ON THE α-SPECTRAL RADIUS OF GRAPHS

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For $0 \leq \alpha \leq 1$, Nikiforov proposed to study the spectral properties of the family of matrices $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$ of a graph G, where $D(G)$ is the degree diagonal matrix and $A(G)$ is the adjacency matrix of G. The α-spectral radius of G is the largest eigenvalue of $A_\alpha(G)$. For a graph with two pendant paths at a vertex or at two adjacent vertices, we prove results concerning the behavior of the α-spectral radius under relocation of a pendant edge in a pendant path. We give upper bounds for the α-spectral radius for unicyclic graphs G with maximum degree $\Delta \geq 2$, connected irregular graphs with given maximum degree and some other graph parameters, and graphs with given domination number, respectively. We determine the unique tree with the second largest α-spectral radius among trees, and the unique tree with the largest α-spectral radius among trees with given diameter. We also determine the unique graphs so that the difference between the maximum degree and the α-spectral radius is maximum among trees, unicyclic graphs and non-bipartite graphs, respectively.

1. INTRODUCTION

We consider simple and undirected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex u of G, denote by $d_G(u)$ or simply d_u the degree of u in G. Let $A(G)$ be the adjacency matrix and $D(G)$ the diagonal matrix of the degrees of G. The signless Laplacian matrix of G is known as $Q(G) = D(G) + A(G)$. The spectral properties of the adjacency matrix and the signless Laplacian matrix of a graph have been investigated for a long time, see, e.g., [9,10].

For any real $\alpha \in [0, 1]$, Nikiforov [25] proposed to study the spectral properties of the family of matrices $A_\alpha(G)$ defined as the convex linear combination:

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

Obviously, $A(G) = A_0(G)$ and $Q(G) = 2A_{1/2}(G)$. For any real $\alpha \in [0, 1]$, $A_\alpha(G)$ is a symmetric nonnegative matrix, and thus its eigenvalues are all real. We call the largest eigenvalue of $A_\alpha(G)$ the α-spectral radius of G, denoted by $\rho_\alpha(G)$. Among other results, Nikiforov [25] showed that the r-partite Turán graph is the unique graph with the largest α-spectral radius for $0 \le \alpha < 1 - \frac{1}{r}$ among K_{r+1}-free graphs on n vertices with $r \ge 2$, where K_s is a complete graph with s vertices. For a tree T with maximum degree $\Delta \ge 2$, Nikiforov et al. [26] found an interesting bound for its α-spectral radius: $\rho_\alpha(T) < \alpha\Delta + 2(1 - \alpha)\sqrt{\Delta - 1}$ when $0 \le \alpha < 1$. This implies some previous results in [16,32]. They also showed in [26] that for $0 \le \alpha \le 1$, if T is a tree on n vertices, then $\rho_\alpha(P_n) \le \rho_\alpha(T) \le \rho_\alpha(S_n)$ with left (right, respectively) equality if and only if $T \cong P_n$ ($T \cong S_n$, respectively), where S_n and P_n are the star and the path on n vertices, respectively. Very recently, Nikiforov and Rojo [27] determined the unique graph with the largest α-spectral radius among connected graphs on n vertices with diameter (at least) k.

For $u, v \in V(G)$, the distance between u and v in G, denoted by $d_G(u, v)$, is the length of a shortest path from u to v in G. The diameter of G is the maximum distance between all vertex pairs of G.

A dominating set of G is a vertex subset S of G such that each vertex of $V(G) \setminus S$ is adjacent to at least one vertex of S. The domination number of G, denoted by $\gamma(G)$, is the minimum cardinality of dominating sets of G.

In this article, we study the α-spectral radius of graphs. For a graph with two pendant paths at a vertex or at two adjacent vertices, we prove two results concerning the behavior of the α-spectral radius under relocation of a pendant edge in a pendant path, which were conjectured in [27]. We show that the upper bound for the α-spectral radius of trees with maximum degree $\Delta \ge 2$ in [26] holds also for unicyclic graphs, and we give upper bounds for the α-spectral radius of connected irregular graphs with fixed maximum degree and some other graph parameters, and of graphs with fixed domination number, respectively. We determine the unique tree with the second largest α-spectral radius among trees, and the unique tree with the largest α-spectral radius among trees with given diameter. We also determine the unique graphs so that the difference between the maximum degree and the α-spectral radius is maximum among trees, unicyclic graphs and non-bipartite graphs, respectively.

2. PRELIMINARIES

For a graph G with $u \in V(G)$, $N_G(u)$ denotes the set of vertices that are adjacent to u in G. For undefined notation and terminology for graphs, the readers are referred to [5].

Let G be a graph with $V(G) = \{v_1, \ldots, v_n\}$. A vector $x = (x_{v_1}, \ldots, x_{v_n})^\top \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex v_i to x_{v_i}, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \ldots, n$. Then

$$x^\top A_\alpha(G) x = \alpha \sum_{u \in V(G)} d_G(u) x_u^2 + 2(1-\alpha) \sum_{uv \in E(G)} x_u x_v.$$

Moreover, λ is an eigenvalue of $A_\alpha(G)$ if and only if $x \neq 0$ and we have the following eigenequation at u for each $u \in V(G)$:

$$\lambda x_u = \alpha d_u x_u + (1-\alpha) \sum_{v \in N_G(u)} x_v.$$

If $0 \leq \alpha < 1$ and G is connected, then $A_\alpha(G)$ is irreducible, and by the well known Perron-Frobenius theorem, it has a unique unit positive x eigenvector corresponding to $\rho_\alpha(G)$. We call such a vector x the Perron vector of $A_\alpha(G)$, see [25].

For a graph G on n vertices and a unit nonnegative vector x of dimension n, we have $\rho_\alpha(G) \geq x^\top A_\alpha(G) x$ with equality if G is connected if and only if x is the Perron vector of $A_\alpha(G)$.

If G is connected, and H is a proper subgraph of G, then by [23, Corollary 2.2, p. 38], $\rho_\alpha(H) < \rho_\alpha(G)$ for $0 \leq \alpha < 1$.

The following lemma is somewhat similar to [25, Proposition 15].

Lemma 2.1. *[27] Let G be a connected graph with $u, v \in V(G)$. Suppose that $v_1, \ldots, v_s \in (N_G(v) \setminus N_G(u)) \setminus \{u\}$, where $1 \leq s \leq d_G(v)$. Let $G' = G - \{vv_i : 1 \leq i \leq s\} + \{uv_i : 1 \leq i \leq s\}$. Let $0 \leq \alpha < 1$ and let x be the Perron vector of $A_\alpha(G)$. If $x_u \geq x_v$, then $\rho_\alpha(G) < \rho_\alpha(G')$.*

Corollary 2.1. *Let G be a connected graph and $e = uv$ a cut edge of G. Suppose that $G - \{e\}$ consists of two nontrivial components G_1 and G_2 with $u \in V(G_1)$ and $v \in V(G_2)$. Let G' be a graph obtained from G by identifying u of G_1 with v of G_2, and adding a pendant edge to this common vertex. Then $\rho_\alpha(G) < \rho_\alpha(G')$ for $0 \leq \alpha < 1$.*

Proof. Let x be the Perron vector of $A_\alpha(G)$. We may assume that $x_u \geq x_v$. Let $N_{G_2}(v) = \{v_1, \ldots, v_s\}$, where $s = d_G(v) - 1 \geq 1$. Let $G^* = G - \{vv_i : 1 \leq i \leq s\} + \{uv_i : 1 \leq i \leq s\}$. Obviously, $G^* \cong G'$. By Lemma 2.1, $\rho_\alpha(G) < \rho_\alpha(G^*) = \rho_\alpha(G')$. $\qquad\square$

The following lemma is an extended version of Theorem 6.4.2 in [11, p. 145].

Lemma 2.2. *Let G be a connected graph with edges $u_1 u_2$ and $v_1 v_2$, where u_1, u_2, v_1 and v_2 are four distinct vertices of G, and $u_1 v_2, v_1 u_2 \notin E(G)$. Let x be the Perron vector of $A_\alpha(G)$, where $0 \leq \alpha < 1$. Let $G' = G - \{u_1 u_2, v_1 v_2\} + \{u_1 v_2, v_1 u_2\}$. If $x_{u_1} \geq x_{v_1}$, $x_{u_2} \leq x_{v_2}$ and one inequality is strict, then $\rho_\alpha(G) < \rho_\alpha(G')$.*

Proof. Note that

$$
\begin{aligned}
\rho_\alpha(G') - \rho_\alpha(G) &\geq x^\top A_\alpha(G')x - x^\top A_\alpha(G)x \\
&= 2(1-\alpha) \sum_{uv \in E(G')} x_u x_v - 2(1-\alpha) \sum_{uv \in E(G)} x_u x_v \\
&= 2(1-\alpha)(x_{v_1} x_{u_2} + x_{u_1} x_{v_2} - x_{u_1} x_{u_2} - x_{v_1} x_{v_2}) \\
&= 2(1-\alpha)(x_{u_1} - x_{v_1})(x_{v_2} - x_{u_2}) \\
&\geq 0.
\end{aligned}
$$

Thus $\rho_\alpha(G') \geq \rho_\alpha(G)$. Suppose that $\rho_\alpha(G') = \rho_\alpha(G)$. Then x is the Perron vector of $A_\alpha(G')$. We may assume that $x_{u_2} < x_{v_2}$. From the eigenequations of G' and G at u_1, we have

$$
\begin{aligned}
\rho_\alpha(G')x_{u_1} &= \alpha d_{u_1} x_{u_1} + (1-\alpha) \sum_{wu_1 \in E(G')} x_w \\
&= \alpha d_{u_1} x_{u_1} + (1-\alpha) \left(\sum_{wu_1 \in E(G)} x_w - x_{u_2} + x_{v_2} \right) \\
&> \alpha d_{u_1} x_{u_1} + (1-\alpha) \sum_{wu_1 \in E(G)} x_w \\
&= \rho_\alpha(G)x_{u_1},
\end{aligned}
$$

which is impossible. It follows that $\rho_\alpha(G') > \rho_\alpha(G)$. $\qquad\square$

The following lemmas follows easily because as a quadratic function in t, $at^2 + b(t-c)^2$ for $a, b > 0$ achieves its minimum value $\frac{abc^2}{a+b}$ when $t = \frac{bc}{a+b}$.

