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Numerical Range of Simple Graphs and Some Bounds for their Eigenvalues

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Abstract. The numerical range of a simple graph $\mathbf{G}$, named $\mathbf{F}(\mathbf{G})$, is the numerical range of its adjacency matrix $\mathbf{A}(\mathbf{G})$. The main purpose of this paper is to approximate $\mathbf{F}(\mathbf{G})$. Then, using this approximation, bounds for the largest and the smallest eigenvalues of $\mathbf{G}$ are proposed. In fact, lower bounds for the largest eigenvalues of $\mathbf{G}$ are presented in terms of disjoint induced subgraphs of $\mathbf{G}$ and the numerical range of the square of $\mathbf{A}(\mathbf{G})$.

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1. Introduction

All graphs considered here are simple and undirected. A graph can be represented in various forms. Adjacency matrix is one of the various representations of a graph. The adjacency matrix of a graph $\mathbf{G}$ with vertex set $\mathbf{V}(\mathbf{G}) = \{v_1, ..., v_n\}$, written $\mathbf{A}(\mathbf{G})$, is the n-by-n matrix in which entry a_{ij} is the number of edges in $\mathbf{G}$ with endpoints $\{v_i, v_j\}$. So $\mathbf{A}(\mathbf{G})$ is Hermitian with entries 0 or 1 and 0s on the diagonal. The

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eigenvalues of a graph $\mathbf{G}$ are the eigenvalues of $\mathbf{A}(\mathbf{G})$. There have been many papers published on the eigenvalues of graphs. A series of articles in graph eigenvalues were collected by Stanic in [8].

The *classic numerical range* or simply *numerical range* $\mathbf{F}(.)$ is a set of complex numbers naturally associated with a given n-by-n matrix $\mathbf{A}$. The numerical range of a Hermitian matrix is an interval dependent on its largest and smallest eigenvalues. See [3, 4] for more properties of the numerical range of matrices. Nakazato [7] tried to determine the numerical range of adjacency matrix of some directed graphs. It is the result obtained by Marcus and Pesce [6] that the numerical range of any n-square matrix $\mathbf{A}$ is the union of the numerical ranges of all 2-square real compressions of $\mathbf{A}$.

In this paper, the researchers have changed their view on the eigenvalues of graphs compared to what has been done so far. They have looked at the largest and smallest eigenvalues of graphs in terms of the numerical range of graphs. The researchers propound a subset for the numerical range of graphs by Marcus and Pesce theorem. This subset gives a lower bound for the largest eigenvalues and an upper bound for the smallest eigenvalues of $\mathbf{G}$ solely based on structural properties of the graph. In addition, by applying Marcus and Pesce theorem to the square of the adjacency matrix of $\mathbf{G}$, a new lower bound for the largest eigenvalues of the graph is obtained.

2. Preliminaries

This section is divided into two parts. In the first part, familiarity with the basic theory of graphs is assumed. The second part presents the numerical range of a matrix and some of the related objects.

First, we recall a few basic notions of graphs which can be found in [9]. Let $\mathbf{G}$ be a graph with vertex set $\mathbf{V}(\mathbf{G})$. When $\mathbf{T} \subseteq \mathbf{V}(\mathbf{G})$, the induced subgraph $\mathbf{G}[\mathbf{T}]$ consists of $\mathbf{T}$ and all edges whose endpoints are contained in $\mathbf{T}$.

The following theorems determine the eigenvalues of bicliques, complete graphs, cycles and paths thoroughly.

Theorem 2.1. ([9]) *The eigenvalues of complete graph* $\mathbf{K}_n$ *are* $\lambda_1 = n-1 > \lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$ *and the eigenvalues of the biclique* $\mathbf{K}_{r,s}$ *are* $\lambda_1 = \sqrt{rs} > \lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = 0 > \lambda_n = -\sqrt{rs}$.

Theorem 2.2. ([1]) *For* $n \geqslant 2$, *the eigenvalues of* $\mathbf{C}_n$ *are* $2cos\dfrac{2k\pi}{n}$, $k = 1, ..., n$. *Also, for* $n \geqslant 1$, *the eigenvalues of* $\mathbf{P}_n$ *are* $2cos\dfrac{k\pi}{n+1}$, $k = 1, ..., n$.

We follow three theorems about bounds of the largest eigenvalue of a graph $\mathbf{G}$ and a theorem about its subgraph $\mathbf{G}-\mathrm{e}$. Let d_i is the degree of vertex v_i and $\Delta(\mathbf{G}) = \mathbf{max}_{v_i \in \mathbf{G}}\ d_i$.

Theorem 2.3. ([9]) *If* $\mathbf{G}$ *is a graph with* n *vertices,* e *edges and eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, *then* $(2e/n) \leqslant \lambda_1 \leqslant \Delta(\mathbf{G})$.

Theorem 2.4. ([1]) *If* $\mathbf{G}$ *is a graph with* n *vertices,* e *edges and eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, *then* $\lambda_1 \leqslant \sqrt{2e(n-1)/n}$.

Theorem 2.5. ([5]) *If* $\mathbf{G}$ *is a graph with* $n \geqslant 2$ *vertices, then*

$$\lambda_1 \geqslant \frac{1}{\sqrt{2}}\mathbf{max}_{j<i}\sqrt{d_i + d_j + \sqrt{(d_i - d_j)^2 + 4{c_{ij}}^2}},$$

where c_{ij} *is the number of common neighbors of vertices* v_i *and* v_j.

Theorem 2.6. ([2]) *If* e *is an edge of a connected graph* $\mathbf{G}$, *then the largest eigenvalue of* $\mathbf{G}$ *is strictly greater than the largest eigenvalue of* $\mathbf{G} - \mathrm{e}$.

