TWO CONJECTURES IN SPECTRAL GRAPH THEORY INVOLVING THE LINEAR COMBINATIONS OF GRAPH EIGENVALUES

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ABSTRACT. We prove two conjectures in spectral extremal graph theory involving the linear combinations of graph eigenvalues. Let $\lambda_1(G)$ be the largest eigenvalue of the adjacency matrix of a graph $G$, and $\overline{G}$ be the complement of $G$. A nice conjecture states that the graph on $n$ vertices maximizing $\lambda_1(G) + \lambda_1(\overline{G})$ is the join of a clique and an independent set, with $\lfloor n/3 \rfloor$ and $\lceil 2n/3 \rceil$ (also $\lfloor n/3 \rfloor$ and $\lceil 2n/3 \rceil$ if $n \equiv 2 \pmod{3}$) vertices, respectively. We resolve this conjecture for sufficiently large $n$ using analytic methods. Our second result concerns the $Q$-spread $s_Q(G)$ of a graph $G$, which is defined as the difference between the largest eigenvalue and least eigenvalue of the signless Laplacian of $G$. It was conjectured by Cvetković, Rowlinson and Simić in 2007 that the unique $n$-vertex connected graph of maximum $Q$-spread is the graph formed by adding a pendant edge to $K_{n-1}$. We confirm this conjecture for sufficiently large $n$.

1. Introduction

Spectral extremal graph theory seeks to maximize or minimize some function of graph eigenvalues or eigenvectors over a given family of graphs. In this paper we focus on two problems in spectral extremal graph theory. Before the statement of the results, we introduce some notation and definitions. Consider a simple graph $G = (V, E)$ with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix of $G$ is defined to be a matrix $A(G) = [a_{ij}]$ of order $n$, where $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$, and $a_{ij} = 0$ otherwise. The signless Laplacian of $G$ is defined by $Q(G) := D(G) + A(G)$, where $D(G)$ is the diagonal matrix whose entries are the degrees of the vertices of $G$. The eigenvalues of $A(G)$ and $Q(G)$ are denoted by $\lambda_1(G) \geq \cdots \geq \lambda_n(G)$ and $q_1(G) \geq \cdots \geq q_n(G)$, respectively. Recall that a complete split graph with parameters $n$, $\omega$ ($\omega \leq n$), denoted by $CS_{n,\omega}$, is the graph on $n$ vertices obtained from a clique on $\omega$ vertices and an independent set on the remaining $n - \omega$ vertices in which each vertex of the clique is adjacent to each vertex of the independent set. We study the following two conjectures.

Conjecture 1.1 ([2, 4, 3, 5, 14]). Let $G$ be a graph on $n$ vertices. Then

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \begin{cases} \frac{4}{3}n - \frac{5}{3} - \frac{1}{6} & n \equiv 0 \pmod{3}, \\
3n - 1 - \sqrt{9n^2 - 6n + 9} & n \equiv 1 \pmod{3}, \\
3n - 2 - \sqrt{9n^2 - 12n + 12} & n \equiv 2 \pmod{3}, \\
0 & \text{otherwise}. \end{cases}$$
Equality holds if and only if $G$ (or $\overline{G}$) is the complete split graph with a clique on $\lfloor n/3 \rfloor$ vertices, and also on $\lceil n/3 \rceil$ vertices if $n \equiv 2 \pmod{3}$.

**Conjecture 1.2** ([9, 4, 23]). Over all connected graphs on $n \geq 6$ vertices, $s_Q(G)$ is maximized by $K_{n-1}^+$, the graph formed by adding a pendant edge to the complete graph $K_{n-1}$. Furthermore, $s_Q(G)$ is minimized by the path $P_n$ and, in the case that $n$ is odd, by the cycle $C_n$.

It is worth mentioning that the second part of Conjecture 1.2 was proved by Das [12] and Fan et al. [15] independently using different proof techniques.

In this paper we confirm Conjecture 1.1 in Section 3 and the first part of Conjecture 1.2 in Section 4 for sufficiently large $n$.

1.1. **Nordhaus–Gaddum type inequality.** The study of Nordhaus–Gaddum type inequality has a long history, dating back to a classical paper of Nordhaus and Gaddum [21]. The following inequalities for the chromatic numbers $\chi(G)$ and $\chi(\overline{G})$ has been established.

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n + 1,$$
$$n \leq \chi(G) \cdot \chi(\overline{G}) \leq \frac{(n+1)^2}{4},$$

where $\overline{G}$ is the complement of $G$. Since then, any bound on the sum or the product of an invariant in a graph $G$ and the same invariant in $\overline{G}$ is called a *Nordhaus–Gaddum type inequality*. For an exhaustive survey of such relations see Aouchiche and Hansen [5] and the references therein. Many of those inequalities involve eigenvalues of adjacency, Laplacian and signless Laplacian matrices of graphs. The first known spectral Nordhaus–Gaddum results belong to Nosal [22], and to Amin–Hakimi [1], who proved that for each graph $G$ of order $n$,

$$\lambda_1(G) + \lambda_1(\overline{G}) < \sqrt{2(n-1)}.$$

Nikiforov [20] enhanced the above bound to $(\sqrt{2} - c)n$, where $c$ is some constant not less than $10^{-7}$. In the same paper, Nikiforov also conjectured that

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \frac{4}{3}n + O(1).$$

In [8], Csikvári improved Nikiforov’s bound to $(1 + \sqrt{3})n/2 - 1$. Later, Terpai [25] resolved Nikiforov’s conjecture using graph limit method.