Lemma 2.3. *[29] If $a, b > 0$, then $at^2 + b(t-c)^2 \geq \frac{abc^2}{a+b}$ with equality if and only if $t = \frac{bc}{a+b}$.*

3. TWO CONJECTURES ON THE α-SPECTRAL RADIUS

Nikiforov and Rojo [27] proposed two conjectures (Conjectures 18 and 19) concerning the behavior of the α-spectral radius under relocation of a pendant edge in a pendant path.

For positive integer p and a graph G with $u \in V(G)$, let $G(u; p)$ be the graph obtained from G by attaching a pendant path of length p at u. That is, $G(u; p)$ is obtained by adding an edge connecting u and a terminal vertex of a path on p vertices. Let $G(u, 0) = G$, and in this case a pendant path of length 0 is understood the trivial path consisting of a single vertex u.

For nonnegative integers p, q and a graph G, let $G_u(p, q)$ or simply $G_{p,q}$ be the graph $H(u; q)$ with $H = G(u; p)$. Nikiforov and Rojo [27] conjectured

that $\rho_\alpha(G_{p,q}) > \rho_\alpha(G_{p+1,q-1})$ for a nontrivial connected graph G and integers p and q with $p \geq q \geq 2$, and mentioned that they can show it is true when $\rho_\alpha(G_{p+1,q-1}) \geq \frac{9}{4}$. We show that it is really true.

Theorem 3.1. *Let G be a connected graph with $|E(G)| \geq 1$ and $u \in V(G)$. For integers $p \geq q \geq 1$ and $0 \leq \alpha < 1$, $\rho_\alpha(G_u(p,q)) > \rho_\alpha(G_u(p+1,q-1))$.*

Proof. Let $uu_1 \ldots u_{p+1}$ and $uv_1 \ldots v_{q-1}$ be the two pendant paths in $G_u(p+1,q-1)$ at u of lengths $p+1$ and $q-1$, respectively. Let x be the Perron vector of $A_\alpha(G_u(p+1,q-1))$. Let $v_0 = u$. Suppose that $\rho_\alpha(G_u(p,q)) \leq \rho_\alpha(G_u(p+1,q-1))$.
Claim. $x_{u_{p-i}} > x_{v_{q-i-1}}$ for all $i = 0,1,\ldots,q-1$.
　　We prove the claim by induction on i. If $x_{v_{q-1}} \geq x_{u_p}$, then for $H = G_u(p+1,q-1) - u_p u_{p+1} + v_{q-1}u_{p+1}$, we have $H \cong G_u(p,q)$, and thus by Lemma 2.1, $\rho_\alpha(G_u(p,q)) = \rho_\alpha(H) > \rho_\alpha(G_u(p+1,q-1))$, a contradiction. Thus $x_{u_p} > x_{v_{q-1}}$. This proves the claim for $i = 0$. If $q = 1$, then $i = 0$ and the claim follows. Suppose that $q \geq 2$, and $x_{u_{p-i}} > x_{v_{q-i-1}}$ where $0 \leq i \leq q-2$. If $x_{v_{q-(i+1)-1}} \geq x_{u_{p-(i+1)}}$, then for

$$
\begin{aligned}
H' &= G_u(p+1,q-1) - \{u_{p-(i+1)}u_{p-i}, v_{q-(i+1)-1}v_{q-i-1}\} \\
&\quad + \{u_{p-i}v_{q-(i+1)-1}, u_{p-(i+1)}v_{q-i-1}\},
\end{aligned}
$$

we have $H' \cong G_u(p,q)$ and thus by Lemma 2.2 that $\rho_\alpha(G_u(p,q)) = \rho_\alpha(H') > \rho_\alpha(G_u(p+1,q-1))$, a contradiction. Thus $x_{u_{p-(i+1)}} > x_{v_{q-(i+1)-1}}$. Therefore, the claim follows.
　　By the claim for $i = q-1$, we have $x_{u_{p-(q-1)}} > x_u$. Since $G_u(p+1,q-1) - \{uw : w \in N_G(u)\} + \{u_{p-(q-1)}w : w \in N_G(u)\} \cong G_u(p,q)$, we have by Lemma 2.1 that $\rho_\alpha(G_u(p,q)) > \rho_\alpha(G_u(p+1,q-1))$, a contradiction.
　　Therefore $\rho_\alpha(G_u(p,q)) > \rho_\alpha(G_u(p+1,q-1))$. □

　　Let G be a connected graph with $uv \in E(G)$. For nonnegative integers p and q, let $G_{u,v}(p,q)$ be the graph $H(v;q)$ with $H = G(u;p)$. It was conjectured in [27] that if the degrees of u and v are at least two in G, then for $p \geq q \geq 2$ and $0 \leq \alpha < 1$, $\rho_\alpha(G_{u,v}(p,q)) > \rho_\alpha(G_{u,v}(p+1,q-1))$. Now we show that this is also indeed true.

Theorem 3.2. *Let G be a connected graph, and let u and v be adjacent vertices of G of degree at least 2. For $p \geq q \geq 1$ and $0 \leq \alpha < 1$, $\rho_\alpha(G_{u,v}(p,q)) > \rho_\alpha(G_{u,v}(p+1,q-1))$.*

Proof. Let $uu_1 \ldots u_{p+1}$ and $vv_1 \ldots v_{q-1}$ be the two pendant paths at u and v in $G_{u,v}(p+1,q-1)$, respectively. Let x be the Perron vector of $A_\alpha(G_{u,v}(p+1,q-1))$. Let $u_0 = u, v_0 = v$. Suppose that $\rho_\alpha(G_{u,v}(p,q)) \leq \rho_\alpha(G_{u,v}(p+1,q-1))$.
　　By argument as in the proof of Theorem 3.1, we have $x_{u_{p-i}} > x_{v_{q-i-1}}$ for all $i = 0,1,\ldots,q-1$. Thus $x_{u_{p-(q-1)}} > x_v$. Let $G' = G_{u,v}(p+1,q-1) - \{vw : w \in N_G(v) \setminus \{u\}\} + \{u_{p-(q-1)}w : w \in N_G(v) \setminus \{u\}\}$. By Lemma 2.1, we have $\rho_\alpha(G') > \rho_\alpha(G_u(p+1,q-1))$. If $p = q$, then $G' \cong G_{u,v}(p,q)$ and thus $\rho_\alpha(G_{u,v}(p,q)) >$

$\rho_\alpha(G_{u,v}(p+1, q-1))$, a contradiction. Thus $p > q$. Let x' be the Perron vector of $A_\alpha(G')$. Note that $x'_{u_{p-(q-1)}} > x'_v$; Otherwise, we have by Lemma 2.1 that $\rho_\alpha(G') < \rho_\alpha(G_u(p+1, q-1))$, a contradiction.

If $x'_{u_{p-q}} \geq x'_u$, then since $G' - \{uw : w \in N_G(u) \setminus \{v\}\} + \{u_{p-q}w : w \in N_G(u) \setminus \{v\}\} \cong G_{u,v}(p, q)$, we have by Lemma 2.1 that $\rho_\alpha(G_{u,v}(p, q)) > \rho_\alpha(G') > \rho_\alpha(G_{u,v}(p+1, q-1))$, a contradiction. Thus we may assume that $x'_{u_{p-q}} < x'_u$. Since $G' - \{uv, u_{p-q}u_{p-(q-1)}\} + \{uu_{p-(q-1)}, vu_{p-q}\} \cong G_{u,v}(p, q)$, we have by Lemma 2.2 that $\rho_\alpha(G_{u,v}(p, q)) > \rho_\alpha(G') > \rho_\alpha(G_{u,v}(p+1, q-1))$, also a contradiction.

Therefore, $\rho_\alpha(G_{u,v}(p, q)) > \rho_\alpha(G_{u,v}(p+1, q-1))$. □

4. BOUNDS FOR THE α-SPECTRAL RADIUS

Let $B = (b_{ij})$ be an $n \times n$ nonnegative matrix with row sums $r_1, \ldots, r_n$, where $r_1 \geq \cdots \geq r_n$. Let M be the largest diagonal entry and N the largest non-diagonal entry of B, where $N > 0$. Let $\rho(B)$ be the spectral radius of B. It is proved in [14] that for $1 \leq \ell \leq n$,

$$\rho(B) \leq \frac{r_\ell + M - N + \sqrt{(r_\ell - M + N)^2 + 4N \sum_{i=1}^{\ell-1}(r_i - r_\ell)}}{2}$$

with equality when B is irreducible if and only if either $r_1 = \cdots = r_n$ or for some $2 \leq t \leq \ell$, $b_{ii} = M$ for $1 \leq i \leq t-1$, $b_{ik} = N$ for $1 \leq i \leq n$ and $1 \leq k \leq t-1$ with $k \neq i$, and $r_t = \cdots = r_n$. For a graph G and $0 \leq \alpha < 1$, we have $\rho_\alpha(G) = \rho(A_\alpha(G))$ and applying this result in [14] to $A_\alpha(G)$, we have the following result.

Let G be a graph on $n \geq 2$ vertices with degree sequence $d_1, \ldots, d_n$, where $d_1 \geq \cdots \geq d_n$. Then for $0 \leq \alpha < 1$ and $1 \leq \ell \leq n$,

$$\rho_\alpha(G) \leq \frac{d_\ell + \alpha d_1 - (1-\alpha) + \sqrt{(d_\ell - \alpha d_1 + 1 - \alpha)^2 + 4(1-\alpha) \sum_{i=1}^{\ell-1}(d_i - d_\ell)}}{2}$$

with equality when G is connected if and only if either G is regular or G is a graph with $d_1 = \cdots = d_{t-1} = n - 1 > d_t = \cdots = d_n$ for some $2 \leq t \leq \ell$.

4.1 A bound for the α-spectral radius of trees and unicyclic graphs using maximum degree

By calculating the A_α-spectra of certain Bethe trees, Nikiforov et al. [26] showed that, for $0 \leq \alpha \leq 1$, $\rho_\alpha(T) < \alpha\Delta + 2(1-\alpha)\sqrt{\Delta - 1}$ for a tree T with maximum degree $\Delta \geq 2$. We extend this result to trees and unicyclic graphs.

Theorem 4.3. *Let G be a tree or unicyclic graph with maximum degree $\Delta \geq 2$. For $0 \leq \alpha \leq 1$, we have*

$$\rho_\alpha(G) \leq \alpha\Delta + 2(1-\alpha)\sqrt{\Delta - 1}$$

with equality for $0 \leq \alpha < 1$ if and only if G is a cycle.

