On the sum of the largest $A_\alpha$-eigenvalues of graphs *

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Abstract

For every real $0 \leq \alpha \leq 1$, Nikiforov defined the $A_\alpha$-matrix of a graph $G$ as $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$, where $A(G)$ and $D(G)$ are the adjacency matrix and the degree diagonal matrix of a graph $G$, respectively. The eigenvalues of $A_\alpha(G)$ are called the $A_\alpha$-eigenvalues of $G$. Let $S_k(A_\alpha(G))$ be the sum of $k$ largest $A_\alpha$-eigenvalues of $G$. In this paper, we present several upper and lower bounds on $S_k(A_\alpha(G))$ and characterize the extremal graphs for certain cases, which can be regard as a common generalization of the sum of $k$ largest eigenvalues of adjacency matrix and signless Laplacian matrix of graphs. In addition, some graph operations on $S_k(A_\alpha(G))$ are presented.

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1 Introduction

Let $G$ be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $K_n$, $P_n$, $C_n$ and $K_{1,n-1}$ the complete graph, path, cycle and star with $n$ vertices, respectively. Let $d_v = d_G(v)$ be the degree of vertex $v$ of the graph $G$. The minimum and maximum degree of a vertex in $G$ are denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. For a graph $G$, the first Zagreb index $Z_1 = Z_1(G)$ is defined as the sum of the squares of the vertices degrees. There is a wealth of literature relating to the first Zagreb index, see for example [5, 16] and the references therein.

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Let $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ be the eigenvalues of the real symmetric matrix $M$. Let $S_k(M)$ be the sum of $k$ largest eigenvalues of $M$. The investigation on the sum of $k$ largest eigenvalues of a real symmetric matrix is a topic of interest in matrix theory. The following classical theorem is due to Fan [15].

**Theorem 1.1 ([15])** Let $M$ and $N$ be two real symmetric matrices of order $n$. Then

$$
\sum_{i=1}^{k} \lambda_i(M + N) \leq \sum_{i=1}^{k} \lambda_i(M) + \sum_{i=1}^{k} \lambda_i(N)
$$

for any $1 \leq k \leq n$.

Rojo et al. [41] obtained some upper bounds for the sum of the $k$ largest eigenvalues of the matrix $M$ in terms of the trace of $M$. Mohar [33] showed that $S_k(M)$ is at most $\frac{1}{2} (\sqrt{k} + 1)n$ when the entries of $M$ are between 0 and 1. Meanwhile, he gave an upper bound on the sum of the $k$ largest eigenvalues of arbitrary symmetric matrices. Nikiforov [35] obtained strengthen the upper bound and extend it to arbitrary $(0, 1)$-matrices.

Let $A(G)$ be the adjacency matrix of a graph $G$. For a graph $G$, Mohar [33] showed that $S_k(A(G))$ is at most $\frac{1}{2} (\sqrt{k} + 1)n$. This bound is shown to be best possible in the sense that for every $k$ there exist graphs whose sum is $\frac{1}{2} (\sqrt{k} + \frac{1}{2})n - o(k^{-2/5})n$.

Das et al. [13] proved an upper bound on $S_k(A(G))$ in terms of vertex number and negative inertia index. Moreover, Gernert [17] showed that $S_2(A(G)) \leq n$ if $G$ is a regular graph with $n$ vertices. He conjectured that this inequality holds for all graphs.

Gernert’s conjecture was disproved by Nikiforov [36], who gave examples of graphs with $S_2(A(G)) \geq 2n + \sqrt{52n} - 25 > 1.122n - 25$ and proved that $S_2(A(G)) \leq 2\sqrt{\frac{n}{3}} < 1.155n$.

Ebrahimi et al. [14] showed that $S_2(A(G)) \leq (\frac{1}{2} + \sqrt{\frac{5}{12}})n < 1.145n$.

Let $Q(G)$ be the signless Laplacian matrix of a graph $G$. Ashraf et al. [3] proposed the following conjecture on $S_k(Q(G))$.

**Conjecture 1.2 ([3])** Let $G$ be a graph with $n$ vertices and $e(G)$ edges. Then

$$
S_k(Q(G)) \leq e(G) + \binom{k + 1}{2}
$$

for $1 \leq k \leq n$. 

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This conjecture has been proved to be correct for all graphs with at most ten vertices [24], all graphs with $k = 1, 2, n - 2, n - 1, n$ [31, 7], regular graphs [3], trees [22], unicyclic graphs [42], bicyclic graphs [42], tricyclic graphs when $k \neq 3$ [42] and so on. Later, Amaro et al. [2] presented a strongly conjecture as follows.

**Conjecture 1.3** ([2]) Let $G$ be a graph with $n \geq 5$ vertices and $3 \leq k \leq n - 2$ edges. Then

$$S_k(Q(G)) \leq S_k(Q(H_{n,k})) < e(G) + \left(\frac{k + 1}{2}\right)$$

with equality if and only if $G = H_{n,k}$, where $H_{n,k}$ is the $P_3$-join graph isomorphic to $P_3[(n - k - 1)K_1, K_{k-1}, K_2]$ for $3 \leq k \leq n - 2$.

Moreover, Oliveira et al. [10] showed that the inequality $S_2(Q(G)) \leq e(G) + 3$ is tighter for the graph $K^+_{1,n-1}$ among all firefly graphs, where $K^+_{1,n-1}$ is the star graph with an additional edge. Meanwhile, they conjectured that $K^+_{1,n-1}$ minimizes $f(G) = e(G) - S_2(Q(G))$ among all graphs $G$ with $n$ vertices. Recently, Du [12] proved that $S_2(Q(G)) < e(G) + 3 - \frac{2}{n}$ when $G$ is a tree, or a unicyclic graph whose unique cycle is not a triangle. This implies that the conjecture of Oliveira et al. is true for trees and unicyclic graphs whose unique cycle is not a triangle. Oliveira and Lima [39] showed that $S_2(Q(G)) \geq d_1 + d_2 + 1$ with equality if and only if $G$ is the star $K_{1,n-1}$ or the complete graph $K_3$, where $d_i$ is the $i$-largest degree of a vertex of $G$.

Another motivation to study $S_k(A(G))$ and $S_k(Q(G))$ came from the energy $\varepsilon(A(G))$ and signless Laplacian energy $\varepsilon(Q(G))$ of a graph $G$, which is very popular in mathematical chemistry. Let $G$ be a graph with $n$ vertices and $m$ edges. Then

$$\varepsilon(A(G)) = \sum_{k=1}^{n} |\lambda_k(A(G))| = 2S_{\sigma}(A(G)) = \max_{1 \leq k \leq n} \{2S_k(A(G))\}$$

and

$$\varepsilon(Q(G)) = \sum_{k=1}^{n} \left|\lambda_k(Q(G)) - \frac{2m}{n}\right| = 2S_{\sigma}(Q(G)) - \frac{4\sigma m}{n} = \max_{1 \leq k \leq n} \left\{2S_k(Q(G)) - \frac{4km}{n}\right\},$$

where $\sigma$ denotes the number of the eigenvalues of $M$ greater than or equal to $tr(M)/n$. Thus $S_k(A(G))$ and $S_k(Q(G))$ are close relation with the energy and signless Laplacian energy, respectively. For more details in this field, we refer the reader to [1, 13, 18, 29].
In addition, $S_k(A(G))$ is related to Ky Fan norms of graphs introduced by Nikiforov [35], which is a fundamental matrix parameter anyway.

For any real $\alpha \in [0, 1]$, Nikiforov [34] defined the matrix $A_\alpha(G)$ as

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G),$$

where $D(G)$ is the diagonal matrix of its vertex degrees and $A(G)$ is the adjacency matrix. It is easy to see that $A_0(G) = A(G)$ and $2A_{1/2}(G) = Q(G)$. The new matrix $A_\alpha(G)$ not only can underpin a unified theory of $A(G)$ and $Q(G)$, but it also brings many new interesting problems, see for example [24, 27, 28, 34, 38]. This matrix has recently attracted the attention of many researchers, and there are several research papers published continually, see for example [8, 9, 19, 21, 23-28, 30-32, 34, 37, 38] and the references therein.

