Notes on the sum of powers of the signless Laplacian eigenvalues of graphs *

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Abstract

For a graph G and a non-zero real number α, the graph invariant $S_\alpha(G)$ is the sum of the α^{th} power of the non-zero signless Laplacian eigenvalues of G. In this paper, we obtain sharp bounds of $S_\alpha(G)$ for a connected bipartite graph G on n vertices and a connected graph G on n vertices having a connectivity less than or equal to k, respectively, and propose some open problems for future research.

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1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and d_i be the degree of the vertex v_i for $i \in \{1, 2, \ldots, n\}$. The Laplacian matrix and the signless Laplacian matrix of G are defined as $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ respectively, where $A(G)$ is the adjacent matrix and $D(G)$ is the diagonal matrix of vertex degrees of G. It is well known that both $L(G)$ and $Q(G)$ are symmetric and positive semidefinite, then we can denote the eigenvalues of $L(G)$ and $Q(G)$, called respectively the Laplacian eigenvalues and the signless eigenvalues of G, by $\mu_1(G) \geq \mu_2(G) \geq \ldots \geq \mu_n(G) = 0$ and $q_1(G) \geq q_2(G) \geq \ldots \geq q_n(G) \geq 0$. If no confusion, we write $\mu_i(G)$ as μ_i, and $q_i(G)$ as q_i, respectively.

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Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $A(G)$. The famous graph energy $E(G)$, introduced by Gutman [6], is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. This quantity has a long known application in molecular-orbital theory of organic molecules and has been much investigated(see [7], [8]).

In [12], Klein and Randić defined the Kirchhoff index as $Kf(G) = \sum_{i<j} r_{ij}$, where r_{ij} is the effective resistance between v_i and v_j. It was proved later by Zhu et al.[26], Gutman and Mohar [10] that $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$. The Kirchhoff index was widely used in electric circuit, probabilistic theory and chemistry(see [10, 17, 24]). Most of its results can be found in the survey [25].

Recently, the so-called Laplacian energy $E_L(G)$ [13] and the Laplacian-energy-like invariant $LEL(G)$ [16] defined respectively as $E_L(G) = \sum_{i=1}^{n} \mu_i^2$, $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$ have been investigated. Stevanović et al. [19] showed that the LEL-variant is a well designed molecular descriptor, which has great applications in chemistry. For more details on $LEL(G)$, we refer readers to the survey [14].

Motivated by the definition of $LEL(G)$, Jooyandeh et al.[11] introduced the incidence energy $IE(G)$ of G, which is defined as $IE(G) = \sum_{i=1}^{n} \sqrt{q_i}$. In [9], relations between $IE(G)$ and $LEL(G)$ and several sharp upper bounds for $IE(G)$ are obtained.

Since the definition of $LEL(G)$ and Kirchhoff index, Zhou [22] put forward a general form $s_\alpha(G)$, i.e., $s_\alpha(G) = \sum_{i=1}^{h} \mu_i^\alpha$, where α is a non-zero real number and h is the number of non-zero Laplacian eigenvalues of G. Zhou called it the sum of powers of Laplacian eigenvalues of G, achieved some properties and bounds for s_α where $\alpha \neq 0, 1$, and discuss further properties for s_2 and $s_{\frac{1}{2}}$. In the sequel, some bounds of s_α for connected bipartite graphs were obtained in [20], which improve some known results of [22]. Moreover, Zhou [23] established some bounds for s_α in terms of degree sequences and Chen et al. [4] presented a lot of bounds of $s_\alpha(G)$ for a connected graph G in terms of its number of vertices and edges, connectivity and chromatic number respectively, some of which generalize those results in [24]. Recently, Das et al. [5] obtained some lower and upper bounds on $s_\alpha(G)$ for G in terms of n, the number of edges, maximum degree, clique number, independence number and the number of spanning trees, and presented some Nordhaus-Gaddum-type results for $s_\alpha(G)$ of G.