Proof. If $\alpha = 1$, then $A_\alpha(G) = D(G)$, and thus $\rho_\alpha(G) = \Delta = \alpha\Delta + 2(1-\alpha)\sqrt{\Delta - 1}$.

Suppose that $0 \le \alpha < 1$.

If G is a tree, then we may add an edge between two vertices of degree one to form a unicyclic graph G' with maximum degree Δ, and for $0 \le \alpha < 1$, by [23, Corollary 2.2, p. 38], we have $\rho_\alpha(G) < \rho_\alpha(G')$. Thus we may assume that G is a unicyclic graph. Let x be the Perron vector of $A_\alpha(G)$. Let C be the unique cycle of G and let k be its length. We label the vertices of G so that $V(G) = \{v_1, \dots, v_n\}$ and $V(C) = \{v_1, \dots, v_k\}$. For $w \in V(G)$, let $d_G(w, C)$ denote the minimum distance between w and vertices of C. We orient the edges of C as arcs $(v_1, v_2), \dots, (v_{k-1}, v_k), (v_k, v_1)$ and an edge uv outside C as (u, v) if $d_G(u, C) > d_G(v, C)$. Now, for any $i = 1, \dots, n$, there is a unique arc from v_i to some other vertex v_i'. Consider the multiple set $\{x_{v_1'}^2, \dots, x_{v_n'}^2\}$. For $i = 1, \dots, n$, the number of times of $x_{v_i}^2$ appearing in this multiple set is equal to the number of arcs to v_i under the above orientation, which is $d_G(v_i) - 1$. Thus

$$\sum_{i=1}^{n} x_{v_i'}^2 = \sum_{i=1}^{n} (d_G(v_i) - 1)x_{v_i}^2.$$

Therefore

$$
\begin{aligned}
\rho_\alpha(G) &= x^\top A_\alpha(G)x \\
&= \alpha \sum_{u \in V(G)} d_G(u)x_u^2 + 2(1-\alpha) \sum_{uv \in E(G)} x_u x_v \\
(4.1) \quad &\le \alpha \sum_{u \in V(G)} \Delta x_u^2 + 2(1-\alpha) \sum_{uv \in E(G)} x_u x_v \\
&= \alpha\Delta + 2(1-\alpha) \sum_{i=1}^{n} x_{v_i} x_{v_i'} \\
(4.2) \quad &\le \alpha\Delta + 2(1-\alpha)\sqrt{\sum_{i=1}^{n} x_{v_i}^2 \sum_{i=1}^{n} x_{v_i'}^2} \\
&= \alpha\Delta + 2(1-\alpha)\sqrt{\sum_{i=1}^{n} x_{v_i'}^2} \\
&= \alpha\Delta + 2(1-\alpha)\sqrt{\sum_{i=1}^{n} (d_G(v_i) - 1)x_{v_i}^2} \\
(4.3) \quad &\le \alpha\Delta + 2(1-\alpha)\sqrt{\sum_{i=1}^{n} (\Delta - 1)x_{v_i}^2} \\
&= \alpha\Delta + 2(1-\alpha)\sqrt{\Delta - 1}.
\end{aligned}
$$

In the above, inequalities (4.1) and (4.3) follow from the fact that $d_G(u) \le \Delta$ for any $u \in V(G)$ and (4.2) follows from the Cauchy-Schwarz inequality.

If $\rho_\alpha(G) = \alpha\Delta + 2(1-\alpha)\sqrt{\Delta-1}$, then (4.3) is an equality, implying that G is Δ-regular, and thus $\Delta = 2$ and $G = C$. Conversely, if G is a cycle, then $\Delta = 2$ and $\rho_\alpha(G) = 2 = \alpha\Delta + 2(1-\alpha)\sqrt{\Delta-1}$. $\qquad\square$

Let G be a unicyclic graph with maximum degree $\Delta \geq 2$. By setting $\alpha = 0, \frac{1}{2}$ in the previous theorem respectively, we have $\rho_0(G) \leq 2\sqrt{\Delta-1}$ and $\rho_{1/2}(G) \leq \frac{1}{2}(\Delta + 2\sqrt{\Delta-1})$ with either equality if and only if G is a cycle. The bound for $\rho_0(G)$ has been known in [20], and actually, we use techniques borrowed from there. Let $\mu(G)$ be the largest eigenvalue of the Laplacian matrix of a graph G. Note that $\mu(G) \leq 2\rho_{1/2}(G)$ with equality if and only if G is bipartite [3]. Thus $\mu(G) \leq \Delta + 2\sqrt{\Delta-1}$ with equality if and only if G is an even cycle, see [20].

4.2 Bounds for the α-spectral radius of irregular graphs

If G is a graph with maximum degree Δ and $0 \leq \alpha \leq 1$, then $\rho_\alpha(G) \leq \Delta$ with equality if and only if $\alpha = 1$ or G has a component that is regular of degree Δ, see [26, Proposition 11].

For a connected irregular graph G with n vertices, maximum degree Δ and diameter D, Cioabă [7] proved a conjecture in [8] stated as

$$\rho_0(G) < \Delta - \frac{1}{Dn},$$

and Ning et al. [24] showed that

$$2\rho_{1/2}(G) < 2\Delta - \frac{1}{\left(D - \frac{1}{4}\right)n}.$$

We follow the techniques in [7, 24] to prove the following result.

Theorem 4.4. *Let G be a connected irregular graph on n vertices with maximum degree Δ and diameter D. For $0 \leq \alpha < 1$, we have*

$$\rho_\alpha(G) < \Delta - \frac{2(1-\alpha)}{(2D - \alpha)n}.$$

Proof. Let x be the Perron vector of $A_\alpha(G)$. Let $x_z = \max\{x_i : i \in V(G)\}$. Then $x_z > \frac{1}{\sqrt{n}}$.

If $d_z < \Delta$, then from the eigenequation at z, we have

$$
\begin{aligned}
\rho_\alpha(G)x_z \;&=\; \alpha d_z x_z + (1-\alpha) \sum_{j \in N_G(z)} x_j \\
&\leq\; \alpha d_z x_z + (1-\alpha) \sum_{j \in N_G(z)} x_z \\
&\leq\; \alpha(\Delta-1)x_z + (1-\alpha)(\Delta-1)x_z
\end{aligned}
$$

$$= (\Delta - 1)x_z,$$

and thus $\rho_\alpha(G) \leq \Delta - 1 < \Delta - \frac{2(1-\alpha)}{(2D-\alpha)n}$.

Assume that $d_z = \Delta$. Let $V_1 = \{v \in V(G) : d_v < \Delta\}$. Obviously, $V_1 \neq \emptyset$.

Suppose that there is a vertex $u \in V_1$ such that $d_G(u, z) \leq D - 1$. Let $P = v_0 v_1 \ldots v_p$ be a shortest path from u to z, where $v_0 = u$ and $v_p = z$. Then

$$\begin{aligned}
\Delta - \rho_\alpha(G) &= \Delta \sum_{i \in V(G)} x_i^2 - x^\top A_\alpha x \\
&= \sum_{i \in V(G)} (\Delta - d_i)x_i^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_u^2 + (1-\alpha) \sum_{j=0}^{p-1} \left(x_{v_j} - x_{v_{j+1}}\right)^2.
\end{aligned}$$

By the Cauchy-Schwarz inequality and Lemma 2.3, we have

$$\begin{aligned}
\Delta - \rho_\alpha(G) &\geq x_u^2 + \frac{(1-\alpha)(x_u - x_z)^2}{p} \\
&\geq \frac{1-\alpha}{p+1-\alpha} x_z^2 \\
&\geq \frac{1-\alpha}{D-\alpha} x_z^2 \\
&> \frac{2(1-\alpha)}{(2D-\alpha)n},
\end{aligned}$$

as desired.

Now assume that for every vertex $v \in V_1$, $d(v, z) = D$. We consider the cases $|V_1| \geq 2$ and $|V_1| = 1$ separately.

Suppose first that $|V_1| \geq 2$. Let $u, v \in V_1$, and $P = v_0 v_1 \ldots v_D$ be a shortest path from u to z, where $v_0 = u$ and $v_D = z$. Let Q be a shortest path from v to z. Let $\ell = \min\{j : v_j \in V(Q)\}$. Then $\ell \in \{1, \ldots, D\}$ and $\ell = d_G(u, v_\ell) = d_G(v, v_\ell)$. Let Q_{v,v_ℓ} be the sub-path of Q from v to v_ℓ. If $\ell \neq D$, i.e., $\ell \leq D - 1$, then by the Cauchy-Schwarz inequality and Lemma 2.3, we have

$$\begin{aligned}
\Delta - \rho_\alpha(G) &= \sum_{i \in V(G)} (\Delta - d_i)x_i^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_u^2 + x_v^2 + (1-\alpha) \left(\sum_{j=0}^{\ell-1} \left(x_{v_j} - x_{v_{j+1}}\right)^2 \right. \\
&\quad + \sum_{kj \in E(Q_{v,v_\ell})} (x_k - x_j)^2 + \left. \sum_{j=\ell}^{D-1} \left(x_{v_j} - x_{v_{j+1}}\right)^2 \right)
\end{aligned}$$

$$\geq \left(x_u^2 + \frac{(1-\alpha)\,(x_u - x_{v_\ell})^2}{\ell}\right) + \left(x_v^2 + \frac{(1-\alpha)\,(x_v - x_{v_\ell})^2}{\ell}\right)$$

$$+ \frac{(1-\alpha)\,(x_{v_\ell} - x_z)^2}{D - \ell}$$

$$\geq \frac{2(1-\alpha)}{\ell + 1 - \alpha}x_{v_\ell}^2 + \frac{(1-\alpha)\,(x_{v_\ell} - x_z)^2}{D - \ell}$$

$$\geq \frac{2(1-\alpha)}{2D - \ell + 1 - \alpha}x_z^2$$

$$\geq \frac{2(1-\alpha)}{2D - \alpha}x_z^2$$

$$> \frac{2(1-\alpha)}{(2D - \alpha)n}.$$

If $\ell = D$, i.e., $v_\ell = z$, then as above and noting that $D > 1$, we have

$$\Delta - \rho_\alpha(G) \;=\; \sum_{i \in V(G)} (\Delta - d_i)x_i^2 + (1-\alpha)\sum_{ij \in E(G)} (x_i - x_j)^2$$

$$\geq \; x_u^2 + x_v^2 + (1-\alpha)\left(\sum_{j=0}^{D-1}\left(x_{v_j} - x_{v_{j+1}}\right)^2 + \sum_{ij \in E(Q)}(x_i - x_j)^2\right)$$

$$\geq \; \left(x_u^2 + \frac{(1-\alpha)(x_u - x_z)^2}{D}\right) + \left(x_v^2 + \frac{(1-\alpha)(x_v - x_z)^2}{D}\right)$$

$$\geq \; \frac{2(1-\alpha)}{D + 1 - \alpha}x_z^2$$

$$> \; \frac{2(1-\alpha)}{(2D - \alpha)n}.$$

Thus, the result follows when $|V_1| \geq 2$.

