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Research article

On the sum of the largest A_α-eigenvalues of graphs

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Abstract: Let $A(G)$ and $D(G)$ be the adjacency matrix and the degree diagonal matrix of a graph G, respectively. For any real number $\alpha \in [0, 1]$, Nikiforov defined the A_α-matrix of a graph G as $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$. Let $S_k(A_\alpha(G))$ be the sum of the k largest eigenvalues of $A_\alpha(G)$. In this paper, some bounds on $S_k(A_\alpha(G))$ are obtained, which not only extends the results of the sum of the k largest eigenvalues of the adjacency matrix and signless Laplacian matrix, but it also gives new bounds on graph energy.

Keywords: A_α-matrix; sum of A_α-eigenvalues; energy; graph operation
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1. Introduction

Let G be a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For $v_i \in V(G)$, $d_i = d_G(v_i)$ denotes the degree of vertex v_i, and $M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2$ is called the first Zagreb index. The minimum and the maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$, or simply δ and Δ, respectively. Denote by K_n, C_n and $K_{s,n-s}$ the complete graph, cycle and complete bipartite graph with n vertices, respectively. The positive inertia index $p = p(M)$ and the negative inertia index of a matrix M are the number of positive and negative eigenvalues of M, respectively. For other undefined notations and terminology from graph theory, the readers are referred to [6].

For a graph G, $S_k(A(G))$ is the sum of the k largest eigenvalues of adjacency matrix $A(G)$. Mohar [23] showed that $S_k(A(G))$ is at most $\frac{1}{2}(\sqrt{k} + 1)n$. This bound is shown to be the 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. [11] proved an upper bound on $S_k(A(G))$ in terms of vertex number and negative inertia index. Let $L(G) = D(G) - A(G)$ be the Laplacian matrix of a graph G. Based on the famous Grone-Merris-Bai theorem [3,14], Brouwer et al. [5] proposed the following conjecture.

Conjecture 1.1. *(Brouwer's conjecture) Let G be a graph with n vertices and $e(G)$ edges. For $1 \leq k \leq n$, we have*

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

Inspired by Brouwer's conjecture, Ashraf et al. [2] proposed a similar conjecture as follows.

Conjecture 1.2. *[2] Let G be a graph with n vertices and $e(G)$ edges. For $1 \leq k \leq n$, we have*

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

where $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix of G.

The above two conjectures have been proven to be correct for all graphs with at most ten vertices [2], all graphs with $k = 1, 2, n-2, n-1, n$ [2,7], regular graphs [2], trees [17], unicyclic graphs [31,32], bicyclic graphs [31,32], tricyclic graphs [31,32] and so on. In particular, Haemers et al. [17] proved that $S_k(L(T)) \leq e(T) + 2k - 1$ when T is a tree with n vertices.

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, m edges and the positive inertia index p. Then we have

$$\varepsilon(G) = \varepsilon(A(G)) = \sum_{k=1}^{n} |\lambda_k(A(G))| = 2S_p(A(G)),$$

and

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

where $\lambda_k(M)$ is the k-th largest eigenvalue of the matrix M. 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 [1,11,13,22]. In addition, $S_k(A(G))$ is related to Ky Fan norms of graphs introduced by Nikiforov [25], which are a fundamental matrix parameter anyway.

For any real $\alpha \in [0, 1]$, Nikiforov [24] 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 [18–20,24,26]. This matrix has recently attracted the attention of many researchers, and there are several research papers published recently, see [4,20,21,29] and the references therein.

Motivated by the above works, we study the sum of the 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

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

where $\varepsilon_\alpha(G)$ is the α-energy of G defined by Guo and Zhou [15]. Thus, $S_k(A_\alpha(G))$ is a close relation with the α-energy of G. It is not difficult to see that $\varepsilon_0(G) = \varepsilon(A(G))$ and $2\varepsilon_{1/2}(G) = \varepsilon(Q(G))$.