Based on the definition of LEL, s_α, and IE, Liu and Liu [15] put forward the sum of powers of the signless Laplacian eigenvalues of G, denoted by $S_\alpha(G) = \sum_{i=1}^{h} q_i^\alpha$, where α is a non-zero real number and h is the number of non-zero signless Laplacian eigenvalues of G. Obviously, $S_1(G) = 2m$, $S_{\frac{1}{2}}(G) = IE(G)$. They determined the graphs on n vertices with the first, second, or third largest value of S_α when $\alpha > 0$ and presented some bounds for S_α in terms of $\{n, m, Z_\alpha(G)\}$ where m is the number of edges in G and $Z_\alpha(G) = \sum_{i=1}^{n} d_i^\alpha$, especially in terms of $\{n, m, Z_2(G)\}$ ($Z_2(G)$ usually written as $M_1(G)$, is called the first Zagreb index). According to the relations between S_α and $\{n, m, Z_2(G)\}$, some bounds for IE are also presented. In [18], Oscar Rojo and Eber Lenes derived an upper bound for $IE(G)$ of G on n vertices having a connectivity less than or equal to k, and showed that this upper bound is attained if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$, where $G_1 \vee G_2$ is the graph obtained by starting with a disjoint union of G_1 and G_2 and adding edges joining every vertex of G_1 to every vertex of G_2, called the join of G_1 and G_2. Moreover, Saieed Akbari et al. [1] established some relations between $s_\alpha(G)$ and $S_\alpha(G)$ when α belongs to different intervals, that is, $S_\alpha(G) \geq s_\alpha(G)$ if $0 < \alpha \leq 1$ or $2 \leq \alpha \leq 3$, while $S_\alpha(G) \leq s_\alpha(G)$ if $1 \leq \alpha \leq 2$, and the equality holds if and only if G is a bipartite graph.

The vertex connectivity(or just connectivity) of a graph G, denoted by $\kappa(G)$, is the minimum number of vertices of G whose deletion disconnects G. It is conventional to define $\kappa(K_n) = n - 1$.

Let $\mathcal{B}_n$ be the family of the connected bipartite graphs on n vertices, $\mathcal{F}_n$ be the family of the simple connected graphs on n vertices, respectively. Let $\mathcal{V}_n^k = \{G \in \mathcal{F}_n | \kappa(G) \leq k\}$. In this paper, we will derive a sharp bound of $S_\alpha(G)$ with $\alpha \leq 1$ in $\mathcal{B}_n$ in Section 3, and derive a sharp bound of $S_\alpha(G)$ with $\alpha \geq 1$ in $\mathcal{V}_n^k$ in Section 4, respectively, and propose some open problems in these sections for future research.

2 Preliminaries

In this section, we introduce some basic properties which we need to use in the proofs of our main results.

Lemma 2.1. ([2]) *Let G be a graph with n vertices and e be an edge of G. Then $0 \leq q_n(G-e) \leq q_n(G) \leq q_{n-1}(G-e) \leq q_{n-1}(G) \leq \cdots \leq q_1(G-e)$ $\leq q_1(G)$.*

Note that $\sum_{i=1}^{n} q_i(G) - \sum_{i=1}^{n} q_i(G-e) = 2$, by Lemma 2.1, we have the following result immediately.

Theorem 2.1. *Let e be an edge of G. Then $S_\alpha(G) > S_\alpha(G-e)$ for $\alpha > 0$, and $S_\alpha(G) < S_\alpha(G-e)$ for $\alpha < 0$.*

Lemma 2.2. ([3]) *If G is bipartite, then $Q(G)$ and $L(G)$ share the same eigenvalues.*

3 Bounding $S_\alpha(G)$ in $\mathcal{B}_n$

In this section, we derive a sharp bound of $S_\alpha(G)$ with $\alpha \le 1$ for a connected bipartite graph G on n vertices, and propose an open problem about $S_\alpha(G)$ with $\alpha > 1$.

We can see that $S_\alpha(G) = s_\alpha(G)$ for a bipartite graph G by Lemma 2.2, so the following results in this section also hold for s_α.

