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Sum of the k Largest Signless Laplacian Eigenvalues

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Abstract. Let G be a simple graph with n vertices, and $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0$ be the signless Laplacian eigenvalues of G. Let $S_k^+(G) = \sum_{i=1}^{k} q_i(G)$, where $1 \leq k \leq n$. In this work, we present upper bounds for $S_k^+(G)$ for $K_{2,s+1}$-free graphs, for even cycle-free graphs and for odd cycle-free graphs.

Keywords. Eigenvalue sum, Upper bound, Signless Laplacian matrix.

1 Introduction

Let $G = (V(G), E(G))$ be a *simple graph*, where $V(G) = \{v_1, v_2, ..., v_n\}$ is the *vertex set* and $E(G)$ is the *edge set*. Denote the set of *neighbors* of v_i by $N_G(v_i)$ and the *degree* of v_i by $d_i = |N_G(v_i)|$. The non-increasing sequence $d_1 \geq d_2 \geq \cdots \geq d_n$ is called *degree sequence* of G.

The *signless Laplacian matrix* of G is defined as $Q(G) = D(G) + A(G)$, where $A(G) = [a_{ij}]$ is the *adjacency matrix* and $D(G) = [d_{ij}]$ is the diagonal matrix with the degree sequence in its main diagonal.

It is well known that $A(G)$ and $Q(G)$ are symmetric and positive semidefinite matrices, then we can denote the eigenvalues of $A(G)$ and $Q(G)$, called respectively the *adjacency eigenvalues* and the *signless Laplacian eigenvalues* of G, by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ and $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0$. The largest eigenvalue of $Q(G)$ is called the *Q-index*.

Consider $M(G)$ a matrix representation of a graph G of order n and let k be a natural number such that $1 \leq k \leq n$. *"How large can the sum of the k largest eigenvalues of $M(G)$ be?"* is a natural question related to G and $M(G)$. In this work we investigate bounds for the sum

$$S_k^+(G) = q_1(G) + q_2(G) + \cdots + q_k(G).$$

Ebrahimi et al. [3] studied bounds for the sum of the two largest adjacency eigenvalues. For general $k \geq 2$, the sum $\Lambda_k(G) = \lambda_1(G) + \lambda_2(G) + \cdots \lambda_k(G)$ has been investigated by Mohar [5], where it was shown that for a simple graph G of order n we have

$$\frac{1}{2}\left(\sqrt{k} + \frac{1}{2}\right) - o(k^{-2/5}) \leq \Lambda_k(G) \leq \frac{1}{2}(1 + \sqrt{k}).$$

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This value is of interest in theoretical chemistry due to, roughly speaking, the sum of the largest adjacency eigenvalues, which correspond to orbitals with lowest energy levels, determine the total energy of the electrons [5].

Motivated by studies of Mohar, Jin et al. [4] investigated the sum of the k largest signless Laplacian eigenvalues and showed that for a graph G of order n we have

$$S_k^+(G) \leq n + \sqrt{k\left(n^2 + \sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right)}, \text{ for } k > 1 + \frac{1}{n^2}\left(\sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right)$$

and

$$S_k^+(G) \leq 2n + \sqrt{(k-1)\left(\sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right)}, \text{ for } k \leq 1 + \frac{1}{n^2}\left(\sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right).$$

In this work, we generalize the result presented by Jin for graphs that have a specific bound for the largest signless Laplacian eigenvalue. In particular, as our main contribution, we present upper bounds for $S_k^+(G)$ for $K_{2,s+1}$-free graphs, for even cycle-free graphs and for odd cycle-free graphs.

This paper is organized as follows. In Section 2, we show known results of real symmetric matrices and eigenvalues inequalities. In Section 3, we present a generalization of Jin's argument. In Section 4, we give upper bounds for the sum of the k largest signless Laplacian eigenvalues for different families of graphs. Finally, in section 5 we discuss and compare the results achieved.

2 Preliminaries

In this section, we show some definitions and known results of real symmetric matrices which are used in the proof of Jin's result and in our generalization.

Given a real symmetric matrix $M = [m_{ij}]$, we define the quantity

$$\sigma_2(M) = \sqrt{\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} |m_{ij}|^2}.$$

Let us observe that $\sigma_2(M)$ is proportional to the usual 2-norm of the matrix M.

The following lemma provides a representation of $\sigma_2(M)$ in terms of the eigenvalues of M.

Lemma 2.1 ([5]). *If M is a real symmetric matrix with eigenvalues $\lambda_1, ..., \lambda_n$, then $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} |m_{ij}|^2 = 2\sigma_2(M)$.*

Let $v = (v_1, ..., v_n)^T$ and $V = vv^T$. Then V is a symmetric matrix of rank 1 with its only nontrivial eigenvalue $tr(V) = \|v\|^2$. Clearly, the corresponding eigenvector is v.