Let us note that there are also some Nordhaus–Gaddum type inequalities for (signless) Laplacian eigenvalues of graphs. Most of the results on Laplacian eigenvalues are around the following conjecture which was posed in [26, 27]: for any graph $G$ on $n$ vertices,

$$\mu_1(G) + \mu_1(\overline{G}) \leq 2n - 1,$$

with equality if and only if $G$ or $\overline{G}$ is isomorphic to the join of an isolated vertex and a disconnected graph of order $n - 1$. Here, $\mu_1(G)$ and $\mu_1(\overline{G})$ are the largest eigenvalues of Laplacian matrices $L(G)$ and $L(\overline{G})$, respectively. Recently, Einollahzadeh and Karkhaneei [13] resolve the conjecture. For signless Laplacian eigenvalues, Ashraf and Tayfeh-Rezaie [6] prove that $q_1(G) + q_1(\overline{G}) \leq 3n - 4$ and equality holds if and only if $G$ is the star $K_{1,n-1}$, which confirms a conjecture in [5].
We now turn to our topic. Using AutoGraphiX, Aouchiche et al. [2] posed Conjecture 1.1 which also appeared in [4, 3, 5, 14]. As mentioned above, Terpai [25] proved a tight upper bound on $\lambda_1(G) + \lambda_1(\overline{G})$ using analytical methods. To be precise, he showed that
\[ \lambda_1(G) + \lambda_1(\overline{G}) \leq \frac{4}{3}n - 1. \]
According to our knowledge, this is the best result until now.

1.2. Q-spread of graphs. The spread $s(M)$ of an arbitrary $n \times n$ matrix $M$ is defined as the maximum modulus over the difference of all pairs of eigenvalues of $M$. When considering the adjacency matrix of a graph $G$, the spread is simply the distance between $\lambda_1$ and $\lambda_n$, denoted by $s(G) := \lambda_1(G) - \lambda_n(G)$. The adjacency spread of a graph has received much attention. In [16], the authors investigated a number of properties regarding the spread of a graph, determining upper and lower bounds on $s(G)$. Recently, Breen et al. [7] determine the unique graph maximizing the spread among all $n$-vertex graphs, which resolves a conjecture in [16].

With regard to the spread for signless Laplacian, we denote $s_Q(G) := q_1(G) - q_n(G)$ and refer it as Q-spread of $G$. Oliveira et al. [23] present some upper and lower bounds for signless Laplacian spread. Liu et al. [17] determine the unique graph with maximum signless Laplacian spread among the class of connected unicyclic graphs of order $n$. Das [12] and Fan et al. [15] confirm the second part of Conjecture 1.2 independently. We prove the first part for $n$ large enough.

2. Preliminaries

2.1. Notation. Given a subset $X$ of the vertex set $V(G)$ of a graph $G$, the subgraph of $G$ induced by $X$ is denoted by $G[X]$, and the graph obtained from $G$ by deleting $X$ is denoted by $G \setminus X$. We use $E(X)$ to denote the set of edges in the induced subgraph $G[X]$. As usual, for a vertex $v$ of $G$ we write $d_G(v)$ and $N_G(v)$ for the degree of $v$ and the set of neighbors of $v$ in $G$, respectively. If the underlying graph $G$ is clear from the context, simply $d(v)$ and $N(v)$.

We denote the maximum degree and minimum degree of $G$ by $\Delta(G)$ and $\delta(G)$, respectively. For a vector $x \in \mathbb{R}^n$, we denote by $x_{\max} := \{|x_i| : 1 \leq i \leq n\}$.

2.2. Graphons and graphon operators. A graphon is a symmetric measurable function $W : [0, 1]^2 \to [0, 1]$ (by symmetric, we mean $W(x, y) = W(y, x)$ for all $(x, y) \in [0, 1]^2$). Let $W$ denote the space of all graphon. Given a graph $G$ with $n$ vertices labeled $1, 2, \ldots, n$, we define its associated graphon $W_G : [0, 1]^2 \to [0, 1]$ by first partitioning $[0, 1]$ into $n$ equal-length intervals $I_1, I_2, \ldots, I_n$ and setting $W_G$ to be 1 on all $I_i \times I_j$ where $ij$ is an edge of $G$, and 0 on all other $I_i \times I_j$’s. Clearly, associated graphon is not unique due to different labeling of vertices. Using an equivalence relation on $W$ derived from the so-called cut metric, we can identify associated graphons that are equivalent up to relabelling, and up to any differences on a set of measure zero. The cut norm of a measurable function $W : [0, 1]^2 \to \mathbb{R}$ is defined as
\[ \|W\| := \sup_{S, T \subseteq [0, 1]} \left| \int_{S \times T} W(x, y) \, dx \, dy \right|, \]
where the supremum is taken over all measurable subsets $S$ and $T$. Given two symmetric measurable functions $U, W : [0, 1]^2 \to \mathbb{R}$, we define their cut metric to be

$$\delta(\square(U, W) := \inf_{\phi} \|U - W\phi\|_\square,$$

where the infimum is taken over all invertible measure preserving maps $\phi : [0, 1] \to [0, 1]$, and $W\phi(x, y) := W(\phi(x), \phi(y))$. For more results on graphons, we refer to [18] for details.