Let $\sigma(M)$ be the spectrum of the square matrix M. By simple calculation, $\sigma(Q(K_{r,s})) = \{r+s, r^{[s-1]}, s^{[r-1]}, 0\}$ where $\lambda^{[t]}$ means that λ is an eigenvalue with multiplicity t.

Thus, by Theorem 2.1, the following result is obvious.

Theorem 3.1. *Let G be a bipartite graph with r and s vertices in its two partite sets. (1) If $\alpha > 0$, then $S_\alpha(G) \le (r+s)^\alpha + (r-1)s^\alpha + (s-1)r^\alpha$, with equality if and only if $G = K_{r,s}$; (2) If $\alpha < 0$, then $S_\alpha(G) \ge (r+s)^\alpha + (r-1)s^\alpha + (s-1)r^\alpha$, with equality if and only if $G = K_{r,s}$.*

Theorem 3.2. *Let G be a bipartite graph with n vertices and $\alpha \le 1$. (1) If $\alpha < 0$, then $S_\alpha(G) \ge n^\alpha + (\lfloor \frac{n}{2} \rfloor - 1)\lceil \frac{n}{2} \rceil^\alpha + (\lceil \frac{n}{2} \rceil - 1)\lfloor \frac{n}{2} \rfloor^\alpha$, with equality if and only if $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$; (2) If $0 < \alpha \le 1$, then $S_\alpha(G) \le n^\alpha + (\lfloor \frac{n}{2} \rfloor - 1)\lceil \frac{n}{2} \rceil^\alpha + (\lceil \frac{n}{2} \rceil - 1)\lfloor \frac{n}{2} \rfloor^\alpha$, with equality if and only if $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.*

Proof. The proof of (2) is similar to (1). Now we show (1) holds.

If $\alpha < 0$, let G_* be a bipartite graph with r and s vertices in its two partite sets, having the minimum value of S_α among all the connected bipartite graphs with n vertices. Without loss of generality, assume that $1 \le r \le s$. By Theorem 3.1, $G_* = K_{r,s}$ for some $r \in \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ with $r + s = n$. Note that $\sigma(Q(K_{r,s})) = \{r+s, r^{[s-1]}, s^{[r-1]}, 0\}$. Thus

$$\begin{aligned} S_\alpha(K_{r,s}) &= n^\alpha + (r-1)s^\alpha + (s-1)r^\alpha \\ &= n^\alpha + (r-1)(n-r)^\alpha + (n-r-1)r^\alpha \\ &= n^\alpha - [(n-r)^{\alpha+1} + r^{\alpha+1}] + (n-1)[(n-r)^\alpha + r^\alpha]. \end{aligned}$$

Let $f(r) = -[(n-r)^{\alpha+1} + r^{\alpha+1}] + (n-1)[(n-r)^\alpha + r^\alpha]$ with $1 \le r \le \lfloor \frac{n}{2} \rfloor$. Then $f'(r) = (\alpha+1)[(n-r)^\alpha - r^\alpha] - \alpha(n-1)[(n-r)^{\alpha-1} - r^{\alpha-1}]$.

If $r = \lfloor \frac{n}{2} \rfloor = \frac{n}{2}$, then $n - r = r$, and therefore $f'(r) = 0$.

Otherwise, $r < \frac{n}{2}$, i.e., $n - r > r$. By Cauchy mean-value Theorem, there exists $\xi \in (r, n-r)$ satisfying $\frac{(n-r)^{\alpha-1} - r^{\alpha-1}}{(n-r)^\alpha - r^\alpha} = \frac{(\alpha-1)\xi^{\alpha-2}}{\alpha\xi^{\alpha-1}} = \frac{\alpha-1}{\alpha\xi}$. Thus we have

$$f'(r) = [(n-r)^\alpha - r^\alpha][(\alpha+1) - \alpha(n-1) \cdot \frac{(n-r)^{\alpha-1} - r^{\alpha-1}}{(n-r)^\alpha - r^\alpha}]$$

$= [(n-r)^\alpha - r^\alpha][(\alpha+1) - (\alpha-1)\cdot\frac{n-1}{\xi}]$.