Given a real symmetric matrix M, we define its *v-complement* as the matrix M', defined by $M' = V - M$, where $V = vv^T$ is as above. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of M in the decreasing order, and let $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_n$ be the eigenvalues of M'.

The following lemma shows a relation between the eigenvalues of M and M'.

Lemma 2.2 ([5]). *For any real symmetric matrix M, and its v-complement M', we have*

(a) $\lambda_1 + \lambda'_1 \geq \|v\|^2$ **(b)** $\lambda_i + \lambda'_{n-i+2} \leq 0$ *for* $i = 2, 3, ...n$.

3 Generalization of the Argument

In this section, we discuss a generalization of Jin's argument which will be used to obtain upper bounds for the sum of the k largest signless Laplacian eigenvalues.

Let $a \in \mathbb{R}$ and $v = (\sqrt{a}, ..., \sqrt{a})^T$, so $V = vv^T$ is the all-a-matrix, and $\|v\|^2 = an$. For $Q(G)$ and $Q(G)'$, where $Q(G)'$ is the v-complement of $Q(G)$, we have

$$\begin{aligned}
(2\sigma_2(Q(G)))^2 \quad + \quad (2\sigma_2(Q(G)'))^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n}[q_{ij}^2 + (a - q_{ij})^2] \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n}[(d_{ij} + a_{ij})^2 + (a - d_{ij} - a_{ij})^2] \\
&= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}^2 + \sum_{i=1}^{n}(a - d_i)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n}(a - a_{ij})^2 - a^2 n \\
&= 2\sum_{i=1}^{n} d_i^2 + (2 - 4a)\sum_{i=1}^{n} d_i + a^2 n^2.
\end{aligned}$$

Let, respectively, $q_1 \geq q_2 \geq \cdots \geq q_n$ and $q'_1 \geq q'_2 \geq \cdots \geq q'_n$ be the eigenvalues of $Q(G)$ and $Q(G)'$. Follows from **Lemma 2.2(b)** that $q_i^2 \leq {q'}_{n-i+2}^2$ for $i = 2, ..., n$.

Let α_1 be an upper bound for the Q-index of a family of graphs $\mathcal{F}$, that is, if $G \in \mathcal{F}$ then $q_1 \leq \alpha_1$. From **Lemma 2.2(a)** we have $q_1 + q'_1 \geq an$. By letting $q_1 = \alpha t$, with $0 \leq t \leq \beta$, and $\alpha\beta = \alpha_1$, we derive therefrom that ${q_1}^2 + {q'_1}^2 \geq \alpha^2 t^2 + (an - \alpha t)^2$.

The above inequalities imply the following estimates

$$\begin{aligned}
2\sum_{i=1}^{n} d_i^2 + (2 - 4a)\sum_{i=1}^{n} d_i \quad + \quad a^2 n^2 &= \sum_{i=1}^{n} {q_i}^2 + \sum_{i=1}^{n} {q'_i}^2 \\
&\geq {q_1}^2 + {q'_1}^2 + \sum_{i=2}^{k} {q_i}^2 + \sum_{i=2}^{k} {q'_{n-i+2}}^2 \\
&\geq {q_1}^2 + {q'_1}^2 + 2\sum_{i=2}^{k} {q_i}^2 \geq \alpha^2 t^2 + (an - \alpha t)^2 + 2\sum_{i=2}^{k} {q_i}^2.
\end{aligned}$$

This shows that

$$\sum_{i=2}^{k} {q_i}^2 \leq \frac{2\sum_{i=1}^{n} d_i^2 + (2 - 4a)\sum_{i=1}^{n} d_i + a^2 n^2 - \alpha^2 t^2 - (an - \alpha t)^2}{2}.$$

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An application of the Cauchy-Schwartz inequality now yields

$$\sum_{i=2}^{k} q_i \leq \sqrt{(k-1)\left(\frac{2\sum_{i=1}^{n} d_i^2 + (2-4a)\sum_{i=1}^{n} d_i + a^2n^2 - \alpha^2t^2 - (an-\alpha t)^2}{2}\right)}.$$

Finally, we conclude that

$$\sum_{i=1}^{k} q_i \leq \alpha t + \sqrt{(k-1)\left(\frac{2\sum_{i=1}^{n} d_i^2 + (2-4a)\sum_{i=1}^{n} d_i + a^2n^2 - \alpha^2t^2 - (an-\alpha t)^2}{2}\right)}.$$

