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EXTREMAL GRAPHS FOR THE SUM OF THE TWO LARGEST SIGNLESS LAPLACIAN EIGENVALUES*

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Abstract. Let G be a simple graph on n vertices and $e(G)$ edges. Consider the signless Laplacian, $Q(G) = D + A$, where A is the adjacency matrix and D is the diagonal matrix of the vertices degree of G. Let $q_1(G)$ and $q_2(G)$ be the first and the second largest eigenvalues of $Q(G)$, respectively, and denote by S_n^+ the star graph with an additional edge. It is proved that inequality $q_1(G) + q_2(G) \leq e(G) + 3$ is tighter for the graph S_n^+ among all firefly graphs and also tighter to S_n^+ than to the graphs $K_k \vee \overline{K}_{n-k}$ recently presented by Ashraf, Omidi and Tayfeh-Rezaie. Also, it is conjectured that S_n^+ minimizes $f(G) = e(G) - q_1(G) - q_2(G)$ among all graphs G on n vertices.

Key words. Signless Laplacian, Sum of eigenvalues, Extremal graphs.

AMS subject classifications. 05C50, 15A42.

1. Introduction. Given a simple graph G with vertex set $V(G)$ and edge set $E(G)$, let A be the adjacency matrix of G and D be the diagonal matrix of the row-sums of A, i.e., the degrees of G. The maximum degree of G is denoted by $\Delta = \Delta(G)$. Let $e(G) = |E(G)|$ be the number of edges and let $n = |V(G)|$ be the number of vertices of G. The matrix $Q(G) = A + D$ is called the *signless Laplacian* or the Q-matrix of G. As usual, we shall index the eigenvalues of $Q(G)$ in non-increasing order and denote them as $q_1(G), q_2(G), \ldots, q_n(G)$. Denote the graph obtained from the star on n vertices by inserting an additional edge by S_n^+; the complement of G by $\overline{G}$ and the complete graph on n vertices by K_n. If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are graphs on disjoint sets of vertices, their graph sum is $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. The join $G_1 \vee G_2$ of G_1 and G_2 is the graph obtained from $G_1 + G_2$ by inserting

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new edges from each vertex in G_1 to every vertex of G_2. Consider $M(G)$ as a matrix of a graph G of order n and let k be a natural number such that $1 \leq k \leq n$. A general question related to G and $M(G)$ can be raised: *"How large can the sum of the k largest eigenvalues of $M(G)$ be ?"* Usually, solving cases $k = 1, n-1$ and n are simple but the general case for any k is not easy to be solved. The natural next case to be studied is $k = 2$ and some work has been recently done in order to prove this case. For instance, Ebrahimi et al., [6], for the adjacency matrix; Haemers et al., [7], for the Laplacian matrix and Ashraf et al., [2], for the signless Laplacian matrix. In particular, the latter denoted the sum of the two largest signless Laplacian by $S_2(G)$ and proved that

$$S_2(G) \leq e(G) + 3 \tag{1.1}$$

for any graph G. Additionally, if G is isomorphic to $K_k \vee \overline{K}_t$ they show that $e(G) + 3 - S_2(G) < 1/\sqrt{t}$. Consequently, inequality (1.1) is asymptotically tight.

Given a graph G with $e(G)$ edges, define the function

$$f(G) = e(G) + 3 - S_2(G).$$

Since inequality (1.1) is asymptotically tight for the graphs $K_k \vee \overline{K}_t$, it means that $f(K_k \vee \overline{K}_t)$ converges to zero when n goes to infinity. In this paper, we prove the following facts:

(A) the function $f(S_n^+)$ converges to zero when n goes to infinity and the graph S_n^+ is the graph within the firefly graphs such that inequality (1.1) is asymptotically tight within the firefly graphs;
(B) the function $f(S_n^+)$ converges to zero faster than $f(K_k \vee \overline{K}_t)$ does.

Additionally, based on computational experiments from AutoGraphiX [3], we conjecture that S_n^+ minimizes $f(G)$ among all graphs G on n vertices.

2. Preliminaries. In this section, we present some known results about $q_1(G)$ and $q_2(G)$ and define some classes of graphs that will be useful to our purposes.