Now, suppose that $\mathbf{M}_n$ is the algebra of all $n \times n$ complex matrices, then the *field of values* or *numerical range* of $\mathbf{A} \in \mathbf{M_n}$ is

$$\mathbf{F}(\mathbf{A}) := \{\mathbf{x}^*\mathbf{A}\mathbf{x} : \mathbf{x} \in \mathbb{C}^n, \mathbf{x}^*\mathbf{x} = 1\}.$$

If $\mathbf{A}$ is Hermitian, then $\mathbf{F}(\mathbf{A})$ is an interval whose endpoints are the largest and the smallest eigenvalues of $\mathbf{A}$. If $\mathbf{A}_1, ..., \mathbf{A}_n \in \mathbf{M}_n$, then $\mathbf{F}(\sum_{k=1}^{n} \mathbf{A}_k) \subseteq \sum_{k=1}^{n} \mathbf{F}(\mathbf{A}_k)$. For all $\mathbf{A} \in \mathbf{M}_{n_1}$ and $\mathbf{B} \in \mathbf{M}_{n_2}$, $\mathbf{F}(\mathbf{A} \oplus \mathbf{B}) = \mathbf{Co}(\mathbf{F}(\mathbf{A}) \cup \mathbf{F}(\mathbf{B}))$. For more details of matrix theory and the numerical range of matrices, one may refer [3, 4]. As a final result, consider the interlacing eigenvalues theorem for bordered matrices.

Theorem 2.7. ([3]) *Let* $\mathbf{A} \in \mathbf{M}_n$ *be a given Hermitian matrix with eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$*, and let* $y \in \mathbb{R}^n$ *be a given vector. Let* $\hat{\mathbf{A}} \in \mathbf{M}_{n+1}$ *be the Hermition matrix as follows:*

$$\hat{\mathbf{A}} \equiv \begin{bmatrix} \mathbf{A} & | & y \\ --- & | & --- \\ y^T & | & 0 \end{bmatrix}.$$

Let eigenvalues of $\hat{\mathbf{A}}$ *be* $\hat{\lambda}_1 \geqslant \hat{\lambda}_2 \geqslant \cdots \geqslant \hat{\lambda}_{n+1}$*. Then*

$$\hat{\lambda}_1 \geqslant \lambda_1 \geqslant \hat{\lambda}_2 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n \geqslant \hat{\lambda}_{n+1}.$$

3. Numerical Range of Graphs

In this section, we present the numerical range of a graph $\mathbf{G}$ and some of its properties.

Definition 3.1. *If* $\mathbf{G}$ *is a graph,* $\mathbf{F}(\mathbf{G})$ *is the numerical range of the adjacency matrix of* $\mathbf{G}$ *i.e.* $\mathbf{F}(\mathbf{G}) = \mathbf{F}(\mathbf{A}(\mathbf{G}))$*.*

Theorem 3.2. *Two isomorphic graphs have the same numerical range.*

Proof. Suppose $\mathbf{G}$ is isomorphic to $\mathbf{H}$, i.e. $\mathbf{G} \cong \mathbf{H}$, so there exists a permutation matrix $\mathbf{P}$ such that $\mathbf{A}(\mathbf{G}) = \mathbf{P}^{-1}\mathbf{A}(\mathbf{H})\mathbf{P}$. Therefore $\mathbf{G}$ and $\mathbf{H}$ have both the same eigenvalues and the same numerical range. $\square$

The next corollary is an immediate result of Definition 3.1 since $\mathbf{A}(\mathbf{G})$ is Hermitian.

Corollary 3.3. *If* $\mathbf{G}$ *is a graph with* n *vertices and eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$*, then* $\mathbf{F}(\mathbf{G}) = [\lambda_n, \lambda_1]$*.*

The following example follows from Corollary 3.3, Theorem 2.1 and 2.2.

Example 3.4. $\mathbf{F}(\mathbf{K}_n) = [-1, n-1]$ and $\mathbf{F}(\mathbf{K}_{r,s}) = [-\sqrt{rs}, \sqrt{rs}]$.
$\mathbf{F}(\mathbf{P}_n) = \left[-2cos(\frac{\pi}{n+1}), 2cos(\frac{\pi}{n+1})\right]$ and $\mathbf{F}(\mathbf{C}_n) = \left[2cos(\lfloor\frac{n}{2}\rfloor\frac{2\pi}{n}), 2\right]$, where the floor $\lfloor x \rfloor$ of x is the largest integer at most x.

Corollary 3.5. *Let* $\mathbf{G}$ *be a graph with* n *vertices and eigenvalues* $\lambda_1(\mathbf{G}) \geqslant \lambda_2(\mathbf{G}) \geqslant \cdots \geqslant \lambda_n(\mathbf{G})$ *and let* $\mathbf{H}$ *be an induced subgraph of* $\mathbf{G}$ *with* p *vertices and eigenvalues* $\lambda_1(\mathbf{H}) \geqslant \lambda_2(\mathbf{H}) \geqslant \cdots \geqslant \lambda_p(\mathbf{H})$. *Then* $\lambda_1(\mathbf{G}) \geqslant \lambda_1(\mathbf{H})$ *and* $\lambda_n(\mathbf{G}) \leqslant \lambda_p(\mathbf{H})$ *and so* $\mathbf{F}(\mathbf{H}) \subseteq \mathbf{F}(\mathbf{G})$.

Proof. $\mathbf{A}(\mathbf{H})$ is a principle submatrix of $\mathbf{A}(\mathbf{G})$ and so $\lambda_1(\mathbf{G}) \geqslant \lambda_1(\mathbf{H})$ and $\lambda_n(\mathbf{G}) \leqslant \lambda_p(\mathbf{H})$. □

Note that if $\mathbf{H}$ is a subgraph of $\mathbf{G}$ that is not an induced subgraph, then Corollary 3.5 is not always true, although Theorem 2.6 and 2.7 say $\lambda_1(\mathbf{H}) \leqslant \lambda_1(\mathbf{G})$. For example, $\mathbf{P}_3$ is a subgraph of $\mathbf{C}_3$ but $\mathbf{F}(\mathbf{P}_3) = \left[-\sqrt{2}, \sqrt{2}\right]$ and $\mathbf{F}(\mathbf{C}_3) = [-1, 2]$.