With $W \in \mathcal{W}$ we associate a graphon operator acting on $\mathcal{L}^2[0, 1]$, defined as the linear integral operator

$$(A_W f)(x) := \int_0^1 W(x, y)f(y)\,dy$$

for all $f \in \mathcal{L}^2[0, 1]$. Since $W$ is symmetric and bounded, $A_W$ is a compact Hermitian operator. In particular, $A_W$ has a discrete, real spectrum whose only possible accumulation point is zero.

Let $\mu(W)$ be the maximum eigenvalue of $A_W$. The following proposition establish a connection between $\lambda_1(G)$ and $\mu(W_G)$.

**Proposition 2.1** ([25]). Let $G$ be a graph on $n$ vertices. Then $\lambda_1(G) = n \cdot \mu(W_G)$.

**Proposition 2.2** ([18, Theorem 11.54]). Let $\{W_n\}$ be a sequence of graphons converging to $W$ with respect to $\delta$. Then $\lim_{n \to \infty} \mu(W_n) = \mu(W)$.

3. **Nordhaus–Gaddum Type Inequality for Spectral Radius of Graphs**

The aim of this section is to give a proof of Conjecture 1.1. Throughout this section, we always assume that $G$ is a graph such that $p(G)$ attaining the maximum among all graphs on $n$ vertices, where $p(G) := \lambda_1(G) + \lambda_1(\overline{G})$. Observe that at least one of $G$ and $\overline{G}$ is connected. Without loss of generality, we assume $G$ is connected. Let $\mathbf{x}$ and $\overline{\mathbf{x}}$ be the nonnegative eigenvectors with unit length corresponding to $\lambda_1(G)$ and $\lambda_1(\overline{G})$, respectively. For convenience, we set $\lambda_1 := \lambda_1(G)$ and $\overline{\lambda}_1 := \lambda_1(\overline{G})$.

First we prove a number of properties of $G$.

**Lemma 3.1.** For any vertices $u$ and $v$, $x_u x_v - \overline{x}_u \overline{x}_v > 0$ if and only if $u$ and $v$ are adjacent.

**Proof.** We first show that $x_u x_v - \overline{x}_u \overline{x}_v \neq 0$ by contradiction. Denote by $H$ the graph formed by adding or deleting the edge $uv$ from $G$. By Rayleigh principle we see

$$\lambda_1(H) \geq \mathbf{x}^T A(H) \mathbf{x} = \lambda_1(G) + 2(-1)^{a_{uv}} \cdot x_u x_v,$$

$$\lambda_1(\overline{H}) \geq \overline{\mathbf{x}}^T A(\overline{H}) \overline{\mathbf{x}} = \lambda_1(\overline{G}) - 2(-1)^{a_{uv}} \cdot \overline{x}_u \overline{x}_v.$$

Therefore, if $x_u x_v - \overline{x}_u \overline{x}_v = 0$, then

$$p(H) = \lambda_1(H) + \lambda_1(\overline{H}) \geq \lambda_1(G) + \lambda_1(\overline{G}) + 2(-1)^{a_{uv}} \cdot (x_u x_v - \overline{x}_u \overline{x}_v) = p(G).$$

Hence, each inequality above must be equality. So $\mathbf{x}$, $\overline{\mathbf{x}}$ are also eigenvectors of $H$ and $\overline{H}$ corresponding to $\lambda_1(H)$ and $\lambda_1(\overline{H})$, respectively. In particular, $A(H) \mathbf{x} = \lambda_1(H) \mathbf{x}$. $A(H) \overline{\mathbf{x}} = \lambda_1(\overline{H}) \overline{\mathbf{x}}$. We immediately obtain that

$$(\lambda_1(G) - \lambda_1(H)) \mathbf{x} = (A(G) - A(H)) \mathbf{x}. \quad (3.2)$$
Choose a vertex \( w \notin \{u, v\} \) and consider the eigenvalue equations with respect to \( w \). We deduce that
\[
(\lambda_1(G) - \lambda_1(H))x_w = 0,
\]
which yields \( \lambda_1(G) = \lambda_1(H) \). Combining with (3.2) we get a contradiction.

Finally, if \( x_u x_v - \bar{x}_u \bar{x}_v > 0 \) and \( a_{uv} = 0 \), then \( p(H) > p(G) \) by (3.1), a contradiction. Conversely, if \( a_{uv} = 1 \) and \( x_u x_v - \bar{x}_u \bar{x}_v < 0 \), then \( p(H) > p(G) \) by (3.1), a contradiction. This completes the proof of this lemma. \( \square \)

**Lemma 3.2.** \( x_{\text{max}} = \Theta(n^{-1/2}) \) and \( \bar{x}_{\text{max}} = \Theta(n^{-1/2}) \).

**Proof.** Consider the complete bipartite graph \( K_{\lfloor n/3 \rfloor \lceil 2n/3 \rceil} \). One can check that \( p(K_{\lfloor n/3 \rfloor \lceil 2n/3 \rceil}) > 1.1n \). Thus, \( \lambda_1 + \bar{\lambda}_1 > 1.1n \) due to the maximality. On the other hand, \( \lambda_1 < n \) and \( \bar{\lambda}_1 < n \), we have \( \lambda_1 = \Theta(n) \) and \( \bar{\lambda}_1 = \Theta(n) \).