In this paper, we obtain some upper and lower bounds on the sum of the k largest eigenvalues of $A_\alpha(G)$, which extend the results of $S_k(A(G))$ and $S_k(Q(G))$. In particular, we give new bounds on the energy of graphs in terms of the positive inertia index and the first Zagreb index. In addition, some graph operations on $S_k(A_\alpha(G))$ are presented, which provides new bounds for the energy of graph operations.

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 terms of A_α-spectral radius and the first Zagreb index. Similarly to Conjecture 1.2, a conjecture is proposed for $\frac{1}{2} \le \alpha < 1$. In Section 4, the line graph and the square of graphs on $S_k(A_\alpha(G))$ are presented.

2. Preliminaries

The line graph $\mathcal{L}(G)$ is the graph whose vertex set is the edges in G, where two vertices are adjacent if the corresponding edges in G have a common vertex. The square G^2 of a graph G is a graph with the same set of vertices as G such that two vertices are adjacent in G^2 if and only if their distance in G is at most 2. The second smallest eigenvalue of the Laplacian of a graph G, best-known as the algebraic connectivity of G, is denoted by $a(G)$.

Lemma 2.1. *[12] Let M and N be two real symmetric matrices of order n. Then we have*

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

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

Lemma 2.2. *[24] Let G be a graph with n vertices. Then we have*

$$\sqrt{\frac{M_1}{n}} \le \lambda_1(A_\alpha(G)) \le \Delta.$$

Lemma 2.3. *[9] Let G be a graph with n vertices and $m \ge 1$ edges. Then, $\lambda_i(Q(G)) = \lambda_i(A(\mathcal{L}(G))) + 2$, $i = 1, 2, \ldots, s$, where $s = \min\{n, m\}$. Further, if $m > n$, we have $\lambda_i(A(\mathcal{L}(G))) = -2$ for $i \ge n+1$, and if $n > m$, we have $\lambda_i(Q(G)) = 0$ for $i \ge m+1$.*

Lemma 2.4. *[8] For any C_3-free and C_4-free graph G, $A(G^2) = A^2(G) - L(G)$.*

3. Bounds on the sum of the largest A_α-eigenvalues

Theorem 3.1. *Let G be a graph with n vertices.*

(i) *If $0 \le \alpha < \frac{1}{2}$, then*

$$(1-\alpha)S_k(Q(G)) + (2\alpha - 1)S_k(D(G)) \le S_k(A_\alpha(G)) \le \alpha S_k(Q(G)) + (1-2\alpha)S_k(A(G))$$

for $1 \le k \le n$.

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

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

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

If G is r-regular, then the equality in the above inequalities must hold.

Proof. (i) Since $A_\alpha(G) = \alpha Q(G) + (1-2\alpha)A(G)$ for $0 \leq \alpha < \frac{1}{2}$, by Lemma 2.1, we have

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

If $0 \leq \alpha < \frac{1}{2}$, then $\frac{1}{2} \leq 1-\alpha \leq 1$. Note that $A_{1-\alpha}(G) = \alpha Q(G) + (1-2\alpha)D(G)$. Since $A_\alpha(G) + A_{1-\alpha}(G) = Q(G)$, by Lemma 2.1, we have

$$\begin{aligned} S_k(A_\alpha(G)) &\geq S_k(Q(G)) - S_k(A_{1-\alpha}(G)) \\ &\geq S_k(Q(G)) - \alpha S_k(Q(G)) - (1-2\alpha)S_k(D(G)) \\ &\geq (1-\alpha)S_k(Q(G)) + (2\alpha-1)S_k(D(G)). \end{aligned}$$

(ii) Since $A_\alpha(G) = (1-\alpha)Q(G) + (2\alpha-1)D(G)$ for $\frac{1}{2} \leq \alpha < 1$, by Lemma 2.1, we have

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

If $\frac{1}{2} \leq \alpha \leq 1$, then $0 \leq 1-\alpha \leq \frac{1}{2}$. Note 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 Lemma 2.1, we have

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

If G is r-regular, from [24], we have $S_k(A_\alpha(G)) = \alpha kr + (1-\alpha)S_k(A(G))$ and $S_k(Q(G)) = kr + S_k(A(G))$. Thus, the two above equations hold. This completes the proof. □

It is well known that the spectrum of any symmetric matrix majorizes its main diagonal, that is, $S_k(Q(G)) \geq S_k(D(G))$, and by Theorem 3.1, we have the following corollary.