Definition 2.1. A firefly graph $F_{r,s,t}$ is a graph on $2r + s + 2t + 1$ vertices that consists of r triangles, s pendant edges and t pendant paths of length 2, all of them sharing a common vertex.

Let v be a vertex of G and let P_{q+1} and P_{r+1} be two paths, say, $v_{q+1}v_q \cdots v_2v_1$ and $u_{r+1}u_r \cdots u_2u_1$. The graph $G_{q,r}$ is obtained by identifying v_{q+1} and u_{r+1} at the same vertex v of G. The graph $G_{q+1,r-1}$ can be obtained from $G_{q,r}$ by removing the edge (u_1, u_2) and placing the edge (v_1, u_1).

The Figure 2.1 displays the firefly graphs and Figure 2.2 illustrates the grafting operation.

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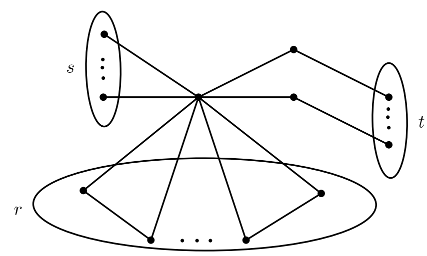

FIG. 2.1. *Firefly graph $F_{r,s,t}$ with r triangles, s pendant vertices and t pendant paths of length 2.*

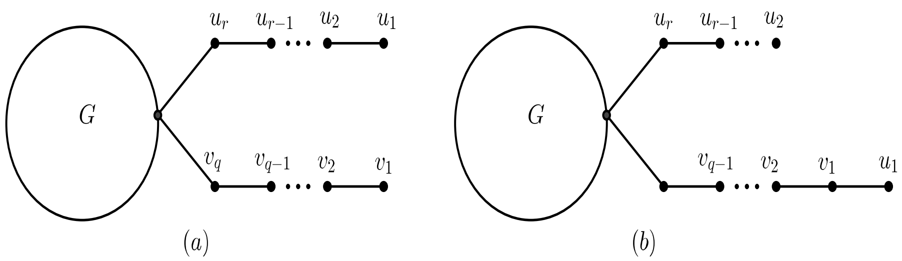

FIG. 2.2. *(a) $G_{q,r}$ (b) $G_{q+1,r-1}$ obtained by grafting an edge of $G_{q,r}$.*

If G is connected with $e(G) = n + c - 1$, then G is called a $c-$cyclic graph.

LEMMA 2.2. [8] *Suppose $c \geq 1$ and G is a $c-$cyclic graph on n vertices with $\Delta \leq n - 3$. If $n \geq 2c + 5$, then $q_1(G) \leq n - 1$.*

LEMMA 2.3. [1] *Let G be a connected graph on $n \geq 7$ vertices. Then*

(i) $3 - \frac{2.5}{n} < q_2(G) < 3$ *if and only if G is a firefly with one triangle.*
(ii) $q_2(G) = 3$ *if and only if G is a firefly and has at least two triangles.*

LEMMA 2.4. [5] *Let G be a connected graph on $n \geq 2$ vertices. For $q \geq r \geq 1$, consider the graphs $G_{q,r}$ and $G_{q+1,r-1}$. Then,*

$$q_1(G_{q,r}) > q_1(G_{q+1,r-1}).$$

3. Main results. In this section, we present the proofs of facts (A) and (B) presented in the introduction. In order to prove fact (A), we firstly present Lemma 3.1. From this point on, we will use $F_{1,n-3,0}$ to denote the graph S_n^+ since they are

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isomorphic and e_i to denote the i-th standard unit basis vector for each $i = 1, \dots, n$.