Motivated by the above works, we study the sum of $k$ largest eigenvalues of $A_\alpha(G)$. Since $S_k(A_0(G)) = S_k(A(G))$ and $2S_k(A_{1/2}(G)) = S_k(Q(G))$, $S_k(A_\alpha(G))$ can be regard as a common generalization of $S_k(A(G))$ and $S_k(Q(G))$. Moreover, if $G$ is a graph with $n$ vertices and $m$ edges, then

$$\varepsilon_\alpha(G) = \sum_{k=1}^{n} \left| \lambda_k(A_\alpha(G)) - \frac{2\alpha m}{n} \right| = 2S_\sigma(A_\alpha(G)) - \frac{4\alpha \sigma m}{n} = \max_{1 \leq k \leq n} \left\{ 2S_k(A_\alpha(G)) - \frac{4\alpha km}{n} \right\},$$

where $\varepsilon_\alpha(G)$ is the $\alpha$-energy of $G$ defined by Guo and Zhou [19]. Thus $S_k(A_\alpha(G))$ is close relation with the $\alpha$-energy of $G$. In this paper, we obtain some upper and lower bounds on the sum of $k$ largest eigenvalues of $A_\alpha(G)$, which extend the results of $S_k(A(G))$ and $S_k(Q(G))$. In particular, the following problems and conjecture are proposed, repectively.

**Problem 1.4** For a given $k$, which graph(s) minimize (or maximize) the sum of $k$ largest eigenvalues of $A_\alpha(G)$ among all graphs with $n$ vertices?

**Conjecture 1.5** Let $G$ be a graph with $n$ vertices and $e(G)$ edges. If $\frac{1}{2} \leq \alpha < 1$, then

$$S_k(A_\alpha(G)) \leq \alpha e(G) + \alpha \left( k + 1 \right) \binom{k + 1}{2}$$

for $1 \leq k \leq n$.

**Problem 1.6** Which graph(s) minimize $f(G) = \alpha e(G) + \alpha + 1 - S_2(A_\alpha(G))$ for $\frac{1}{2} \leq \alpha < 1$?
The remainder of this paper is organized as follows. In Section 2, we recall some useful notions and lemmas used further. In Section 3, some upper bounds on $S_k(A_\alpha(G))$ are obtained. In Section 4, some upper bounds on the sum of the $k$ largest $A_\alpha(G)$-eigenvalues of a tree are presented. In Section 5, some lower bounds on $S_k(A_\alpha(G))$ are given. Moreover, we prove that path is the minimum $S_2(A_\alpha(G))$ among all connected graphs for $\frac{1}{2} \leq \alpha < 1$, which is concerned with Problem 1.4. In Section 6, some graph operations on $S_k(A_\alpha(G))$ are presented.

2 Preliminaries

Let $\overline{G}$ be the complement of a graph $G$. The line graph $L(G)$ is the graph whose vertex set are the edges in $G$, where two vertices are adjacent if the corresponding edges in $G$ have a common vertex. The $k$-th power $G^k$ of a graph $G$ is a graph with the same set of vertices as $G$ such that two vertices are adjacent in $G^k$ if and only if their distance in $G$ is at most $k$. The double graph $D(G)$ of $G$ is a graph obtained by taking two copies of $G$ and joining each vertex in one copy with the neighbors of corresponding vertex in another copy. A clique of a graph $G$ is the maximal complete subgraph of the graph $G$. The independence number of $G$ is the maximum size of a subset of vertices of $G$ that contains no edge. A matching $\mathcal{M}$ of $G$ is a subset of $E(G)$ such that no two edges in $\mathcal{M}$ share a common vertex. The matching number of $G$ is the maximum number of edges of a matching in $G$. The chromatic number of a graph $G$ is the minimum number of colors such that $G$ can be colored in a way such that no two adjacent vertices have the same color. The nullity of a graph is the multiplicity of the eigenvalue zero in its spectrum. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of $G$. The second smallest eigenvalue of the Laplacian of a graph $G$, best-known as the algebraic connectivity of $G$, denoted by $a(G)$.

Lemma 2.1 ([33]) If $a$, $b$ are real numbers, where $a < b$, and $n$ is an integer, let $S_{a,b}^n$ be the set of all symmetric matrices whose entries are between $a$ and $b$. Then for every integer $k$, $2 \leq k \leq n$, and every $M \in S_{a,b}^n$, we have

$$S_k(M) \leq \frac{(b - a)n}{2} (1 + \sqrt{k}) + \max\{0, a\}.$$ 

Lemma 2.2 ([41]) Let $M$ be an $n \times n$ matrix with nonnegative eigenvalues. Let $1 \leq k \leq \sqrt{n}$
$n - 1$. Then

$$S_k(M) \leq \frac{k(tr(M))}{n} + \sqrt{\frac{k(n-k)}{n} f(M)},$$

where

$$f(M) = \sum_{i=1}^{n} \sum_{k=1}^{n} m_{ik} m_{ki} - \frac{(tr(M))^2}{n}.$$

Lemma 2.3 ([5, 16]) Let $G$ be a graph with $n$ vertices and $m$ edges. Then

$$\frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2 \leq Z_1(G) \leq \frac{4m^2}{n} + \frac{n}{4}(\Delta - \delta)^2.$$

Lemma 2.4 ([34]) Let $G$ be a graph with $n$ vertices. Then

$$\sqrt{\frac{Z_1}{n}} \leq \lambda_1(A_\alpha(G)) \leq \Delta.$$

Lemma 2.5 ([8]) Let $G$ be a graph of with $n$ vertices and $\Delta(G) < n - 1$. If $\frac{1}{2} < \alpha < 1$, then

$$\lambda_2(A_\alpha(G)) \leq \alpha(n - 2)$$

If the equality holds, then the complement of $G$ has at least one component isomorphic to $K_2$.

Lemma 2.6 ([22]) Let $T$ be a tree with $n$ vertices. Then $S_k(L(T)) \leq n + 2k - 2$ for $1 \leq k \leq n$.

Lemma 2.7 ([4]) Let $M$ be an $n \times n$ Hermitian matrix. Then for $1 \leq k \leq n$,

$$\sum_{i=1}^{k} \lambda_i(M) = \max \sum_{i=1}^{k} \langle MX_i, X_i \rangle,$$

where the maximum is taken over all orthonormal $k$-tuples of vectors $\{X_1, \ldots, X_k\}$ in $\mathbb{C}^n$.

Lemma 2.8 ([32]) Let $G$ be a graph with $n$ vertices. If $e \in E(G)$ and $\alpha \geq \frac{1}{2}$, then

$$\lambda_i(A_\alpha(G)) \geq \lambda_i(A_\alpha(G - e))$$

for $1 \leq i \leq n$. 
Lemma 2.9 ([23]) Let \( G \) be a graph with \( n \) vertices and degree sequence \( d_1 \geq d_2 \geq \cdots \geq d_n \). Then
\[
\lambda_k(A_\alpha(G)) \leq \alpha d_k + (1 - \alpha)(n - k) \quad (2.1)
\]
If equality in (2.1) holds and \( 0 < \alpha < 1 \), then \( G \) has an induced subgraph \( H \cong K_{n-k+1} \) such that \( d(v_i) = \delta \) for all \( v_i \in V(H) \).

Lemma 2.10 ([11]) Let \( G \) be a graph with \( n \) vertices and \( m \geq 1 \) edges. Then \( \lambda_i(Q(G)) = \lambda_i(A(L(G))) + 2, i = 1, 2, \ldots, s \), where \( s = \min\{n, m\} \). Further if \( m > n \), we have \( \lambda_i(A(L(G))) = -2 \) for \( i \geq n + 1 \) and if \( n > m \), we have \( \lambda_i(Q(G)) = 0 \) for \( i \geq m + 1 \).

Lemma 2.11 ([9]) For any \( K_3 \)-free and \( C_4 \)-free graph \( G \), \( A(G^2) = A^2(G) - L(G) \).

Lemma 2.12 If \( 1 \leq k \leq n \), then
\[
\sum_{i=1}^{k} \cos \frac{i\pi}{n} = \frac{1}{2} \csc \frac{\pi}{2n} \sin \left( \frac{(2k+1)\pi}{2n} \right) - \frac{1}{2}.
\]

Proof. For \( 1 \leq k \leq n \), we have
\[
\sum_{i=1}^{k} \cos \frac{i\pi}{n} = \frac{(1 + \cos \frac{\pi}{n}) \sin \frac{k\pi}{n}}{2 \sin \frac{\pi}{n}} + \frac{1}{2} \cos \frac{k\pi}{n} - \frac{1}{2}
\]
\[
= \frac{1}{2} \cot \frac{\pi}{2n} \sin \frac{k\pi}{n} + \frac{1}{2} \cos \frac{k\pi}{n} - \frac{1}{2}
\]
\[
= \frac{1}{2} \csc \frac{\pi}{2n} \sin \left( \frac{(2k+1)\pi}{2n} \right) - \frac{1}{2}.
\]
The proof is completed. \( \square \)

Lemma 2.13 If \( 0 \leq \beta < \alpha \leq 1 \) and \( G \) is a graph with \( n \) vertices, then
\[
S_k(A_\beta(G)) \leq S_k(A_\alpha(G))
\]
for \( 1 \leq k \leq n \). If \( G \) is connected, then inequality is strict, unless \( k = 1 \) and \( G \) is regular.