Let \( u \) be a vertex such that \( x_u = x_{\text{max}} \). By eigenvalue equation and Cauchy–Schwarz inequality,
\[
\lambda_1^2 x_u^2 = \left( \sum_{uw \in E(G)} x_w \right)^2 \leq d(u) \sum_{uw \in E(G)} x_w^2 \leq d(u),
\]
which yields that
\[
x_{\text{max}} = x_u < \sqrt{\frac{d(u)}{\lambda_1}} = O\left( \frac{1}{\sqrt{n}} \right).
\]
On the other hand, it is clear that \( n^{-1/2} \leq x_{\text{max}} \geq n^{-1/2} \). Hence, we see \( x_{\text{max}} = \Theta(n^{-1/2}) \). Likewise, we have \( \bar{x}_{\text{max}} = \Theta(n^{-1/2}) \). \( \square \)

**Lemma 3.3.** For any pair of vertices \( u \) and \( v \), we have
\[
|\langle \lambda_1 x_u^2 + \bar{\lambda}_1 \bar{x}_u^2, \lambda_1 x_v^2 + \bar{\lambda}_1 \bar{x}_v^2 \rangle - \langle \lambda_1 x_u^2 + \bar{\lambda}_1 \bar{x}_u^2, \lambda_1 x_v^2 + \bar{\lambda}_1 \bar{x}_v^2 \rangle| = O\left( \frac{1}{n} \right).
\]

**Proof.** Let \( H \) be the graph obtained from \( G \) by deleting all edges incident with \( u \), and adding edges \( \{uw : w \in N_G(v)\} \). That is,
\[
E(H) = E(G) \setminus \{uw : w \in N_G(u)\} \cup \{uw : w \in N_G(v)\}.
\]
Define two vectors \( z \) and \( \bar{x} \) for \( H \) by
\[
z_w = \begin{cases} x_w, & w \neq u, \\ x_v, & w = u, \end{cases}
\]
and
\[
\bar{x}_w = \begin{cases} \bar{x}_w, & w \neq u, \\ \bar{x}_v, & w = u. \end{cases}
\]
Noting that \( \lambda_1 = x^T A(G)x \) we deduce that
\[
z^T A(H)z - \lambda_1 = 2z_u \sum_{w \in N_G(v) \setminus \{u\}} x_w - 2x_u \sum_{w \in N_G(u)} x_w
\]
\[
= 2x_v \sum_{w \in N_G(v)} x_w - 2x_u \sum_{w \in N_G(u)} x_w - 2a_{uv}x_u x_v
\]
\[
= 2\lambda_1 x_u^2 - 2\lambda_1 x_v^2 - 2a_{uv}x_u x_v.
\]
Similarly, we have
\[ z^T A(H) z - \lambda_1 = 2\bar{\lambda}_1 x_v^2 - 2\bar{\lambda}_1 x_u^2 + 2\bar{x}_u^2 - 2(1 - a_{uv})x_u x_v. \]

Combining the above equations gives
\[
0 \geq \frac{z^T A(H) z}{z^T z} + \frac{\bar{x}_u^2}{\bar{x}_u^2} - (\lambda_1 + \bar{\lambda}_1)
= \frac{\lambda_1 + 2\bar{\lambda}_1 x_v^2 - 2\bar{\lambda}_1 x_u^2 - 2a_{uv}x_u x_v}{1 - x_u^2 + x_v^2}
+ \frac{\bar{\lambda}_1 + 2\bar{x}_u^2 - 2\bar{\lambda}_1 x_u^2 + 2\bar{x}_v^2 - 2(1 - a_{uv})x_u x_v}{1 - \bar{x}_u^2 + \bar{x}_v^2} - (\lambda_1 + \bar{\lambda}_1)
= \frac{\lambda_1 x_v^2 - \lambda_1 x_u^2 - 2a_{uv}x_u x_v + \bar{\lambda}_1 \bar{x}_u^2 - \bar{\lambda}_1 \bar{x}_v^2 + 2\bar{x}_v^2 - 2(1 - a_{uv})x_u x_v}{1 - \bar{x}_u^2 + \bar{x}_v^2}.
\]

By Lemma 3.2, \( x_u, x_v, \bar{x}_u \) and \( \bar{x}_v \) are all \( O(n^{-1/2}) \). Therefore,
\[
(\lambda_1 x_v^2 - \lambda_1 x_u^2) + (\bar{\lambda}_1 \bar{x}_u^2 - \bar{\lambda}_1 \bar{x}_v^2) < O\left(\frac{1}{n}\right).
\]
Similarly, we also have
\[
(\lambda_1 x_u^2 - \lambda_1 x_v^2) + (\bar{\lambda}_1 \bar{x}_u^2 - \bar{\lambda}_1 \bar{x}_v^2) < O\left(\frac{1}{n}\right).
\]
The desired result follows from the above two inequalities. \( \square \)

The following theorem describes the approximate structure of the extremal graph \( G \) except for \( o(n) \) vertices, which are the main results in \([25]\).

**Theorem 3.4 ([25])**. Let \( W \) and \( \overline{W} \) be the graphons of \( G \) and \( \overline{G} \), respectively. Then for all \( (x, y) \in [0, 1]^2 \),
\[
W(x, y) = \begin{cases} 
0, & (x, y) \in [1/3, 1]^2, \\
1, & \text{otherwise},
\end{cases}
\]
and the maximum eigenvalues of \( W \) and \( \overline{W} \) are \( \mu = \overline{\mu} = 2/3 \). Furthermore, if \( f, g \) are nonnegative unit eigenfunctions associated to \( \mu, \overline{\mu} \) respectively, then for every \( x \in [0, 1] \),
\[
f(x) = \begin{cases} 
\sqrt{2}, & x \in [0, 1/3], \\
\sqrt{2}/2, & \text{otherwise},
\end{cases} \quad g(x) = \begin{cases} 
0, & x \in [0, 1/3], \\
\sqrt{6}/2, & \text{otherwise}.
\end{cases}
\]

Combining Theorem 3.4 and the arguments in \([7]\) we obtain the following result.