Now assume that $|V_1| = 1$. Let w be a vertex of G such that $x_w = \min\{x_i : i \in V(G)\}$. Since

$$\Delta x_w > \rho_\alpha(G)x_w = \alpha d_w x_w + (1-\alpha)\sum_{j \in N_G(w)} x_j \geq d_w x_w,$$

we have $d_w < \Delta$, implying that $V_1 = \{w\}$.

Since $\rho_\alpha(G)x_i = \alpha d_i x_i + (1-\alpha)\sum_{j \in N_G(i)} x_j$ for $i \in V(G)$, we have

$$\rho_\alpha(G)\sum_{i \in V(G)} x_i \;=\; \alpha \sum_{i \in V(G)} d_i x_i + (1-\alpha)\sum_{i \in V(G)}\sum_{j \in N_G(i)} x_j$$

$$=\; \sum_{i \in V(G)} d_i x_i = \Delta \sum_{i \neq w} x_i + d_w x_w,$$

i.e., $(\Delta - \rho_\alpha(G)) \sum_{i \in V(G)} x_i = (\Delta - d_w) x_w$, from which we get

$$\Delta - \rho_\alpha(G) = \frac{(\Delta - d_w) x_w}{\sum_{i \in V(G)} x_i} > \frac{x_w}{n x_z}.$$

Let $\gamma = \frac{x_z}{x_w}$. If $\gamma \leq \frac{2D - \alpha}{2(1-\alpha)}$, then

$$\Delta - \rho_\alpha(G) > \frac{1}{n\gamma} \geq \frac{2(1-\alpha)}{(2D - \alpha)n},$$

as desired.

In the following, we assume that $\gamma > \frac{2D - \alpha}{2(1-\alpha)}$.

Since $d_G(w, z) = D$, we can choose a vertex $z' \in N_G(z)$ such that $d_G(w, z') = D - 1$. Let $v_0 \ldots v_{D-1}$ be a shortest path from w to z' with $v_0 = w$ and $v_{D-1} = z'$. Then as above, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &= x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_w^2 + (1-\alpha) \sum_{j=0}^{D-2} \left(x_{v_j} - x_{v_{j+1}}\right)^2 \\
&\geq x_w^2 + \frac{(1-\alpha)(x_w - x_{z'})^2}{D - 1} \\
&\geq \frac{1 - \alpha}{D - \alpha} x_{z'}^2.
\end{aligned}
$$

If $x_{z'} > \frac{1}{\sqrt{n}}$, then

$$\Delta - \rho_\alpha(G) > \frac{1 - \alpha}{(D - \alpha)n} \geq \frac{2(1-\alpha)}{(2D - \alpha)n},$$

as desired.

Thus, we assume that there is a vertex $z' \in N_G(z)$ such that $x_{z'} \leq \frac{1}{\sqrt{n}}$. Then

$$\rho_\alpha(G) x_z = \alpha \Delta x_z + (1-\alpha) \sum_{i \in N_G(z)} x_i \leq (\Delta - 1 + \alpha) x_z + (1-\alpha) \frac{1}{\sqrt{n}},$$

which implies $\Delta - \rho_\alpha(G) \geq (1-\alpha) \left(1 - \frac{1}{x_z \sqrt{n}}\right)$.

If $(1-\alpha) \left(1 - \frac{1}{x_z \sqrt{n}}\right) > \frac{2(1-\alpha)}{(2D - \alpha)n}$, then we are done. Thus, we assume that $(1-\alpha)(1 - \frac{1}{x_z \sqrt{n}}) \leq \frac{2(1-\alpha)}{(2D-\alpha)n}$, i.e.,

$$x_z \leq \frac{(2D - \alpha)\sqrt{n}}{(2D - \alpha)n - 2}.$$

This, together with the fact that $(n-1)x_z^2 + x_w^2 \geq \sum_{i \in V(G)} x_i^2 = 1$, implies that

$$\gamma^2 = \left(\frac{x_z}{x_w}\right)^2 \leq \frac{1}{\frac{1}{x_z^2} - (n-1)} \leq \frac{(2D-\alpha)^2 n}{(2D-\alpha)(2D-\alpha-4)n + 4}.$$

If $D \geq 3$, then $(2D-\alpha)(2D-\alpha-4)n + 4 \geq (\alpha^2 - 8\alpha + 12)n + 4 > 4n$, and thus

$$\gamma^2 < \frac{(2D-\alpha)^2 n}{4n} \leq \frac{(2D-\alpha)^2}{4(1-\alpha)^2} < \gamma^2,$$

which is a contradiction. Thus, it follows that $D = 2$.

By Lemma 2.3 and the fact that $x_z^2 > \frac{1}{n}$, we have $x_w^2 + (1-\alpha)(x_w - x_z)^2 \geq \frac{1-\alpha}{2-\alpha}x_z^2 > \frac{2(1-\alpha)}{(2D-\alpha)n}$.

Suppose that there are two paths, say wuz and wvz, from w to z. Note that $(x_w - t)^2 + (t - x_z)^2 \geq \frac{1}{2}(x_w - x_z)^2$. As earlier, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &= x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_w^2 + (1-\alpha)\left((x_w - x_u)^2 + (x_u - x_z)^2 \right. \\
&\qquad \left. + (x_w - x_v)^2 + (x_v - x_z)^2\right) \\
&\geq x_w^2 + (1-\alpha)\left(\frac{(x_w - x_z)^2}{2} + \frac{(x_w - x_z)^2}{2}\right) \\
&= x_w^2 + (1-\alpha)(x_w - x_z)^2 \\
&> \frac{2(1-\alpha)}{(2D-\alpha)n},
\end{aligned}
$$

as desired.

Thus, we assume that there is a unique path, say wuz, from w to z. Let $N_1 = N_G(z) \setminus \{u\}$ and let N_2 the set of vertices of distance 2 from z except w. Then $V(G) \setminus \{z, u, w\} = N_1 \cup N_2$, and for every vertex $v \in N_1$, $d_G(v, w) = 2$. We consider three cases.

Case 1. u is adjacent to at least two vertices in N_1.

We choose $v, v' \in N_1 \cap N_G(u)$. Since $d_u = d_z = \Delta$, there is a vertex in $N_1 \setminus \{v, v'\}$, say v_1, such that $uv_1 \notin E(G)$. Note that $d_G(v_1, w) = 2$. Then there is a path, say $v_1 v_2 w$, connecting v_1 and w, where $v_2 \in N_2$. Then as earlier, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &= x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_w^2 + (1-\alpha)\left((x_w - x_u)^2 + (x_u - x_z)^2 \right. \\
&\qquad + (x_u - x_v)^2 + (x_v - x_z)^2 + (x_u - x_{v'})^2 + (x_{v'} - x_z)^2 \\
&\qquad \left. + (x_w - x_{v_2})^2 + (x_{v_2} - x_{v_1})^2 + (x_{v_1} - x_z)^2\right) \\
&\geq x_w^2 + (1-\alpha)\left((x_w - x_u)^2 + (x_u - x_z)^2 \right.
\end{aligned}
$$

$$+ \frac{(x_u - x_z)^2}{2} + \frac{(x_u - x_z)^2}{2} + \frac{(x_w - x_z)^2}{3} \Big)$$

$$= \ x_w^2 + (1 - \alpha) \left((x_w - x_u)^2 + 2(x_u - x_z)^2 + \frac{(x_w - x_z)^2}{3} \right).$$

By Lemma 2.3,

$$\Delta - \rho_\alpha(G) \geq x_w^2 + (1 - \alpha)(x_w - x_z)^2 > \frac{2(1 - \alpha)}{(2D - \alpha)n},$$

as desired.

Case 2. u is adjacent to exactly one vertex in N_1.

Let v be the unique vertex in $N_1 \cap N_G(u)$. Since $d_u = d_z = \Delta$, there is a vertex in $N_1 \setminus \{v\}$, say v_1, such that $uv_1 \notin E(G)$. Note that $d_G(v_1, w) = 2$. Then there is a path, say $v_1 v_2 w$, connecting v_1 and w where $v_2 \in N_2$. Since $w, u, z, v, v_1, v_2 \in V(G)$, we have $n \geq 6$. If $n = 6$, then $\Delta = d_z = 3$, $d_w = 2$, and thus $2|E(G)| = 5\Delta + d_w = 17$, a contradiction. Thus $n \geq 7$.

Case 2.1. $\Delta \geq 4$.

Since $|N_1| = d_z - 1 = \Delta - 1 \geq 3$, we may choose $s \in N_1 \setminus \{v, v_1\}$. Since $D = 2$, there is a path, say $ss'w$, connecting s and w, where $s' \in N_2$.

If $s' = v_2$, then as above, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) \ &= \ x_w^2 + (1 - \alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq \ x_w^2 + (1 - \alpha) \big((x_w - x_u)^2 + (x_u - x_z)^2 + (x_w - x_{v_2})^2 \\
&\quad + (x_{v_2} - x_{v_1})^2 + (x_{v_1} - x_z)^2 \\
&\quad + (x_{v_2} - x_s)^2 + (x_s - x_z)^2 \big) \\
&\geq \ x_w^2 + (1 - \alpha) \left(\frac{(x_w - x_z)^2}{2} + (x_w - x_{v_2})^2 + \frac{(x_{v_2} - x_z)^2}{2} \cdot 2 \right) \\
&\geq \ x_w^2 + (1 - \alpha)(x_w - x_z)^2 \\
&> \ \frac{2(1 - \alpha)}{(2D - \alpha)n},
\end{aligned}
$$

as desired.

