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BOUNDS ON THE A_α-SPREAD OF A GRAPH*

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Abstract. Let G be a simple undirected graph. For any real number $\alpha \in [0,1]$, Nikiforov defined the A_α-matrix of 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 G, respectively. The A_α-spread of a graph is defined as the difference between the largest eigenvalue and the smallest eigenvalue of the associated A_α-matrix. In this paper, some lower and upper bounds on A_α-spread are obtained, which extend the results of A-spread and Q-spread. Moreover, the trees with the minimum and the maximum A_α-spread are determined, respectively.

Key words. Graph, A_α-matrix, A_α-eigenvalue, A_α-spread, Bound.

AMS subject classifications. 05C50.

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 $v_i \in V(G)$, $d(v_i) = d_i(G)$ denotes the degree of vertex v_i in G. The minimum and the maximum degree of G are denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. For any real number $\alpha \in [0,1]$, Nikiforov [25] defined the A_α-matrix of G as

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

where $D(G)$ is the diagonal matrix of the vertex degrees of G and $A(G)$ is the adjacency matrix. It is easy to see that $A_\alpha(G)$ is the adjacency matrix $A(G)$ if $\alpha = 0$, and $A_\alpha(G)$ is essentially equivalent to signless Laplacian matrix $Q(G)$ if $\alpha = 1/2$. The new matrix not only can underpin a unified theory of $A(G)$ and $Q(G)$, but it also brings many new interesting problems (see [25, 27, 28]). There are a considerable results regarding $A_\alpha(G)$ in the literature. For related results, one may refer to [3, 5, 12, 18, 20, 21, 25, 32, 34] and references therein.

Let $\lambda_i(M)$ be the i-th largest eigenvalue of a symmetric matrix M. The spread of M is defined by

$$S_M = \lambda_1(M) - \lambda_n(M).$$

There is a considerable literature on the spread of a symmetric matrix [14, 15, 22, 30]. For a graph G, Gregory et al. [10] investigated the spread of the adjacency matrix of G, called the A-spread, defined as

$$S_A(G) = \lambda_1(A(G)) - \lambda_n(A(G)).$$

Liu et al. [17] and Oliveira et al. [31] proposed the signless Laplacian spread of a graph G, called the Q-spread, defined as

$$S_Q(G) = \lambda_1(Q(G)) - \lambda_n(Q(G)).$$

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There are several results concerning A-spread and Q-spread, see for example [1, 2, 7, 10, 17, 31] and the references therein.

Motivated by the definition of A-spread and Q-spread, we define A_α-spread of a graph G as

$$S_\alpha(G) = \lambda_1(A_\alpha(G)) - \lambda_n(A_\alpha(G)).$$

Since $S_0(G) = S_A(G)$ and $S_{1/2}(G) = \frac{1}{2}S_Q(G)$, the A_α-spread can be regard as a common generalization of A-spread and Q-spread.

The primary purpose of this paper is to establish the bounds of A_α-spread of graphs, which extend the results of A-spread and Q-spread. The rest of the paper is organized as follows. In Section 2, we recall some useful notions and lemmas used further. In Section 3, some upper bounds on the A_α-spread are obtained. In Section 4, some lower bounds on the A_α-spread are presented. In Section 5, the trees with the minimum and the maximum A_α-spread are determined, respectively.

2. Preliminaries. Let $K_{1,\,n-1}$ and K_n denote the star and the complete graph with n vertices, respectively. Let $K_{r,\,s}$ denote the complete bipartite graph with $r+s$ vertices. Let P_n and C_n denote the path and the cycle with n vertices, respectively. A subset I of $V(G)$ is called an independent set of a graph G if no two vertices in I are adjacent in G. A clique of a graph G is a subset of vertices such that it induces a complete subgraph of G. Given a graph G, the independence number $a = a(G)$ and the clique number $\omega = \omega(G)$ of G are the numbers of vertices of the largest independent set and the largest clique in G, respectively. The chromatic number $\chi = \chi(G)$ 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. Denote by $\overline{G}$ the complement of a graph G.

Lemma 2.1. ([22]) *Let H be an $n \times n$ matrix. Then*

$$S_H = \left(2||H||_F^2 - \frac{2}{n}(trH)^2\right)^{\frac{1}{2}}$$

with equality if and only if H is normal and the eigenvalues $h_1, h_2, \ldots, h_n$ of H satisfy the following condition

$$h_2 = \cdots = h_{n-1} = \frac{h_1 + h_n}{2}.$$

Lemma 2.2. ([33]) *Let A and B be Hermitian matrices of order n, and let $1 \le i \le n$ and $1 \le j \le n$. Then*

$$\lambda_i(A) + \lambda_j(B) \le \lambda_{i+j-n}(A+B), \quad if\, i+j \ge n+1,$$

$$\lambda_i(A) + \lambda_j(B) \ge \lambda_{i+j-1}(A+B), \quad if\, i+j \le n+1.$$

In either of these inequalities, the equality holds if and only if there exists a nonzero n-vector that is an eigenvector to each of the three eigenvalues involved.