Proof. If \( 0 \leq \beta < \alpha \leq 1 \), from Proposition 4 in [34], then \( \lambda_k(A_\beta(G)) \leq \lambda_k(A_\alpha(G)) \) for \( 1 \leq k \leq n \). Thus \( S_k(A_\beta(G)) \leq S_k(A_\alpha(G)) \), and the proof follows. \( \square \)
3 Upper bounds on the sum of the largest $A_\alpha$-eigenvalues in terms of vertex degrees

Nikiforov [34] showed that $A_\alpha(G)$ is a positive semi-definite matrix for $\frac{1}{2} \leq \alpha < 1$. Further, $G$ has no isolated vertices, then $A_\alpha(G)$ is positive definite. Let $\alpha_0(G)$ be the smallest $\alpha$ such that $A_\alpha(G)$ is positive semidefinite for $\alpha_0(G) \leq \alpha \leq 1$. Nikiforov and Rojo [38] found $\alpha_0(G)$ if $G$ is regular or $G$ contains a bipartite component and given a lower bound on $\alpha_0(G)$ of $\chi$-colorable graphs.

**Theorem 3.1** Let $G \neq K_n$ be a graph with $n$ vertices and maximum degree $\Delta$.

(i) If $0 \leq \alpha < \frac{1}{\Delta + 1}$, then $S_k(A_\alpha(G)) \leq \frac{(1-\alpha)n}{2}(1 + \sqrt{k})$ for $2 \leq k \leq n$.

(ii) If $\frac{1}{\Delta + 1} \leq \alpha < 1$, then $S_k(A_\alpha(G)) \leq \frac{\alpha \Delta n}{2}(1 + \sqrt{k})$ for $2 \leq k \leq n$.

**Proof.** In this proof we use Lemma 2.1 with $a = 0$ and $b = 1 - \alpha$ for $0 \leq \alpha < \frac{1}{\Delta + 1}$. Then

$$S_k(A_\alpha(G)) \leq \frac{(1-\alpha)n}{2}(1 + \sqrt{k}).$$

By a similar reasoning as above, the second part of the theorem follows. □

**Theorem 3.2** Let $\frac{1}{2} \leq \alpha < 1$ and $G$ be a graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$S_k(A_\alpha(G)) \leq \frac{2\alpha km}{n} + \sqrt{k(n-k)}\left(\frac{\alpha^2 Z_1 + 2m(1-\alpha)^2 - \frac{4\alpha^2 m^2}{n}}{n}\right).$$

**Proof.** Since $tr(A_\alpha(G)) = 2\alpha m$, $\sum_{i=1}^{n} \sum_{k=1}^{n} a_{ik}a_{ki} = \alpha^2 Z_1 + 2m(1-\alpha)^2$ and $A_\alpha(G)$ is a positive semi-definite matrix for $\frac{1}{2} \leq \alpha < 1$, by Lemma 2.2 we have the proof. □

The following result is direct corollary of Lemma 2.3 and Theorem 3.2.

**Corollary 3.3** Let $\frac{1}{2} \leq \alpha < 1$ and $G$ be a graph with $n$ vertices and $m$ edges. If $1 \leq k \leq n - 1$, then

$$S_k(A_\alpha(G)) \leq \frac{2\alpha km}{n} + \sqrt{k(n-k)}\left(\frac{2m(1-\alpha)^2 + \frac{\alpha^2 n}{4}(\Delta - \delta)^2}{n}\right).$$
Theorem 3.4 Let $\frac{1}{2} < \alpha < 1$ and $G$ be a graph with $n$ vertices. If $1 \leq k \leq n - 1$ and $G$ has no isolated vertices, then

$$S_k(A_\alpha(G)) \leq 2\alpha m - (n - k) \left( \frac{|\det(A_\alpha(G))|}{\lambda_1(A_\alpha(G))\lambda_2^{k-1}(A_\alpha(G))} \right)^{\frac{1}{n-k}} \tag{3.1}$$

with equality if and only if $\lambda_2(A_\alpha(G)) = \cdots = \lambda_k(A_\alpha(G))$ and $\lambda_{k+1}(A_\alpha(G)) = \cdots = \lambda_n(A_\alpha(G))$.

**Proof.** Since $\frac{1}{2} < \alpha < 1$ and $G$ has no isolated vertices, we know that $A_\alpha(G)$ is positive definite. By the arithmetic-geometric mean inequality, we have

$$S_k(A_\alpha(G)) = \lambda_1(A_\alpha(G)) + \lambda_2(A_\alpha(G)) + \cdots + \lambda_k(A_\alpha(G))$$

$$\leq 2\alpha m - (\lambda_{k+1}(A_\alpha(G)) + \lambda_{k+2}(A_\alpha(G)) + \cdots + \lambda_n(A_\alpha(G)))$$

$$\leq 2\alpha m - (n - k) \left( \prod_{i=k+1}^{n} \lambda_i(A_\alpha(G)) \right)^{\frac{1}{n-k}}$$

$$= 2\alpha m - (n - k) \left( \frac{|\det(A_\alpha(G))|}{\prod_{i=1}^{k} \lambda_i(A_\alpha(G))} \right)^{\frac{1}{n-k}}$$

with equality if and only if $\lambda_2(A_\alpha(G)) = \cdots = \lambda_k(A_\alpha(G))$ and $\lambda_{k+1}(A_\alpha(G)) = \cdots = \lambda_n(A_\alpha(G))$. This completes the proof. \(\Box\)

If $G$ is a complete graph $K_n$, then equality holds in (3.1). However, there are many other cases of equality some of which are rather complicated and their complete description seems difficult.

**Problem 3.5** Characterize the graphs for which equality holds in (3.1).

**Corollary 3.6** Let $\frac{1}{2} < \alpha < 1$ and $G$ be a graph with $n$ vertices and maximum degree $\Delta < n - 1$. If $1 \leq k \leq n - 1$ and $G$ has no isolated vertices, then

$$S_k(A_\alpha(G)) \leq 2\alpha m - (n - k) \left( \frac{|\det(A_\alpha(G))|}{\alpha^{k-1}\Delta(n - 2)^{k-1}} \right)^{\frac{1}{n-k}}.$$
Proof. By Lemma 2.4 we have $\lambda_1(A_\alpha(G)) \leq \Delta$. By Lemma 2.5 and Theorem 3.4 we have the proof. □

Corollary 3.7 Let $G$ be a connected non-bipartite graph. Then

$$S_k(Q(G)) \leq 2m - (n - k) \left( \frac{\det(Q(G))}{\lambda_1(Q(G)) \lambda_{k+1}^{-1}(Q(G))} \right)^{1/n}.$$  

Theorem 3.8 Let $0 \leq \alpha < \alpha_0(G)$ and $G$ be a graph with $n$ vertices and $m$ edges, and let $p$ be the positive inertia index of $A_\alpha(G)$. Then

$$S_p(A_\alpha(G)) \leq 2\alpha m + \frac{1}{2}(2m(1 - \alpha)^2 + \alpha^2 Z_1) \sqrt{n(n - p)} \frac{Z_1}{Z}.$$  

Proof. By Lemma 2.4 we have $\lambda_1(A_\alpha(G)) \geq \sqrt{\frac{Z_1}{n}}$. We assume that

$$\sum_{i=1}^{n-p} \lambda_{n-i+1}^2(A_\alpha(G)) > \frac{n(2m(1 - \alpha)^2 + \alpha^2 Z_1)^2}{4Z_1},$$

in which case

$$2m(1 - \alpha)^2 + \alpha^2 Z_1 = \sum_{i=1}^p \lambda_i^2(A_\alpha(G)) + \sum_{i=1}^{n-p} \lambda_{n-i+1}^2(A_\alpha(G)) \geq \lambda_1^2(A_\alpha(G)) + \sum_{i=1}^{n-p} \lambda_{n-i+1}^2(A_\alpha(G)) > \frac{Z_1}{n} + \frac{n(2m(1 - \alpha)^2 + \alpha^2 Z_1)^2}{4Z_1}.$$  

This implies that

$$\left( \sqrt{\frac{Z_1}{n}} - \frac{1}{2}(2m(1 - \alpha)^2 + \alpha^2 Z_1) \sqrt{n/Z_1} \right)^2 < 0,$$

which is a contradiction. Thus

$$\sum_{i=1}^{n-p} \lambda_{n-i+1}^2(A_\alpha(G)) \leq \frac{n(2m(1 - \alpha)^2 + \alpha^2 Z_1)^2}{4Z_1},$$
By the Cauchy-Schwarz inequality, we have

\[ S_p(A_\alpha(G)) = 2\alpha m - \sum_{i=1}^{n-p} \lambda_{n-i+1}(A_\alpha(G)) \]

\[ \leq 2\alpha m + \sqrt{(n-p) \sum_{i=1}^{n-p} \lambda_{n-i+1}^2(A_\alpha(G))} \]

\[ \leq 2\alpha m + \frac{1}{2}(2m(1-\alpha)^2 + \alpha^2 Z_1) \sqrt{\frac{n(n-p)}{Z_1}}. \]

This completes the proof. \( \blacksquare \)

By Lemma 2.3 and Theorem 3.8, we obtain the following corollary.

