y = \frac{n-1+c}{d_2} > \frac{n}{2}$. Noting that $c \leq \frac{n-1}{2}$, we have $d_2 \leq 2$.

If $d_2 = 1$, then G is the star $K_{1,n-1}$. It is well known that $q_1(K_{1,n-1}) = n$. However, in this case,

$$\max \left\{ 2 + \frac{n-1}{2}, \Delta(G) + \frac{n-1}{\Delta(G)} \right\} + 1 = n + 1 > n = q_1(K_{1,n-1}).$$

This is a contradiction.

If $d_2 = 2$, by (2), we have

$$\frac{n-1+c}{d_1} + \frac{n-1+c}{2} = n.$$

Since $c \leq \frac{n-1}{2}$, it follows that $d_1 \leq 5$. In the case when $d_1 = 3$, by Lemma 2.5, we have

$$q_1(G) \leq 5 < \max \left\{ 2 + \frac{n-1}{2}, 3 + \frac{n-1}{3} \right\} + 1 = 3 + \frac{n-1}{2}$$

for $n > 7$, a contradiction. In the cases when $d_1 = 4$ or 5 , we can derive a contradiction similarly.

From the above arguments, we have

$$q_1(G) < \max \left\{ 2 + \frac{n-1}{2}, \Delta(G) + \frac{n-1}{\Delta(G)} \right\} + 1.$$

This completes the proof. □

4. A proof of Theorem 1.1.

LEMMA 4.1. *Let $n > 11$, $G \in \mathcal{C}_n$. If $\Delta(G) \leq n - 2$, then $q_1(G) < n - \frac{1}{2}$.*

Proof. *Case 1.* $\Delta(G) \leq n - 3$. By Theorem 3.1, we have

$$q_1(G) < \max \left\{ 2 + \frac{n-1}{2}, n-3 + \frac{n-1}{n-3} \right\} + 1 = n - 1 + \frac{2}{n-3} < n - \frac{1}{2}.$$

Case 2. $\Delta(G) = n - 2$. Then G must be the double star $S(n - 3, 1)$ or one of the graphs G_i^k ($i = 1, 2, 3$), shown in Fig. 1.1, where $G_1^k := C_n(k) - v_0v_1 + v_{n-1}v_1$, $G_2^k := C_n(k) - v_0v_{n-2}$, $G_3^k := C_n(k) - v_{n-2}v_{n-1} - v_0v_1 + v_1v_{n-2} + v_1v_{n-1}$. By Lemma 2.4, we have $q_1(G) > n - 1$. If $G = S(n - 3, 1)$, by Lemma 2.6, we have $q_1(G) \leq q_1(G_1^1)$ or $q_1(G) \leq q_1(G_2^0)$. Next we will prove that $q_1(G_i^k) < n - \frac{1}{2}$ for $i = 1, 2, 3$.

If $G = G_1^k$ and n is an even number, by Lemma 2.6, we have $q_1(G_1^k) \leq q_1(G_1^1)$. Obviously, we have

$$Q(G_1^1) = \begin{pmatrix} n-2 & 0 & 1 & 1 & 1 & 1 & \cdots & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \\ 1 & 0 & 2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 2 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 2 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 3 \end{pmatrix}.$$

It can be written as follows:

$$Q(G_1^1) = \begin{pmatrix} (n-3)J_1 + I_1 & 0 & J_{1,2} & \cdots & J_{1,2} & J_1 & J_1 \\ 0 & I_1 & 0 & \cdots & 0 & 0 & J_1 \\ J_{2,1} & 0 & J_2 + I_2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ J_{2,1} & 0 & 0 & \cdots & J_2 + I_2 & 0 & 0 \\ J_1 & 0 & 0 & \cdots & 0 & J_1 + I_1 & J_1 \\ J_1 & J_1 & 0 & \cdots & 0 & J_1 & 2J_1 + I_1 \end{pmatrix}.$$

Let $B_1(G_1^1)$ be the corresponding quotient matrix of $Q(G_1^1)$. Then

$$B_1(G_1^1) = \begin{pmatrix} n-2 & 0 & 2 & \cdots & 2 & 1 & 1 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 3 & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 2 & 1 \\ 1 & 1 & 0 & \cdots & 0 & 1 & 3 \end{pmatrix}.$$