**Lemma 3.5**. The extremal graph \( G \) is a complete split graph.

**Proof**. Let \( \mu \) and \( \overline{\mu} \) be the maximum eigenvalues of \( W \) and \( \overline{W} \), respectively. For every positive integer \( n \), let \( G_n \) denote a graph on \( n \) vertices attaining \( \max\{p(H) : H \text{ is an } n\text{-vertex graph}\} \), and let \( W_n \) be any associated graphon corresponding to \( G_n \). Denote by \( \mu_n, \overline{\mu}_n \) the maximum eigenvalues of \( W_n \) and \( \overline{W}_n \), respectively. By Proposition 2.2,
\[
\lim_{n \to \infty} \mu(W_n) = \mu, \quad \lim_{n \to \infty} \mu(\overline{W}_n) = \overline{\mu}.
\]
Furthermore, let \( f_n \) be a nonnegative unit \( \mu_n \)-eigenfunction for \( W_n \) and let \( \overline{f}_n \) be a nonnegative unit \( \overline{\mu}_n \)-eigenfunction for \( \overline{W}_n \). Moreover, we may apply measure-preserving transformations to each \( W_n \) such that without loss of generality, \( ||W - W_n||_\Box \to 0 \). By Lemma 2 of \([24]\), \( f_n \) and \( \overline{f}_n \) converge to \( f \) and \( \overline{f} \) in \( L^2 \) sense, respectively.
For convenience, we let \( \alpha_1 = \sqrt{2}, \beta_1 = \sqrt{2}/2, \alpha_2 = 0 \) and \( \beta_2 = \sqrt{3}/2 \). For any \( \varepsilon_0 > 0 \), we define

\[
S_n := \{ x \in [0, 1] : |f_n(x) - \alpha_1| < \varepsilon_0, \quad |\overline{f}_n(x) - \alpha_2| < \varepsilon_0 \},
\]

\[
L_n := \{ x \in [0, 1] : |f_n(x) - \beta_1| < \varepsilon_0, \quad |\overline{f}_n(x) - \beta_2| < \varepsilon_0 \},
\]

\[
T_n := [0, 1] \setminus (S_n \cup L_n).
\]

One can show that the Lebesgue measure \( m(T_n) \) of \( T_n \) goes to zero, and \( m(L_n) \to 2/3 \). Indeed, we have

\[
\int_{|f_n - f|^2 \geq \varepsilon_0} |f_n - f|^2 \, dx \leq \int_0^1 |f_n - f|^2 \, dx \to 0,
\]

and

\[
\int_{|\overline{f}_n - \overline{f}|^2 \geq \varepsilon_0} |\overline{f}_n - \overline{f}|^2 \, dx \leq \int_0^1 |\overline{f}_n - \overline{f}|^2 \, dx \to 0,
\]

as desired.

For all \( u \in V(G_n) \), let \( I_u \) be the subinterval of \([0, 1]\) corresponding to \( u \) in \( W_n \), and denote by \( f_n(u) \) and \( \overline{f}_n(u) \) the constant values of \( f_n \) and \( \overline{f}_n \) on \( I_u \), respectively. For convenience, we define the following discrete analogues of \( S_n, L_n, T_n \):

\[
S_n := \{ u \in V(G_n) : |f_n(u) - \alpha_1| < \varepsilon_0, \quad |\overline{f}_n(u) - \alpha_2| < \varepsilon_0 \},
\]

\[
L_n := \{ u \in V(G_n) : |f_n(u) - \beta_1| < \varepsilon_0, \quad |\overline{f}_n(u) - \beta_2| < \varepsilon_0 \},
\]

\[
T_n := V(G_n) \setminus (S_n \cup L_n).
\]

For any \( \varepsilon_1 > 0 \). By Proposition 2.2, \( \mu_n \to \mu \) and \( \overline{\mu}_n \to \overline{\mu} \). It follows from Lemma 3.3 and Proposition 2.1 that

\[
|\mu f_n^2(u) + \overline{\mu} \overline{f}_n^2(u) - (\mu + \overline{\mu})| < \varepsilon_1,
\]

for sufficiently large \( n \).

**Claim 3.6.** Let \( \varepsilon'_0 > 0 \) and \( n \) be sufficiently large in terms of \( \varepsilon_0' \). For each \( v \in T_n \),

\[
\max \{ |f_n(v) - \beta_1|, \quad |\overline{f}_n(v) - \beta_2| \} < \varepsilon'_0.
\]

**Proof.** Without loss of generality, we assume \( G_n \) is connected. Hence, \( \alpha_1 f_n(v) - \alpha_2 \overline{f}_n(v) > 0 \).