Note that $\alpha < 0$, $n-r > r$ and $0 < r < \xi < n-r \le n-1$, we have $\alpha - 1 < 0$, $(n-r)^\alpha - r^\alpha < 0$, $\frac{n-1}{\xi} > 1$ and $(\alpha+1) - (\alpha-1)\frac{n-1}{\xi} > (\alpha+1) - (\alpha-1) = 2 > 0$. Hence, $f'(r) < 0$, that is, $f(r)$ is decreasing for $1 \le r \le \lfloor \frac{n}{2} \rfloor$.

Therefore, $S_\alpha(K_{r,n-r}) = n^\alpha + f(r)$ with $1 \le r \le \lfloor \frac{n}{2} \rfloor$ is minimum if and only if $r = \lfloor \frac{n}{2} \rfloor$. It follows that $G_* = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ and $S_\alpha(G) \ge n^\alpha + (\lfloor \frac{n}{2} \rfloor - 1) \lceil \frac{n}{2} \rceil^\alpha + (\lceil \frac{n}{2} \rceil - 1) \lfloor \frac{n}{2} \rfloor^\alpha$. □

Remark 3.1. By Lemma 2.2, $LEL(G) = S_{\frac{1}{2}}(G)$ and $Kf(G) = nS_{-1}(G)$ for G is a bipartite graph. Hence, Theorem 3.1 and Theorem 3.2 generalize the results of Liu and Huang for the Laplacian-energy-like invariant (Corollary 2.4, [14]) and the results of Yang for the Kirchhoff index (Theorem 3.1, [21]). In our proof, some techniques in [4] are referred.

Comparing the results of Theorem 3.1 and Theorem 3.2, we put forward the following conjecture to close this section.

Conjecture 3.1. *Let G be a bipartite graph with n vertices. If $\alpha > 1$, then*

$$S_\alpha(G) \le n^\alpha + (\lfloor \tfrac{n}{2} \rfloor - 1) \lceil \tfrac{n}{2} \rceil^\alpha + (\lceil \tfrac{n}{2} \rceil - 1) \lfloor \tfrac{n}{2} \rfloor^\alpha,$$

with equality if and only if $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

4 Bounding $S_\alpha(G)$ in $\mathcal{V}_n^k$

In this section, we characterize the extremal graph of $S_\alpha(G)$ in $\mathcal{V}_n^k$ and derive a sharp upper bound of $S_\alpha(G)$ with $\alpha \ge 1$ in $\mathcal{V}_n^k$. Moreover, we propose an open problem about $S_\alpha(G)$ with $\alpha < 1$.

By simple calculation, $\sigma(Q(K_n)) = \{2n-2, (n-2)^{[n-1]}\}$. Actually, Theorem 2.1 implies that

Theorem 4.1. *Let $G \in \mathcal{F}_n$. (1) If $\alpha > 0$, then $S_\alpha(G) \le 2^\alpha(n-1)^\alpha + (n-1)(n-2)^\alpha$ with equality if and only if $G = K_n$. (2) If $\alpha < 0$, then $S_\alpha(G) \ge 2^\alpha(n-1)^\alpha + (n-1)(n-2)^\alpha$ with equality if and only if $G = K_n$.*

Throughout the following paper, let G^*, G_* be the graphs having the maximum and the minimum value of $S_\alpha(G)$ among the graphs in $\mathcal{V}_n^k$, respectively. Let $|U|$ be the cardinality of a finite set U, and $G(i) = K_k \vee (K_i \cup K_{n-k-i})$ where $i \in \{1, 2, \ldots, \lfloor \frac{n-k}{2} \rfloor\}$.

Theorem 4.2. *Let n, k be positive integers with $1 \le k \le n-1$, $G^*(G_*)$ be defined as above. Then (1) $G^* \in \{G(1), G(2), \cdots, G(\lfloor \frac{n-k}{2} \rfloor)\}$ when $\alpha > 0$; (2) $G_* \in \{G(1), G(2), \cdots, G(\lfloor \frac{n-k}{2} \rfloor)\}$ when $\alpha < 0$.*

Proof. The proof of (2) is similar to (1). Now we show (1) holds.