If $s' \neq v_2$, then as above, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) \ &= \ x_w^2 + (1 - \alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq \ x_w^2 + (1 - \alpha) \big((x_w - x_u)^2 + (x_u - x_z)^2 \\
&\quad + (x_w - x_{v_2})^2 + (x_{v_2} - x_{v_1})^2 + (x_{v_1} - x_z)^2 \\
&\quad + (x_w - x_{s'})^2 + (x_{s'} - x_s)^2 + (x_s - x_z)^2 \big) \\
&\geq \ x_w^2 + (1 - \alpha) \left(\frac{(x_w - x_z)^2}{2} + \frac{2(x_w - x_z)^2}{3} \right)
\end{aligned}
$$

$$\geq \quad x_w^2 + \frac{7(1-\alpha)(x_w - x_z)^2}{6}$$

$$> \quad x_w^2 + (1-\alpha)(x_w - x_z)^2$$

$$> \quad \frac{2(1-\alpha)}{(2D-\alpha)n},$$

as desired.

Case 2.2. $\Delta = 3$.

Suppose that $n \geq 8$. Then there are two vertices, say $s_1, s_2 \in V(G) \setminus \{w, u, z, v, v_1, v_2\}$. Since $D = 2$, $d_u = 3$ and $d_w = 2$, we have $d_G(s_1, w) = d_G(s_2, w) = 2$, and thus s_1 and s_2 can only be adjacent to v_2, which is impossible because $d_{v_2} = 3$. Thus $n = 7$. Let s be the vertex different from w, u, z, v, v_1, v_2. Then $E(G) = \{wu, uz, uv, vz, wv_2, v_2v_1, v_1z, v_2s, sv, sv_1\}$, see Fig. 1. Note that
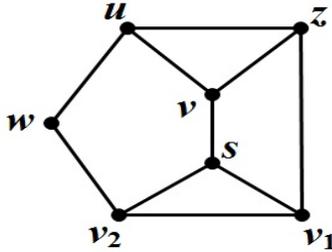

Fig. 1: The only possible graph G in Case 2.2.

there is an automorphism σ such that $\sigma(s) = z$. By [25, Proposition 16], $x_s = x_z$. Thus as above, we have

$$\begin{aligned}
\Delta - \rho_\alpha(G) &= x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq x_w^2 + (1-\alpha)\left((x_w - x_u)^2 + (x_u - x_z)^2 \right. \\
&\quad \left. + (x_w - x_{v_2})^2 + (x_{v_2} - x_s)^2\right) \\
&\geq x_w^2 + (1-\alpha)(x_w - x_z)^2 \\
&> \frac{2(1-\alpha)}{(2D-\alpha)n},
\end{aligned}$$

as desired.

Case 3. u is not adjacent to any vertex in N_1.

Since $d_w < \Delta$, there are two vertices, say v_1 and v_2 in N_1, such that some vertex v^* in N_2 is adjacent to w, v_1 and v_2. Thus, we have

$$\Delta - \rho_\alpha(G) = x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2$$

$$
\begin{aligned}
\geq \ & x_w^2 + (1-\alpha)\left((x_w - x_u)^2 + (x_u - x_z)^2 + (x_w - x_{v^*})^2 \right. \\
& \left. + (x_{v^*} - x_{v_1})^2 + (x_{v_1} - x_z)^2 + (x_{v^*} - x_{v_2})^2 + (x_{v_2} - x_z)^2\right) \\
\geq \ & x_w^2 + (1-\alpha)\left(\frac{(x_w - x_z)^2}{2} + (x_w - x_{v^*})^2 + \frac{(x_{v^*} - x_z)^2}{2} \cdot 2\right) \\
\geq \ & x_w^2 + (1-\alpha)(w_w - x_z)^2 \\
> \ & \frac{2(1-\alpha)}{(2D-\alpha)n},
\end{aligned}
$$

as desired.

Now by combining the above three cases, we complete the proof.   □

Besides those considerations in [7, 24], the proof of Theorem 4.4 needs more detailed analysis in the case of diameter two.

By the Perron-Frobenius Theorem, if $\lambda_\alpha(G)$ is the least eigenvalue $A_\alpha(G)$, then $\rho_\alpha(G) \geq -\lambda_\alpha(G)$. Thus, for a connected irregular graph G on n vertices with maximum degree Δ and diameter D,

$$
\Delta + \lambda_\alpha(G) > \frac{2(1-\alpha)}{(2D-\alpha)n}.
$$

Recall that Alon and Sudakov [2] proved that for a connected graph G on n vertices with maximum degree Δ and diameter D, if it is not bipartite (but possibly regular), then

$$
\Delta + \lambda_0(G) > \frac{1}{(D+1)n}.
$$

For a connected irregular graph G on n vertices with maximum degree Δ, minimum degree δ, average d and diameter D, Shi [29] showed that

$$
\rho_0(G) < \Delta - \frac{1}{(n-\delta)D - \binom{D}{2} + \frac{1}{\Delta - d}}
$$

and

$$
\mu(G) < 2\Delta - \frac{1}{(n-\delta)D - \binom{D}{2} + \frac{1}{2(\Delta - d)}},
$$

where $\mu(G)$ is the the largest eigenvalue of the Laplacian matrix of G. For a connected graph G, since $\mu(G) \leq 2\rho_{1/2}(G)$, upper bounds for $2\rho_{1/2}(G)$ result in upper bounds for $\mu(G)$.

We remark that the argument in [29] applies easily to prove the following result. For completeness, however, we include a proof here.

Theorem 4.5. *Let G be a connected irregular graph on n vertices with maximum degree Δ, minimum degree δ, average degree d and diameter D. For $0 \leq \alpha < 1$, we have*

$$
\rho_\alpha(G) < \Delta - \frac{1}{\frac{D(n-\delta)}{1-\alpha} - \frac{\binom{D}{2}}{1-\alpha} + \frac{1}{\Delta - d}}
$$

Proof. Let x be the Perron vector of $A_\alpha(G)$. Let $x_z = \max\{x_i : i \in V(G)\}$ and $x_w = \min\{x_i : i \in V(G)\}$. Let $v_0 \ldots v_p$ be a shortest path connecting w and z, where $v_0 = w$ and $v_p = z$. Now for $\ell = 1, \ldots, p$, by the Cauchy-Schwarz inequality,

$$\sum_{ij \in E(G)} (x_i - x_j)^2 \geq \sum_{j=0}^{\ell-1} \left(x_{v_j} - x_{v_{j+1}}\right)^2 \geq \frac{(x_w - x_{v_\ell})^2}{\ell}.$$

Thus, for $\ell = 1, \ldots, p$, we have by Lemma 2.3 that

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &= \sum_{u \in V(G)} (\Delta - d_u)x_u^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq (n\Delta - 2m)x_w^2 + (1-\alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq (n\Delta - 2m)x_w^2 + (1-\alpha)\frac{(x_w - x_{v_\ell})^2}{\ell} \\
&\geq \frac{(1-\alpha)(n\Delta - 2m)x_{v_\ell}^2}{\ell(n\Delta - 2m) + 1 - \alpha}.
\end{aligned}
$$

(4.4)

It is known that $D + \Delta \leq n + 1$. Since $\delta < \Delta$, we have $D + \delta \leq n$. Since $1 \leq p \leq D$ and $\delta \leq d_w \leq \Delta$, we have

$$p(n - d_w) - \binom{p}{2} \leq p(n - \delta) - \binom{p}{2} \leq D(n - \delta) - \binom{D}{2}.$$

Let

$$\beta = \frac{1}{\frac{p(n-d_w)-\binom{p}{2}}{1-\alpha} + \frac{1}{\Delta-d}}.$$

Then it suffices to show that $\Delta - \rho_\alpha(G) > \beta$.

If $x_w^2 > \frac{\beta}{n\Delta-2m}$, then $\Delta - \rho_\alpha(G) \geq (n\Delta - 2m)x_w^2 > \beta$.

If $x_{v_\ell}^2 > \frac{\ell(n\Delta-2m)+1-\alpha}{(1-\alpha)(n\Delta-2m)}\beta$ for some $\ell = 1, \ldots, p$, then from (4.4) we have $\Delta - \rho_\alpha(G) > \beta$.

If $\sum_{v \in N_G(w)} x_v^2 > \frac{d_w(1-\alpha)+n\Delta-2m}{(1-\alpha)(n\Delta-2m)}\beta$, then by Lemma 2.3,

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &\geq (n\Delta - 2m)x_w^2 + (1-\alpha) \sum_{v \in N_G(w)} (x_v - x_w)^2 \\
&\geq \sum_{v \in N_G(w)} \left(\frac{(n\Delta - 2m)x_w^2}{d_w} + (1-\alpha)(x_v - x_w)^2 \right) \\
&\geq \sum_{v \in N_G(w)} \frac{(1-\alpha)(n\Delta - 2m)}{d_w(1-\alpha) + (n\Delta - 2m)}x_v^2 > \beta.
\end{aligned}
$$

Thus, we can assume that $x_w^2 \leq \frac{\beta}{n\Delta-2m}$, $\sum_{v \in N_G(w)} x_v^2 \leq \frac{d_w(1-\alpha)+n\Delta-2m}{(1-\alpha)(n\Delta-2m)}\beta$ and $x_{v_\ell}^2 \leq \frac{\ell(n\Delta-2m)+1-\alpha}{(1-\alpha)(n\Delta-2m)}\beta$ for $\ell = 1, \ldots, p$. Then

$$
\begin{aligned}
(n-p-d_w+1)x_z^2 &\geq 1 - x_w^2 - \sum_{\ell=2}^{p-1} x_{v_\ell}^2 - \sum_{v \in N_G(w)} x_v^2 \\
&\geq 1 - \frac{\beta}{n\Delta-2m} - \frac{\sum_{\ell=2}^{p-1}(\ell(n\Delta-2m)+1-\alpha)}{(1-\alpha)(n\Delta-2m)}\beta \\
&\quad - \frac{d_w(1-\alpha)+n\Delta-2m}{(1-\alpha)(n\Delta-2m)}\beta \\
&= 1 - \left(\frac{d_w+p-1}{n\Delta-2m} + \frac{\binom{p}{2}}{1-\alpha}\right)\beta
\end{aligned}
$$

with equality only if $x_w^2 = \frac{\beta}{n\Delta-2m}$. From (4.4), we have

$$
\Delta - \rho_\alpha(G) \geq \frac{(1-\alpha)(n\Delta-2m)\left(1-\left(\frac{d_w+p-1}{n\Delta-2m}+\frac{\binom{p}{2}}{1-\alpha}\right)\beta\right)}{(p(n\Delta-2m)+1-\alpha)(n-p-d_w+1)} = \beta.
$$

Suppose that $\Delta - \rho_\alpha(G) = \beta$. Then by Lemma 2.3, we have $x_w = \frac{1-\alpha}{p(n\Delta-2m)+1-\alpha}x_{v_p}$. Note that we also have $x_w^2 = \frac{\beta}{n\Delta-2m}$. Thus

$$
\left(\frac{p(n\Delta-2m)+1-\alpha}{1-\alpha}\right)^2 \frac{\beta}{n\Delta-2m} = x_{v_p}^2 \leq \frac{p(n\Delta-2m)+1-\alpha}{(n\Delta-2m)(1-\alpha)}\beta,
$$

implying that $p(n\Delta-2m) \leq 0$, a contradiction. Therefore $\Delta - \rho_\alpha(G) > \beta$. □

For a k-connected irregular graph G on $n \geq 3$ vertices with m edges and maximum degree Δ, Chen and Hou [6] (see also Shiu et al. [30]) showed that

$$
\rho_0(G) < \Delta - \frac{(n\Delta-2m)k^2}{(n\Delta-2m)(n^2-(\Delta-k+2)(n-k))+nk^2},
$$

and Shiu et al. [30] showed that

$$
2\rho_{1/2}(G) < 2\Delta - \frac{(n\Delta-2m)k^2}{2(n\Delta-2m)(n^2-(\Delta-k+2)(n-k))+nk^2}.
$$

The argument in [6,30] leads easily to the following result. For completeness, however, we include a proof here.