By Lemma 2.2, we have $\sigma(Q(G_1^1)) = \sigma(B_1(G_1^1)) \cup \{1^{\lfloor \frac{n-4}{2} \rfloor}\}$. Further, we can write $B_1(G_1^1)$ as follows:

$$B_1(G_1^1) = \begin{pmatrix} (n-3)J_1 + I_1 & 0 & 2J_{1, \frac{n-4}{2}} & J_1 & J_1 \\ 0 & I_1 & 0 & 0 & J_1 \\ J_{\frac{n-4}{2}, 1} & 0 & 3I_{\frac{n-4}{2}} & 0 & 0 \\ J_1 & 0 & 0 & J_1 + I_1 & J_1 \\ J_1 & J_1 & 0 & J_1 & 2J_1 + I_1 \end{pmatrix}.$$

Let $B_2(G_1^1)$ be the corresponding quotient matrix of $B_1(G_1^1)$. Then

$$B_2(G_1^1) = \begin{pmatrix} n-2 & 0 & n-4 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 3 & 0 & 0 \\ 1 & 0 & 0 & 2 & 1 \\ 1 & 1 & 0 & 1 & 3 \end{pmatrix}. \quad (3)$$

By Lemma 2.2, we have $\sigma(B_1(G_1^1)) = \sigma(B_2(G_1^1)) \cup \{3^{\lfloor \frac{n-6}{2} \rfloor}\}$. Thus, we have

$$\sigma(Q(G_1^1)) = \sigma(B_2(G_1^1)) \cup \{1^{\lfloor \frac{n-4}{2} \rfloor}, 3^{\lfloor \frac{n-6}{2} \rfloor}\}, \quad (4)$$

and by direct computing, we know the characteristic polynomial of (3) is as follows:

$$\det(xI_n - B_2(G_1^1)) = (x-2)[x^4 - (n+5)x^3 + (6n+1)x^2 - (9n-13)x + 3n-6]. \quad (5)$$

Combining (4) and (5), we have

$$\phi(G_1^1, x) = (x-2)(x-1)^{\frac{n-4}{2}}(x-3)^{\frac{n-6}{2}}[x^4 - (n+5)x^3 + (6n+1)x^2 - (9n-13)x + 3n-6].$$

This implies that $q_1(G_1^1)$ is the largest root of the polynomial

$$f_1(x) := x^4 - (n+5)x^3 + (6n+1)x^2 - (9n-13)x + 3n-6.$$

Noting that $f_1'(x) > 0$ for $x \in [n-1, +\infty)$, we know that $f_1(x)$ is strictly increasing in the interval $[n-1, +\infty)$. Since $f_1(n-1) = -(n-4)(2n-3) < 0$ and

$$f_1\left(n - \frac{1}{2}\right) = \frac{1}{16}[4n(n-12)(2n+1) + 318n - 185] > 0$$

for $n > 11$, it follows that $q_1(G_1^1) < n - \frac{1}{2}$. This means that $q_1(G_1^k) < n - \frac{1}{2}$.

If $G = G_1^k$ and n is an odd number, by Lemma 2.6, we have $q_1(G_1^k) \leq q_1(G_1^2)$. By a similar reasoning as the above, we have

$$\begin{aligned} \phi(G_1^2, x) &= (x-1)^{\frac{n-5}{2}}(x-3)^{\frac{n-7}{2}}[x^6 - (n+8)x^5 + 9(n+2)x^4 - (29n-2)x^3 \\ &\quad + (42n-55)x^2 - (27n-62)x + 6n-18]. \end{aligned}$$

This implies that $q_1(G_1^2)$ is the largest root of the polynomial

$$\begin{aligned} f_2(x) &:= x^6 - (n+8)x^5 + 9(n+2)x^4 - (29n-2)x^3 \\ &\quad + (42n-55)x^2 - (27n-62)x + 6n-18. \end{aligned}$$

Noting that $f_2'(x) > 0$ for $x \in [n-1, +\infty)$, we know that $f_2(x)$ is strictly increasing in $[n-1, +\infty)$. Since $f_2(n-1) = -(2n-5)[n^2(n-9) + 26n-22] < 0$ and

$$f_2\left(n - \frac{1}{2}\right) = \frac{1}{64}[16n^3(n-12)(2n-7) + 1456n^2(n-6) + 1336n^2 + 9026n - 3943] > 0$$

for $n > 11$, it follows that $q_1(G_1^2) < n - \frac{1}{2}$. This means that $q_1(G_1^k) < n - \frac{1}{2}$.