Let $G \in \mathcal{V}_n^k$ and $\alpha > 0$.

Case 1: $k = n-1$.

From Theorem 4.1, $S_\alpha(G) \le S_\alpha(K_n)$ with equality if and only if $G = K_n$. Note that $K_n = G(1)$, the result is true for $k = n-1$.

Case 2: $1 \le k \le n-2$.

By Theorem 2.1, there is a graph G^* with the maximum value of $S_\alpha(G)$ in $\mathcal{V}_n^k$. Let $U \subseteq V(G^*)$ such that $G^* - U$ is a disconnected graph and $|U| = \kappa(G^*)$. Hence, $|U| \le k$. Let $G_1, G_2, \ldots, G_r$ be the connected components of $G^* - U$.

We claim that $r = 2$. If $r > 2$, then we can construct a new graph $H = G^* + e$ where e is an edge connecting a vertex in G_1 with a vertex in G_2. Clearly, $\kappa(H) \le |U| \le k$ since H is connected and $H - U = G^* + e - U$ is disconnected. Thus, $H \in \mathcal{V}_n^k$ and $G^* = H - e$. By Theorem 2.1, $S_\alpha(G^*) < S_\alpha(H)$, which is a contradiction. Therefore $r = 2$, that is, $G^* - U = G_1 \cup G_2$.

We claim that $\kappa(G^*) = k$. If $\kappa(G^*) < k$, then $|U| < k$. Construct a new graph $H = G^* + e$ where e is an edge joining a vertex $u \in V(G_1)$ with a vertex $v \in V(G_2)$. Hence, $\kappa(H) \le |U| + 1 \le k$ since $H - U$ is a connected graph and $H - U \cup \{u\}$ is disconnected. Therefore $H \in \mathcal{V}_n^k$. By Theorem 2.1, $S_\alpha(G^*) < S_\alpha(H)$, which is also a contradiction. Thus, $\kappa(G^*) = k$.

Let $|V(G_1)| = i$. Then $|V(G_2)| = n - k - i$. Repeating application of Theorem 2.1 enables to write $G^* = K_k \vee (K_i \cup K_{n-k-i}) = G(i)$ where $i \in \{1, 2, \ldots, \lfloor \frac{n-k}{2} \rfloor\}$. □

Remark 4.1. In our proofs of Theorem 4.2, some techniques in [18] are referred.

When $\alpha \ge 1$, we search for the value of i for which $S_\alpha(G(i))$ ($i \in \{1, 2, \ldots, \lfloor \frac{n-k}{2} \rfloor\}$) is maximum. In this proof, we need the spectrum of $Q(G(i))$, which is given in [18].

Lemma 4.1. ([18]) *The spectrum of* $Q(G(i))$ *is*

$$\sigma(Q(G(i))) = \{q_1(i), q_2, q_3(i), (n-2)^{[k-1]}, (k+i-2)^{[i-1]}, (n-i-2)^{[n-k-i-1]}\},$$

where $q_1(i) = n - 2 + \frac{k}{2} + \frac{1}{2}\sqrt{(k-2n)^2 + 16i(k-n+i)}$, $\quad q_2 = n-2$, *and* $q_3(i) = n - 2 + \frac{k}{2} - \frac{1}{2}\sqrt{(k-2n)^2 + 16i(k-n+i)}$.