Theorem 4.6. *Let G be a k-connected irregular graph on n vertices with m edges, maximum degree Δ. For $0 \leq \alpha < 1$, we have*

$$
\rho_\alpha(G) < \Delta - \frac{(1-\alpha)(n\Delta-2m)k^2}{(n\Delta-2m)(n^2-(\Delta-k+2)(n-k))+(1-\alpha)nk^2}.
$$

Proof. Let

$$\beta = \frac{(1-\alpha)(n\Delta - 2m)k^2}{(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + (1-\alpha)nk^2}.$$

Note that $n^2 - (\Delta - k + 2)(n - k) \geq nk > k^2$. Then $\beta < 1$.

Let x be the Perron vector of $A_\alpha(G)$. Let $x_z = \max\{x_i : i \in V(G)\}$. Then $x_z > \frac{1}{\sqrt{n}}$.

If $d_z < \Delta$, then as in the proof of Theorem 4.4, we have $\rho_\alpha(G) \leq \Delta - 1 < \Delta - \beta$.

Assume that $d_z = \Delta$. Let w be a vertex of G such that $x_w = \min\{x_i : i \in V(G)\}$. From the eigenequation at w, we have $d_w < \Delta$. As G is k-connected, by Menger's Theorem, we can choose k vertex-disjoint paths, say $Q_1, \ldots, Q_k$, connecting w and z in G so that $\sum_{s=1}^k |V(Q_s)|$ is as small as possible. Then $\bigcup_{s=1}^k V(Q_s)$ contains exactly k vertices in $N_G(z)$, implying that $\left|\bigcup_{s=1}^k V(Q_s)\right| \leq n - (\Delta - k)$, and thus $\sum_{s=1}^k (|V(Q_s)| - 1) = \left|\bigcup_{s=1}^k V(Q_s)\right| + 2(k-1) - k \leq n - \Delta + 2k - 2$. By the Cauchy-Schwarz inequality,

$$
\begin{aligned}
\sum_{ij \in E(G)} (x_i - x_j)^2 &\geq \sum_{s=1}^k \sum_{ij \in E(Q_s)} (x_i - x_j)^2 \\
&\geq \sum_{s=1}^k \frac{1}{|V(Q_s)| - 1} \left(\sum_{ij \in E(Q_s)} (x_i - x_j) \right)^2 \\
&= (x_w - x_z)^2 \sum_{s=1}^k \frac{1}{|V(Q_s)| - 1} \\
&\geq (x_w - x_z)^2 \frac{k^2}{\sum_{s=1}^k (|V(Q_s)| - 1)} \\
&\geq \frac{k^2}{n - \Delta + 2k - 2} (x_w - x_z)^2.
\end{aligned}
$$

Therefore, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) &= \sum_{u \in V(G)} (\Delta - d_u) x_u^2 + (1 - \alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq (n\Delta - 2m) x_w^2 + (1 - \alpha) \sum_{ij \in E(G)} (x_i - x_j)^2 \\
&\geq (n\Delta - 2m) x_w^2 + \frac{(1-\alpha)k^2}{n - \Delta + 2k - 2} (x_w - x_z)^2.
\end{aligned}
$$

Note that $x_w \neq x_z$ as G is irregular.

If $x_w^2 \geq \frac{\beta}{n\Delta - 2m}$, then $\Delta - \rho_\alpha(G) > (n\Delta - 2m) x_w^2 \geq \beta$, as desired.

Assume that $x_w^2 < \frac{\beta}{n\Delta - 2m}$. By Lemma 2.3,

$$(4.5) \qquad \Delta - \rho_\alpha(G) \geq \frac{(1-\alpha)(n\Delta - 2m)k^2}{(n\Delta - 2m)(n - \Delta + 2k - 2) + (1-\alpha)k^2} x_z^2.$$

If $k = 1$, then $(n-1)x_z^2 \geq 1 - x_w^2 > 1 - \frac{\beta}{n\Delta - 2m}$, and thus from (4.5), we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) \ &> \ \frac{(1-\alpha)(n\Delta - 2m)}{(n\Delta - 2m)(n - \Delta) + 1 - \alpha} \cdot \frac{1}{n-1} \cdot \left(1 - \frac{\beta}{n\Delta - 2m}\right) \\
&= \ \beta \cdot \frac{(n\Delta - 2m)\left(\frac{n^2}{n-1} - (\Delta + 1)\right) + 1 - \alpha}{(n\Delta - 2m)(n - \Delta) + 1 - \alpha} \\
&> \ \beta,
\end{aligned}
$$

as desired.

Now assume that $k \geq 2$. Since $d_w \geq k$, we may choose $k - 1$ vertices, say $v_1, \ldots, v_{k-1}$, in $N_G(w)$ different from z. Then as above, we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) \ &\geq \ (n\Delta - 2m)x_w^2 + (1-\alpha)\sum_{i=1}^{k-1}(x_{v_i} - x_w)^2 \\
&= \ \sum_{i=1}^{k-1}\left(\frac{n\Delta - 2m}{k-1}x_w^2 + (1-\alpha)(x_{v_i} - x_w)^2\right) \\
&\geq \ \sum_{i=1}^{k-1}\frac{(1-\alpha)(n\Delta - 2m)}{n\Delta - 2m + (1-\alpha)(k-1)}x_{v_i}^2 \\
&= \ \frac{(1-\alpha)(n\Delta - 2m)}{n\Delta - 2m + (1-\alpha)(k-1)}\sum_{i=1}^{k-1}x_{v_i}^2.
\end{aligned}
$$

If $\sum_{i=1}^{k-1}x_{v_i}^2 > \frac{n\Delta - 2m + (1-\alpha)(k-1)}{(1-\alpha)(n\Delta - 2m)}\beta$, then $\Delta - \rho_\alpha(G) > \beta$, as desired.

Assume that $\sum_{i=1}^{k-1}x_{v_i}^2 \leq \frac{n\Delta - 2m + (1-\alpha)(k-1)}{(1-\alpha)(n\Delta - 2m)}\beta$. Recall that $x_w^2 < \frac{\beta}{n\Delta - 2m}$. Then

$$(n-k)x_z^2 \geq 1 - x_w^2 - \sum_{i=1}^{k-1}x_{v_i}^2 > 1 - \frac{n\Delta - 2m + (1-\alpha)k}{(1-\alpha)(n\Delta - 2m)}\beta.$$

Therefore, from (4.5), we have

$$
\begin{aligned}
\Delta - \rho_\alpha(G) \ &\geq \ \frac{(1-\alpha)(n\Delta - 2m)k^2}{(n\Delta - 2m)(n - \Delta + 2k - 2) + (1-\alpha)k^2}x_z^2 \\
&> \ \frac{(1-\alpha)(n\Delta - 2m)k^2}{(n\Delta - 2m)(n - \Delta + 2k - 2) + (1-\alpha)k^2} \\
&\qquad \cdot \frac{1}{n-k}\left(1 - \frac{n\Delta - 2m + (1-\alpha)k}{(1-\alpha)(n\Delta - 2m)}\beta\right)
\end{aligned}
$$

$$= \quad \beta,$$

as desired. □

By direct check, the upper bound in Theorem 4.4 is less than or equal to the upper bound in Theorem 4.5 if and only if

$$(\Delta - d)\,(2D\delta + D(D-1) - \alpha n) \leq 2(1 - \alpha),$$

the upper bound in Theorem 4.4 is less than or equal to the upper bound in Theorem 4.6 if and only if

$$2n^2 + \frac{2(1-\alpha)nk^2}{n\Delta - 2m} \geq n(2D - \alpha)k^2 + 2(\Delta - k + 2)(n - k),$$

and the upper bound in Theorem 4.5 is less than or equal to the upper bound in Theorem 4.6 if and only if

$$k^2 D(2n - 2\delta - D + 1) \leq 2n^2 - 2(\Delta - k + 2)(n - k).$$

4.3   A bound for the α-spectral radius of graphs with fixed domination number

For a graph G with $u \in V(G)$, let $R_u = V(G) \setminus N_G(u)$. The following result concerning the domination number unifies the results in [33, 34] on spectral radius and signless Laplacian spectral radius of a graph. We note that the bound is independent of the parameter α. By $\overline{G}$ we denote the complement of G.

Theorem 4.7. *Let G be a graph with n vertices and domination number γ, where $1 \leq \gamma \leq n - 1$. For $0 \leq \alpha < 1$, we have $\rho_\alpha(G) \leq n - \gamma$ with equality if and only if $G \cong K_{n-\gamma+1} \cup (\gamma-1)K_1$ or when $\gamma \geq 2$ and $n-\gamma$ is even, $G \cong \frac{n-\gamma+2}{2}K_2 \cup (\gamma-2)K_1$.*

Proof. Let Δ be the maximum degree of G. For $u \in V(G)$ with $d_G(u) = \Delta$, it is easily seen that R_u is a dominating set of G, and thus $\gamma \leq |R_u| = n - \Delta$, implying that $\Delta(G) \leq n - \gamma$ with equality if and only if R_u is a minimum dominating set of G. Thus $\rho_\alpha(G) \leq \Delta \leq n - \gamma$.