In order to facilitate, we rewrite the expression as

$$\frac{\sum_{i=1}^{k} q_i}{\alpha} \leq t + \sqrt{(k-1)\left[-t^2 + \left(\frac{an}{\alpha}\right)t + \frac{\sum_{i=1}^{n} d_i^2 + (1-2a)\sum_{i=1}^{n} d_i}{\alpha^2}\right]}.$$

Observe that to obtain an upper bound for the sum of the k largest signless Laplacian eigenvalues of the graph G we must determine the maximum value of the function

$$f(t) = t + \sqrt{(k-1)(-t^2 + Bt + C)}, \tag{1}$$

in the interval $(0, \beta)$, where $B = \frac{an}{\alpha}$ and $C = \frac{\sum_{i=1}^{n} d_i^2 + (1-2a)\sum_{i=1}^{n} d_i}{\alpha^2}$.

A routine calculation, similar to that presented in [4], shows that $f(t)$ has maximum value for some t. In the results presented in the next section we find this value of t for specific values of the parameters a, α_1 and β, associated with different graph families.

4 Upper Bounds for $S_k^+(G)$

Now, we present the upper bounds for $S_k^+(G)$ for different graph families.

In this section we consider that K_t is the *complete graph* of order t, and $K_{t,s}$ is the *complete bipartite graph* with vertex classes of sizes t and s. Let's use these definitios in the next results.

4.1 $K_{2,s+1}$-free Graphs

The problem *"What is the maximum $q_1(G)$ of a graph G of order n containing no $K_{t,s}$?"* has been intensively studied [2]. This question is a spectral version of the famous Zarankiewicz problem, which turned out to be one of the most difficult problems in modern Discrete Mathematics. In [2], de Freitas et al. investigated this topic and obtained the following result:

Lemma 4.1 ([2]). *Let $s \geq 1$, and let G be a graph of order n, with $d_1 = n-1$. If G is $K_{2,s+1}$-free, then*

$$q_1(G) \leq \frac{n + 2s + \sqrt{(n-2s)^2 + 8s}}{2}.$$

Equality holds if and only if $G = K_1 \vee H$, and H is an s-regular graph.

Using the upper bound given in **Lemma 4.1** for the parameter α_1, $\beta = \frac{1}{2}$ and $a = 1$ we obtain the next result. The proof is made by the calculations for the maximization of the function (1), and will be omitted due to lack of space.

Theorem 4.1. *Let $s \geq 1$, and let G be a graph of order n, with $d_1 = n-1$. If G is $K_{2,s+1}$-free, then*

$$S_k^+(G) \leq n + \sqrt{k\left(n^2 + \sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right)}, \text{ for } k > \theta$$

and

$$S_k^+(G) \leq \frac{n + 2s + \sqrt{(n-2s)^2 + 8s}}{2} + \frac{\sqrt{2(k-1)\left[n^2 + 4s(n-s-1) + (n-2s)\sqrt{(n-2s)^2+8s} + 2\sum_{i=1}^{n} {d_i}^2 - 6\sum_{i=1}^{n} d_i\right]}}{2},$$

for $k \leq \theta$, where $\theta = \dfrac{4n^2 + 4\sum_{i=1}^{n} {d_i}^2 - 12\sum_{i=1}^{n} d_i}{\left(2s - n + \sqrt{(n-2s)^2 + 8s}\right)^2}$.

4.2 Even/Odd Cycle-free Graphs

The generalized problem *"Given a graph H, what is the maximum $q_1(G)$ of a graph G of order n containing no H?"* was intensively studied for several cases. In [1], de Freitas et al. studied the case for graphs with no cycles of length 4 and 5, and two conjectures are formulated for the maximum $q_1(G)$ of even/odd cycle-free graphs.

Let $S_{n,t} = K_t \vee \overline{K_{n-t}}$, and $S_{n,t}^+$ be the graph obtained by adding an edge to $S_{n,t}$. As usual, let C_t be the cycle of size t.

Yuan [7] studied how large can $q_1(G)$ be if G is a graph of order n and contains no cycle of given odd length, and presented the following result:

Lemma 4.2 ([7]). *Let $s \geq 3$, $n \geq 110s^2$, and let G be a graph of order n. If G has no cycle of length $2s+1$, then* $q_1(G) < q_1(S_{n,s}) = \dfrac{n + 2s - 2 + \sqrt{(n-2)^2 + 4s(n-s)}}{2}$, *unless $G = S_{n,s}$.*

Using the upper bound given in **Lemma 4.2** for the parameter α_1, $\beta = \frac{1}{2}$ and $a = 2$, we obtain the next result. The proof is made by the calculations for the maximization of the function (1), and will be omitted due to lack of space.