Corollary 3.1. *Let G be a graph with n vertices. If* $\frac{1}{2} \leq \alpha < 1$*, then*

$$S_k(A_\alpha(G)) \leq \alpha S_k(Q(G))$$

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

From Corollary 3.1 and Conjecture 1.1, we give a new conjecture.

Conjecture 3.1. *Let G be a graph with n vertices and* $e(G)$ *edges. If* $\frac{1}{2} \leq \alpha < 1$*, then*

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

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

Theorem 3.2. *Let G be a graph with n vertices and m edges. If $0 \leq \alpha < 1$, then*

$$S_k(A_\alpha(G)) \leq \frac{(n-k)\lambda_1(A_\alpha(G)) + 2\alpha(k-1)m + \sqrt{(k-1)(n-k)\Upsilon}}{n-1}, \tag{3.1}$$

where $\Upsilon = (n-1)(\alpha^2 M_1 + 2m(1-\alpha)^2 - \lambda_1^2(A_\alpha(G))) - (2\alpha m - \lambda_1(A_\alpha(G)))^2$. The equality holds for $k = 1$. Moreover, the equality holds if and only if $\lambda_2(A_\alpha(G)) = \cdots = \lambda_k(A_\alpha(G))$ and $\lambda_{k+1}(A_\alpha(G)) = \cdots = \lambda_n(A_\alpha(G))$ for $k \geq 2$.

Proof. Let $\lambda_i(A_\alpha(G)) = \lambda_i$ and $S_k(A_\alpha(G)) = S_k$ for $i = 1, 2, \ldots, n$. Since $\sum_{i=1}^{n} \lambda_i = 2\alpha m$, $\sum_{i=1}^{n} \lambda_i^2 = \alpha^2 M_1 + 2m(1-\alpha)^2$, and by the Cauchy-Schwarz inequality, we have

$$\begin{aligned} S_k &\leq \lambda_1 + \sqrt{(k-1)(\lambda_2^2 + \cdots + \lambda_k^2)} \\ &= \lambda_1 + \sqrt{(k-1)\left(\alpha^2 M_1 + 2m(1-\alpha)^2 - \lambda_1^2 - \sum_{i=k+1}^{n} \lambda_i^2\right)} \\ &\leq \lambda_1 + \sqrt{(k-1)\left(\alpha^2 M_1 + 2m(1-\alpha)^2 - \lambda_1^2 - \frac{1}{n-k}(2\alpha m - S_k)^2\right)} \end{aligned}$$

with equality if and only if $\lambda_2 = \cdots = \lambda_k$ and $\lambda_{k+1} = \cdots = \lambda_n$ for $k \geq 2$. Thus,

$$(n-k)(S_k - \lambda_1)^2 + (k-1)(S_k - 2\alpha m)^2 \leq (k-1)(n-k)(\alpha^2 M_1 + 2m(1-\alpha)^2 - \lambda_1^2),$$

that is,

$$S_k \leq \frac{(n-k)\lambda_1 + 2\alpha(k-1)m + \sqrt{(k-1)(n-k)\Upsilon}}{n-1},$$

where

$$\begin{aligned} \Upsilon &= (n-1)(\alpha^2 M_1 + 2m(1-\alpha)^2 - \lambda_1^2) - (2\alpha m - \lambda_1)^2 \\ &= (n-1)\sum_{i=2}^{n} \lambda_i^2 - \left(\sum_{i=2}^{n} \lambda_i\right)^2 \\ &\geq 0. \end{aligned}$$

This completes the proof. □

Remark 3.1. *If the equality in* (3.1) *holds, then this implies that G has at most three distinct A_α-eigenvalues. If G is a connected graph with two distinct A_α-eigenvalues, then $G \cong K_n$. Clearly, the equality in* (3.1) *holds for K_n. If G is a graph with three distinct A_α-eigenvalues, then we refer to [30].*

Corollary 3.2. *Let G be a graph with n vertices and m edges. If p is the positive inertia index of $A(G)$, then*

$$\mathcal{E}(G) \leq \frac{2(n-p)\lambda_1(A(G)) + 2\sqrt{(p-1)(n-p)[2(n-1)m - n\lambda_1^2(A(G))]}}{n-1}. \tag{3.2}$$

The equality holds for K_n and $K_{s,t}$ ($s + t = n$).