Theorem 4.3. *Let n, k be positive integers with $1 \le k \le n-1$, $G \in \mathcal{V}_n^k$ and $\alpha \ge 1$. Then*

$$S_\alpha(G) \le b_\alpha(n,k) \tag{4.1}$$

where

$$b_\alpha(n,k) = k(n-2)^\alpha + (n-k-2)(n-3)^\alpha + \left[n - 2 + \frac{k}{2} + \frac{1}{2}\sqrt{(k-2n)^2 + 16(k-n+1)}\right]^\alpha$$

$$+\left[n-2+\tfrac{k}{2}-\tfrac{1}{2}\sqrt{(k-2n)^2+16(k-n+1)}\right]^{\alpha}.$$

The equality (4.1) *holds if and only if* $G = K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let G^* be defined as above. Then $G^* = G(i)$ for some $i \in \{1, 2, \ldots, \lfloor\frac{n-k}{2}\rfloor\}$ by $\alpha \geq 1$ and Theorem 4.2. By Lemma 4.1, we have

$$\begin{aligned}S_\alpha(G(i)) &= k(n-2)^\alpha + (i-1)(k+i-2)^\alpha + (n-k-i-1)(n-i-2)^\alpha \\ &+ \left[n-2+\tfrac{k}{2}+\tfrac{1}{2}\sqrt{(k-2n)^2+16i(k-n+i)}\right]^\alpha \\ &+ \left[n-2+\tfrac{k}{2}-\tfrac{1}{2}\sqrt{(k-2n)^2+16i(k-n+i)}\right]^\alpha \\ &= k(n-2)^\alpha + (k+i-2)^{\alpha+1} + (n-i-2)^{\alpha+1} \\ &-(k-1)[(k+i-2)^\alpha + (n-i-2)^\alpha] \\ &+ \left[n-2+\tfrac{k}{2}+\tfrac{1}{2}\sqrt{(k-2n)^2+16i(k-n+i)}\right]^\alpha \\ &+ \left[n-2+\tfrac{k}{2}-\tfrac{1}{2}\sqrt{(k-2n)^2+16i(k-n+i)}\right]^\alpha.\end{aligned}$$

Let

$$\begin{aligned}f(x) &= (x+k-2)^{\alpha+1}+(n-2-x)^{\alpha+1}-(k-1)\left[(x+k-2)^\alpha+(n-2-x)^\alpha\right] \\ &+ \left[n-2+\tfrac{k}{2}+\tfrac{1}{2}\sqrt{(k-2n)^2+16x(k-n+x)}\right]^\alpha \\ &+ \left[n-2+\tfrac{k}{2}-\tfrac{1}{2}\sqrt{(k-2n)^2+16x(k-n+x)}\right]^\alpha\end{aligned}$$

with $1 \leq x \leq \lfloor\frac{n-k}{2}\rfloor$. Then

$$\begin{aligned}f'(x) &= \alpha(k-1)[(n-2-x)^{\alpha-1}-(x+k-2)^{\alpha-1}] \\ &-(\alpha+1)[(n-2-x)^\alpha-(x+k-2)^\alpha] \\ &+\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4+\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1} \\ &-\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4-\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1}.\end{aligned}$$

If $x = \lfloor\frac{n-k}{2}\rfloor = \frac{n-k}{2}$, then $n-x = x+k$, so $f'(x) = 0$.

Otherwise, $x < \frac{n-k}{2}$, i.e., $n-x > x+k$ and therefore $n-x-2 > x+k-2$. By Cauchy mean-value Theorem, there exists $\xi \in (x+k-2, n-x-2)$ satisfying $\frac{(n-2-x)^{\alpha-1}-(x+k-2)^{\alpha-1}}{(n-2-x)^\alpha-(x+k-2)^\alpha} = \frac{(\alpha-1)\xi^{\alpha-2}}{\alpha\xi^{\alpha-1}} = \frac{\alpha-1}{\alpha\xi}$. Thus we have

$$\begin{aligned}&f'(x) \\ &= [(n-2-x)^\alpha-(x+k-2)^\alpha]\cdot\left[\alpha(k-1)\cdot\frac{(n-2-x)^{\alpha-1}-(x+k-2)^{\alpha-1}}{(n-2-x)^\alpha-(x+k-2)^\alpha}-(\alpha+1)\right] \\ &+\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4+\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1} \\ &-\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4-\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1} \\ &= [(n-2-x)^\alpha-(x+k-2)^\alpha]\cdot[(\alpha-1)\cdot\tfrac{k-1}{\xi}-(\alpha+1)] \\ &+\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4+\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1}\end{aligned}$$

$$-\frac{4\alpha[2x-(n-k)]}{\sqrt{(k-2n)^2+16x(k-n+x)}}\cdot\left[\frac{2n+k-4-\sqrt{(k-2n)^2+16x(k-n+x)}}{2}\right]^{\alpha-1}.$$