Suppose that $\rho_\alpha(G) = n - \gamma$. Then $\Delta = n - \gamma$. Obviously, $\rho_\alpha(G) = \rho_\alpha(G_1)$ for some nontrivial component G_1 of G. Let Δ_1 be the maximum degree of G_1. Note that $\rho_\alpha(G) = \rho_\alpha(G_1) \leq \Delta_1 \leq \Delta = n - \gamma$. Thus G_1 is regular, $\Delta_1 = n - \gamma$, and R_u is a minimum dominating set of G for some $u \in V(G_1)$. Thus, R_u is an independent set of G, and if G is not connected, then any component different from G_1 is trivial. If $\gamma = 1$, then $G \cong K_n$. Suppose that $\gamma \geq 2$.

Suppose that $d_{G_1}(u) \leq |V(G_1)| - 3$ for some $u \in V(G_1)$. Then there exists $v, w \in V(G_1)$ such that $uv, uw \notin E(G_1)$. Since G_1 is $(n - \gamma)$-regular and R_u is an independent set of G, v and w are both adjacent to each vertex of $N_{G_1}(u)$, implying that, for a vertex $z \in N_{G_1}(u)$, $(R_u \setminus \{v, w\}) \cup \{z\}$ is a dominating set of G with

cardinality $\gamma - 1$, a contradiction. Thus $d_{G_1}(u) = |V(G_1)| - 1$ or $|V(G_1)| - 2$. If $d_{G_1}(u) = |V(G_1)| - 1$, then since G_1 is $(n - \gamma)$-regular, we have $G_1 \cong K_{n-\gamma+1}$, and thus $G \cong K_{n-\gamma+1} \cup (\gamma - 1)K_1$. Suppose that $d_{G_1}(u) = |V(G_1)| - 2$. Then there is unique vertex, say v, in $V(G_1)\setminus\{u\}$ that is not adjacent to u, and $N_{G_1}(u) = N_{G_1}(v)$. For any $w \in N_{G_1}(u)$, since w is adjacent to both u and v, there is a unique vertex in $N_{G_1}(u) \setminus \{w\}$ that is not adjacent to w in G_1. Thus $n - \gamma$ is even, $G_1 \cong \overline{\frac{n-\gamma+2}{2}K_2}$, and thus $G \cong \overline{\frac{n-\gamma+2}{2}K_2} \cup (\gamma - 2)K_1$.

If $G \cong K_{n-\gamma+1} \cup (\gamma - 1)K_1$, or if $\gamma \geq 2$, $n - \gamma$ is even and $G \cong \overline{\frac{n-\gamma+2}{2}K_2} \cup (\gamma - 2)K_1$, then G has a unique nontrivial regular component of degree $n - \gamma$, and thus $\rho_\alpha(G) = n - \gamma$. $\square$

5. TREES WITH LARGE α-SPECTRAL RADIUS

If T is a tree on n vertices, then, for $0 \leq \alpha < 1$, we have by Corollary 2.1 that $\rho_\alpha(T) \leq \rho_\alpha(S_n)$ with equality if and only if $T \cong S_n$, see [26].

For $n \geq 4$ and $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$, let $D_{n,a}$ be the tree obtained from vertex-disjoint S_{a+1} with center u and S_{n-a-1} with center v by adding an edge uv.

Theorem 5.8. *Let T be a tree on $n \geq 4$ vertices. Suppose that $T \not\cong S_n$. Then for $0 \leq \alpha < 1$, $\rho_\alpha(T) \leq \rho_\alpha(D_{n,1})$ with equality if and only if $T \cong D_{n,1}$.*

Proof. The statement is trivial for $n = 4$. Suppose that $n \geq 5$. Let T be a tree with the largest α-spectral radius among trees on n vertices except the star S_n.

Let d be the diameter of T. Since $T \not\cong S_n$, we have $d \geq 3$. Suppose that $d \geq 4$. Let $v_0v_1 \ldots v_d$ be a diametral path of T. Let $N_1 = N_T(v_{d-1}) \setminus \{v_{d-2}\}$ Let $T' = T - \{v_{d-1}v : v \in N_1\} + \{v_{d-2}v : v \in N_1\}$. Obviously, $T' \not\cong S_n$. By Corollary 2.1, we have $\rho_\alpha(T) < \rho_\alpha(T')$, a contradiction. Thus $d = 3$ and $T \cong D_{n,a}$, where $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$. By Lemma 2.1, we have $a = 1$ and $T \cong D_{n,1}$. $\square$

For $3 \leq d \leq n - 1$, let $T_{n,d}$ be the tree obtained from a path $v_0v_1 \cdots v_d$ with length d by attaching $n - 1 - d$ pendant edges at vertex $v_{\lfloor \frac{d}{2} \rfloor}$.

Theorem 5.9. *Let T be a tree with n vertices and diameter $d \geq 3$. For $0 \leq \alpha < 1$, $\rho_\alpha(T) \leq \rho_\alpha(T_{n,d})$ with equality if and only if $T \cong T_{n,d}$.*

Proof. Let T be a tree with the largest α-spectral radius among trees with n vertices and diameter d. Let $P = v_0 \ldots v_d$ be a diametral path of T. For any $u \in V(T)$, let $d_T(u, P) = \min\{d_T(u, v_i) : i = 0, \ldots, d\}$.

Suppose that uv is an edge outside P that is not a pendant edge. Assume that $d_T(u, P) < d_T(v, P)$. Let w be the vertex on P with $d_T(u, P) = d_T(u, w)$. Let $T^* = T - \{vz : vz \in E(T), z \neq u\} + \{wz : vz \in E(T), z \neq u\}$ if $x_w \geq x_v$, and $T^* = T - \{wz : wz \in E(T) \setminus \{e\}\} + \{vz : zw \in E(T) \setminus \{e\}\}$ otherwise, where e is the edge incident with w in the path connecting w and v. Obviously, T^* is a tree

with n vertices and diameter d. By Lemma 2.1, $\rho_\alpha(T^*) > \rho_\alpha(T)$, a contradiction. Every edge outside P is a pendant edge at some vertex of P except v_0 and v_d.

Suppose that there are two vertices, say u and v, on P with degree greater than two. We may assume that $x_u \geq x_v$. Let $T^* = T - \{vz : vz \in E(T) \setminus E(P)\} + \{uz : vz \in E(T) \setminus E(P)\}$. By Lemma 2.1, we have $\rho_\alpha(T^*) > \rho_\alpha(T)$, a contradiction. It follows that there is at most one vertex on P with degree greater than two.

Therefore T is obtainable from P by attaching $n - d - 1$ pendant edges at a vertex different from v_0 and v_d. By Theorem 3.1, we have $T \cong T_{n,d}$. $\square$

It is known that $T_{n,d}$ is the unique tree with maximum 0-spectral radius among trees with n vertices and diameter $d \geq 3$, see [17, 31].

6. THE DIFFERENCE BETWEEN MAXIMUM DEGREE AND THE α-SPECTRAL RADIUS

Recall that for a graph G with maximum degree Δ and $0 \leq \alpha < 1$, $\rho_\alpha(G) \leq \Delta$ with equality if and only if G has a component that is regular of degree Δ. Let $\gamma_\alpha(G) = \Delta - \rho_\alpha(G)$. We may view $\gamma_\alpha(G)$ as a measure of irregularity of the graph G. The case when $\alpha = 0$ has been studied in [28].

Theorem 6.10. *Let G be a graph on $n \geq 2$ vertices. For $0 \leq \alpha < 1$, we have*

$$\gamma_\alpha(G) \leq n - 1 - \frac{\alpha n}{2} - \frac{\sqrt{\alpha^2 n^2 + 4(1 - 2\alpha)(n - 1)}}{2}$$

with equality if and only if $G \cong S_n$.

Proof. Let Δ be the maximum degree of G. Then $S_{\Delta+1}$ is a subgraph of G. By [23, Corollary 2.2, p. 38],

$$\rho_\alpha(G) \geq \rho_\alpha(S_{\Delta+1})$$

with equality when G is connected if and only if $G \cong S_{\Delta+1}$. From [25], we have

$$\rho_\alpha(S_{\Delta+1}) = \frac{\alpha(\Delta + 1) + \sqrt{\alpha^2(\Delta + 1)^2 + 4(1 - 2\alpha)\Delta}}{2}.$$

Thus

$$\gamma_\alpha(G) \leq f(\Delta),$$

where

$$f(t) = t - \frac{\alpha(t + 1)}{2} - \frac{\sqrt{\alpha^2(t + 1)^2 + 4(1 - 2\alpha)t}}{2}.$$

Note that

$$f'(t) = 1 - \frac{\alpha}{2} - \frac{\alpha^2(t + 1) + 2(1 - 2\alpha)}{2\sqrt{\alpha^2(t + 1)^2 + 4(1 - 2\alpha)t}}.$$

It can be seen that $f'(t) > 0$ if and only if $g(t) > 0$, where

$$g(t) = \alpha^2 t^2 + 2(\alpha^2 - 4\alpha + 2)t - \alpha^2 + 3\alpha - 1.$$

Since $0 \le \alpha < 1$, we have $-\frac{2(\alpha^2 - 4\alpha + 2)}{2\alpha^2} < 1$. Thus $g(t)$ is strictly increasing for $t \ge 1$. Now it follows that for $t \ge 1$,

$$g(t) \ge g(1) = (\alpha - 1)(2\alpha - 3) > 0,$$

or equivalently, $f'(t) > 0$. Thus $f(t)$ is strictly increasing for $t \ge 1$. Therefore

$$\gamma_\alpha(G) \le f(\Delta) \le f(n-1) = n - 1 - \frac{\alpha n}{2} - \frac{\sqrt{\alpha^2 n^2 + 4(1 - 2\alpha)(n-1)}}{2}$$

with equalities if and only if $\Delta = n-1$ (implying that G is connected) and $\rho_\alpha(G) = \rho_\alpha(S_{\Delta+1})$, or equivalently, $G \cong S_n$. $\qquad\square$

For connected graph G, if there is an automorphism σ such that $\sigma(u) = v$, then $x_u = x_v$, where x is the Perron vector of $A_\alpha(G)$ with $0 \le \alpha < 1$, see [25, Proposition 16].

For $n \ge 3$, let $S_n + e$ be the unicyclic graph obtained from the star by adding an edge to connect two vertices of degree one.