Lemma 2.3. ([26]) *Let M be a Hermitian matrix partitioned into $r \times r$ blocks so that all diagonal blocks are zero. Then for every real diagonal matrix N of the same size as M,*

$$\lambda_1(N - M) \ge \lambda_1\left(N + \frac{1}{r-1}M\right).$$

Lemma 2.4. ([25]) *Let G be a graph with n vertices. If $0 \le \alpha \le 1/2$, then $\lambda_1(A_\alpha) \ge \alpha(\Delta+1)$. If $1/2 \le \alpha < 1$, then $\lambda_1(A_\alpha) \ge \alpha\Delta + \frac{(1-\alpha)^2}{\alpha}$.*

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Lemma 2.5. ([25]) *Let G be a graph with n vertices. If $0 \leq \alpha \leq 1$, then $\lambda_n(A_\alpha) \leq \alpha\delta$.*

Lemma 2.6. ([16]) *Let G be a graph of order n with m edges and $1/2 \leq \alpha \leq 1$. If G has isolated vertices, then $\lambda_n(A_\alpha(G)) = 0$. Otherwise,*

$$\lambda_n(A_\alpha(G)) \leq \left(\frac{2m}{n} + 1\right)\alpha - 1$$

with equality if and only if $G \cong tK_q$ with $\alpha < 1$, where $n = qt$, $t \geq 1$ and $q > 1$, or G is a regular graph with $\alpha = 1$.

Lemma 2.7. ([25]) *If G is a connected graph of diameter D, then $A_\alpha(G)$ has at least $D + 1$ distinct eigenvalues.*

Lemma 2.8. ([9]) *Let M be a Hermitian matrix of order n with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ as eigenvalues, and B a principal submatrix of order p, and let B have eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_p$. Then the inequalities $\lambda_{n-p+i} \leq \mu_i \leq \lambda_i$ hold.*

Lemma 2.9. ([1]) *Let M be a real symmetric matrix of order n. Then*

$$S_M \geq 2 \max_{X \in B_n} \sqrt{X^T M^2 X - (X^T M X)^2},$$

where B_n denote the unit ball in R^n, that is, the set of vectors in R^n such that $||X|| \leq 1$.

The first Zagreb index are defined as $M_1 = M_1(G) = \sum_{i=1}^n d_i^2(G)$. There is a wealth of literature relating to the first Zagreb index, the reader is referred to the survey [4, 8] and the references therein.

Lemma 2.10. ([4, 8]) *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \leq \frac{4m^2}{n} + \frac{n}{4}(\Delta - \delta)^2.$$

Lemma 2.11. ([4, 24]) *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2$$

with equality if and only if G has the property $d_2 = d_3 = \cdots = d_{n-1} = (\Delta + \delta)/2$, which includes also the regular graphs.

Lemma 2.12. ([23]) *Let $(a_1, \ldots, a_n)$ and $(b_1, \ldots, b_n)$ be two vectors with $0 < a \leq a_i \leq A$ and $0 < b \leq b_i \leq B$, for $i = 1, \ldots, n$, for some constants a, b, A and B. Then*

$$\left(\sum_{i=1}^n a_i^2\right)\left(\sum_{i=1}^n b_i^2\right) - \left(\sum_{i=1}^n a_i b_i\right)^2 \leq \frac{n^2}{4}(AB - ab)^2.$$

Lemma 2.13. ([15]) *Let $M = (m_{ij})$ be an $n \times n$ Hermitian matrix. Then*

$$S_M \geq \max_{i \neq j} \left[(m_{ii} - m_{jj})^2 + 2\sum_{k \neq i} |m_{ik}|^2 + 2\sum_{k \neq j} |m_{jk}|^2 + 4e_{ij}\right]^{\frac{1}{2}},$$

where $e_{ij} = 2f_{ij}$ if $m_{ii} = m_{jj}$ and otherwise

$$e_{ij} = \min\left\{(m_{ii} - m_{jj})^2 + 2|(m_{ii} - m_{jj})^2 - f_{ij}|, \frac{f_{ij}^2}{(m_{ii} - m_{jj})^2}\right\}$$

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with

$$f_{ij} = \left| \sum_{k\neq i} |m_{ik}|^2 - \sum_{k\neq j} |m_{jk}|^2 \right|.$$

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

LEMMA 2.14. ([11]) *Let A 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 $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_m$ and $n > m$. Then $\xi_i \geq \eta_i \geq \xi_{n-m+i}$ for $i = 1, 2, \ldots, m$.*

LEMMA 2.15. ([29, 35]) *Let G be a connected graph with $\alpha \in [0, 1)$. For $u, v \in V(G)$, suppose $N \subseteq N(v) \setminus (N(u) \cup \{u\})$. Let $G' = G - \{vw : w \in N\} + \{uw : w \in N\}$. Let X be a unit eigenvector of $A_\alpha(G)$ corresponding to $\lambda_1(A_\alpha(G))$. If $N \neq \Phi$ and $x_u \geq x_v$, then $\lambda_1(A_\alpha(G')) > \lambda_1(A_\alpha(G))$.*

3. Upper bounds for A_α-spread.

THEOREM 3.1. *Let G be a graph with n vertices and m edges. If $0 \leq \alpha \leq 1$, then*

$$S_\alpha(G) \leq \sqrt{2\alpha^2 M_1 + 4m(1-\alpha)^2 - \frac{8\alpha^2 m^2}{n}}. \tag{3.1}$$

If G is a complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$, then equality holds.

Proof. Since $A_\alpha(G)$ is a normal matrix, by Lemma 2.1, we have

$$S_\alpha(G) \leq \left(2||A_\alpha(G)||_F^2 - \frac{2}{n}(trA_\alpha(G))^2\right)^{\frac{1}{2}} = \sqrt{2\alpha^2 M_1 + 4m(1-\alpha)^2 - \frac{8\alpha^2 m^2}{n}}.$$

It is easy to verify that the equality holds when G is a complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$. ∎

PROBLEM 3.2. *Find all cases of equality in (3.1).*

COROLLARY 3.3. *Let G be a connected k-regular graph with n vertices. If $0 \leq \alpha \leq 1$, then*

$$S_\alpha(G) \leq (1-\alpha)\sqrt{2kn}.$$

If G is a complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$, then equality holds.