If $G = G_2^k$ and n is an even number, by Lemma 2.6, then

$$q_1(G_2^k) \leq q_1(G_2^1) \leq q_1(G_1^1) < n - \frac{1}{2}.$$

If $G = G_2^k$ and n is an odd number, by Lemma 2.6, we have $q_1(G_2^k) \leq q_1(G_2^0)$. By a similar reasoning as the above, we have

$$\phi(G_2^0, x) = (x - 1)^{\frac{n-3}{2}}(x - 3)^{\frac{n-5}{2}}[x^4 - (n + 4)x^3 + 5nx^2 - (7n - 12)x + 2n - 6].$$

This implies that $q_1(G_2^0)$ is the largest root of the polynomial

$$f_3(x) := x^4 - (n + 4)x^3 + 5nx^2 - (7n - 12)x + 2n - 6.$$

Noting that $f_3'(x) > 0$ for $x \in [n - 1, +\infty)$, we know that $f_3(x)$ is strictly increasing in $[n - 1, +\infty)$. Since $f_3(n - 1) = -[(n - 12)(2n + 13) + 169] < 0$ and

$$f_3\left(n - \frac{1}{2}\right) = \frac{1}{16}[4n(n - 12)(2n + 3) + 390n - 183] > 0$$

for $n > 11$, it follows that $q_1(G_2^0) < n - \frac{1}{2}$. This means that $q_1(G_2^k) < n - \frac{1}{2}$.

If $G = G_3^k$ and n is an even number, by Lemma 2.6, we have $q_1(G_3^k) \leq q_1(G_3^1)$. By a similar reasoning as the above, we have

$$\phi(G_3^1, x) = (x - 2)^2(x - 1)^{\frac{n-4}{2}}(x - 3)^{\frac{n-6}{2}}[x^3 - (n + 3)x^2 + 4(n - 1)x - 2n + 8].$$

This implies that $q_1(G_3^1)$ is the largest root of the polynomial

$$f_4(x) := x^3 - (n + 3)x^2 + 4(n - 1)x - 2n + 8.$$

Noting that $f_4'(x) > 0$ for $x \in [n - 1, +\infty)$, we know that $f_4(x)$ is strictly increasing in $[n - 1, +\infty)$. Since $f_4(n - 1) = -2n + 8 < 0$ and $f_4(n - \frac{1}{2}) = \frac{1}{8}[4(n - 12)(n + 3) + 217] > 0$ for $n > 11$, it follows that $q_1(G_3^1) < n - \frac{1}{2}$. This means that $q_1(G_3^k) < n - \frac{1}{2}$.

If $G = G_3^k$ and n is an odd number, by Lemma 2.6, we have $q_1(G_3^k) \leq q_1(G_3^2)$. By a similar reasoning as the above, we have

$$\begin{aligned} \phi(G_3^2, x) &= (x - 2)(x - 3)^{\frac{n-7}{2}}(x - 1)^{\frac{n-5}{2}}[x^5 - (n + 6)x^4 + 7(n + 1)x^3 \\ &\quad - 16(n - 1)x^2 + 2(7n - 20)x - 4n + 20]. \end{aligned}$$

This implies that $q_1(G_3^2)$ is the largest root of the polynomial

$$f_5(x) := x^5 - (n + 6)x^4 + 7(n + 1)x^3 - 16(n - 1)x^2 + 2(7n - 20)x - 4n + 20.$$

Noting that $f_5'(x) > 0$ for $x \in [n - 1, +\infty)$, we know that $f_5(x)$ is strictly increasing in $[n - 1, +\infty)$. Since $f_5(n - 1) = -[2n(n - 12)(n + 2) + 112n - 62] < 0$ and

$$f_5\left(n - \frac{1}{2}\right) = \frac{1}{32}[16n^2(n - 1)(n - 12) + 800n(n - 3) + 372n + 1367] > 0$$

for $n > 11$, it follows that $q_1(G_3^2) < n - \frac{1}{2}$. This means that $q_1(G_3^k) < n - \frac{1}{2}$.

From the above arguments, we have $q_1(G) < n - \frac{1}{2}$. This completes the proof. \square

Proof of Theorem 1.1. Let $n > 11$, $G \in \mathcal{C}_n$. If $\Delta(G) \leq n - 2$, by Lemma 4.1, we have $S_Q(G) < q_1(G) < n - \frac{1}{2}$.