Let x be the Perron vector of $A_\alpha(S_n + e)$. Let x_1 be the entry of x corresponding to the vertex of degree $n - 1$. The entry of x corresponding to the either vertex of degree 2 is equal, which is denoted by x_2, the entry of each vertex of degree 1 is equal, which is denoted by x_3. Let $\rho = \rho_\alpha(S_n + e)$. Thus

$$\begin{aligned} (\rho - \alpha(n-1))x_1 &= 2(1 - \alpha)x_2 + (n-3)(1-\alpha)x_3, \\ (\rho - 1 - \alpha)x_2 &= (1 - \alpha)x_1, \\ (\rho - \alpha)x_3 &= (1 - \alpha)x_1. \end{aligned}$$

Therefore $h(\rho) = 0$ with

$$\begin{aligned} h(t) &= t^3 - (\alpha(n+1) + 1)t^2 + ((\alpha^2 + 3\alpha - 1)(n-1) + \alpha(\alpha+1))t \\ &\quad + (1 - 2\alpha)(\alpha+1)(n-1) - 2(1-\alpha)^2. \end{aligned}$$

It follows that $\rho_\alpha((S_n + e))$ is the largest root of $h(t) = 0$.

Theorem 6.11. *Let G be a unicyclic graph with $n \ge 4$ vertices. For $0 \le \alpha < 1$, we have*

$$\gamma_\alpha(G) \le \gamma_\alpha(S_n + e)$$

with equality if and only if $G \cong S_n + e$.

Proof. Let Δ be the maximum degree of G. Let

$$t_0 = 1 + \frac{\alpha(n-1)}{2} + \frac{\sqrt{\alpha^2(n-1)^2 + 4(1 - 2\alpha)(n-2)}}{2}.$$

If $\Delta \leq n - 2$, then by the argument as in the proof of Theorem 6.10, we have

$$\gamma_\alpha(G) \leq f(\Delta) \leq f(n-2) = n - 1 - t_0.$$

If $\Delta = n - 1$, then $G \cong S_n + e$, and

$$\gamma_\alpha(G) = n - 1 - \rho_\alpha(S_n + e),$$

where $\rho_\alpha(S_n + e)$ is the largest root of $h(t) = 0$.

Let t_1 be the larger root of $h'(t) = 0$, i.e.,

$$t_1 = \frac{\alpha(n+1) + 1 + \sqrt{\alpha^2 n^2 - (\alpha^2 + 7\alpha - 3)n + \alpha^2 + 8\alpha - 2}}{3}.$$

It may be checked that $t_0 > t_1$. Thus $h(t)$ is strictly increasing for $t \geq t_0$.

Case 1. $0 \leq \alpha \leq \frac{1}{2}$.

Note that

$$\begin{aligned} h(t_0) &= \alpha(1-\alpha)(n-2)\frac{\alpha(n-1) + \sqrt{\alpha^2(n-1)^2 + 4(1-2\alpha)(n-2)}}{2} \\ &\quad + (3n-8)\alpha^2 + (14-5n)\alpha + 2n - 6. \end{aligned}$$

We view $h(t_0)$ as a function of n, denoted by $H(n)$. Then

$$\begin{aligned} 2H'(n) &= (2n-3)\alpha^2(1-\alpha) + \alpha(1-\alpha)\sqrt{\alpha^2(n-1)^2 + 4(1-2\alpha)(n-2)} \\ &\quad + \frac{\alpha(1-\alpha)(n-2)(\alpha^2(n-1) + 2(1-2\alpha))}{\sqrt{\alpha^2(n-1)^2 + 4(1-2\alpha)(n-2)}} + 6\alpha^2 - 10\alpha + 4. \end{aligned}$$

For $n \geq 4$, since $0 \leq \alpha \leq \frac{1}{2}$, we have $H'(n) > 0$, and thus $H(n)$ is strictly increasing for $n \geq 4$. Therefore

$$h(t_0) = H(n) \geq H(4) = \alpha(1-\alpha)\sqrt{9\alpha^2 + 8(1-2\alpha)} + (1-\alpha)(3\alpha^2 - 4\alpha + 2) > 0.$$

Case 2. $\frac{1}{2} < \alpha < 1$.

Note that

$$\sqrt{\alpha^2(n-1)^2 + 4(1-2\alpha)(n-2)} \geq \alpha(n-3) + \frac{2(1-\alpha)^2}{\alpha}.$$

Then

$$h(t_0) \geq \alpha^2(1-\alpha)(n-2)^2 + ((1-\alpha)^3 + 3\alpha^2 - 5\alpha + 2)(n-2) - 2(1-\alpha)^2.$$

Let $H(n)$ be the expression in the right hand side of the above inequality, which is a function of n. Then

$$H'(n) = 2\alpha^2(1-\alpha)n + 3\alpha^3 + 2\alpha^2 - 8\alpha + 3,$$

which is strictly increasing for $n \geq 4$. It follows that

$$H'(n) \geq H'(4) = (1 - \alpha)(5\alpha^2 - 5\alpha + 3) > 0.$$

Therefore

$$h(t_0) \geq H(n) \geq H(4) = 2(1 - \alpha)(3\alpha^2 - 4\alpha + 2) > 0.$$

Now combining Cases 1 and 2, we have $h(t_0) > 0$. Thus, for $t \geq t_0$, we have $h(t) > h(t_0) > 0$, implying that $\rho_\alpha(S_n + e) < t_0$. Now the result follows. $\square$

Theorem 6.12. *Let G be a graph on $n \geq 4$ vertices. If G is not bipartite, then for $0 \leq \alpha < 1$, we have*

$$\gamma_\alpha(G) \leq \gamma_\alpha(S_n + e)$$

with equality if and only if $G \cong S_n + e$.

Proof. Let Δ be the maximum degree of G. If $\Delta = n - 1$, then $S_n + e$ is a subgraph of G, and thus

$$\gamma_\alpha(G) = n - 1 - \rho_\alpha(G) \leq n - 1 - \rho_\alpha(S_n + e)$$

with equality if and only if $G \cong S_n + e$. Now the result follows as in the proof of Theorem 6.11. $\square$

7. COMMENTS

Because of the work of Nikiforov [25], we may study the (adjacency) spectral properties and signless Laplacian spectral properties of a graph in a unified way. Thus, we may also study those parameters based on the spectrum of $A_\alpha(G)$ of a graph G for $0 \leq \alpha < 1$. We give two such examples.

Let G be a graph with n vertices and m edges. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $A_\alpha(G)$, arranged in a non-increasing manner. Obviously, $\lambda_1 = \rho_\alpha(G)$.

The first is the α-energy of G, which is defined as

$$\mathcal{E}_\alpha(G) = \sum_{i=1}^{n} \left| \lambda_i - \frac{2\alpha m}{n} \right|.$$

Note that $\mathcal{E}_0(G)$ is the energy of G, which has been studied extensively [18, 21], and $\mathcal{E}_{1/2}(G)$ is half of the signless Laplacian energy of G, which has received some attention in recent years [1]. Let $A_\alpha = A_\alpha(G)$. Note that $\sum_{i=1}^{n} \lambda_i = \text{tr}(A_\alpha) = 2\alpha m$ and $\sum_{i=1}^{n} \lambda_i^2 = \text{tr}(A_\alpha^2) = 2(1 - \alpha)^2 m + \alpha^2 Z(G)$, where $Z(G) = \sum_{u \in V(G)} d_u^2$. By the Cauchy-Schwarz inequality, we have

$$\mathcal{E}_\alpha(G) \leq \sqrt{n \sum_{i=1}^{n} \left| \lambda_i - \frac{2\alpha m}{n} \right|^2}$$

$$= \sqrt{n\sum_{i=1}^{n}\lambda_i^2 - 4\alpha^2 m^2}$$

$$= \sqrt{2(1-\alpha)^2 mn + \alpha^2(nZ(G) - 4m^2)}.$$

For $\mathcal{E}_0(G)$, this is just McClelland's upper bound in [22]. On the other hand, it is easily seen that $\mathcal{E}_\alpha(G) \geq 2(\lambda_1 - \frac{2\alpha m}{n})$. Note that $\lambda_1 \geq \rho_0(G)$ [25, Proposition 18]. Lower bounds for $\rho_0(G)$, for example, $\lambda_1 \geq \sqrt{\frac{Z(G)}{n}} \geq \frac{2m}{n}$, may be used to derive lower bounds for $\mathcal{E}_\alpha(G)$. Furthermore, let $s_i = \lambda_i - \frac{2\alpha m}{n}$ for $i = 1, \ldots, n$. Then $\sum_{i=1}^{n} s_i = 0$, implying that $\sum_{i=1}^{n} s_i^2 \leq 2\sum_{1\leq i<j\leq n} |s_i||s_j|$. Thus $\mathcal{E}_\alpha(G)^2 = \sum_{i=1}^{n} s_i^2 + 2\sum_{1\leq i<j\leq n} |s_i||s_j| \geq 2\sum_{i=1}^{n} s_i^2$, i.e.,

$$\mathcal{E}_\alpha(G) \geq \sqrt{2\left(2(1-\alpha)^2 m + \alpha^2\left(Z(G) - \frac{4m^2}{n}\right)\right)}.$$

The second one is the α-Estrada index of a graph G, defined as $EE_\alpha(G) = \sum_{i=1}^{n} e^{\lambda_i}$. Obviously, $EE_0(G)$ is just the much studied Estrada index of G, see, e.g., [12, 13, 15]. Note also that $EE_{1/2}(G)$ is somewhat different from the so called signless Laplacian Estrada index [4, 19], which is defined to be $\sum_{i=1}^{n} e^{2\lambda_i}$ (with λ_i's being the eigenvalues of $A_{1/2}(G)$). For a graph G with n vertices and m edges, it is easily seen that

$$EE_\alpha(G) = n + 2\alpha m + \sum_{k\geq 2} \frac{\sum_{i=1}^{n}\lambda_i^k}{k!}.$$

As in [35], we have $\sum_{i=1}^{n}\lambda_i^k \leq \left(\sum_{i=1}^{n}\lambda_i^2\right)^{k/2} = \left(\sqrt{2(1-\alpha)^2 m + \alpha^2 Z(G)}\right)^k$ for $k \geq 2$. Thus

$$EE_\alpha(G) \leq n - 1 + 2\alpha m - \sqrt{2(1-\alpha)^2 m + \alpha^2 Z(G)} + e^{\sqrt{2(1-\alpha)^2 m + \alpha^2 Z(G)}}.$$

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