The following result is direct corollary of Lemma 2.10 and Theorem 3.1.

COROLLARY 3.4. *Let G be a graph with n vertices and m edges. If $0 \leq \alpha \leq 1$, then*

$$S_\alpha(G) \leq \frac{\sqrt{2}}{2}\sqrt{\alpha^2 n(\Delta-\delta)^2 + 8m(1-\alpha)^2}.$$

If G is a complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$, then equality holds.

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THEOREM 3.5. *Let G be a graph with n vertices.*

(i) *If $0 \le \alpha \le 1$, then $S_\alpha(G) \le \alpha(\Delta - \delta) + (1-\alpha)S_A(G)$;*

(ii) *If $0 \le \alpha < 1/2$, then $S_\alpha(G) \le \alpha S_Q(G) + (1-2\alpha)S_A(G)$;*

(iii) *If $1/2 \le \alpha \le 1$, then $S_\alpha(G) \le (1-\alpha)S_Q(G) + (2\alpha-1)(\Delta-\delta)$;*

(iv) *If $0 \le \alpha \le 1$, then $S_{1-\alpha}(G) - S_\alpha(G) \le S_Q(G) \le S_{1-\alpha}(G) + S_\alpha(G)$;*

(v) *If $0 \le \beta \le \alpha \le 1$, then $S_\alpha(G) + S_\beta(G) \ge (\alpha-\beta)\lambda_1(L(G))$, where $L(G) = D(G) - A(G)$ is the Laplacian matrix of G.*

If G is a regular graph, then equality holds in (i)–(iii).

Proof. (i) Since $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$, by Lemma 2.2, we have

$$\lambda_1(A_\alpha(G)) \le \alpha\lambda_1(D(G)) + (1-\alpha)\lambda_1(A(G))$$

and

$$\lambda_n(A_\alpha(G)) \ge \alpha\lambda_n(D(G)) + (1-\alpha)\lambda_n(A(G)).$$

Thus, $S_\alpha(G) \le \alpha(\Delta-\delta) + (1-\alpha)S_A(G)$.

(ii) Since $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G) = \alpha Q(G) + (1-2\alpha)A(G)$, by Lemma 2.2, we have

$$\lambda_1(A_\alpha(G)) \le \alpha\lambda_1(Q(G)) + (1-2\alpha)\lambda_1(A(G))$$

and

$$\lambda_n(A_\alpha(G)) \ge \alpha\lambda_n(Q(G)) + (1-2\alpha)\lambda_n(A(G))$$

for $0 \le \alpha < 1/2$. Thus, $S_\alpha(G) \le \alpha S_Q(G) + (1-2\alpha)S_A(G)$.

(iii) Since $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G) = (1-\alpha)Q(G) + (2\alpha-1)D(G)$, by Lemma 2.2, we have

$$\lambda_1(A_\alpha(G)) \le (1-\alpha)\lambda_1(Q(G)) + (2\alpha-1)\lambda_1(D(G))$$

and

$$\lambda_n(A_\alpha(G)) \ge (1-\alpha)\lambda_n(Q(G)) + (2\alpha-1)\lambda_n(D(G))$$

for $1/2 \le \alpha \le 1$. Thus, $S_\alpha(G) \le (1-\alpha)S_Q(G) + (2\alpha-1)(\Delta-\delta)$.

(iv) Since $A_{1-\alpha}(G) + A_\alpha(G) = Q(G)$, by Lemma 2.2, we have

$$\lambda_1(A_{1-\alpha}(G)) + \lambda_n(A_\alpha(G)) \le \lambda_1(Q(G)) \le \lambda_1(A_{1-\alpha}(G)) + \lambda_1(A_\alpha(G))$$

and

$$\lambda_n(A_{1-\alpha}(G)) + \lambda_n(A_\alpha(G)) \le \lambda_n(Q(G)) \le \lambda_1(A_\alpha(G)) + \lambda_n(A_{1-\alpha}(G))$$

for $0 \le \alpha \le 1$. Thus, $S_{1-\alpha}(G) - S_\alpha(G) \le S_Q(G) \le S_{1-\alpha}(G) + S_\alpha(G)$.

(v) Since $A_\alpha(G) - A_\beta(G) = (\alpha-\beta)L(G)$, by Lemma 2.2, we have

$$(\alpha-\beta)\lambda_1(L(G)) \le \lambda_1(A_\alpha(G)) - \lambda_n(A_\beta(G))$$

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and

$$(\alpha-\beta)\lambda_n(L(G)) \geq \lambda_n(A_\alpha(G)) - \lambda_1(A_\beta(G))$$

for $0 \leq \beta \leq \alpha \leq 1$. It is well known that $\lambda_n(L(G)) = 0$. Thus, $S_\alpha(G) + S_\beta(G) \geq (\alpha-\beta)\lambda_1(L(G))$. This completes the proof. ∎

COROLLARY 3.6. *Let P_n denote the path with n vertices.*

(i) *If $0 \leq \alpha \leq 1$, then $S_\alpha(P_n) \leq \alpha + 4(1-\alpha)cos\left(\frac{\pi}{n+1}\right)$;*

(ii) *If $0 \leq \alpha < 1/2$, then $S_\alpha(P_n) \leq 2\alpha\left(1 + cos\left(\frac{\pi}{n}\right)\right) + 4(1-2\alpha)cos\left(\frac{\pi}{n+1}\right)$;*

(iii) *If $1/2 \leq \alpha \leq 1$, then $S_\alpha(P_n) \leq 1 + 2(1-\alpha)cos\left(\frac{\pi}{n}\right)$.*

Gregory et al. [10] proved that $S_A(G) \leq \lambda_1(A(G)) + \sqrt{2m - \lambda_1^2(A(G))}$ with equality if and only if $G = K_{r,\,s}$ for some r, s with $r+s=n$. Let χ be the chromatic number of G. Nikiforov and Rojo [28] showed that $A_\alpha(G)$ is not positive semi-definite for $\alpha < 1/\chi$. In this case, we give an upper bound on A_α-spread under chromatic number condition.