By Lemma 3.1, \( S_n \subseteq N_{G_n}(v) \) for sufficiently large \( n \). Write

\[
\mathcal{U}_n := \bigcup_{w \in N_{G_n}(v)} I_w
\]

and recall that \( f_n \) is an eigenfunction of \( W_n \) corresponding to \( \mu_n \). Then

\[
\mu_n f_n(v) = \int_0^1 W_n(v, y) f_n(y) \, dy
\]

\[
= \int_{y \in L_n \cap \mathcal{U}_n} f_n(y) \, dy + \int_{y \in S_n} f_n(y) \, dy + \int_{y \in T_n \cap \mathcal{U}_n} f_n(y) \, dy.
\]

Denote the Lebesgue measure \( m(L_n \cap \mathcal{U}_n) \) of \( L_n \cap \mathcal{U}_n \) by \( \gamma_n \). For any \( \varepsilon_2 > 0 \), if \( n \) is sufficiently large and \( \varepsilon_1 \) is sufficiently small, then

\[
|f_n(v) - 3\gamma_n \beta_1 + \alpha_1| < \varepsilon_2.
\]

(3.4)
Similarly, we have
\[
\mathbf{\pi}_n f_n(v) = \int_0^1 W_n(v, y) \mathbf{\bar{f}}_n(y) \, dy \\
= \int_{y \in \mathcal{L}_n \cap \mathcal{U}_n} \mathbf{\bar{f}}_n(y) \, dy + \int_{y \in \mathcal{S}_n \cap \mathcal{U}_n} \mathbf{\bar{f}}_n(y) \, dy + \int_{y \in \mathcal{T}_n \cap \mathcal{U}_n} \mathbf{\bar{f}}_n(y) \, dy,
\]
where \( \mathcal{U}_n := [0, 1] \setminus \mathcal{U}_n \). Then
\[
\left| \mathbf{\bar{f}}_n(v) - \frac{(2 - 3\gamma_n)\beta_2}{3\mathbf{\pi}} \right| < \varepsilon_2. \tag{3.5}
\]
Let \( \varepsilon_3 > 0 \). Combining (3.4), (3.5) and (3.3), we obtain
\[
\left| \mu \cdot \frac{(3\gamma_n\beta_1 + \alpha_1)^2}{3\mu} + \frac{(2 - 3\gamma_n)\beta_2}{3\mathbf{\pi}} \right| < \varepsilon_3.
\]
Substituting the values of \( \alpha_1, \alpha_2, \beta_1, \beta_2 \) and simplifying, we deduce that
\[
|\gamma_n(3\gamma_n - 2)| < \varepsilon_3.
\]
It follows that if \( n \) is sufficiently large and \( \varepsilon_3 \) is sufficiently small, then
\[
\min\{\gamma_n, |3\gamma_n - 2|\} < \varepsilon_4
\]
for any \( \varepsilon_4 > 0 \). Combining with (3.4) and (3.5), we have either
\[
\max\left\{|f_n(v) - \alpha_1|, \left| \mathbf{\bar{f}}_n(v) - \frac{2\beta_2}{3\mathbf{\pi}} \right|\right\} < \varepsilon'_0
\]
or
\[
\max\left\{|f_n(v) - \alpha_1 + \frac{2\beta_1}{3\mu}|, \left| \mathbf{\bar{f}}_n(v) \right|\right\} < \varepsilon'_0.
\]
Notice that \( (\alpha_1 + 2\beta_1)/(3\mu) = \alpha_1 \) and \( v \in \mathcal{T}_n \), the second inequality does not hold. So we obtain the desired claim by observing that \( \alpha_1/(3\mu) = \beta_1 \) and \( 2\beta_2/(3\mathbf{\pi}) = \beta_2 \).

Next, according to the definition of \( S_n \) and \( L_n \) and Claim 3.6, we see for \( n \) sufficiently large,
\[
\max\{|f_n(v) - \alpha_1|, \left| \mathbf{\bar{f}}_n(v) - \alpha_2 \right|\} < \varepsilon_0, \quad v \in S_n
\]
\[
\max\{|f_n(v) - \beta_1|, \left| \mathbf{\bar{f}}_n(v) - \beta_2 \right|\} < \varepsilon_0, \quad v \in L_n
\]
\[
\max\{|f_n(v) - \beta_1|, \left| \mathbf{\bar{f}}_n(v) - \beta_2 \right|\} < \varepsilon'_0, \quad v \in \mathcal{T}_n.
\]
Let \( \varepsilon_0, \varepsilon'_0 \) be sufficiently small. Then for sufficiently large \( n \) and for all \( u, v \in V(G_n) \), \( f_n(u)f_n(v) > \mathbf{\bar{f}}_n(u)\mathbf{\bar{f}}_n(v) \) if and only if \( u, v \in S_n \) or \( (u,v) \in (S_n \cup (L_n \cup \mathcal{T}_n)) \cup ((L_n \cup \mathcal{T}_n) \cap S_n) \). Finally, using Lemma 3.1, we get the required result.

Now we are ready to prove Conjecture 1.1.

\textbf{Proof of Conjecture 1.1.} By Lemma 3.5, we assume \( G = CS_{n,\omega} \). By easy algebraic computation, we find
\[
\lambda_1(G) = \frac{\omega - 1 + \sqrt{-3\omega^2 + (4n - 2)\omega + 1}}{2}.
\]
Therefore, we immediately have
\[
\lambda_1(G) + \lambda_1(G) = \frac{\sqrt{-3\omega^2 + (4n - 2)\omega + 1 - \omega}}{2} + n - \frac{3}{2}.
\]
For convenience, denote \( f(x) := \sqrt{-3x^2 + (4n-2)x + 1} - x \). To complete the proof, we need to determine the value \( \omega \) maximizing \( f(\omega) \).