Next corollary provides two bounds for the numerical range of a graph depending only on n, e and Δ.

Corollary 3.6. *Let* $\mathbf{G}$ *be a graph with* n *vertices,* $e \geqslant 1$ *edges and eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. *Also suppose that*

$$\gamma = min\{\Delta(\mathbf{G}), \sqrt{2e(n-1)/n}\}$$

and

$$\sigma = max\{(2e/n), \sqrt{\Delta(\mathbf{G})}\}$$

then

$$[-1, 1] \subseteq [-1, \sigma] \subseteq \mathbf{F}(\mathbf{G}) \subseteq [-\gamma, \gamma].$$

Proof. Let $\mathbf{H}$ be an induced subgraph of $\mathbf{G}$ which contains exactly two incident vertices. So $\mathbf{H}$ is a path with two vertices and by Theorem 2.2, $\mathbf{F}(\mathbf{H}) = [-1, 1]$. Now, by Corollary 3.5, $[-1, 1] = \mathbf{F}(\mathbf{H}) \subseteq \mathbf{F}(\mathbf{G})$. Clearly $\Delta(\mathbf{G}) \geqslant 1$ and $\mathbf{K}_{1,\Delta(\mathbf{G})}$ is a subgraph of $\mathbf{G}$ and $\lambda_1(\mathbf{K}_{1,\Delta(\mathbf{G})}) = \sqrt{\Delta(\mathbf{G})} \leqslant \lambda_1(\mathbf{G})$ by Theorem 2.1. Therefore, by Theorem 2.3, $\lambda_1(\mathbf{G}) \geqslant \sigma$ and $[-1, 1] \subseteq [-1, \sigma] \subseteq \mathbf{F}(\mathbf{G})$. The third inclusion follows from Theorem 2.3 and 2.4. □

Remark 3.7. *If* $\mathbf{G}$ *has* m *components,* $\mathbf{H}_1, \mathbf{H}_2, \cdots, \mathbf{H}_m$, *then each component is an induced subgraph of* $\mathbf{G}$ *and the adjacency matrix of* $\mathbf{G}$ *can be written as* $\mathbf{A}(\mathbf{G}) = \mathbf{A}(\mathbf{H}_1) \oplus \mathbf{A}(\mathbf{H}_2) \oplus \cdots \oplus \mathbf{A}(\mathbf{H}_m)$, *so*

$\mathbf{F}(\mathbf{G}) = \mathbf{Co}(\mathbf{F}(\mathbf{H}_1) \cup \mathbf{F}(\mathbf{H}_2) \cup \cdots \cup \mathbf{F}(\mathbf{H}_m))$. *By Corollary 3.6 for all* $j \in \{1, ..., m\}$, $\mathbf{F}(\mathbf{H}_j)$ *is an interval which contains 0, so*

$$\mathbf{Co}(\mathbf{F}(\mathbf{H}_1) \cup \mathbf{F}(\mathbf{H}_2) \cup \cdots \cup \mathbf{F}(\mathbf{H}_m)) = \mathbf{F}(\mathbf{H}_1) \cup \mathbf{F}(\mathbf{H}_2) \cup \cdots \cup \mathbf{F}(\mathbf{H}_m).$$

Therefore, for each $j \in \{1, ..., m\}$, *if* $\mathbf{I}_j$ *is an interval such that* $\mathbf{I}_j \subseteq \mathbf{F}(\mathbf{H}_j)$, *then* $\bigcup \mathbf{I}_j \subseteq \mathbf{F}(\mathbf{G})$.

Beineke and Wilson [2] proved that if $\mathbf{G}$ is neither complete nor null, then $\lambda_n(\mathbf{G}) \leqslant -\sqrt{2}$. In the next theorem, we aim to extend this result as far as possible and obtain a better upper bound for λ_n.

Theorem 3.8. *If* $\mathbf{G}$ *is an* n *vertices graph with the star* $\mathbf{K}_{1,m}$ *as an induced subgraph, then* $\lambda_n \leqslant -\sqrt{m}$. *In particular,* $[-\sqrt{m}, \sqrt{m}\ ] \subseteq \mathbf{F}(\mathbf{G})$.

Proof. It follows from Theorem 2.1 that $-\sqrt{m}$ and $\sqrt{m}$ are the smallest and the largest eigenvalues of $\mathbf{K}_{1,m}$. Now, by Corollary 3.5, the result is clear. $\square$

Theorem 3.9. *If* $\mathbf{G}$ *is a graph with* n *vertices and eigenvalues* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, *then there exists a positive integer* $m \leqslant n$ *such that*

$$\left[2cos(\lfloor \frac{m}{2} \rfloor \frac{2\pi}{m}), 2\right] \subseteq \mathbf{F}(\mathbf{G}),$$

or

$$\left[-2cos(\frac{\pi}{m+1}), 2cos(\frac{\pi}{m+1})\right] \subseteq \mathbf{F}(\mathbf{G}).$$

Proof. If $\mathbf{G}$ has no cycle, then consider $\mathbf{P}_m$ as a path in $\mathbf{G}$ that is not contained in a longer path; called a *maximal path.* Since $\mathbf{G}$ has no cycles, $\mathbf{P}_m$ is an induced subgraph of $\mathbf{G}$ and by Corollary 3.5, $\mathbf{F}(\mathbf{P}_m) \subseteq \mathbf{F}(\mathbf{G})$. Now, by Theorem 2.2,

$$\left[2cos(\frac{m\pi}{m+1}), 2cos(\frac{\pi}{m+1})\right] = \left[-2cos(\frac{\pi}{m+1}), 2cos(\frac{\pi}{m+1})\right] \subseteq \mathbf{F}(\mathbf{G}).$$

Otherwise, $\mathbf{G}$ contains a cycle $\mathbf{C}_m$ which is an induced subgraph of $\mathbf{G}$ and $m \geqslant p$ for all the cycles $\mathbf{C}_p$ that are induced subgraphs of $\mathbf{G}$. By

Corollary 3.5, $\mathbf{F}(\mathbf{C}_m) \subseteq \mathbf{F}(\mathbf{G})$. Similar to the previous case, by Theorem 2.2

$$\left[2cos(\lfloor\frac{m}{2}\rfloor\frac{2\pi}{m}), 2\right] \subseteq \mathbf{F}(\mathbf{G}). \quad \Box$$

Applying the decompositions of graphs, we obtain an upper bound for $\mathbf{F}(\mathbf{G})$ in continuation of this section.