THEOREM 3.7. *Let $0 < \alpha \leq 1/\chi$, and G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$S_\alpha(G) \leq \lambda_1(A_\alpha(G)) + \sqrt{2(1-\alpha)^2 m + \alpha^2 M_1 - \lambda_1^2(A_\alpha(G))}.$$

The equality holds if and only if G is a complete graph K_n and $\alpha = \frac{1}{n}$.

Proof. Since $\lambda_1^2(A_\alpha(G)) + \lambda_2^2(A_\alpha(G)) + \cdots + \lambda_n^2(A_\alpha(G)) = Tr(A_\alpha^2(G))$, it follows that $\lambda_1^2(A_\alpha(G)) + \lambda_n^2(A_\alpha(G)) \leq 2(1-\alpha)^2 m + \alpha^2 M_1$. Noting that $0 < \alpha \leq 1/\chi$, we have

$$S_\alpha(G) = \lambda_1(A_\alpha(G)) + |\lambda_n(A_\alpha(G))| \leq \lambda_1(A_\alpha(G)) + \sqrt{2(1-\alpha)^2 m + \alpha^2 M_1 - \lambda_1^2(A_\alpha(G))}.$$

If the equality holds, then $\lambda_2(A_\alpha(G)) = \cdots = \lambda_{n-1}(A_\alpha(G)) = 0$. Let D be the diameter of G. By Lemma 2.7, we have $D \leq 2$. In the case when $D = 2$, let $u, v \in V(G)$ such that $uv \notin E(G)$, and A_2' be the principal submatrix of $A_\alpha(G)$ corresponding to vertices u and v. Namely,

$$A_2' = \begin{pmatrix} \alpha d(u) & 0 \\ 0 & \alpha d(v) \end{pmatrix}.$$

Without loss of generality, we may assume that $d(u) \geq d(v)$. By Lemma 2.8, we have $0 = \lambda_2(A_\alpha(G)) \geq \alpha d(v)$ for $\alpha > 0$, a contradiction. Hence, $D = 1$, that is, $G = K_n$. From Proposition 36 in [25], we have $\lambda_i(K_n) = \alpha n - 1$ for $i = 2, \ldots, n$. Since $\lambda_i(A_{1/n}(K_n)) = 0$ for $i = 2, \ldots, n-1$, it follows that $\alpha = \frac{1}{n}$. Conversely, it is easy to verify that the equality holds when $G = K_n$ and $\alpha = \frac{1}{n}$. The proof is completed. ∎

THEOREM 3.8. *Let G be a graph with n vertices. If $(1-\alpha)(\chi-1) = 1$, then*

$$S_\alpha(G) \leq \alpha(\Delta - \delta) - (2-\alpha)\lambda_n(A(G)).$$

Proof. In this proof, we use Lemma 2.3 with $r = \chi$, $N = \alpha D(G)$ and $M = A(G)$. Since $(1-\alpha)(\chi-1) = 1$, it follows that

$$\lambda_1(A_\alpha(G)) = \lambda_1(\alpha D(G) + (1-\alpha)A(G)) \leq \lambda_1(\alpha D(G) - A(G)).$$

By Lemma 2.2, we have

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$$\lambda_1(A_\alpha(G)) \leq \alpha\Delta - \lambda_n(A(G)) \text{ and } \lambda_n(A_\alpha(G)) \geq \alpha\delta + (1-\alpha)\lambda_n(A(G)).$$

Thus, $S_\alpha(G) \leq \alpha(\Delta-\delta) - (2-\alpha)\lambda_n(A(G))$. The proof is completed. ◻

For a graph G, Hong and Shu [13] showed that $\lambda_n(A(G)) \geq -\sqrt{2(n-\chi)}$ for $n \geq 3$. By Theorem 3.8, we have

Corollary 3.9. *Let G be a graph with $n \geq 3$ vertices. If $(1-\alpha)(\chi-1) = 1$, then*

$$S_\alpha(G) \leq \alpha(\Delta-\delta) + (2-\alpha)\sqrt{2(n-\chi)}.$$

4. Lower bounds for A_α-spread.

Theorem 4.1. *Let G be a graph with n vertices. If $0 \leq \alpha \leq 1/2$, then*

$$S_\alpha(G) \geq \alpha(\Delta-\delta) + \alpha.$$

If $1/2 \leq \alpha < 1$, then

$$S_\alpha(G) \geq \alpha(\Delta-\delta) + \frac{(1-\alpha)^2}{\alpha}.$$

Proof. By Lemmas 2.4 and 2.5, we have the proof. ◻

Theorem 4.2. *Let $1/2 \leq \alpha \leq 1$, and G be a graph with n vertices and m edges. If G has no isolated vertices, then*

$$S_\alpha(G) \geq (1-\alpha)\left(\frac{2m}{n}+1\right)$$

with equality if and only if $G \cong tK_q$ with $\alpha < 1$, where $n = qt$, $t \geq 1$ and $q > 1$, or G is a regular graph with $\alpha = 1$.