The following can be found in [2], we include it here for completeness. Letting \( f'(x) = 0 \), we obtain

\[
x_0 = \frac{2n - 3 - \sqrt{n^2 - n + 1}}{3}, \quad x_1 = \frac{2n - 3 + \sqrt{n^2 - n + 1}}{3}.
\]

It is easy to see that \( f(\omega) \) attains its maximum value at \([x_0] \) or \([x_0]\). Notice that

\[
[x_0] = \frac{1}{3} \begin{cases} n - 3, & n \equiv 0 \pmod{3}, \\ n - 1, & n \equiv 1 \pmod{3}, \\ n - 2, & n \equiv 2 \pmod{3}, \end{cases}
\]

and

\[
[x_0] = \frac{1}{3} \begin{cases} n, & n \equiv 0 \pmod{3}, \\ n + 2, & n \equiv 1 \pmod{3}, \\ n + 1, & n \equiv 2 \pmod{3}. \end{cases}
\]

Finally, we obtain the desired result by comparing \( f([x_0]) \) and \( f([x_0]) \).

\[ \square \]

4. CONNECTED GRAPHS OF MAXIMUM Q-SPREAD

For unit vectors \( x, z \in \mathbb{R}^n \), two basic inequalities can be obtained from the following well-known inequality for the Rayleigh quotient,

\[
q_1(G) \geq x^T Q(G)x \quad \text{and} \quad q_n(G) \leq z^T Q(G)z.
\]

Hence, the Q-spread of a graph can be expressed as

\[
s_Q(G) = \max_{x, z} \sum_{uv \in E(G)} ((x_u + x_v)^2 - (z_u + z_v)^2), \tag{4.1}
\]

where the maximum is taken over all unit vectors \( x \) and \( z \).

Throughout this section, we always assume that \( G \) is a graph attaining maximum Q-spread among all connected \( n \)-vertex graphs. Let \( x \) and \( z \) be the unit eigenvectors of \( Q(G) \) corresponding to \( q_1(G) \) and \( q_n(G) \), respectively. By the Perron–Frobenius theorem for non-negative matrices, we may assume that \( x \) is a positive vector. We also set \( q_1 := q_1(G) \) and \( q_n := q_n(G) \) for short.

**Lemma 4.1.** \( q_1 > 2n - 5 \) and \( q_n < 3 \).

**Proof.** Consider the graph \( K_{n-1}^+ \). Clearly, \( q_1(K_{n-1}^+) > q_1(K_{n-1}) = 2(n - 2) \). On the other hand, we have \( q_n(K_{n-1}) \leq 1 \) (see [11]). Indeed, we define a unit vector \( y \) for \( K_{n-1}^+ \) by

\[
y_u = \begin{cases} 1, & d(u) = 1, \\ 0, & \text{otherwise}. \end{cases}
\]

It follows that \( q_n(K_{n-1}^+) \leq y^T Q(K_{n-1}^+) y = 1 \). By maximality of \( G \), we conclude that \( s_Q(G) \geq s_Q(K_{n-1}^+) > 2n - 5 \).

Notice that \( Q(G) \) is a positive semidefinite matrix. Hence, \( q_1 \geq s_Q(G) > 2n - 5 \). On the other hand, it follows from \( q_1 \leq 2\Delta(G) \) that \( 2n - 5 < q_1 - q_n \leq 2(n - 1) - q_n \), which yields that \( q_n < 3 \). This completes the proof of the lemma. \[ \square \]

**Lemma 4.2.** \( |E(G)| > (n - 1)(n - 3)/2 \).
Proof. By Theorem 3.1 in [10] and the main result in [19], we deduce that
\[ q_1 \leq \frac{2|E(G)|}{n-1} + n - 2. \]
As shown in Lemma 4.1, \( q_1 > 2n - 5 \). Therefore,
\[ \frac{2|E(G)|}{n-1} + n - 2 > 2n - 5, \]
as desired. \( \square \)

Lemma 4.3. For any vertices \( u \) and \( v \), if \( x_u + x_v > |z_u + z_v| \), then \( u \) and \( v \) are adjacent; if \( x_u + x_v < |z_u + z_v| \) and \( G - uv \) is connected, then \( u \) and \( v \) are non-adjacent.

Proof. By (4.1), if \( x_u + x_v > |z_u + z_v| \) and \( u \), \( v \) are non-adjacent, then
\[ s_Q(G + uv) - s_Q(G) \geq (x_u + x_v)^2 - (z_u + z_v)^2 > 0, \]
a contradiction implies that \( u \) and \( v \) are adjacent. Likewise, if \( x_u + x_v < |z_u + z_v| \) and \( u \), \( v \) are adjacent, then
\[ s_Q(G - uv) - s_Q(G) \geq (z_u + z_v)^2 - (x_u + x_v)^2 > 0, \]
a contradiction implies that \( u \) and \( v \) are non-adjacent. \( \square \)

Lemma 4.4. For each \( v \in V(G) \), \( x_v < \frac{\sqrt{n}}{n-3} \).

Proof. By eigenvalue equation and Cauchy–Schwarz inequality we have
\[ q_1x_v = d(v)x_v + \sum_{u \in N(v)} x_u \leq (d(v) - 1)x_v + \sqrt{n} \leq (n - 2)x_v + \sqrt{n}, \]
which, together with Lemma 4.1, gives the desired result. \( \square \)

Fix a sufficiently small constant \( \varepsilon > 0 \), whose value will be chosen later. Let
\[ S := \{ v \in V(G) : |z_v| < \frac{\varepsilon}{\sqrt{n}} \}, \quad T := \{ v \in V(G) : x_v < \frac{1}{2\sqrt{n}} \}, \]
and \( L := V(G) \setminus S \).