Theorem 3.10. *Let $\mathcal{H} = \{\mathbf{G}_1, \mathbf{G}_2, ..., \mathbf{G}_k\}$ be a decomposition of an n-vertices graph $\mathbf{G}$ such that $\mathbf{G}_i$ is n-vertices subgraph of $\mathbf{G}$ and $\lambda_{i_1} \geqslant \lambda_{i_2} \geqslant \cdots \geqslant \lambda_{i_n}$ are the eigenvalues of $\mathbf{G}_i$, for each i=1,...,k. Then $\mathbf{F}(\mathbf{G}) \subseteq [\alpha_\mathcal{H}, \beta_\mathcal{H}]$, where $\alpha_\mathcal{H} = \sum_{i=1}^k \lambda_{i_n}$ and $\beta_\mathcal{H} = \sum_{i=1}^k \lambda_{i_1}$.*

Proof. By the hypothesis that $\mathbf{G}_i$ is an n-vertices subgraph of $\mathbf{G}$ for each i=1,...,k, $\mathbf{A}(\mathbf{G}) = \mathbf{A}(\mathbf{G}_1) + \mathbf{A}(\mathbf{G}_2) + ... + \mathbf{A}(\mathbf{G}_k)$. So

$$\begin{aligned} \mathbf{F}(\mathbf{G}) &\subseteq \mathbf{F}(\mathbf{G}_1) + \mathbf{F}(\mathbf{G}_2) + ... + \mathbf{F}(\mathbf{G}_k) \\ &= [\lambda_{1_n}, \lambda_{1_1}] + [\lambda_{2_n}, \lambda_{2_1}] + ... + [\lambda_{k_n}, \lambda_{k_1}] \\ &= \left[\sum_{i=1}^k \lambda_{i_n}, \sum_{i=1}^k \lambda_{i_1}\right] = [\alpha_\mathcal{H}, \beta_\mathcal{H}]. \quad \Box \end{aligned}$$

Now, we have the following obvious corollary.

Corollary 3.11. *Let $\mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_m$ be m decompositions of $\mathbf{G}$ in the same condition of Theorem 3.10. Then for every j=1,2,...,m, $\mathbf{F}(\mathbf{G}) \subseteq \left[\alpha_{\mathcal{H}_j}, \beta_{\mathcal{H}_j}\right]$, and so*

$$\mathbf{F}(\mathbf{G}) \subseteq \bigcap_{j=1}^m \left[\alpha_{\mathcal{H}_j}, \beta_{\mathcal{H}_j}\right].$$

Remark 3.12. *If $\mathbf{G}$ is a graph with e edges and $\mathcal{H} = \{\mathbf{G}_1, \mathbf{G}_2, ..., \mathbf{G}_e\}$ is a decomposition of $\mathbf{G}$ such that $\mathbf{E}(\mathbf{G}_i) \cap \mathbf{E}(\mathbf{G})$ has exactly one member, for each $i \in \{1, 2, ...e\}$, then $\mathbf{F}(\mathbf{G}_i) = [-1, 1]$ for all $i \in \{1, 2, ..., e\}$ and by Theorem 3.10, $\mathbf{F}(\mathbf{G}) \subseteq [-e, e]$. Now, without loss of generality, suppose that $\mathbf{G}_1, \mathbf{G}_2$ are two members of $\mathcal{H}$ such that their edges are disjoint, i.e. their edges have distinct endpoints. So we can make a new decomposition $\mathcal{H}' = \{\mathbf{G'}_1, \mathbf{G}_3, ..., \mathbf{G}_e\}$ such that $\mathbf{G'}_1$ is a subgraph of $\mathbf{G}$ and $\mathbf{E}(\mathbf{G'}_1) = \mathbf{E}(\mathbf{G}_1) \cup \mathbf{E}(\mathbf{G}_2)$. $\mathbf{F}(\mathbf{G'}_1) = [-1, 1]$ and by Theorem 3.10,*

$$\mathbf{F}(\mathbf{G}) \subseteq \mathbf{F}(\mathbf{G'}_1) + \mathbf{F}(\mathbf{G}_3) + ... + \mathbf{F}(\mathbf{G}_e) = [-(e-1), e-1],$$

which is a superset of $\mathbf{F}(\mathbf{G})$ *such that it is a subset of* $[-e, e]$. *Also, without loss of generality, suppose that* $\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3$ *are three members of* $\mathcal{H}$ *such that every two distinct edges of* $\mathbf{E}(\mathbf{G}_1) \cup \mathbf{E}(\mathbf{G}_2) \cup \mathbf{E}(\mathbf{G}_3)$ *have exactly one common endpoint. So the new* n*-vertices subgraph* $\mathbf{G}'_1$ *of* $\mathbf{G}$ *contains one copy of* $\mathbf{C}_3$ *and for the new decomposition* $\mathcal{H}'' = \{\mathbf{G}'_1, \mathbf{G}_4, ..., \mathbf{G}_e\}$, *we have*

$$\begin{aligned}\mathbf{F}(\mathbf{G}) &\subseteq \mathbf{F}(\mathbf{G}'_1) + \mathbf{F}(\mathbf{G}_4) + ... + \mathbf{F}(\mathbf{G}_e) \\ &\subseteq [-1, 2] + [-1, 1] + \cdots + [-1, 1] = [-(e-2), e-1],\end{aligned}$$

which again is a superset of $\mathbf{F}(\mathbf{G})$ *such that it is a subset of* $[-(e-1), e-1]$. *Therefore for finding a superset of* $\mathbf{F}(\mathbf{G})$ *with smaller length it is enough to concentrate on those decompositions that have the minimum number subgraphs between all the decompositions of graph* $\mathbf{G}$. *Additionally, decompositions whose subgraphs are disjoint edges, disjoint paths, disjoint cycles, disjoint cliques or disjoint bicliques will attaine an interval with a smaller length compair with those decompositions whose subgraphs are not chosen in such a way.*