Proof. From [6] and [25], we have $\lambda_1(A_\alpha(G)) \geq \lambda_1(A(G)) \geq \frac{2m}{n}$ with equality if and only if G is a regular graph. By Lemma 2.6, we have

$$S_\alpha(G) = \lambda_1(A_\alpha(G)) - \lambda_n(A_\alpha(G)) \geq \frac{2m}{n} - \left(\frac{2m}{n}+1\right)\alpha + 1 = (1-\alpha)\left(\frac{2m}{n}+1\right)$$

with equality if and only if $G \cong tK_q$ with $\alpha < 1$, where $n = qt$, $t \geq 1$ and $q > 1$, or G is a regular graph with $\alpha = 1$. The proof is completed. ◻

Theorem 4.3. *Let G be a graph with n vertices. If $0 \leq \alpha \leq 1$, then*

$$S_\alpha(G) \geq \frac{2}{n}\sqrt{nM_1 - 4m^2}.$$

Proof. Let $X = \frac{1}{\sqrt{n}}(1,\ldots,1)^T$. Then

$$\begin{aligned} X^TA_\alpha^2(G)X &= X^T(\alpha D(G) + (1-\alpha)A(G))^2X \\ &= \alpha^2X^TD^2(G)X + (1-\alpha)^2X^TA^2(G)X \\ &\quad + \alpha(1-\alpha)X^TD(G)A(G)X + \alpha(1-\alpha)X^TA(G)D(G)X \\ &= \frac{M_1}{n} \end{aligned}$$

and

$$X^TA_\alpha(G)X = X^T(\alpha D(G) + (1-\alpha)A(G))X = \alpha X^TD(G)X + (1-\alpha)X^TA(G)X = \frac{2m}{n}.$$

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By Lemma 2.9, we have

$$S_\alpha(G) \geq 2 \max_{X \in B_n} \sqrt{X^T A_\alpha^2(G) X - (X^T A_\alpha(G) X)^2} = \frac{2}{n}\sqrt{nM_1 - 4m^2}.$$

This completes the proof. ∎

THEOREM 4.4. *Let G be a connected graph with n vertices. If $1/2 < \alpha \leq 1$, then*

$$S_\alpha(G) \geq \frac{2}{n}\sqrt{2(1-\alpha)^2 mn + \alpha^2 n M_1 - 4\alpha^2 m^2}.$$

Proof. In this proof, we use Lemma 2.12 with $a_i = \lambda_i(A_\alpha(G))$ and $b_i = 1$ for $1 \leq i \leq n$. Since $0 < \lambda_n(A_\alpha(G)) \leq a_i \leq \lambda_1(A_\alpha(G))$, and $b_i = 1$, $1 \leq i \leq n$. Thus, $AB = \lambda_1(A_\alpha(G))$ and $ab = \lambda_n(A_\alpha(G))$. By Lemma 2.12, we have

$$\sum_{i=1}^n \lambda_i^2(A_\alpha(G)) \sum_{i=1}^n 1^2 - \left(\sum_{i=1}^n \lambda_i(A_\alpha(G))\right)^2 \leq \frac{n^2}{4}(\lambda_1(A_\alpha(G)) - \lambda_n(A_\alpha(G)))^2.$$

Then

$$n(2(1-\alpha)^2 m + \alpha^2 M_1) - 4\alpha^2 m^2 \leq \frac{n^2}{4} S_\alpha^2(G),$$

that is,

$$S_\alpha(G) \geq \frac{2}{n}\sqrt{2(1-\alpha)^2 mn + \alpha^2 n M_1 - 4\alpha^2 m^2}.$$

Thus, the result follows. ∎

By Lemma 2.11, Theorems 4.3 and 4.4, we get the following corollaries, respectively.

COROLLARY 4.5. *Let G be a graph with n vertices. If $0 \leq \alpha \leq 1$, then*

$$S_\alpha(G) \geq (\Delta - \delta)\sqrt{\frac{2}{n}}.$$

COROLLARY 4.6. *Let G be a connected graph with n vertices and m edges. If $1/2 < \alpha \leq 1$, then*

$$S_\alpha(G) \geq \frac{1}{n}\sqrt{8(1-\alpha)^2 mn + 2\alpha^2 n(\Delta - \delta)^2}.$$

THEOREM 4.7. *Let G be a connected graph. If $0 \leq \alpha \leq 1$ and $\Delta - \delta \geq (1 - \frac{1}{\alpha})^2$, then*

$$S_\alpha(G) \geq \sqrt{\alpha^2(\Delta-\delta)^2 + 2(1-\alpha)^2(\Delta+\delta) + \frac{4(1-\alpha)^4}{\alpha^2}}.$$

If $0 \leq \alpha \leq 1$ and $\Delta - \delta < (1 - \frac{1}{\alpha})^2$, then

$$S_\alpha(G) \geq \sqrt{2(1-\alpha)^2(5\Delta - 3\delta) - 3\alpha^2(\Delta-\delta)^2}.$$

Proof. Let $V(\Delta) = \{v \in V(G) : d(v) = \Delta\}$ and $V(\delta) = \{v \in V(G) : d(v) = \delta\}$. By Lemma 2.13, we have

$$S_\alpha(G) = S(A_\alpha(G)) \geq \Upsilon,$$

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where

$$\Upsilon = \max_{i\neq j}\left[(a_{ii}-a_{jj})^2 + 2\sum_{k\neq i}|a_{ik}|^2 + 2\sum_{k\neq j}|a_{jk}|^2 + 4e_{ij}\right]^{\frac{1}{2}}$$

and e_{ij} and f_{ij} are given in Lemma 2.13.