Remark 3.2. *There are many graphs such that the equality in* (3.2) *holds, we may refer to [10, 28].*

Let α_0 be the smallest α such that $A_\alpha(G)$ is positive semidefinite for $\alpha_0 \leq \alpha \leq 1$. Recently, Nikiforov et al. [27] and Brondani et al. [4] found α_0 for some special classes of graphs.

Theorem 3.3. *Let* $0 \leq \alpha < \alpha_0$ *and* G *be a graph with* n *vertices and* m *edges. Then we have*

$$S_k(A_\alpha(G)) \leq 2\alpha m + \frac{1}{2}(2m(1-\alpha)^2 + \alpha^2 M_1)\sqrt{\frac{n(n-k)}{M_1}}$$

with equality if and only if $|\lambda_{k+1}(A_\alpha(G))| = \cdots = |\lambda_n(A_\alpha(G))| = \frac{2m(1-\alpha)^2+\alpha^2 M_1}{2}\sqrt{\frac{n}{(n-k)M_1}}$.

Proof. By Lemma 2.2, we have $\lambda_1(A_\alpha(G)) \geq \sqrt{\frac{M_1}{n}}$. We assume that

$$\sum_{i=1}^{n-k} \lambda_{n-i+1}^2(A_\alpha(G)) > \frac{n(2m(1-\alpha)^2 + \alpha^2 M_1)^2}{4M_1},$$

in which case

$$\begin{aligned} 2m(1-\alpha)^2 + \alpha^2 M_1 &= \sum_{i=1}^{k} \lambda_i^2(A_\alpha(G)) + \sum_{i=1}^{n-k} \lambda_{n-i+1}^2(A_\alpha(G)) \\ &\geq \lambda_1^2(A_\alpha(G)) + \sum_{i=1}^{n-k} \lambda_{n-i+1}^2(A_\alpha(G)) \\ &> \frac{M_1}{n} + \frac{n(2m(1-\alpha)^2 + \alpha^2 M_1)^2}{4M_1}. \end{aligned}$$

This implies that

$$\left(\sqrt{\frac{M_1}{n}} - \frac{1}{2}(2m(1-\alpha)^2 + \alpha^2 M_1)\sqrt{\frac{n}{M_1}}\right)^2 < 0,$$

which is a contradiction. Thus,

$$\sum_{i=1}^{n-k} \lambda_{n-i+1}^2(A_\alpha(G)) \leq \frac{n(2m(1-\alpha)^2 + \alpha^2 M_1)^2}{4M_1}.$$

By the Cauchy-Schwarz inequality, we have

$$\begin{aligned} S_k(A_\alpha(G)) &= 2\alpha m - \sum_{i=1}^{n-k} \lambda_{n-i+1}(A_\alpha(G)) \\ &\leq 2\alpha m + \sqrt{(n-k)\sum_{i=1}^{n-k} \lambda_{n-i+1}^2(A_\alpha(G))} \\ &\leq 2\alpha m + \frac{1}{2}(2m(1-\alpha)^2 + \alpha^2 M_1)\sqrt{\frac{n(n-k)}{M_1}} \end{aligned}$$

with equality if and only if $|\lambda_{k+1}(A_\alpha(G))| = \cdots = |\lambda_n(A_\alpha(G))| = \frac{2m(1-\alpha)^2+\alpha^2 M_1}{2}\sqrt{\frac{n}{(n-k)M_1}}$. This completes the proof. □

Corollary 3.3. *Let G be a graph with n vertices and m edges. If p is the positive inertia index of $A(G)$, then*

$$\mathcal{E}(G) \leq 2m\sqrt{\frac{n(n-p)}{M_1}}$$

with equality if and only if $|\lambda_{p+1}(A(G))| = \cdots = |\lambda_n(A(G))| = m\sqrt{\frac{n}{(n-p)M_1}}$.