Example 3.13. Consider the 3-regular graph $\mathbf{G}$, as in Figure 1, and the decomposition $\mathcal{H} = \{\mathbf{G}_1, \mathbf{G}_2\}$ of $\mathbf{G}$, as in Figure 2. By Theorem 3.10, $\mathbf{F}(\mathbf{G}) \subseteq [-1, 2] + [-1, 1] = [-2, 3]$. In Example 4.4, it will be shown that this decomposition identifies exactly $\mathbf{F}(\mathbf{G})$, in fact, $\mathbf{F}(\mathbf{G}) = [-2, 3]$.

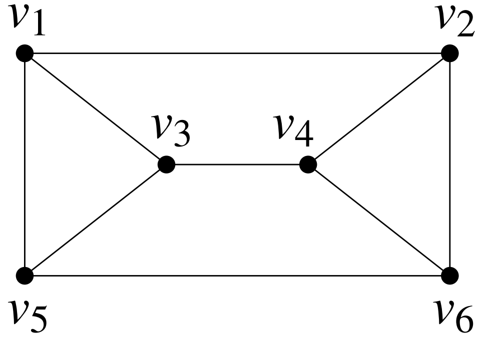

Figure 1. 3-regular graph $\mathbf{G}$

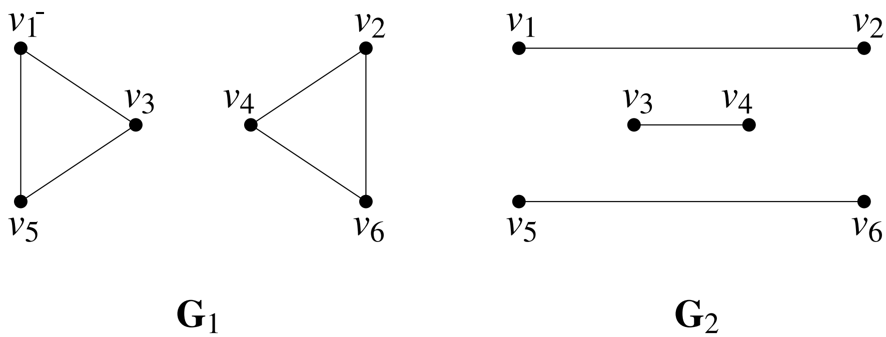

Figure 2. Decomposition $\mathcal{H}$ of **G**

4. Main Results

In this section, we looked at the largest and smallest eigenvalues of graphs in terms of the numerical range of graphs. Throughout this section, it is supposed that **G** is a connected n-vertices graph with $n > 1$. Also, $\mathbf{V}(\mathbf{G}) = \{v_1, v_2, ..., v_n\}$, d_i is the degree of vertex v_i and **A** is the adjacency matrix of **G**.

M. Marcus and C. Pesce [6] showed that for each $\mathbf{A} \in \mathbf{M}_n$,

$$\mathbf{F}(\mathbf{A}) = \bigcup \mathbf{F}(\mathbf{A}_{xy}), \tag{1}$$

where $\mathbf{A}_{xy}$ is the 2-square matrix

$$\mathbf{A}_{xy} = \begin{bmatrix} x^*Ax & x^*Ay \\ y^*Ax & y^*Ay \end{bmatrix}, \tag{2}$$

and x and y run over all pairs of real orthonormal vectors. The purpose of the next theorem is to construct a subset of $\mathbf{F}(\mathbf{G})$. Since x and y are real vectors and $\mathbf{A}(\mathbf{G})$, or simply **A**, is Hermitian,

$$\mathbf{A}_{xy} = \begin{bmatrix} x^TAx & x^TAy \\ x^TAy & y^TAy \end{bmatrix}. \tag{3}$$

The main result needs two lemmas in which x^TAx, x^TAy and y^TAy are introduced by induced subgraphs of **G**. In order to find the desired subset, special pairs of real orthonormal vectors are considered and an induced subgraph of $\mathbf{G}$ is attributed to each vector.

Lemma 4.1. *Let* $x = [x_1, x_2, ..., x_n]^T$ *be a real vector such that for* $1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant n$, $x_{i_1} = x_{i_2} = \cdots = x_{i_k} = 1/\sqrt{k}$ *and* $x_j = 0$ *when* $1 \leqslant j \leqslant n$ *and* $j \notin \{i_1, i_2, ..., i_k\}$. *Then* $x^T Ax$ *is* $2/k$ *times the number of edges in the induced subgraph* $\mathbf{G}[\{v_{i_1}, v_{i_2}, ..., v_{i_k}\}]$.