**Corollary 3.9** Let \( 0 \leq \alpha < \alpha_0(G) \) and \( G \) be a graph with \( n \) vertices and \( m \) edges, and let \( p \) be the positive inertia index of \( A_\alpha(G) \). Then

\[ S_p(A_\alpha(G)) \leq 2\alpha m + \left( mn(1-\alpha)^2 + 2\alpha^2 m^2 + \frac{\alpha^2 n^2}{8} (\Delta - \delta)^2 \right) \sqrt{\frac{2(n-p)}{8m^2 + n(\Delta - \delta)^2}}. \]

### 4 On the sum of the \( k \) largest \( A_\alpha \)-eigenvalues of a tree

**Theorem 4.1** Let \( G \) be a bipartite graph with \( n \) vertices and \( m \) edges, and let \( \eta \) be the nullity of \( G \). Then

\[ S_k(A(G)) \leq \begin{cases} 
\sqrt{km}, & \text{if } 1 \leq k \leq \left\lfloor \frac{n-\eta}{2} \right\rfloor; \\
\sqrt{\left\lfloor \frac{n-\eta}{2} \right\rfloor m}, & \text{if } \left\lfloor \frac{n-\eta}{2} \right\rfloor < k \leq \left\lfloor \frac{n+\eta}{2} \right\rfloor; \\
\sqrt{(n-k)m}, & \text{if } \left\lfloor \frac{n+\eta}{2} \right\rfloor < k \leq n.
\end{cases} \]

**Proof.** Since \( G \) is a bipartite graph, we know that eigenvalues of \( A(G) \) are symmetric with respect to the origin, that is \( S_k(A(G)) = S_{n-k}(A(G)) \) for \( \left\lfloor \frac{n+\eta}{2} \right\rfloor < k \leq n-1 \). Since \( \sum_{i=1}^{n} \lambda_i^2(A(G)) = 2m \), we have \( \sum_{i=1}^{\left\lfloor \frac{n+\eta}{2} \right\rfloor} \lambda_i^2(A(G)) = m \). By the Cauchy-Schwarz inequality,
we have
\[ S_k(A(G)) = \sum_{i=1}^{k} \lambda_i(A(G)) \leq \sqrt{k \sum_{i=1}^{k} \lambda_i^2(A(G))} \leq \sqrt{k m} \]
for \(1 \leq k \leq \left\lfloor \frac{n-\eta}{2} \right\rfloor\). This completes the proof. \(\square\)

If \(T\) is a tree with \(n\) vertices and matching number \(\beta\), Cvetković and Gutman [6] showed that \(\eta = n - 2\beta\). Thus we have

**Corollary 4.2** Let \(T\) be a tree with \(n\) vertices and matching number \(\beta\). Then
\[
S_k(A(T)) \leq \begin{cases} 
\sqrt{k(n-1)}, & \text{if } 1 \leq k \leq \beta; \\
\sqrt{\beta(n-1)}, & \text{if } \beta < k \leq n - \beta; \\
\sqrt{(n-k)(n-1)}, & \text{if } n - \beta < k \leq n.
\end{cases}
\]

**Theorem 4.3** Let \(T\) be a tree with \(n\) vertices.

(i) If \(0 \leq \alpha < \frac{1}{2}\), then
\[
S_k(A_\alpha(T)) \leq \begin{cases} 
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{k(n-1)}, & \text{if } 1 \leq k \leq \beta; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{\beta(n-1)}, & \text{if } \beta < k \leq n - \beta; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{(n-k)(n-1)}, & \text{if } n - \beta < k \leq n.
\end{cases}
\]

(ii) If \(\frac{1}{2} \leq \alpha < 1\), then
\[
S_k(A_\alpha(T)) \leq \alpha(n + 2k - 2)
\]
for \(1 \leq k \leq n\).

**Proof.** (i) From Proposition 2.5 in [10], we know that \(Q(G)\) and \(L(G)\) share the same eigenvalues if and only if \(G\) is bipartite. By Lemma 2.6, we have \(S_k(Q(T)) \leq n + 2k - 2\) for \(1 \leq k \leq n\). Since \(A_\alpha(T) = \alpha Q(T) + (1 - 2\alpha)A(T)\) for \(0 \leq \alpha < \frac{1}{2}\), by Theorem 1.1 and Corollary 4.2, we have
\[
S_k(A_\alpha(T)) \leq \alpha S_k(Q(T)) + (1 - 2\alpha)S_k(A(T))
\]
\[
\leq \begin{cases} 
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{k(n-1)}, & \text{if } 1 \leq k \leq \beta; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{\beta(n-1)}, & \text{if } \beta < k \leq n - \beta; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{(n-k)(n-1)}, & \text{if } n - \beta < k \leq n.
\end{cases}
\]
(ii) Since \( Q(G) \) is a real symmetric matrix, the spectrum of \( Q(G) \) majorizes its main diagonal, that is, \( S_k(Q(G)) \geq S_k(D(G)) \). Since \( A_\alpha(T) = (1 - \alpha)Q(T) + (2\alpha - 1)D(T) \) for \( \frac{1}{2} \leq \alpha < 1 \), by Theorem 1.1 and Lemma 2.6, we have

\[
S_k(A_\alpha(T)) \leq (1 - \alpha)S_k(Q(T)) + (2\alpha - 1)S_k(D(T))
\]

\[
\leq (1 - \alpha)S_k(Q(T)) + (2\alpha - 1)S_k(Q(T))
\]

\[
= \alpha S_k(Q(T))
\]

\[
\leq \alpha(n + 2k - 2).
\]

The proof is completed. \( \square \)

**Theorem 4.4** Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges, and let \( \beta' \) be the matching number of the spanning tree of \( G \).

(i) If \( 0 \leq \alpha < \frac{1}{2} \), then

\[
S_k(A_\alpha(G)) \leq \begin{cases} 
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{k(n - 1)} + m - n + 1, & \text{if } 1 \leq k \leq \beta' \; ; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{\beta'(n - 1)} + m - n + 1, & \text{if } \beta' < k \leq n - \beta' \; ; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{(n - k)(n - 1)} + m - n + 1, & \text{if } n - \beta' < k \leq n.
\end{cases}
\]

(ii) If \( \frac{1}{2} \leq \alpha < 1 \), then

\[
S_k(A_\alpha(G)) \leq \alpha(2k + 2m - n)
\]

for \( 2 \leq k \leq n \).

**Proof.** (i) Let \( T \) be a spanning tree of \( G \). If \( 0 \leq \alpha < \frac{1}{2} \), by Theorems 1.1 and 1.3, we have

\[
S_k(A_\alpha(G)) \leq S_k(A_\alpha(T)) + (m - n + 1)S_k(A_\alpha(K_2 \cup (n - 2)K_1))
\]

\[
= S_k(A_\alpha(T)) + m - n + 1
\]

\[
\leq \begin{cases} 
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{k(n - 1)} + m - n + 1, & \text{if } 1 \leq k \leq \beta' \; ; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{\beta'(n - 1)} + m - n + 1, & \text{if } \beta' < k \leq n - \beta' \; ; \\
\alpha(n + 2k - 2) + (1 - 2\alpha)\sqrt{(n - k)(n - 1)} + m - n + 1, & \text{if } n - \beta' < k \leq n.
\end{cases}
\]
(ii) If $\frac{1}{2} \leq \alpha < 1$, by Theorems 1.1 and 4.3, we have
\[
S_k(A_\alpha(G)) \leq S_k(A_\alpha(T)) + (m - n + 1)S_k(A_\alpha(K_2 \cup (n - 2)K_1)) \\
= S_k(A_\alpha(T)) + 2\alpha(m - n + 1) \\
\leq \alpha(n + 2k - 2) + 2\alpha(m - n + 1) \\
= \alpha(2k + 2m - n)
\]
for $2 \leq k \leq n$.