LEMMA 3.1. *Let G be isomorphic to $F_{1,n-3,0}$ with $n \geq 7$. Then*

$$e(G) + 3 - \frac{2.5}{n} < S_2(G) < e(G) + 3.$$

Proof. The matrix $Q(G)$ can be written as

$$Q(G) = \left[\begin{array}{c|c|c} I+J & \mathbf{1} & \mathbf{0} \\ \hline 1 & n-1 & 1 \\ \hline & & \\ \mathbf{0}^T & \mathbf{1}^T & I \end{array}\right],$$

where the diagonal blocks are of orders 2, 1 and $n-3$, respectively. We find that $e_1 - e_2$ and $e_4 - e_j$, $5 \leq j \leq n$ are eigenvectors for $Q(G)$ corresponding to the eigenvalue 1. Consequently, we see that $Q(G)$ has 1 as an eigenvalue of multiplicity at least $n-3$. Further, since $Q(G)$ has an orthogonal basis of eigenvectors, there are remaining eigenvectors of $Q(G)$ of the form $\left[\begin{array}{c} \alpha\mathbf{1} \\ \hline \beta \\ \hline \gamma\mathbf{1} \end{array}\right]$. We then deduce that the eigenvalues of the 3×3 matrix $M = \begin{bmatrix} 3 & 1 & 0 \\ 2 & n-1 & n-3 \\ 0 & 1 & 1 \end{bmatrix}$ comprise the remaining three eigenvalues of $Q(G)$ that are the roots of the polynomial $\Psi(x) = x^3 - (n+3)x^2 + 3nx - 4$. As Ψ is a continuous function in $\mathbb{R}$ and $\Psi(0) = -4 < 0$, $\Psi(1) = 2n - 6 > 0$, from [1], $\Psi(3 - \frac{2.5}{n}) > 0$, $\Psi(3 - \frac{1}{n}) = -1 - \frac{1}{n^3} + \frac{6}{n^2} - \frac{10}{n} < 0$, $\Psi(n) = -4 < 0$, and for $n \geq 7$, $\Psi(n+\frac{1}{n}) = -7 + \frac{1}{n^3} - \frac{3}{n^2} + \frac{2}{n} + n > 0$, so $3 - \frac{2.5}{n} < q_2(G) < 3 - \frac{1}{n}$ and $n < q_1(G) < n + \frac{1}{n}$ for $n \geq 7$. Thus, $e(G) + 3 - \frac{2.5}{n} < S_2(G) < e(G) + 3$. □

From Lemma 3.1, one can easily see that function $f(F_{1,n-3,0})$ converges to zero when n goes to infinity. To complete the proof of the statement (A) we need to show that $F_{1,n-3,0}$ is the only firefly graph such that inequality (1.1) is asymptotically tight. The proof follows from Lemmas 3.2, 3.3 and 3.5.

LEMMA 3.2. *Let G be isomorphic to $F_{1,n-5,1}$ with $n \geq 9$. Then*

$$e(G) + 2 - \frac{0.8}{\ln n} < S_2(G) < e(G) + 2.$$

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Proof. The matrix $Q(G)$ can be written as

$$Q(G) = \begin{bmatrix} 2 & 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & n-2 & 1 & 0 & 1 & \dots & 1 \\ 0 & 0 & 1 & 2 & 1 & 0 & \dots & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots & \\ 0 & 0 & 1 & 0 & 0 & & \dots & 1 \end{bmatrix}.$$

We find that $e_6 - e_j$, $7 \leq j \leq n$ and $e_1 - e_2$ are eigenvectors for $Q(G)$ corresponding to eigenvalue 1. Consequently, we see that $Q(G)$ has 1 as an eigenvalue of multiplicity at least $n-5$. Further, since $Q(G)$ has an orthogonal basis of eigenvectors, it follows that there are remaining eigenvectors of $Q(G)$ of the form

$$\begin{bmatrix} \alpha\mathbf{1} \\ \hline \beta \\ \hline \gamma \\ \hline \xi \\ \hline \varpi\mathbf{1} \end{bmatrix}.$$

We deduce that the eigenvalues of 5×5 matrix

$$M = \begin{bmatrix} 3 & 1 & 0 & 0 & 0 \\ 2 & n-2 & 1 & 0 & n-5 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

comprise the remaining five eigenvalues of $Q(G)$ that are the roots of the polynomial $\Psi(x) = x^5 - (n+5)x^4 + (6n+4)x^3 - (10n-2)x^2 + (3n+12)x - 4$. As Ψ is a continuous function in $\mathbb{R}$, there are three roots of $\Psi(x)$ in the intervals $[0, 0.3]$, $[0.3, 1]$ and $[1, 2.7]$. For the other two, as