Let $v_{i_0}\in V(\Delta)$ and $v_{j_0}\in V(\delta)$. If $a_{j_0j_0}=a_{i_0i_0}$, then $e_{i_0j_0}=2f_{i_0j_0}$; otherwise

$$e_{i_0j_0} = \min\left\{(a_{i_0i_0}-a_{j_0j_0})^2 + 2|(a_{i_0i_0}-a_{j_0j_0})^2 - f_{i_0j_0}|, \frac{f_{i_0j_0}^2}{(a_{i_0i_0}-a_{j_0j_0})^2}\right\}$$

with

$$f_{i_0j_0} = \left|\sum_{k\neq i_0}|a_{i_0k}|^2 - \sum_{k\neq j_0}|a_{j_0k}|^2\right| = \left|(1-\alpha)^2(d(v_{i_0})-d(v_{j_0}))\right| = (1-\alpha)^2(\Delta-\delta).$$

Therefore,

$$\begin{aligned} e_{i_0j_0} &= \min\left\{\alpha^2(\Delta-\delta)^2 + 2\left|\alpha^2(\Delta-\delta)^2-(1-\alpha)^2(\Delta-\delta)\right|, \frac{(1-\alpha)^4}{\alpha^2}\right\} \\ &= \begin{cases} \frac{(1-\alpha)^4}{\alpha^2}, & if\ \ \Delta-\delta \geq \left(1-\frac{1}{\alpha}\right)^2; \\ 2(1-\alpha)^2(\Delta-\delta)-\alpha^2(\Delta-\delta)^2, & if\ \ \Delta-\delta < \left(1-\frac{1}{\alpha}\right)^2. \end{cases} \end{aligned}$$

Thus,

$$\Upsilon \geq \begin{cases} \sqrt{\alpha^2(\Delta-\delta)^2 + 2(1-\alpha)^2(\Delta+\delta) + \frac{4(1-\alpha)^4}{\alpha^2}}, & if\ \ \Delta-\delta \geq \left(1-\frac{1}{\alpha}\right)^2; \\ \sqrt{2(1-\alpha)^2(5\Delta-3\delta)-3\alpha^2(\Delta-\delta)^2}, & if\ \ \Delta-\delta < \left(1-\frac{1}{\alpha}\right)^2. \end{cases}$$

The proof is completed. □

Let $V(G)=V_1\cup V_2$ be a partition of G. Then $e(V_1,V_2)$ stands for the number of edges joining vertices of V_1 to vertices of V_2.

THEOREM 4.8. *Let G be a connected graph with n vertices, and let $V(G)=V_1\cup V_2$ be a partition of G with $n_i := |V_i|$ for $i=1,2$. If $0\leq\alpha\leq 1$, then*

$$S_\alpha(G) \geq \sqrt{(\overline{d_1}-\overline{d_2})^2 - 2t(1-\alpha)(\overline{d_1}-\overline{d_2})\left(\frac{1}{n_1}-\frac{1}{n_2}\right) + t^2(1-\alpha)^2\left(\frac{1}{n_1}+\frac{1}{n_2}\right)^2},$$

where $t=e(V_1,V_2)$, $\overline{d_1}=\sum_{v\in V_1}d(v)/n_1$ and $\overline{d_2}=\sum_{v\in V_2}d(v)/n_2$.

Proof. Let $\mathcal{B}(G)$ be the quotient matrix of $A_\alpha(G)$ corresponding to the partition $V(G)=V_1\cup V_2$ of G. Then

$$\mathcal{B}(G) = \begin{pmatrix} \overline{d_1}-\frac{t(1-\alpha)}{n_1} & \frac{t(1-\alpha)}{n_1} \\ \frac{t(1-\alpha)}{n_2} & \overline{d_2}-\frac{t(1-\alpha)}{n_2} \end{pmatrix}. \tag{4.1}$$

By direct computing, we know the characteristic polynomial of (4.1) is as follows:

$$\det(xI_n-\mathcal{B}(G)) = x^2 - \left(\overline{d_1}+\overline{d_2}-\frac{t(1-\alpha)}{n_1}-\frac{t(1-\alpha)}{n_2}\right)x + \overline{d_1d_2} - \frac{t(1-\alpha)\overline{d_2}}{n_1} - \frac{t(1-\alpha)\overline{d_1}}{n_2}.$$

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By Lemma 2.14, we have

$$\begin{aligned} S_\alpha(G) &\geq \eta_1(\mathcal{B}) - \eta_2(\mathcal{B}) \\ &= \sqrt{(\eta_1(\mathcal{B}) + \eta_2(\mathcal{B}))^2 - 4\eta_1(\mathcal{B})\eta_2(\mathcal{B})} \\ &= \sqrt{(\overline{d_1} - \overline{d_2})^2 - 2t(1-\alpha)(\overline{d_1} - \overline{d_2})\left(\frac{1}{n_1} - \frac{1}{n_2}\right) + t^2(1-\alpha)^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)^2}. \end{aligned}$$

The proof is completed. □

Corollary 4.9. *Let G be a connected k-regular graph with n vertices, and let $V(G) = V_1 \cup V_2$ be a partition of G with $n_i := |V_i|$ for $i = 1, 2$. Then*

$$S_\alpha(G) \geq t(1-\alpha)\left(\frac{1}{n_1} + \frac{1}{n_2}\right),$$

where $t = e(V_1, V_2)$.

Further, let V_1 in Corollary 4.9 be the largest independent set and the largest clique, respectively. Then the following corollaries are obtained.