Proof. Without loss of generality, suppose that $x = [1/\sqrt{k}, ..., 1/\sqrt{k}, 0, ..., 0]^T$ with exactly k nonzero coordinates. Then $x^T A$ simply is $1/\sqrt{k}$ times a vector whose ith coordinate, for $1 \leqslant i \leqslant k$, is the degree of v_i in $\mathbf{G}[\{v_1, v_2, ..., v_k\}]$ and its ith coordinate, for $k+1 \leqslant i \leqslant n$, is the number of edges incident v_i and their other endpoints are in $\mathbf{G}[\{v_1, v_2, ..., v_k\}]$, and finally $x^T Ax$ is $1/k$ times the sum of degree of vertices in $\mathbf{G}[\{v_1, v_2, ..., v_k\}]$. Since the sum of degree of vertices in a graph is 2 times the number of edges, the result will be followed. □

Lemma 4.2. *Let* $x = [x_1, x_2, ..., x_n]^T$ *and* $y = [y_1, y_2, ..., y_n]^T$ *be two real vectors and* $\xi = \{i_1, i_2, ..., i_k\}$ *and* $\eta = \{j_1, j_2, ..., j_m\}$ *be two subsets of* $\{1, ..., n\}$ *such that* $\xi \cap \eta = \emptyset$. *Let* $x_{i_1} = x_{i_2} = \cdots = x_{i_k} = 1/\sqrt{k}$ *and* $x_i = 0$ *when* $i \notin \xi$ *and also* $y_{j_1} = y_{j_2} = \cdots = y_{j_m} = 1/\sqrt{m}$ *and* $y_j = 0$ *when* $j \notin \eta$. *Then* $x^T Ay$ *is* $1/\sqrt{km}$ *times the number of edges having one endpoint in* $\mathbf{G}[\{v_{i_1}, v_{i_2}, ..., v_{i_k}\}]$ *and the other in* $\mathbf{G}[\{v_{j_1}, v_{j_2}, ..., v_{j_m}\}]$.

Proof. Suppose x is identically the vector of the proof of Lemma 4.1 with exactly k nonzero coordinates. Also, $y = [0, ..., 0, 1/\sqrt{m}, ..., 1/\sqrt{m}]^T$ with exactly m nonzero coordinates. Since $\xi \cap \eta = \emptyset$, $x^T y = 0$. $x^T A$ can be acquired like the proof of Lemma 4.1 and $x^T Ay$ is $1/\sqrt{km}$ times the number of edges having one endpoint in $\mathbf{G}[\{v_1, v_2, ..., v_k\}]$ and the other in $\mathbf{G}[\{v_{n-m+1}, ..., v_n\}]$. □

Theorem 4.3. *For each pair* $T, S \subseteq \mathbf{V}(\mathbf{G})$ *such that* $S \cap T = \emptyset$ *and* $n(T) = k$ *and* $n(S) = m$ *define* β_T *as* $2/k$ *times the number of edges in the induced subgraph* $\mathbf{G}[T]$, β_S *as* $2/m$ *times the number of edges in the induced subgraph* $\mathbf{G}[S]$ *and* $\alpha_{T,S}$ *as* $1/\sqrt{km}$ *times the number of edges having one endpoint in* $\mathbf{G}[T]$ *and the other in* $\mathbf{G}[S]$. *Then* $\bigcup [a_{T,S}, b_{T,S}] \subseteq \mathbf{F}(\mathbf{G})$, *where*

$$a_{T,S} = \frac{(\beta_T + \beta_S) - \sqrt{(\beta_T - \beta_S)^2 + 4\alpha_{T,S}^2}}{2},$$

$$b_{T,S} = \frac{(\beta_T + \beta_S) + \sqrt{(\beta_T - \beta_S)^2 + 4\alpha_{T,S}^2}}{2}$$

and the union runs over all pairs of disjoint subsets T and S of $\mathbf{V}(\mathbf{G})$.

Proof. Without loss of generality, let $T = \{v_1, ..., v_k\}$ and $S = \{v_{n-m+1}, ..., v_n\}$. Now, consider two orthonormal vectors $x, y \in \mathbb{C}^n$ similar to the proof of Lemma 4.2. Then by Lemma 4.1 and 4.2, $\beta_T = x^T Ax$, $\beta_S = y^T Ay$, $\alpha_{T,S} = x^T Ay$. Then by (3),

$$\mathbf{A}_{xy} = \begin{bmatrix} \beta_T & \alpha_{T,S} \\ \alpha_{T,S} & \beta_S \end{bmatrix}$$

and a simple calculation,

$$\mathbf{F}(\mathbf{A}_{xy}) = [a_{T,S}, b_{T,S}] \subseteq \mathbf{F}(\mathbf{G}), \tag{4}$$

by (1). The result is clear, since x and y are a special pair of orthonormal vectors. $\square$

In the next example, it will be tried to construct a subset of $\mathbf{F}(\mathbf{G})$ where $\mathbf{G}$ is the graph of Example 3.13, by using the method of the previous theorem.

Example 4.4. Consider the 3-regular graph $\mathbf{G}$ which was stated in Example 3.13. Two choices of T and S will be stated bellow and then the related interval $[a_{T,S}, b_{T,S}]$ will be calculated.
Case 1: If $T = \{v_1, v_4\}$ and $S = \{v_2, v_3\}$, then $\beta_T = 0$, $\beta_S = 0$, $\alpha_{T,S} = 4/\sqrt{4} = 2$ and $[a_{T,S}, b_{T,S}] = [-2, 2]$.
Case 2: If $T = \{v_1, v_3, v_5\}$ and $S = \{v_2, v_4, v_6\}$, then $\beta_T = 2$, $\beta_S = 2$, $\alpha_{T,S} = 3/\sqrt{9} = 1$ and $[a_{T,S}, b_{T,S}] = [1, 3]$.
Finally by using Theorem 4.3, $[-2, 2] \cup [1, 3] = [-2, 3] \subseteq \mathbf{F}(\mathbf{G})$. Thus by Example 3.13, $\mathbf{F}(\mathbf{G}) = [-2, 3]$.