This completes the proof. $\square$

Theorem 4.5 Let $P_n$ be a path with $n$ vertices.

(i) If $0 \leq \alpha < \frac{1}{2}$, then
\[
S_k(A_\alpha(P_n)) \leq 2\alpha k + \alpha - 1 + \alpha \csc \frac{\pi}{2n} \sin \left(\frac{(2k + 1)\pi}{2n}\right) \\
+ (1 - 2\alpha) \csc \frac{\pi}{2(n + 1)} \sin \left(\frac{(2k + 1)\pi}{2(n + 1)}\right)
\]
for $1 \leq k \leq n$.

(ii) If $\frac{1}{2} \leq \alpha \leq 1$, then
\[
S_k(A_\alpha(P_n)) \leq 2\alpha k + (1 - \alpha) \left(\csc \frac{\pi}{2n} \sin \left(\frac{(2k + 1)\pi}{2n}\right) - 1\right)
\]
for $1 \leq k \leq n$.

Proof. (i) Since $A_\alpha(P_n) = \alpha Q(P_n) + (1 - 2\alpha)A(P_n)$ for $0 \leq \alpha < \frac{1}{2}$, by Theorem 1.1 and Lemma 2.12 we have
\[
S_k(A_\alpha(P_n)) \leq \alpha S_k(Q(P_n)) + (1 - 2\alpha)S_k(A(P_n)) \\
= 2\alpha \sum_{i=1}^{k} \left(1 + \cos \frac{i\pi}{n}\right) + 2(1 - 2\alpha) \sum_{i=1}^{k} \cos \frac{i\pi}{n + 1} \\
= 2\alpha k + \alpha \left(\csc \frac{\pi}{2n} \sin \left(\frac{(2k + 1)\pi}{2n}\right) - 1\right) \\
+ (1 - 2\alpha) \left(\csc \frac{\pi}{2(n + 1)} \sin \left(\frac{(2k + 1)\pi}{2(n + 1)}\right) - 1\right)
\]
for 1 ≤ k ≤ n.

(ii) Since $A_\alpha(P_n) = (1 - \alpha)Q(P_n) + (2\alpha - 1)D(P_n)$ for $\frac{1}{2} \leq \alpha < 1$, by Theorem 1.1 and Lemma 2.12 we have

$$S_k(A_\alpha(P_n)) \leq (1 - \alpha)S_k(Q(P_n)) + (2\alpha - 1)S_k(D(P_n))$$

$$= 2(1 - \alpha)\sum_{i=1}^{k} \left( 1 + \cos \frac{i\pi}{n} \right) + 2(2\alpha - 1)k$$

$$= 2k(1 - \alpha) + (1 - \alpha) \left( \csc \frac{\pi}{2n} \sin \frac{(2k + 1)\pi}{2n} - 1 \right)$$

$$+ 2(2\alpha - 1)k$$

$$= 2\alpha k + (1 - \alpha) \left( \csc \frac{\pi}{2n} \sin \frac{(2k + 1)\pi}{2n} - 1 \right)$$

for 1 ≤ k ≤ n. The proof is completed. □

Corollary 4.6 Let $P_n$ be a path with n vertices. If $0 \leq \alpha < 1$, then $S_k(A_\alpha(P_n)) < 2k$ for 1 ≤ k ≤ n.

5 Lower bounds on the sum of the largest $A_\alpha$-eigenvalues

Theorem 5.1 Let $G$ be a graph with maximum degree $\Delta$.

(i) If $0 \leq \alpha \leq \frac{1}{2}$, then

$$S_k(A_\alpha(G)) \geq (1 - \alpha)S_k(Q(G)) + (2\alpha - 1)k\Delta.$$  

(ii) If $\frac{1}{2} \leq \alpha \leq 1$, then

$$S_k(A_\alpha(G)) \geq \alpha S_k(Q(G)) + (1 - 2\alpha)S_k(A(G)).$$

If $G$ is a regular graph, then the equality in the above inequalities must hold.

Proof. (i) If $0 \leq \alpha \leq \frac{1}{2}$, then $\frac{1}{2} \leq 1 - \alpha \leq 1$. It follows that $A_{1-\alpha}(G) = \alpha Q(G) + (1 - 2\alpha)D(G)$. Since $A_\alpha(G) + A_{1-\alpha}(G) = Q(G)$, by Theorem 1.1 we have

$$S_k(A_\alpha(G)) \geq S_k(Q(G)) - S_k(A_{1-\alpha}(G))$$

$$\geq S_k(Q(G)) - \alpha S_k(Q(G)) - (1 - 2\alpha)S_k(D(G))$$

$$\geq (1 - \alpha)S_k(Q(G)) + (2\alpha - 1)k\Delta.$$  

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(ii) If $\frac{1}{2} \leq \alpha \leq 1$, then $0 \leq 1 - \alpha \leq \frac{1}{2}$. It follows that $A_{1-\alpha}(G) = (1 - \alpha)Q(G) + (2\alpha - 1)A(G)$. Since $A_{\alpha}(G) + A_{1-\alpha}(G) = Q(G)$, by Theorem 1.1, we have

$$S_k(A_{\alpha}(G)) \geq S_k(Q(G)) - S_k(A_{1-\alpha}(G))$$
$$\geq S_k(Q(G)) - (1 - \alpha)S_k(Q(G)) - (2\alpha - 1)S_k(A(G))$$
$$\geq \alpha S_k(Q(G)) + (1 - 2\alpha)S_k(A(G)).$$

This completes the proof. \[\square\]

**Corollary 5.2** Let $P_n$ be a path with $n$ vertices.

(i) If $0 \leq \alpha \leq \frac{1}{2}$, then

$$S_k(A_{\alpha}(P_n)) \geq 2\alpha k + (1 - \alpha) \left( \csc \frac{\pi}{2n} \sin \left( \frac{(2k + 1)\pi}{2n} \right) - 1 \right)$$

for $1 \leq k \leq n$.

(ii) If $\frac{1}{2} \leq \alpha \leq 1$, then

$$S_k(A_{\alpha}(P_n)) \geq 2\alpha k + \alpha - 1 + \alpha \csc \frac{\pi}{2n} \sin \left( \frac{(2k + 1)\pi}{2n} \right)$$
$$+ (1 - 2\alpha) \csc \frac{\pi}{2(n + 1)} \sin \left( \frac{(2k + 1)\pi}{2(n + 1)} \right)$$

for $1 \leq k \leq n$.

**Theorem 5.3** Let $G$ be a $r$-regular graph.

(i) Let $t$ be the number of vertex-disjoint cliques in $G$. If $0 \leq \alpha \leq 1$, then

$$S_k(A_{\alpha}(G)) \geq \alpha kr + (1 - \alpha)(r - k + 1)$$

for $1 \leq k \leq t + 1$.

(ii) Let $g_1 \geq g_2 \geq \cdots \geq g_c$ and $C_{g_1}, C_{g_2}, \ldots, C_{g_c}$ be the vertex-disjoint induced cycles of length even in $G$. If $0 \leq \alpha \leq 1$, then

$$S_k(A_{\alpha}(G)) \geq (\alpha k + 1 - \alpha)r + 2(1 - \alpha)\sum_{i=1}^{k-1} (1 - \frac{4}{g_i})$$

for $1 \leq k \leq c + 1$.  

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Proof. (i) Let $X_1$ be the vector with all entries equal to 1. Then $X_1$ is an eigenvector corresponding to $\lambda_1(A(G))$. Let $K_{\omega_1}, K_{\omega_2}, \ldots, K_{\omega_t}$ be the vertex-disjoint cliques in $G$. Then we take

\[
X_2 = (x_1^{(2)}, x_2^{(2)}, \ldots, x_{\omega_1}^{(2)}, 0, \ldots, 0),
\]

\[
X_3 = (0, \ldots, 0, x_1^{(3)}, x_2^{(3)}, \ldots, x_{\omega_2}^{(3)}, 0, \ldots, 0), \ldots,
\]

\[
X_{t+1} = (0, \ldots, 0, 0, \ldots, x_1^{(t+1)}, x_2^{(t+1)}, \ldots, x_{\omega_t}^{(t+1)}, 0, \ldots, 0)
\]

satisfying

\[
\begin{align*}
&x_1^{(s)} + x_2^{(s)} + \cdots + x_{\omega_{s-1}^{(s)}} = 0 \\
&x_1^{2(s)} + x_2^{2(s)} + \cdots + x_{\omega_{s-1}^{2(s)}} = 1
\end{align*}
\]

for $s = 2, 3, \ldots, t+1$. Thus we have $2 \sum_{i<j} x_i^{(s)} x_j^{(s)} = -1$. Since $G$ is a $r$-regular graph and the vectors $X_1, X_2, \ldots, X_{t+1}$ are orthogonal, by Lemma 2.7, we have

\[
S_k(A_\alpha(G)) = \alpha kr + (1 - \alpha) S_k(A(G))
\]

\[
= \alpha kr + (1 - \alpha) \max \sum_{i=1}^k \langle A(G)X_i, X_i \rangle
\]

\[
\geq \alpha kr + (1 - \alpha) \sum_{i=1}^k \langle A(G)X_i, X_i \rangle
\]

\[
= \alpha kr + (1 - \alpha)(r + 2(k - 1) \sum_{i<j} x_i^{(k-1)} x_j^{(k-1)})
\]

\[
= \alpha kr + (1 - \alpha)(r - k + 1).
\]

for $1 \leq k \leq t + 1$.