Corollary 4.10. *Let G be a connected k-regular graph with n vertices and independence number a. Then*

$$S_\alpha(G) \geq \frac{kn(1-\alpha)}{n-a}.$$

Corollary 4.11. *Let G be a connected k-regular graph with n vertices and clique number ω. Then*

$$S_\alpha(G) \geq \frac{n(1-\alpha)(k-\omega+1)}{n-\omega}.$$

Theorem 4.12. *If $0 \leq \alpha \leq 1$ and G is a graph with n vertices, then*

$$S_\alpha(G) + S_\alpha(\overline{G}) \geq (1-\alpha)n.$$

Proof. From Proposition 36 in [25], we have $\lambda_1(A_\alpha(K_n)) = n - 1$ and $\lambda_n(A_\alpha(K_n)) = \alpha n - 1$. Noting that $A_\alpha(G) + A_\alpha(\overline{G}) = A_\alpha(K_n)$, by Lemma 2.2, we have

$$\lambda_1(A_\alpha(K_n)) \leq \lambda_1(A_\alpha(G)) + \lambda_1(A_\alpha(\overline{G}))$$

and

$$\lambda_n(A_\alpha(K_n)) \geq \lambda_n(A_\alpha(G)) + \lambda_n(A_\alpha(\overline{G})).$$

These imply that $S_\alpha(G) + S_\alpha(\overline{G}) \geq (1-\alpha)n$. The proof is completed. □

The Cartesian product of G_1 and G_2 is the graph $G_1 \Box G_2$, whose vertex set is $V = V_1 \times V_2$ and where two vertices (u_i, v_s) and (u_j, v_t) are adjacent if and only if either $u_i = u_j$ and $v_s v_t \in E(G_2)$ or $v_s = v_t$ and $u_i u_j \in E(G_1)$.

Lemma 4.13. ([19]) *Let G_1 and G_2 be graphs on n_1 and n_2 vertices, respectively. Then the A_α-eigenvalues of $G_1 \Box G_2$ are all possible sums $\lambda_i(A_\alpha(G_1)) + \lambda_j(A_\alpha(G_2))$, $1 \leq i \leq n_1$ and $1 \leq j \leq n_2$.*

Theorem 4.14. *If $0 \leq \alpha \leq 1$ and $G = G_1 \Box G_2$, then*

$$S_\alpha(G) = S_\alpha(G_1) + S_\alpha(G_2).$$

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Proof. As a consequence of Lemma 4.13, we have

$$\lambda_1(A_\alpha(G)) = \lambda_1(A_\alpha(G_1)) + \lambda_1(A_\alpha(G_2)),\ \lambda_n(A_\alpha(G)) = \lambda_n(A_\alpha(G_1)) + \lambda_n(A_\alpha(G_2)).$$

Thus, $S_\alpha(G) = S_\alpha(G_1) + S_\alpha(G_2)$ follows. ∎

5. The A_α-spread of trees. For all connected graphs with n vertices, Gregory et al. [10] showed that $S_0(G) \geq S_0(P_n)$ with equality if and only if $G = P_n$, and Fan and Fallat [7] proved that $S_{1/2}(G) \geq 1+cos\left(\frac{\pi}{n}\right)$ with equality if and only if $G = P_n$ or $G = C_n$ in case of odd n. The union of two graphs G_1 and G_2 is the graph $G_1 \cup G_2$ with vertex set $V_1(G) \cup V_2(G)$ and edge set $E(G_1) \cup E(G_2)$. For two vertex disjoint graphs G_1 and G_2, the join $G_1 \vee G_2$ is obtained from $G_1 \cup G_2$ by adding to it all edges between vertices from $V(G_1)$ and $V(G_2)$. Gregory et al. [10] conjectured the maximum spread $S_0(G)$ of the graphs of order n is attained only by $K_{\lfloor 2n/3 \rfloor} \vee \overline{K}_{n-\lfloor 2n/3 \rfloor}$. For all connected graphs with n vertices, Oliveira et al. [31] conjectured $S_{1/2}(G) \leq S_{1/2}(\overline{K_1 \cup K_{1,\,n-2}})$ with equality if and only if $G = \overline{K_1 \cup K_{1,\,n-2}}$. For A_α-spread, an interesting question naturally arises:

Problem 5.1. *Which graphs minimize (or maximize) the A_α-spread among all graphs with n vertices?*

Based on our numerical calculation, we find that even for all connected graphs with five vertices the problem of finding graphs which minimize or maximum A_α-spread is difficult, even though it may be in sight. Let $\mathcal{T}_n$ be the set of trees with n vertices.

Theorem 5.2. *If $\frac{5+\sqrt{5}}{10} \leq \alpha \leq 1$ and $T \in \mathcal{T}_n$, then $S_\alpha(P_n) \leq S_\alpha(T)$, and the equality holds if and only if $T = P_n$.*

Proof. For $T \in \mathcal{T}_n$ with $\Delta(T) \geq 3$, by Theorem 4.1 and Corollary 3.6, we have

$$S_\alpha(T) \geq 2\alpha + \frac{(1-\alpha)^2}{\alpha} \geq 3 - 2\alpha > 1 + 2(1-\alpha)cos\left(\frac{\pi}{n}\right) \geq S_\alpha(P_n).$$

Therefore, $S_\alpha(T) \geq S_\alpha(P_n)$ for $T \in \mathcal{T}_n$. Clearly, the equality holds if and only if $T = P_n$. This completes the proof. ∎

Let $N(v) = \{w \in V(G) : vw \in E(G)\}$, and let $R(p,\, q)$ be the graph obtained from K_2 by attaching p pendant edges to a vertex and q pendant edges to the other.

Lemma 5.3. *Let $T \in \mathcal{T}_n \setminus \{K_{1,\,n-1}, R(1,\, n-3)\}$. Then $\lambda_1(A_\alpha(T)) < \lambda_1(A_\alpha(R(1,\, n-3)))$.*

Proof. Let $T \in \mathcal{T}_n \setminus \{K_{1,\,n-1}, R(1,\, n-3)\}$ with the largest A_α-spectral radius, and $X = \{x_1, x_2, \ldots, x_n\}$ be a unit eigenvector of $A_\alpha(T)$ corresponding to $\lambda_1(A_\alpha(T))$.