Example 4.5. Let $\mathbf{G}$ and $\mathbf{H}$ be the graphs shown in Figure 3. Choose T and S for $\mathbf{G}$ in the two following ways:

Case 1: If $T = \{v_1, v_2, v_4\}$ and $S = \{v_3\}$, then $\beta_T = 2$, $\beta_S = 0$, $\alpha_{T,S} = 1/\sqrt{3}$ and $[a_{T,S}, b_{T,S}] = \big[1 - 2/\sqrt{3}, 1 + 2/\sqrt{3}\big]$,
Case 2: If $T = \{v_2, v_3, v_4\}$ and $S = \{v_1\}$, then $\beta_T = 2/3$, $\beta_S = 0$, $\alpha_{T,S} = \sqrt{3}$ and $[a_{T,S}, b_{T,S}] = \big[(1 - \sqrt{28})/3, (1 + \sqrt{28})/3\big]$.
Then $\big[(1 - \sqrt{28})/3, 1 + 2/\sqrt{3}\big] \subseteq \mathbf{F}(\mathbf{G})$, $\lambda_1(\mathbf{G}) \geqslant 2.154$ and $\lambda_n(\mathbf{G}) \leqslant -1.430$. Also, by choosing $T = \{v_1, v_2, v_5, v_6\} \subseteq \mathbf{V}(\mathbf{H})$ and $S = \{v_3, v_4\} \subseteq \mathbf{V}(\mathbf{H})$ we have $\beta_T = 2$, $\beta_S = 0$ and $\alpha_{T,S} = 1/\sqrt{2}$. Therefore $\big[1 - \sqrt{6}/2, 1 + \sqrt{6}/2\big] \subseteq \mathbf{F}(\mathbf{H})$. So $\lambda_1(\mathbf{H}) \geqslant 2.224$ and $\lambda_n(\mathbf{H}) \leqslant -2.224$,

since $\lambda_n = -\lambda_1$ in bipartite graphs. By calculating of all cases of T and S, it can be seen that the bounds obtained in this remark are the best possible ones, based on Theorem 4.3.

Remark 4.6. *For each pair $T, S \subseteq \mathbf{V}(\mathbf{G})$ such that $T \cap S = \emptyset$, $[a_{T,S}, b_{T,S}] \subseteq \mathbf{F}(\mathbf{G})$ as stated in the proof of Theorem 4.3. Let $\bigcup [a_{T,S}, b_{T,S}] = [a_{T_1,S_1}, b_{T_2,S_2}]$ where $a_{T_1,S_1} = \mathbf{min}\ a_{T,S}$ and $b_{T_2,S_2} = \mathbf{max}\ b_{T,S}$ and the union, the minimum and the maximum run over all pairs of disjoint subsets of $\mathbf{V}(\mathbf{G})$. We can consider $a_{T,S}$ and $b_{T,S}$ as two functions with three variables β_T, β_S and $\alpha_{T,S}$. Naturally, for each $T \subseteq \mathbf{V}(\mathbf{G})$,*

$$0 \leqslant \beta_T \leqslant \frac{2(e - k\delta)}{n - k}$$

and

$$0 \leqslant \alpha_{T,S} \leqslant \sqrt{\lfloor \frac{n}{2} \rfloor (n - \lfloor \frac{n}{2} \rfloor)},$$

where e is the number of edges of n-vertices graph $\mathbf{G}$, k is the maximum size of an independent set of vertices of degree $\delta = \mathbf{min}_{v_i \in \mathbf{G}}\ d_i$. How to choose T and S, is important to achieve a_{T_1,S_1} and b_{T_2,S_2}. The next corollary suggests a usefull choice to obtain a lower bound for λ_1 based on the graph indices which are easily accessible.

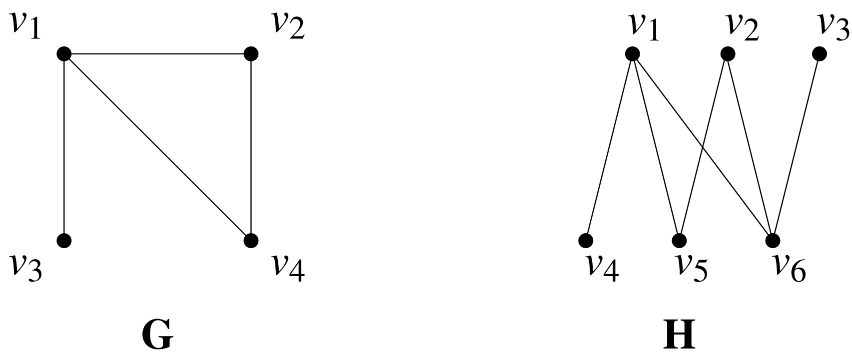

Figure 3. Graphs **G** and **H**

Corollary 4.7. *Let* **G** *be a graph with n vertices and e edges such that* $\delta = \mathbf{min}_{v_i \in \mathbf{G}}\ d_i$. *Then*

$$\lambda_1 \geqslant \frac{(e - k\delta) + \sqrt{e^2 - k\delta(2e - n\delta)}}{n - k},$$

where k is the maximum size of an independent set of vertices of degree δ.

Proof. Recording to the preamble of Remark 4.6, let T be a set of independent vertices of degree δ with $n(T) = k$ and $S = \mathbf{V}(\mathbf{G}) - T$. So $n(S) = n - k$. So $\beta_T = 0$, $\beta_S = \dfrac{2(e - k\delta)}{n - k}$, $\alpha_{T,S} = \dfrac{k\delta}{\sqrt{k(n - k)}}$. Therefore

$$b_{T,S} = \frac{(e - k\delta) + \sqrt{e^2 - 2ke\delta + nk\delta^2}}{n - k}. \quad \square$$

The next corollary results from Corollary 4.7. Recall that a leaf is a vertex of degree 1.

Corollary 4.8. *If* **T** *is an n-vertices tree with* $n > 1$ *and k leaves, then*

$$\lambda_1 \geqslant \frac{(n - k - 1) + \sqrt{(n - k - 1)(n - 1) + k}}{n - k}.$$

In Theorem 4.10, we aim to present a lower bound for λ_1 by replacing $\mathbf{A}^2$ instead of $\mathbf{A}$ in Theorem 4.3. Naturally, we can use Theorem 4.3 for $\mathbf{A}^k$ where $k \geqslant 1$, but, as mentioned in Remark 4.6, our aim is to find a lower bound for λ_1 and an upper bound for λ_n based on structural properties of graph $\mathbf{G}$ and the results for $\mathbf{A}^k$ where $k \geqslant 3$, are not clear in comparison to $\mathbf{A}^2$.
Again, to get the main result, we need two lemmas. Let $\mathbf{A}^2 = [c_{ij}]$, then c_{ii} is the degree of vertex v_i, called d_i, and c_{ij} is the number of common neighbors of vertices v_i and v_j when $i \neq j$. Clearly $\mathbf{A}^2$ is symmetric.