(ii) Let $X_1$ be the vector with all entries equal to 1. Then $X_1$ is an eigenvector corresponding to $\lambda_1(A(G))$. Let $g_1 \geq g_2 \geq \cdots \geq g_c$ and $C_{g_1}, C_{g_2}, \ldots, C_{g_c}$ be the vertex-disjoint induced cycles of length even in $G$. Then we take

\[
X_2 = \frac{1}{\sqrt{g_1}}(1, \ldots, 1, -1, \ldots, -1, 0, \ldots, 0),
\]

\[
X_3 = \frac{1}{\sqrt{g_2}}(0, \ldots, 0, 1, \ldots, 1, -1, \ldots, -1, 0, \ldots, 0), \ldots,
\]
Thus we have

\[ \sum_{v_i v_j \in E(C_{gs})} x_i x_j = 2(1 - \frac{4}{g_s}) \text{ for } s = 1, 2, \ldots, c. \]

Since \( G \) is a \( r \)-regular graph and the vectors \( X_1, X_2, \ldots, X_{c+1} \) are orthogonal, by Lemma 2.7, we have

\[
S_k(A_\alpha(G)) = \alpha kr + (1 - \alpha)S_k(A(G)) \\
= \alpha kr + (1 - \alpha) \max \sum_{i=1}^{k} \langle A(G)X_i, X_i \rangle \\
\geq \alpha kr + (1 - \alpha) \sum_{i=1}^{k} \langle A(G)X_i, X_i \rangle \\
= \alpha kr + (1 - \alpha)(r + 2 \sum_{s=1}^{k-1} \sum_{v_i v_j \in E(C_{gs})} x_i x_j) \\
= \alpha kr + (1 - \alpha) \left( r + 2 \sum_{i=1}^{k-1} (1 - \frac{4}{g_i}) \right) \\
= (\alpha k + 1 - \alpha)r + 2(1 - \alpha) \sum_{i=1}^{k-1} (1 - \frac{4}{g_i})
\]

for \( 1 \leq k \leq c + 1. \)

This completes the proof. \( \square \)

**Theorem 5.4** Let \( G \) be a connected bipartite graph with bipartition \( V(G) = X \cup Y, \) \( |X| = s \) and \( |Y| = t. \) Let \( m \) and \( \beta \) be the number of edges and matching number of \( G, \) respectively. If \( 0 \leq \alpha \leq 1, \) then

\[
S_k(A_\alpha(G)) \geq \frac{\alpha m}{2} \left( \frac{1}{s} + \frac{1}{t} \right) + \frac{(1 - \alpha)m}{\sqrt{st}} + (k - 1) \left( \alpha - \frac{2(1 - \alpha)\sqrt{st}}{s + t} \right)
\]

for \( 1 \leq k \leq \beta + 1. \)

**Proof.** By the hypothesis, we take a set of orthonormal vectors as follows:

\[
X_1 = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{s}}, \ldots, \frac{1}{\sqrt{s}}, \frac{1}{\sqrt{t}}, \ldots, \frac{1}{\sqrt{t}} \right)
\]

\[
X_2 = \sqrt{\frac{t}{s+t}} (1,0,\ldots,0) - \sqrt{\frac{s}{s+t}} (0,\ldots,0)
\]
\[ X_3 = \sqrt{\frac{s}{s+t}} (0,1,\ldots,0,-\sqrt{\frac{t}{s}},0,\ldots,0), \ldots, \]

\[ X_{\beta+1} = \sqrt{\frac{s}{s+t}} (0,\ldots,0,1,0,\ldots,0,0,\ldots,0,-\sqrt{\frac{t}{s}},0,\ldots,0). \]

By Lemma 2.7, we have

\[
S_k(A_\alpha(G)) = \max \sum_{i=1}^{k} (A_\alpha(G)X_i, X_i) \\
\geq \sum_{i=1}^{k} (A_\alpha(G)X_i, X_i) \\
= \sum_{i=1}^{k} \sum_{ uv \in E(G)} (\alpha x^2_u + 2(1-\alpha)x_u x_v + \alpha x^2_v) \\
= m \left( \frac{\alpha}{2s} + 2(1-\alpha) \frac{1}{2\sqrt{st}} + \frac{\alpha}{2t} \right) \\
+ (k-1) \left( \frac{\alpha s}{s+t} + 2(1-\alpha) \frac{-\sqrt{st}}{s+t} + \frac{\alpha t}{s+t} \right) \\
= \frac{am}{2} \left( \frac{1}{s} + \frac{1}{t} \right) + \frac{(1-\alpha)m}{\sqrt{st}} + (k-1) \left( \alpha - \frac{2(1-\alpha)\sqrt{st}}{s+t} \right)
\]

for \(1 \leq k \leq \beta + 1.\) The proof is completed. \(\Box\)

Let \(M\) be a real symmetric partitioned matrix of order \(n\) described in the following block form

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

where the diagonal blocks \(M_{ii}\) are \(n_i \times n_i\) matrices for any \(i \in \{1,2,\ldots,t\}\) and \(n = n_1 + \cdots + n_t.\) For any \(i,j \in \{1,2,\ldots,t\},\) 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 \(M.\)

**Lemma 5.5 ([20])** Let \(M\) be a symmetric partitioned matrix of order \(n\) with eigenvalues \(\xi_1 \geq \xi_2 \geq \cdots \geq \xi_n,\) and let \(B\) its quotient matrix with eigenvalues \(\eta_1 \geq \eta_2 \geq \cdots \geq \eta_r\) and \(n > r.\) Then \(\xi_i \geq \eta_i \geq \xi_{n-r+i}\) for \(i = 1,2,\ldots,r.\)
Corollary 5.6 Let $M$ be a symmetric partitioned matrix of order $n$, and let $B$ be its quotient matrix of order $k$. Then
\[ S_k(M) \geq S_k(B). \]

Let $B$ be the quotient matrix of $A_\alpha(G)$ corresponding to the partition for the color classes of $G$. Then the following corollary is immediate.

Corollary 5.7 Let $G$ be a connected graph with $n$ vertices, $m$ edges, chromatic number $\chi$ and independence number $\theta$. If $0 \leq \alpha < 1$, then
\[ S_\chi(A_\alpha(G)) \geq \frac{2m}{\theta}. \]

Let $U \subseteq V(G)$, $W \subseteq V(G)$ and $\partial(U, W)$ be the set of edges which connect vertices in $U$ with vertices in $W$.

Theorem 5.8 Let $0 \leq \alpha < 1$ and $G$ be a connected graph with $n$ vertices and $m$ edges. For any given vertices subset $U = \{u_1, \ldots, u_{k-1}\}$ with $1 \leq k \leq n$,
\[ S_k(A_\alpha(G)) \geq \left( \alpha - \frac{1}{n-k+1} \right) \sum_{u \in U} d_u + \frac{2m - (1 - \alpha)|\partial(U, V(G) \setminus U)|}{n-k+1}. \]