$$\begin{aligned} \Psi\left(3 - \frac{0.8}{\ln n}\right) &= -4 + (12+3n)\left(3 - \frac{0.8}{\ln n}\right) - (-2+10n)\left(3 - \frac{0.8}{\ln n}\right)^2 \\ &\quad + (4+6n)\left(3 - \frac{0.8}{\ln n}\right)^3 - (5+n)\left(3 - \frac{0.8}{\ln n}\right)^4 + \left(3 - \frac{0.8}{\ln n}\right)^5 \\ &> 0, \end{aligned}$$

$$\begin{aligned} \Psi\left(3 - \frac{5}{4n}\right) &= -\frac{1}{1024n^5}\left(3125 - 25000n + 70500n^2 - 72800n^3 + 12160n^4 + 256n^5\right) \\ &< 0, \end{aligned}$$

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$$\Psi(n-1) = -24 + 25n - 5n^2 < 0$$

and

$$\begin{aligned}\Psi(n-1+\frac{5}{4n}) &= \frac{1}{1024n^5}\big(3125 - 25000n + 78000n^2 - 140000n^3 + 178400n^4 \\ &\quad -142976n^5 + 75520n^6 - 17920n^7 + 1280n^8\big) \\ &> 0.\end{aligned}$$

So, $3 - \frac{0.8}{\ln n} < q_2(G) < 3 - \frac{5}{4n}$ and $n-1 < q_1(G) < n-1+\frac{5}{4n}$. Then,

$$e(G) + 2 - \frac{0.8}{\ln n} < S_2(G) < e(G) + 2. \quad \square$$

From Lemma 3.2, one can easily see that function $f(F_{1,n-5,1})$ converges to 1 when n goes to infinity.

Lemma 3.3. *Let G be isomorphic to $F_{1,s,t}$ a firefly graph such that $s \geq 1$ and $t \geq 2$. Then $S_2(G) < e(G) + 2$.*

Proof. From Lemma 2.2, we have $q_1(G) \leq s + 2t + 2$ and from Lemma 2.3, $q_2(G) < 3$. So, $S_2(G) < s + 2t + 5 = e(G) + 2$. $\square$

From Lemma 3.3, follows that function $f(F_{1,s,t}) > 1$ when $s \geq 1$ and $t \geq 2$.

Lemma 3.4. *For $2r + s + 1 \geq 6$ and $r \geq 2$,*

$$2r + s + 1 < q_1(F_{r,s,0}) < 2r + s + \frac{3}{2}.$$

Proof. The signless Laplacian matrix of the graph $F_{r,s,0}$ can be written as

$$Q(F_{r,s,0}) = \left[\begin{array}{c|c|c} 2r+s & 1 & 1 \\ \hline \mathbf{1}^T & \mathbf{I} & \mathbf{0} \\ \hline \mathbf{1}^T & \mathbf{0} & \mathbf{B} \end{array}\right],$$

where the diagonal blocks are of orders 1, s and $2r$, respectively, and B is a diagonal block matrix and each block has order 2 of the type $I + J$. We find that for each $j = 3, \ldots, s+1, e_2 - e_j$ is an eigenvector for $Q(F_{r,s,0})$ corresponding to eigenvalue 1; also, for each $k = 1, \ldots, r, e_{s+2k} - e_{s+2k+1}$ is an eigenvector for $Q(F_{r,s,0})$ corresponding to eigenvalue 1. So, 1 is an eigenvalue with multiplicity at least $r+s-1$. Further, since $Q(F_{r,s,0})$ has an orthogonal basis of eigenvectors, it follows that there are remaining eigenvectors of $Q(F_{r,s,0})$ of the form

$$\left[\begin{array}{c} \gamma \\ \hline \alpha\mathbf{1} \\ \hline \beta\mathbf{1} \end{array}\right].$$

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We then deduce that the eigenvalues of the 3×3 matrix

$$M = \begin{bmatrix} 2r+s & s & 2r \\ 1 & 1 & 0 \\ 1 & 0 & 3 \end{bmatrix}$$

comprise the remaining three eigenvalues of $Q(F_{r,s,0})$. The eigenvalues of M are the roots of the characteristic polynomial of M given by $g(x) = -(x^3 + (-s-2r-4)x^2 + (3s+6r+3)x - 4r)$. See that $g(2r+s+1) > 0$ and $g(2r+s+3/2) < 0$. Since $q_2(G) \leq n-2 = 2r+s-1$ and $q_1(G) \geq q_2(G)$, we get

$$2r+s+1 < q_1(G) < 2r+s+\frac{3}{2}. \quad \square$$

Lemma 3.5. *Let $G = F_{r,s,t}$ such that $r \geq 2$, $t, s \geq 1$. Then $S_2(G) \leq e(G) + 2.5$.*