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, $\mathcal{B}(M) = (b_{ij})$ (or denoted simply by $\mathcal{B}$) is called the quotient matrix of M.

Lemma 3.1. *[16] Let M be a symmetric partitioned matrix of order n with eigenvalues $\xi_1 \geq \xi_2 \geq \cdots \geq \xi_n$, and let $\mathcal{B}$ be 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 $i = 1, 2, \ldots, r$.*

Let $\mathcal{B}$ 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 3.4. *Let G be a connected graph with n vertices, m edges, chromatic number χ and independence number θ. If $0 \leq \alpha < 1$, then*

$$S_\chi(A_\alpha(G)) \geq \frac{2\alpha m}{\theta}.$$

Theorem 3.4. *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 $1 \leq k \leq n$,*

$$S_k(A_\alpha(G)) \geq \left(\alpha - \frac{1}{n-k+1}\right)\sum_{u\in U} d_u + \frac{2m - (1-\alpha)|\partial(U, V(G)\backslash U)|}{n-k+1},$$

where $\partial(U, V(G)\backslash U)$ is the set of edges which connect vertices in U with vertices in $V(G)\backslash U$.

Proof. If $2 \leq k \leq n$, then the quotient matrix of $A_\alpha(G)$ corresponding to the partition $V(G) = (\bigcup\limits_{x\in U}\{x\}) \cup (V(G)\backslash U)$ of G is

$$\mathcal{B}(G) = \left[\begin{array}{ccc|c} & & & b_{1,k} \\ & A_\alpha(U) & & \vdots \\ & & & b_{k-1,k} \\ \hline b_{k,1} & \cdots & b_{k,k-1} & b_{k,k} \end{array}\right],$$

where $A_\alpha(U)$ is the principal submatrix of $A_\alpha(G)$. By Lemma 3.1, we have

$$\begin{aligned} S_k(A_\alpha(G)) &\geq S_k(\mathcal{B}(G)) \\ &= tr(A_\alpha(U)) + b_{k,k} \\ &= \alpha \sum_{u\in U} d_u + \frac{2m - \sum\limits_{u\in U} d_u - (1-\alpha)|\partial(U, V(G)\backslash U)|}{n-k+1} \\ &= \left(\alpha - \frac{1}{n-k+1}\right)\sum_{u\in U} d_u + \frac{2m - (1-\alpha)|\partial(U, V(G)\backslash U)|}{n-k+1}. \end{aligned}$$

If $k = 1$, then U is an empty set. Thus, $\sum\limits_{u\in U} d_u = 0$ and $|\partial(U, V(G)\backslash U)| = 0$. Taking $X = (1, \ldots, 1)^T$, 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. □

Corollary 3.5. *Let G be a connected graph with n vertices, m edges and the positive inertia index p. Then we have*

$$\mathcal{E}(G) \geq \frac{4m - 2|\partial(U, V(G)\backslash U)|}{n-p+1} - \frac{2\sum_{u\in U} d_u}{n-p+1}.$$

4. On the sum of the largest A_α-eigenvalues of graph operations

Theorem 4.1. *Let G be a graph with n vertices and $m \geq 1$ edges. Then we have*

$$S_k(A_\alpha(\mathcal{L}(G))) \leq 2k(\alpha\Delta - 1) + (1-\alpha)S_k(Q(G))$$