Proof. If $2 \leq k \leq n$, then the quotient matrix of $A_\alpha(G)$ corresponding to the partition $V(G) = U \cup (V(G) \setminus U)$ of $G$ is
\[ B(G) = \begin{bmatrix} A_\alpha(U) & b_{1,k} \\ \vdots & \vdots \\ b_{k,1} & \cdots & b_{k,k-1} & b_{k,k} \end{bmatrix}, \]
where $A_\alpha(U)$ is the principal submatrix of $A_\alpha(G)$. By Lemma 5.5, we have
\[ S_k(A_\alpha(G)) \geq S_k(B(G)) \]
\[ = \text{tr}(A_\alpha(U)) + b_{k,k} \]
\[ = \alpha \sum_{u \in U} d(u) + \frac{2m - \sum_{u \in U} d_u - (1 - \alpha)|\partial(U, V(G) \setminus U)|}{n-k+1} \]
\[ = \left( \alpha - \frac{1}{n-k+1} \right) \sum_{u \in U} d_u + \frac{2m - (1 - \alpha)|\partial(U, V(G) \setminus U)|}{n-k+1}. \]
If \( k = 1 \), then \( U \) is an empty set. Thus \( \sum_{u \in U} d_u = 0 \) and \( |\partial(U, V(G) \setminus U)| = 0 \). Taking a \( n \)-vector \( X = (1, \ldots, 1) \), by Rayleigh’s principle, we have
\[
S_1(A_\alpha(G)) = \lambda_1(A_\alpha(G)) \geq \frac{2m}{n}.
\]
Therefore, the above inequality still holds for \( k = 1 \). This completes the proof. \( \square \)

If \( U \) is a subset of a maximum independent set of \( G \), by Theorem 5.8, we have

**Corollary 5.9** Let \( G \) be a connected graph with \( n \) vertices, \( m \) edges and independence number \( \theta \). If \( 0 \leq \alpha < 1 \), then
\[
S_k(A_\alpha(G)) \geq \alpha(k - 1)\delta + \frac{2m - (2 - \alpha)(k - 1)\delta}{n - k + 1}
\]
for \( 1 \leq k \leq \theta + 1 \).

The next theorem is concerned with Problem 1.4. For \( k = 2 \), we will prove that path is the minimum \( S_k(A_\alpha(G)) \) among all connected graphs for \( \frac{1}{2} \leq \alpha < 1 \). Let the sequence \( (d_1, d_2, \ldots, d_n) \) be the set of a graph with the same degree sequence.

**Theorem 5.10** Let \( G \) be a connected graph with \( n \geq 12 \) vertices. If \( \frac{1}{2} \leq \alpha < 1 \), then
\[
S_2(A_\alpha(G)) \geq S_2(A_\alpha(P_n))
\]
with equality if and only if \( G = P_n \).

**Proof.** By Corollary 4.6, we have \( S_2(A_\alpha(P_n)) < 4 \). Let \( T_n \) be a spanning tree of a connected graph \( G \) with \( n \) vertices. By Lemmas 2.8 and 2.13 we have
\[
S_2(A_\alpha(G)) \geq S_2(A_\alpha(T_n)) \geq S_2(A_{1/2}(T_n)) \geq S_2(A_{1/2}(T_{12}))
\]
for \( \frac{1}{2} \leq \alpha < 1 \) and \( n \geq 12 \).

In the following, we only need to show \( S_2(A_{1/2}(T_{12})) \geq S_2(A_\alpha(P_n)) \) for \( \frac{1}{2} \leq \alpha < 1 \) and \( n \geq 12 \). For \( \alpha = \frac{1}{2} \), we have \( A_{1/2}(G) = \frac{1}{2}Q(G) \). From Theorem 3.1 in [39], we know that \( S_2(Q(G)) \geq S_2(D(G)) + 1 \) with equality if and only if \( G \) is the star \( K_{1, n-1} \) or the complete graph \( K_3 \). Let \( \Delta_2(G) \) be the second largest degree of a graph \( G \).
If $\Delta(T_{12}) \geq 4$ and $\Delta_2(T_{12}) \geq 3$, then we have

$$S_2(A_{1/2}(T_{12})) \geq \frac{1}{2}(S_2(D(G)) + 1) = \frac{1}{2}(4 + 3 + 1) = 4 > S_2(A_n(P_n))$$

for $\frac{1}{2} \leq \alpha < 1$ and $n \geq 12$.

If $\Delta(T_{12}) \geq 5$ and $\Delta_2(T_{12}) \geq 2$, then we have

$$S_2(A_{1/2}(T_{12})) \geq \frac{1}{2}(S_2(D(G)) + 1) = \frac{1}{2}(5 + 2 + 1) = 4 > S_2(A_n(P_n))$$

for $\frac{1}{2} \leq \alpha < 1$ and $n \geq 12$.

If $\Delta(T_{12}) = 4$ and $\Delta_2(T_{12}) = 2$, then $T_{12}$ is one of the trees $(4, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1)$. By computation with computer, we have

$$S_2(A_{1/2}(T_{12})) \geq S_2(A_{1/2}(T')) \geq \frac{1}{2} \times 8.57037 = 4.285185 > S_2(A_n(P_n))$$

for $\frac{1}{2} \leq \alpha < 1$ and $n \geq 12$, where $T'$, shown in Fig. 4.1, is a tree with minimum sum of the two largest $A_{1/2}$-eigenvalues in the set of trees $(4, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1)$. If $\Delta(T_{12}) = \Delta_2(T_{12}) = 3$, then we assume that $x, y$ and $z$ be the number of the vertices of the degree three, the degree two and the degree one, respectively. Thus, we have

$$x + y + z = 12, \quad 3x + 2y + z = 22.$$ Solve the above equations, we get $x = 2, y = 6, z = 4$; $x = 3, y = 4, z = 5$; $x = 4, y = 2, z = 6$; $x = 5, y = 0, z = 7$. Further, we know that $T_{12}$ is one of the trees $(3, 3, 2, 2, 2, 2, 1, 1, 1, 1), (3, 3, 3, 2, 2, 2, 1, 1, 1, 1, 1), (3, 3, 3, 3, 2, 2, 1, 1, 1, 1, 1, 1)$ and $(3, 3, 3, 3, 3, 1, 1, 1, 1, 1, 1, 1)$. By computation with computer, we have

$$S_2(A_{1/2}(T_{12})) \geq S_2(A_{1/2}(T'')) \geq \frac{1}{2} \times 8.31903 = 4.159515 > S_2(A_n(P_n))$$

for $\frac{1}{7} \leq \alpha < 1$ and $n \geq 12$, where $T''$, shown in Fig. 4.1, is a tree with minimum sum of the two largest $A_{1/2}$-eigenvalues in the set of trees $(3, 3, 2, 2, 1, 1, 1, 1, 1, 1, 1), (3, 3, 3, 2, 2, 1, 1, 1, 1, 1, 1), (3, 3, 3, 3, 2, 1, 1, 1, 1, 1, 1, 1)$ and $(3, 3, 3, 3, 3, 3, 1, 1, 1, 1, 1, 1, 1)$. If $\Delta(T_{12}) = 3$ and $\Delta_2(T_{12}) = 2$, then $T_{12}$ is one of the trees $(3, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1)$. By computation with computer, we have

$$S_2(A_{1/2}(T_{12})) \geq S_2(A_{1/2}(T''')) \geq \frac{1}{2} \times 8.02294 = 4.01147 > S_2(A_n(P_n))$$

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for \( \frac{1}{2} \leq \alpha < 1 \) and \( n \geq 12 \), where \( T''' \), shown in Fig. 4.1, is a tree with minimum sum of the two largest \( A_{1/2} \)-eigenvalues in the set of trees \((3, 2, 2, 2, 2, 2, 2, 1, 1, 1) \).

If \( \Delta_2(T_{12}) = 1 \), then \( T_{12} \) is a star \( K_{1,11} \). Thus,

\[
S_2(A_{1/2}(K_{1,11})) \geq \frac{1}{2} \times 13 = 6.5 > S_2(A_\alpha(P_n))
\]

for \( \alpha \in \left[ \frac{1}{2}, 1 \right) \) and \( n \geq 12 \).

Combining the above argument, we have

\[
S_2(A_{1/2}(T_{12})) \geq S_2(A_\alpha(P_n)) \quad \text{for} \quad \alpha \in \left[ \frac{1}{2}, 1 \right) \quad \text{and} \quad n \geq 12.
\]

Further, we get

\[
S_2(A_\alpha(G)) \geq S_2(A_\alpha(P_n)) \quad \text{for} \quad \frac{1}{2} \leq \alpha < 1 \quad \text{and} \quad n \geq 12,
\]

and equality holds if and only if \( G = P_n \), completing the proof. \( \square \)

![Fig. 4.1 Trees \( T ', T '', T ''' \).](image)

**Problem 5.11** For \( 0 \leq \alpha < \frac{1}{2} \), which graph(s) minimize the sum of the two largest of \( A_\alpha \)-eigenvalues among all connected graphs with \( n \) vertices?