Lemma 4.5. \( |T| < 8 \).

Proof. Since \( x \) is a unit vector, it follows from Lemma 4.4 that
\[ 1 = \sum_{u \in T} x_u^2 + \sum_{u \in V(G) \setminus T} x_u^2 < \frac{|T|}{4n} + (n - |T|) \cdot \frac{n}{(n-3)^2}, \]
yielding \( |T| < 8 \), as desired. \( \square \)

Lemma 4.6. There is exactly one vertex with degree \( o(n) \).
Proof. By Lemma 4.2, we know that there exists at most one vertex with degree $o(n)$. Hence, it suffices to rule out the case that $d(v) = \Omega(n)$ for each $v \in V(G)$.

Let $u$ be a vertex such that $|z_u| = \max \{|z_w| : w \in V(G)\}$. Without loss of generality, we assume $z_u < 0$. Consider the following eigenvalue equation with respect to vertex $u$,

$$(q_n - d(u))z_u = \sum_{w \in N(u)} z_w.$$ 

Noting that $q_n < 3$, $d(u) = \Omega(n)$ and $|z_u| \geq n^{-1/2}$, we have

$$\sum_{w \in N(u)} z_w = (q_n - d(u))z_u > \Omega(\sqrt{n}).$$

On the other hand, by Cauchy–Schwarz inequality we find that

$$\sum_{w \in N(u)} z_w \leq \sum_{w \in N(u) \cap L} |z_w| + \sum_{w \in N(u) \setminus L} |z_w|$$

$$\leq \sqrt{|L|} + \frac{\varepsilon}{\sqrt{n}}(n - |L|)$$

$$\leq \sqrt{|L|} + \varepsilon\sqrt{n},$$

which implies that $|L| > \Omega(n)$ for sufficiently small $\varepsilon$. Thus, one of the following two sets

$$B := \{ v \in L : z_v > 0 \}, \quad C := \{ v \in L : z_v < 0 \}$$

(say $B$) has size $\Omega(n)$. Recall that $z$ is a unit eigenvector corresponding to $q_n$. Hence,

$$q_n = \sum_{uv \in E(G)} (z_u + z_v)^2$$

$$= \sum_{uv \in E(G)} (z^2_u + z^2_v + 2z_u z_v)$$

$$\geq 2 \sum_{uv \in E(G)} (|z_u z_v| + z_u z_v)$$

$$= 2 \sum_{uv \in E(G), z_u z_v > 0} (|z_u z_v| + z_u z_v)$$

$$\geq 2 \sum_{uv \in E(B)} (|z_u z_v| + z_u z_v).$$

By Lemma 4.2, $|E(B)| > \Omega(n^2)$. It follows that $q_n > \Omega(n)$, a contradiction completing the proof of Lemma 4.6. $\square$

From now on, we assume $w$ is the unique vertex such that $d(w) = o(n)$.

Lemma 4.7. For each $v \in V(G) \setminus \{w\}$, $x_v = \Theta(n^{-1/2})$.

Proof. Let $v$ be any vertex in $V(G) \setminus \{w\}$. Using the eigenvalue equation with respect to vertex $v$, we deduce that

$$(q_1 - d(v))x_v \geq \sum_{u \in N(v) \setminus T} x_u \geq \frac{d(v) - 8}{2\sqrt{n}} > \Omega(\sqrt{n}).$$
The second inequality follows from Lemma 4.5, and the last inequality is due to Lemma 4.6. On the other hand, \((q_1 - d(v))x_v < 2nx_v\). Therefore, \(x_v > \Omega(n^{-1/2})\). Combining with Lemma 4.4 we get the desired result.

\[\square\]

**Lemma 4.8.** For each \(v \in V(G) \setminus \{w\}\), \(|z_v| = o(n^{-1/2})\).

**Proof.** Suppose on the contrary that there exists a vertex \(v \in V(G) \setminus \{w\}\) such that \(|z_v| > c/\sqrt{n}\) for some \(c > 0\). By eigenvalue equation and Lemma 4.6,

\[\left| \sum_{u \in N(v)} z_u \right| = |(q_n - d(v))z_v| > \Omega(\sqrt{n}).\]

On the other hand, we see

\[\left| \sum_{u \in N(v)} z_u \right| \leq \sum_{u \in N(v) \cap L} |z_u| + \sum_{u \in N(v) \setminus L} |z_u| \leq \sqrt{|L|} + \varepsilon \sqrt{n},\]

which yields that \(|L| > \Omega(n)|\). Using similar arguments in the proof of Lemma 4.6, we have \(q_n > \Omega(n)|\), a contradiction completing the proof. \[\square\]

Now we are in a position to confirm the validity of the first part of Conjecture 1.2.

**Proof of Conjecture 1.2.** By Lemma 4.7 and Lemma 4.8, for any \(u, v \in V(G) \setminus \{w\}\) we have \(x_u + x_v > |z_u + z_v|\). Combining with Lemma 4.3, we deduce that the induce subgraph \(G[V(G) \setminus \{w\}]\) is a complete graph. To complete the proof, we show that \(d(w) = 1\). Indeed, by Lemma 4.8 again,

\[z_w^2 = 1 - \sum_{u \in V(G) \setminus \{w\}} z_u^2 = 1 - o(1).\]

If \(d(w) \geq 2\), then deleting one edge between \(w\) and \(V(G) \setminus \{w\}\) will increase the \(Q\)-spread by Lemma 4.3, a contradiction completing the proof. \[\square\]

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