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

$$S_k(A_\alpha(\mathcal{L}(G))) \leq 2\alpha k(\Delta - 1) + 2(1-\alpha)(m-k)$$

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 $d_{\mathcal{L}(G)}(w) = d_G(u) + d_G(v) - 2$. By Lemmas 2.1 and 2.3, we have

$$\begin{aligned} S_k(A_\alpha(\mathcal{L}(G))) &\leq \alpha S_k(D(\mathcal{L}(G))) + (1-\alpha)S_k(A(\mathcal{L}(G))) \\ &\leq \alpha k(2\Delta - 2) + (1-\alpha)(S_k(Q(G)) - 2k) \\ &= 2k(\alpha\Delta - 1) + (1-\alpha)S_k(Q(G)) \end{aligned}$$

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

$$S_k(A_\alpha(\mathcal{L}(G))) \leq \alpha k(2\Delta - 2) + (1-\alpha)(2m - 2n - 2(k-n)) = 2\alpha k(\Delta - 1) + 2(1-\alpha)(m-k)$$

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

By the special cases of Conjecture 1.2 and Theorem 4.1, we have the following corollaries.

Corollary 4.1. *If T is a tree with n vertices, then $S_k(A_\alpha(\mathcal{L}(T))) \leq 2k\alpha(\Delta-1)+(1-\alpha)(n-2)$ for $1 \leq k \leq n-1$. If U is a unicyclic graph with n vertices, then $S_k(A_\alpha(\mathcal{L}(U))) \leq 2k(\alpha\Delta-1)+(1-\alpha)(n+\frac{k^2+k}{2})$ for $1 \leq k \leq n$. If B is a bicyclic graph with n vertices, then $S_k(A_\alpha(\mathcal{L}(B))) \leq 2k(\alpha\Delta-1)+(1-\alpha)(n+1+\frac{k^2+k}{2})$ for $1 \leq k \leq n$.*

Corollary 4.2. *If T is a tree with n vertices, then $\mathcal{E}(\mathcal{L}(T)) \leq 2(n-2)$. If U is a unicyclic graph with n vertices, then $\mathcal{E}(\mathcal{L}(U))) \leq 2n+p^2-3p$. If B is a bicyclic graph with n vertices, then $\mathcal{E}(\mathcal{L}(B)) \leq 2n+p^2-3p+2$.*

Theorem 4.2. *Let G be a C_3-free and C_4-free graph with n vertices, m edges and the algebraic connectivity $a(G)$. If $0 \leq \alpha \leq 1$, then*

$$S_k(A_\alpha(G^2)) \leq \alpha(M_1(G)-(n-k)\delta^2(G))+(1-\alpha)(k\Delta^2(G)-(k-1)a(G)).$$

Proof. By Lemma 2.2, we have

$$\begin{aligned} S_k(A^2(G)) &= \lambda_1(A^2(G))+\lambda_2(A^2(G))+\cdots+\lambda_k(A^2(G)) \\ &\leq k\lambda_1^2(A(G)) \\ &\leq k\Delta^2(G). \end{aligned}$$

Since $\sum\limits_{u\in V(G^2)} d_u = M_1(G)$, by Lemmas 2.1 and 2.4, we have

$$\begin{aligned} S_k(A_\alpha(G^2)) &\leq \alpha S_k(D(G^2))+(1-\alpha)S_k(A(G^2)) \\ &\leq \alpha S_k(D(G^2))+(1-\alpha)(S_k(A^2(G))+S_k(-L(G))) \\ &\leq \alpha(M_1(G)-(n-k)\delta^2(G))+(1-\alpha)(k\Delta^2(G)-(k-1)a(G)). \end{aligned}$$

This completes the proof. □

Corollary 4.3. *Let G be a C_3-free and C_4-free graph with n vertices, m edges and the algebraic connectivity $a(G)$. If p is the positive inertia index of $A(G^2)$, then*

$$\mathcal{E}(G^2) \leq 2p\Delta^2(G)-2(p-1)a(G).$$

5. Conclusions

In this paper, we study the sum of the k largest eigenvalues of the A_α-matrix of a graph, which not only extends the results of the sum of the k largest eigenvalues of the adjacency matrix and signless Laplacian matrix, but it also gives new bounds on graph energy.

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Conflict of interest

The authors declare no conflicts of interest.

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