Theorem 4.2. *Let $s \geq 3$, $n \geq 110s^2$, and let G be a graph of order n. If G has no cycle of length $2s+1$, then*

$$S_k^+(G) \leq n + \sqrt{k\left(n^2 + \sum_{i=1}^{n} {d_i}^2 - 3\sum_{i=1}^{n} d_i\right)}, \text{ for } k > \theta$$

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and

$$S_k^+(G) \leq \frac{n+2s-2+\sqrt{(n-2)^2+4s(n-s)}}{2} + \frac{\sqrt{2(k-1)\left[n^2+4s-4+(n-2s+2)\sqrt{(n-2)^2+4s(n-s)}+2\sum_{i=1}^n {d_i}^2-6\sum_{i=1}^n d_i\right]}}{2},$$

for $k \leq \theta$, *where* $\theta = \dfrac{4n^2+4\sum_{i=1}^n {d_i}^2-12\sum_{i=1}^n d_i}{\left(2s-2-n+\sqrt{(n-2)^2+4s(n-s)}\right)^2}$.

In [6], Nikiforov and Yuan studied how large can $q_1(G)$ be if G is a graph of order n and contains no cycle of given even length and presented the following result:

Lemma 4.3 ([6])**.** *Let* $s \geq 2$, $n \geq 400s^2$, *and let* G *be a graph of order* n. *If* G *has no cycle of length* $2s+2$, *then* $q_1(G) < q(S_{n,s}^+) \leq n+2s-2-\dfrac{2s(s-1)}{n+2s+2}$, *unless* $G = S_{n,s}^+$.

Using the upper bound given in **Lemma 4.3** for the parameter α_1, $\beta = 1$ and $a = 3$, we obtain the next result. The proof is made by the calculations for the maximization of the function (1), and will be omitted due to lack of space.

Theorem 4.3. *Let* $s \geq 2$, $n \geq 400s^2$, *and let* G *be a graph of order* n. *If* G *has no cycle of length* $2s+2$, *then*

$$S_k^+(G) \leq \frac{3n}{2} + \sqrt{k\left(\frac{9n^2}{4}+\sum_{i=1}^n {d_i}^2-5\sum_{i=1}^n d_i\right)}, \text{ for } k > \theta$$

and

$$S_k^+(G) \leq n+2s-2-\frac{2s(s-1)}{n+2s+2} + \sqrt{(k-1)\left[\left(n+2s-2-\frac{2s(s-1)}{n+2s+2}\right)\left(2n-2s+2+\frac{2s(s-1)}{n+2s+2}\right)+\sum_{i=1}^n {d_i}^2-5\sum_{i=1}^n d_i\right]}$$

for $k \leq \theta$, *where* $\theta = \dfrac{\left(9n^2+4\sum_{i=1}^n {d_i}^2-20\sum_{i=1}^n d_i\right)(n+2s+2)^2}{(n^2+6n-2sn-4s^2-4s+8)^2}$.

5 Conclusion

The results presented in this paper provide upper bounds for the sum of the k largest signless Laplacian eigenvalues for families of graphs that have a specific upper bound for the Q-index.

Consider the graph $G = K_{1,39999}$ and $s = 10$. Note that G is a graph that contains no cycle of length $2s+1$ or $2s+2$, and is $K_{2,s+1}$-free. The following table presents a comparison between the bounds presented in this work.

Table 1: **Bounds for** $S_k^+(K_{1,39999})$**.**

	$k = 10$	$k = 10000$	$k = 20000$	$k = 30000$	$k = 40000$
Jin's Bound	218877,61	5696606,76	8039650,00	9837530,31	11353213,52
$K_{2,11}$**-free**	209698,20	5696323,92	8039450,00	9837367,01	11353072,11
C_{21}**-free**	209716,18	5696341,63	8039467,59	9837384,51	11353089,54
C_{22}**-free**	247870,14	7270797,46	9838017,27	12549467,57	14481594,93

Note that the upper bounds obtained for $K_{2,s+1}$-free graphs, and C_{2s+1}-free graphs, are better than the Jin's bound. This is due to the use of a better bound for the Q-index.

However, the bound for C_{2s+2}-free graphs is worse for all presented case. This happens because we use the value $a = 3$ in bound construction, which is higher than that used for the other bounds, such choice was necessary due to the difficulties to realize the calculations with other values.

We emphasize that the method show in this work enables the elaboration of an upper bound of $S_k^+(G)$ for any family of graphs that have a specific bound for the largest signless Laplacian eigenvalue, making possible the development of future works.

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