### 6 On the sum of the largest \( A_\alpha \)-eigenvalues of graph operations

**Theorem 6.1** Let \( G \) be a graph with \( n \) vertices. If \( 0 \leq \alpha \leq 1 \), then

\[
(1-\alpha)n+(\alpha n-1)k \leq S_k(A_\alpha(G)) + S_k(A_\alpha(\overline{G})) \leq k[(2-\alpha)n+\alpha(\Delta-\delta-1)-(1-\alpha)(k+1)].
\]

**Proof.** From Proposition 36 in [34], we have \( S_k(A_\alpha(K_n)) = (1-\alpha)n+(\alpha n-1)k \). Since \( A_\alpha(G) + A_\alpha(\overline{G}) = A_\alpha(K_n) \), by Theorem 1.1, we have

\[
S_k(A_\alpha(G)) + S_k(A_\alpha(\overline{G})) \geq S_k(A_\alpha(K_n)) = (1-\alpha)n+(\alpha n-1)k.
\]

By Lemma 2.3, we have

\[
S_k(A_\alpha(G)) \leq \alpha(d_1 + d_2 + \cdots + d_k) + (1-\alpha)\left(kn - \frac{k(k+1)}{2}\right).
\]

Thus

\[
S_k(A_\alpha(G)) + S_k(A_\alpha(\overline{G})) \leq \alpha k(n-1) + \alpha \sum_{i=1}^{k} (d_i - d_{n-i+1}) + (1-\alpha)(2kn - k(k+1))
\]

\[
\leq \alpha k(n-1) + \alpha k(\Delta - \delta) + (1-\alpha)(2kn - k(k+1))
\]

\[ 23 \]
This completes the proof. □

**Theorem 6.2** Let \( G \) be a graph with \( n \) vertices and \( m \geq 1 \) edges. Then

\[
S_k(A_\alpha(L(G))) \leq 2k(\alpha \Delta - 1) + (1 - \alpha)S_k(Q(G))
\]

for \( 1 \leq k \leq s \), where \( s = \min \{n, m\} \). If \( m > n \), then

\[
S_k(A_\alpha(L(G))) \leq 2\alpha k(\Delta - 1) + 2(1 - \alpha)(m - k)
\]

for \( n + 1 \leq k \leq m \).

**Proof.** If a vertex \( w \) is in one-to-one correspondence with the edge \( uv \) of the graph \( G \), then \( d_{L(G)}(w) = d_G(u) + d_G(v) - 2 \). By Theorem 1.1 and Lemma 2.10, we have

\[
S_k(A_\alpha(L(G))) \leq \alpha S_k(D(L(G))) + (1 - \alpha)S_k(A(L(G)))
\]

\[
= \alpha k(2\Delta - 2) + (1 - \alpha)(S_k(Q(G)) - 2k)
\]

\[
= 2k(\alpha \Delta - 1) + (1 - \alpha)S_k(Q(G))
\]

for \( 1 \leq k \leq s \), where \( s = \min \{n, m\} \). If \( m > n \), then we have

\[
S_k(A_\alpha(L(G))) \leq \alpha k(2\Delta - 2) + (1 - \alpha)(2m - 2n - 2(k - n)) = 2\alpha k(\Delta - 1) + 2(1 - \alpha)(m - k)
\]

for \( n + 1 \leq k \leq m \). This completes the proof. □

By Lemma 2.6 and Conjecture 1.3, we have

**Corollary 6.3** If \( T \) is a tree with \( n \) vertices, then \( S_k(A_\alpha(L(T))) \leq 2k\alpha(\Delta - 1) + (1 - \alpha)(n-2) \) for \( 1 \leq k \leq n-1 \). If \( U \) is a unicyclic graph with \( n \) vertices, then \( S_k(A_\alpha(L(U))) \leq 2k(\alpha \Delta - 1) + (1 - \alpha)(n + \frac{k^2+k}{2}) \) for \( 1 \leq k \leq n \). If \( B \) is a bicyclic graph with \( n \) vertices, then \( S_k(A_\alpha(L(B))) \leq 2k(\alpha \Delta - 1) + (1 - \alpha)(n + 1 + \frac{k^2+k}{2}) \) for \( 1 \leq k \leq n \).

**Theorem 6.4** Let \( G \) be a \( K_3 \)-free and \( C_4 \)-free graph with \( n \) vertices and \( m \) edges. If \( 0 \leq \alpha \leq 1 \), then

\[
S_k(A_\alpha(G^2)) \leq \alpha(Z_1(G) - (n-k)\delta^2(G)) + (1 - \alpha) \left( 2m - \frac{1}{n-k}S_k^2(A(G)) - (k-1)a(G) \right).
\]
Proof. Since \( \sum_{i=1}^{n} \lambda_i(A(G)) = 0 \) and \( \sum_{i=1}^{n} \lambda_i^2(A(G)) = 2m \), by the Cauchy-Schwarz inequality, we have

\[
S_k(A^2(G)) = \lambda_1^2(A(G)) + \lambda_2^2(A(G)) + \cdots + \lambda_k^2(A(G)) = 2m - \sum_{i=k+1}^{n} \lambda_i^2(A(G))
\]

\[
\leq 2m - \frac{1}{n-k} \left( \sum_{i=k+1}^{n} \lambda_i(A(G)) \right)^2
\]

\[
= 2m - \frac{1}{n-k} \left( \sum_{i=1}^{k} \lambda_i(A(G)) \right)^2
\]

\[
= 2m - \frac{1}{n-k} S_k^2(A(G)).
\]

Since \( \sum_{u \in V(G^2)} d_u = Z_1(G) \), by Theorem 1.1 and Lemma 2.11, we have

\[
S_k(A_\alpha(D(G^2))) \leq \alpha S_k(D(G^2)) + (1-\alpha) S_k(A^2(G))
\]

\[
\leq \alpha S_k(D(G^2)) + (1-\alpha) (S_k(A^2(G)) + S_k(-L(G)))
\]

\[
\leq \alpha(Z_1(G) - (n-k)d^2(G)) + (1-\alpha) \left( 2m - \frac{1}{n-k} S_k^2(A(G)) - (k-1)a(G) \right).
\]

This completes the proof. □

Theorem 6.5 Let \( G \) be a graph with \( n \) vertices. If \( 0 \leq \alpha \leq 1 \), then

\[
S_k(A_\alpha(D(G))) \leq \begin{cases} 
4 \sum_{i=1}^{k/2} d_i(G) + 2(1-\alpha)S_k(A(G)), & \text{if } 1 < k < n \text{ is even;} \\
4 \sum_{i=1}^{(k-1)/2} d_i(G) + 2d_{(k+1)/2} + 2(1-\alpha)S_k(A(G)), & \text{if } 1 \leq k < n \text{ is odd;} \\
4 \sum_{i=1}^{k/2} d_i(G), & \text{if } n \leq k \leq 2n \text{ is even;} \\
4 \sum_{i=1}^{(k-1)/2} d_i(G) + 2d_{(k+1)/2}, & \text{if } n \leq k \leq 2n \text{ is odd},
\end{cases}
\]

where \( d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G) \) is the vertex degree sequence of \( G \).
Proof. By the definition of $\mathcal{D}(G)$, the $A_\alpha$-matrix of the double graph of $G$ is

$$A_\alpha(\mathcal{D}(G)) = \alpha D(\mathcal{D}(G)) + (1 - \alpha) A(D(G))$$

$$= \alpha \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \otimes D(G) + (1 - \alpha) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes A(G),$$

where $M \otimes N$ is the Kronecker product (or tensor product) of $M$ and $N$. Thus the spectrum of $\left(\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \otimes D(G)\right)$ and $\left(\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes A(G)\right)$ are

$$2d_1(G), 2d_1(G), 2d_2(G), 2d_2(G), \ldots, 2d_n(G), 2d_n(G)$$

and

$$2\lambda_1(A), 2\lambda_2(A), \ldots, 2\lambda_n(A), 0, 0, \ldots, 0,$$

respectively. By Theorem 1.1, we have

$$S_k(A_\alpha(\mathcal{D}(G))) \leq \alpha S_k(D(\mathcal{D}(G))) + (1 - \alpha) S_k(A(D(G)))$$

$$= \begin{cases} 4 \sum_{i=1}^{k/2} d_i(G) + 2(1 - \alpha) S_k(A(G)), & \text{if } 1 < k < n \text{ is even;} \\ 4 \sum_{i=1}^{(k-1)/2} d_i(G) + 2d_{(k+1)/2} + 2(1 - \alpha) S_k(A(G)), & \text{if } 1 \leq k < n \text{ is odd;} \\ 4 \sum_{i=1}^{k/2} d_i(G), & \text{if } n \leq k \leq 2n \text{ is even;} \\ 4 \sum_{i=1}^{(k-1)/2} d_i(G) + 2d_{(k+1)/2}, & \text{if } n \leq k \leq 2n \text{ is odd.} \end{cases}$$

This completes the proof. $\blacksquare$

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