Proof. For firefly graphs $F_{r,s,t}$ such that $t \geq 1$, we can obtain any $F_{r,s,t}$ from grafting edges of the graph $F_{r,s,0}$. From Lemma 2.4 and Lemma 3.4 $q_1(F_{r,s,t}) < q_1(F_{r,s+2t,0}) < 2r+s+2t+\frac{3}{2}$. Also, by Lemma 2.3, $q_2(F_{r,s,t}) = 3$ and we get $q_1(F_{r,s,t}) + q_2(F_{r,s,t}) < 2r+s+2t+4.5$. Observe that $e(F_{r,s+2t,0}) = 3r+s+2t$ and then $2r+s+2t+4.5 = e(F_{r,s+2t,0}) + 2.5 + (2-r) \leq e(F_{r,s+2t,0}) + 2.5$ for $r \geq 2$. So, $S_2(G) \leq e(G) + 2.5$. $\square$

From Lemma 3.5, follows that function $f(F_{r,s,t}) \geq 0.5$ when $r \geq 2$. The next proposition proves the statement (B) of the introduction.

Proposition 3.6. *For $n \geq 9$ and $k \geq 2$, the function $f(F_{1,n-3,0})$ converges to zero faster than $f(K_k \vee \overline{K}_{n-k})$.*

Proof. From Lemma 3.1, we have $0 < f(F_{1,n-3,0}) < \frac{2.5}{n}$ and from Remark 8 of [2], $0 < f(K_k \vee \overline{K}_{n-k}) < \frac{1}{\sqrt{n-k}}$. Noting that $\frac{2.5}{n} < \frac{1}{\sqrt{n-k}}$ for $k \geq 2$ completes the proof. $\square$

Therefore, we proved that inequality (1.1) is asymptotically tight for the graph $F_{1,n-3,0}$ within the firefly graphs on $n \geq 9$ vertices. Based on computational experiments with AutoGraphiX, we propose the following conjecture.

Conjecture 3.7. Let G be a graph on $n \geq 9$ vertices. Then

$$f(G) \geq f(F_{1,n-3,0}).$$

Equality holds if and only if G is isomorphic to $F_{1,n-3,0}$.

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REFERENCES

[1] M. Aouchiche, P. Hansen, and C. Lucas. On the extremal values of the second largest Q-eigenvalue. *Linear Algebra Appl.*, 435:2591–2606, 2011.

[2] F. Ashraf, G.R. Omidi, and B. Tayfeh-Rezaie. On the sum of signless Laplacian eigenvalues of a graph. *Linear Algebra Appl.*, 438:4539–4546, 2013.

[3] G. Caporossi and P. Hansen. Variable neighborhood search for extremal graphs: the AutographiX system. *Discrete Math.*, 212:29–34, 2000.

[4] D. Cvetković. Spectral theory of graphs based on the signless Laplacian. Research report, 2010. Available at `http://www.mi.sanu.ac.rs/projects/signless_L_reportApr11.pdf`.

[5] D. Cvetković, P Rowlinson, and S.K. Simić. Eigenvalue bounds for the signless Laplacian. *Publ. Inst. Math. (Beograd)*, 81:11–27, 2007.

[6] J. Ebrahimi, B. Mohar, V. Nikiforov, and A.S. Ahmady. On the sum of two largest eigenvalues of a symmetric matrix. *Linear Algebra Appl.*, 429:2871–2787, 2008.

[7] W.H. Haemers, A. Mohammadian, and B. Tayfeh-Rezaie. On the sum of Laplacian eigenvalues of graphs. *Linear Algebra Appl.*, 432:2214–2221, 2010.

[8] M.H. Liu. Some results on the signless Laplacian spectra of unicyclic graphs. *International Scholarly Research Network Algebra*, 1–10, 2011.