We first show that T has only one non-pendant edge. Otherwise, suppose that T has more than one non-pendant edges, and let uv be a non-pendant edge of T. Without lose the generality, we may assume $x_u \geq x_v$. Let

$$T_1 = T - \sum_{w \in N(v)} vw + \sum_{w \in N(v)} uw.$$

Clearly, $T_1 \in \mathcal{T}_n \setminus \{K_{1,\,n-1}, R(1,\, n-3)\}$. By Lemma 2.15, we have $\lambda_1(A_\alpha(T)) < \lambda_1(A_\alpha(T_1))$, a contradiction. Hence, T has only one non-pendant edge, denoted by uv. Namely, $T = R(s,\, t)$ with $s+t = n-2$, $d(u) = s+1$ and $d(v) = t+1$.

Without loss of the generality, we may assume $s \leq t$. Since $T \neq R(1,\, n-3)$, it follows that $s \geq 2$. By the similar reason as the above, we can prove that $\lambda_1(A_\alpha(T)) < \lambda_1(A_\alpha(R(1,\, n-3)))$. This completes the proof. ∎

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THEOREM 5.4. *If* $n \geq 4$, $\frac{1}{2} \leq \alpha \leq \frac{8}{15}$ *and* $T \in \mathcal{T}_n$, *then*

$$S_\alpha(T) \leq \sqrt{\alpha^2 n^2 + 4(n-1)(1-2\alpha)},$$

and the equality holds if and only if $T = K_{1,\,n-1}$.

Proof. Let $\phi_\alpha(G, x)$ be the characteristic polynomial of $A_\alpha(G)$. By direct computation, we have

$$\phi_\alpha(R(1,\, n-3), x) = (x-\alpha)^{n-4} f(x),$$

where

$$\begin{aligned} f(x) = x^4 &- \alpha(n+2)x^3 + ((3\alpha^2 + 2\alpha - 1)n - 2\alpha^2 - 2\alpha + 1)x^2 \\ &- ((\alpha^3 + 8\alpha^2 - 4\alpha)n - 16\alpha^2 + 8\alpha)x + (2\alpha^3 + 3\alpha^2 - 4\alpha + 1)n \\ &- 2\alpha^3 - 11\alpha^2 + 12\alpha - 3. \end{aligned}$$

Noting that $n \geq 4$ and $\frac{1}{2} \leq \alpha < \frac{8}{15}$, by derivative, we know that $f'(x) > 0$ for $x \in [\alpha n - 1, +\infty)$. Therefore, $f(x)$ is strictly increasing on $x \in [\alpha n - 1, +\infty)$. Since

$$\begin{aligned} f(\alpha n - 1) &= \alpha^2(\alpha^2 + \alpha - 1)n^3 - (3\alpha^4 + 10\alpha^3 - 4\alpha^2 - 2\alpha)n^2 \\ &\quad + (23\alpha^3 + 4\alpha^2 - 11\alpha)n - 2\alpha^3 - 29\alpha^2 + 20\alpha - 1 \\ &< 0 \end{aligned}$$

and

$$\begin{aligned} f(\alpha n - \frac{1}{4}) &= \alpha^2\left(\alpha^2 + \frac{7}{4}\alpha - 1\right)n^3 - \left(3\alpha^4 + 10\alpha^3 - \frac{67}{16}\alpha^2 - \frac{1}{2}\alpha\right)n^2 \\ &\quad + \left(\frac{77}{4}\alpha^3 - \frac{35}{16}\alpha^2 - \frac{347}{64}\alpha + \frac{15}{16}\right)n - 2\alpha^3 - \frac{121}{8}\alpha^2 + \frac{445}{32}\alpha - \frac{751}{256} \\ &> 0, \end{aligned}$$

it follows that $\lambda_1(A_\alpha(R(1,\, n-3))) < \alpha n - \frac{1}{4}$. For $T \in \mathcal{T}_n \setminus \{K_{1,\,n-1}, R(1,\, n-3)\}$, By Lemma 5.3 we have $\lambda_1(A_\alpha(T)) < \lambda_1(A_\alpha(R(1,\, n-3)))$. From Proposition 7 in [25], we know that $A_\alpha(G)$ is a positive semi-definite matrix for $1/2 \leq \alpha \leq 1$. This means that $S_\alpha(T) < \alpha n - \frac{1}{4}$ for $T \in \mathcal{T}_n \setminus \{K_{1,\,n-1}\}$. From Proposition 39 in [25], we have

$$S_\alpha(K_{1,\,n-1}) = \sqrt{\alpha^2 n^2 + 4(n-1)(1-2\alpha)} > \alpha n - \frac{1}{4}$$

for $\frac{1}{2} \leq \alpha \leq \frac{8}{15}$. Therefore, $S_\alpha(T) \leq \sqrt{\alpha^2 n^2 + 4(n-1)(1-2\alpha)}$ for $\frac{1}{2} \leq \alpha \leq \frac{8}{15}$, and the equality holds if and only if $T = K_{1,\,n-1}$. This completes the proof. ☐

In the case when $\alpha = 0$, it is well known that $S_0(T) = S_A(T) \leq S_A(K_{1,\,n-1})$ with equality if and only if $T = K_{1,\,n-1}$. Combining Theorems 5.2 and 5.4, we have the following conjecture.

CONJECTURE 5.5. *If* $0 \leq \alpha \leq 1$ *and* $T \in \mathcal{T}_n$, *then*

$$S_\alpha(P_n) \leq S_\alpha(T) \leq S_\alpha(K_{1,\,n-1}),$$

where the left (right) equality holds if and only if $T = P_n$ $(T = K_{1,\,n-1})$.

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