If $\Delta(G) = n - 1$, then G must be the graph $C_n(k)$ shown in Fig. 1.1, where $0 \leq k \leq n - 1$. By Lemma 2.4, we have $q_1(C_n(k)) \geq n$. By a similar reasoning as the proof of Lemma 4.1, we have

$$\phi(C_n(k), x) = (x - 1)^{\frac{n+k-3}{2}} (x - 3)^{\frac{n-k-3}{2}} [x^3 - (n + 3)x^2 + 3nx - 2n + 2k + 2].$$

For $k = 0$, n must be odd, and we have

$$\phi(C_n(0), x) = (x - 1)^{\frac{n-1}{2}} (x - 3)^{\frac{n-3}{2}} [x^2 - (n + 2)x + 2n - 2].$$

It follows that

$$S_Q(C_n(0)) = q_1(C_n(0)) - q_n(C_n(0)) = \frac{n + 2 + \sqrt{n^2 - 4n + 12}}{2} - 1 < n - \frac{1}{2}.$$

For $1 \leq k \leq n - 1$, by Lemma 2.7, we have $q_n(C_n(k)) < 1$. This implies that $q_1 = q_1(C_n(k))$ and $q_n = q_n(C_n(k))$ are roots of the following polynomial

$$f(x) := x^3 - (n + 3)x^2 + 3nx - 2n + 2k + 2.$$

Let q be the other root of $f(x)$. By derivative, we know that $f'(x) < 0$ for $x \in [2, 3]$. Therefore, $f(x)$ is strictly decreasing in the interval $[2, 3]$. Since $f(2) = 2k - 2 \geq 0$ and $f(3) = -2(n - k - 1) \leq 0$ for $1 \leq k \leq n - 1$, it follows that $q \in [2, 3]$. By the Vieta Theorem, we have

$$\begin{cases} q_1 + q + q_n = n + 3, \\ qq_1 + q_1q_n + qq_n = 3n, \\ qq_1q_n = 2n - 2k - 2. \end{cases} \quad (6)$$

Thus,

$$\begin{aligned} S_Q(C_n(k)) &= q_1 - q_n = \sqrt{(q_1 + q_n)^2 - 4q_1q_n} \\ &= \sqrt{-3q^2 + 2(n + 3)q + (n - 3)^2}. \end{aligned}$$

For $2 \leq q \leq 3$, it is easy to verify that $S_Q(C_n(k))$ is strictly increased with respect to q . By (6), we have

$$k = -\frac{1}{2}[q^3 - (n + 3)q^2 + 3nq - 2n + 2]. \quad (7)$$

By derivative, we know that k is a strictly increasing function on q in the interval $[2, 3]$. By the inverse function theorem, we have that q is a strictly increasing function on k in the interval $[1, n - 1]$. This means that $S_Q(C_n(k))$ is a strictly increasing function on k in $[1, n - 1]$. Thus, if n is odd, then

$$S_Q(C_n(2)) < S_Q(C_n(4)) < \cdots < S_Q(C_n(n - 1));$$

if n is even, then

$$S_Q(C_n(1)) < S_Q(C_n(3)) < \cdots < S_Q(C_n(n - 1)).$$

In order to prove that

$$S_Q(C_n(k)) = \sqrt{-3q^2 + 2(n + 3)q + (n - 3)^2} \geq n - \frac{1}{2}$$

for $2 \leq q \leq 3$, it is sufficient to show that

$$q \geq \frac{2n + 6 - \sqrt{4n^2 - 36n + 141}}{6}.$$

Using (7), it is sufficient to show that

$$k \geq \frac{16n^3 - 72n^2 + 216n - (8n^2 - 33)\sqrt{4n^2 - 36n + 141}}{432} = g(n).$$

Since k_0 is the smallest integer such that $k_0 \geq g(n)$ and $n - k_0$ is odd, it follows that

$$S_Q(C_n(k_0 - 2)) < n - \frac{1}{2} \leq S_Q(C_n(k_0)) < S_Q(C_n(k_0 + 2)) < \dots < S_Q(C_n(n - 1)).$$

Combining the above arguments, we have

$$S_Q(G) < n - \frac{1}{2} \leq S_Q(C_n(k_0)) < S_Q(C_n(k_0 + 2)) < \dots < S_Q(C_n(n - 1))$$

for $G \in \mathcal{C}_n \setminus \{C_n(k_0), C_n(k_0 + 2), \dots, C_n(n - 1)\}$. This completes the proof. \square

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