Note that $\alpha \geq 1$, $x < \frac{n-k}{2}$, $n-x-2 > x+k-2$ and $\xi > x+k-2 \geq k-1$, we have $f'(x) < 0$, that is, $f(x)$ is decreasing for $1 \leq x \leq \lfloor\frac{n-k}{2}\rfloor$.

Therefore, $S_\alpha(G(i)) = k(n-2)^\alpha + f(i)$ with $1 \leq i \leq \lfloor\frac{n-k}{2}\rfloor$ is maximum if and only if $i = 1$. It followings that $G^* = K_k \vee (K_1 \cup K_{n-k-1})$. □

Note that $S_1(G) = 2m$, where m is the number of edges in G. From Theorem 4.3, we have

Corollary 4.1. *Let n, k be positive integers with $1 \leq k \leq n-1$, and G be any graph in $\mathcal{V}_n^k$ with m edges. Then $m \leq \frac{1}{2}b_1(n,k) = \frac{1}{2}(n^2-3n+2k+2)$, with equality if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$.*

The trace of the matrix $X = (x_{ij})_{n\times n}$ is defined as $tr(X) = \sum_{i=1}^n x_{ii}$, which is also equal to the sum of eigenvalues of X. Obviously, $E_L(G) = tr(L(G)^2) = tr[(D(G)-A(G))^2]$, and $S_2(G) = tr(Q(G)^2) = tr[(D(G)+A(G))^2]$. Since $tr[D(G)A(G)] = 0$, $tr[(D(G)+A(G))^2] = tr[(D(G)-A(G))^2]$, which implies that $E_L(G) = S_2(G)$. Thus, we have

Corollary 4.2. *Let n, k be positive integers with $1 \leq k \leq n-1$, and $G \in \mathcal{V}_n^k$. Then $E_L(G) \leq b_2(n,k) = n^3+2n^2+(2k+5)n+k^2-k-2$, with equality if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$.*

The edge connectivity of G, denoted by $\varepsilon(G)$, is the minimum number of edges whose deletion disconnects G. Let $\varepsilon_n^k = \{G \in \mathcal{F}_n | \varepsilon(G) \leq k\}$.

Corollary 4.3. *Let n, k be positive integers with $1 \leq k \leq n-1$, G be any graph in ε_n^k and $\alpha \geq 1$. Then $S_\alpha(G) \leq b_\alpha(n,k)$, with equality if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$.*

Proof. Since $\kappa(G) \leq \varepsilon(G)$, it follows $\varepsilon_n^k \subseteq \mathcal{V}_n^k$. Let $G \in \varepsilon_n^k$, the corollary follows from the fact $K_k \vee (K_1 \cup K_{n-k-1}) \in \varepsilon_n^k$. □

In [18], the authors proved that $S_{\frac{1}{2}}(G) = IE(G) \leq b_{\frac{1}{2}}(n,k)$ for any graph G in $\mathcal{V}_n^k$, and the equality holds if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$, that is, when $\alpha = \frac{1}{2}$, $S_\alpha(G) \leq b_\alpha(n,k)$ also holds for any graph G in $\mathcal{V}_n^k$. Following from the fact, and comparing the results of Theorem 4.1 and Theorem 4.3, we propose the following conjecture.

Conjecture 4.1. *Let n, k be positive integers with $1 \leq k \leq n-1$, $G \in \mathcal{V}_n^k$ and $\alpha < 1$. Then we have*
(1) If $0 < \alpha < 1$, then $S_\alpha(G) \leq b_\alpha(n,k)$ with equality if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$.
(2) If $\alpha < 0$, then $S_\alpha(G) \geq b_\alpha(n,k)$ with equality if and only if $G = K_k \vee (K_1 \cup K_{n-k-1})$.

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