Lemma 4.9. *Let x, y, ξ and η are defined in the same way as Lemma 4.2, then*

$$x^T A^2 x = \frac{1}{k}(\sum_{i\in\xi} d_i + 2\sum_{i,j\in\xi} c_{ij}),$$

and

$$x^T A^2 y = \frac{1}{\sqrt{km}} \sum_{\substack{i\in\xi \\ j\in\eta}} c_{ij}.$$

Proof. Like the proof of Lemma 4.1, without loss of generality, suppose that $x = [1/\sqrt{k}, ..., 1/\sqrt{k}, 0, ..., 0]^T$ with exactly k nonzero coordinates. Then $x^T A^2$ simply is $1/\sqrt{k}$ times a vector whose jth coordinate, for $1 \leqslant j \leqslant k$, is $d_j + \sum_{\substack{i=1 \\ i\neq j}}^k c_{ij}$ and its jth coordinate, for $k+1 \leqslant j \leqslant n$, is $\sum_{i=1}^k c_{ij}$. The result will be followed similar to the proof of Lemma 4.1 and 4.2. $\square$

Theorem 4.10. *For each pair $T, S \subseteq \mathbf{V}(\mathbf{G})$ such that $S \cap T = \emptyset$ and $n(T) = k$ and $n(S) = m$, define*

$$\beta'_T = \frac{1}{k}(\sum_{v_i\in T} d_i + 2\sum_{v_i,v_j\in T} c_{ij}), \quad \beta'_S = \frac{1}{k}(\sum_{v_i\in S} d_i + 2\sum_{v_i,v_j\in S} c_{ij}),$$

and

$$\alpha'_{T,S} = \frac{1}{\sqrt{km}} \sum_{\substack{v_i\in T \\ v_j\in S}} c_{ij}.$$

Then

$$\lambda_1 \geqslant \sqrt{\mathbf{max}_{T,S}\frac{(\beta'_T+\beta'_S)+\sqrt{(\beta'_T-\beta'_S)^2+4\alpha'^2_{T,S}}}{2}}.$$

Proof. Without loss of generality, let $T=\{v_1,...,v_k\}$ and $S=\{v_{n-m+1},...,v_n\}$. Now, consider two orthonormal vectors $x,y\in\mathbb{C}^n$ similar to the proof of Lemma 4.2. Then by Lemma 4.9, $\beta'_T = x^TA^2x$, $\beta'_S=y^TA^2y$ and $\alpha'_{T,S}=x^TA^2y$. Then by (3) and similar to the proof of Theorem 4.3,

$$\lambda_1^2 \geqslant \mathbf{max}_{T,S}\frac{(\beta'_T+\beta'_S)+\sqrt{(\beta'_T-\beta'_S)^2+4\alpha'^2_{T,S}}}{2}. \quad \square$$

In particular, if $T=\{v_i\}\subseteq\mathbf{V}(\mathbf{G})$ and $S=\{v_j\}\subseteq\mathbf{V}(\mathbf{G})$ where $i\neq j$, then the inequality of Theorem 2.5 is a consequence of Theorem 4.10. The next theorem is another application of Marcus and Pesce theorem to obtain a subset of $\mathbf{F}(\mathbf{G})$ and consequently a lower bound and an upper bound for λ_1 and λ_2, respectively. Let w_i be a arbitrary positive real number, called weight, corresponding to vertex v_i for each $i=1,...,n$.

Theorem 4.11. *Let $T,S\subseteq\mathbf{V}(\mathbf{G})$ such that $S\cap T=\emptyset$. For each $1\leqslant i,j\leqslant n$, let*

$$e_{ij}=\begin{cases} w_iw_j & \text{if } v_i \textit{is adjacent to } v_j\\ 0 & \text{if } v_i \textit{ is not adjacent to } v_j.\end{cases}$$

Now, define

$$\beta_T=\frac{2\sum_{v_i,v_j\in T}e_{ij}}{\sum_{v_i\in T}w_i^2},\quad \beta_S=\frac{2\sum_{v_i,v_j\in S}e_{ij}}{\sum_{v_i\in S}w_i^2},\quad \alpha_{T,S}=\frac{\sum_{v_i\in T,v_j\in S}e_{ij}}{\sqrt{(\sum_{v_i\in T}w_i^2)(\sum_{v_j\in S}w_j^2)}}.$$

Then $\bigcup[a_{T,S},b_{T,S}]\subseteq\mathbf{F}(\mathbf{G})$, *where*

$$a_{T,S}=\frac{(\beta_T+\beta_S)-\sqrt{(\beta_T-\beta_S)^2+4\alpha_{T,S}^2}}{2},$$

$$b_{T,S}=\frac{(\beta_T+\beta_S)+\sqrt{(\beta_T-\beta_S)^2+4\alpha_{T,S}^2}}{2},$$

and the union runs over all pairs of disjoint subsets T and S of $\mathbf{V}(\mathbf{G})$. Also $\lambda_1 \geqslant b_{T,S}$ and $\lambda_n \leqslant a_{T,S}$ for each disjoint pair of T and S.

Proof. For $1 \leqslant i \leqslant n$, let

$$x_i = \begin{cases} \dfrac{w_i}{\sum_{v_i \in T} w_i^2} & v_i \in T \\ \\ 0 & v_i \notin T \end{cases}$$

and

$$y_i = \begin{cases} \dfrac{w_i}{\sum_{v_i \in S} w_i^2} & v_i \in S \\ \\ 0 & v_i \notin S. \end{cases}$$

Also $x = [x_1, x_2, ..., x_n]^T$ and $y = [y_1, y_2, ..., y_n]^T$. Corresponding to the proof of Theorem 4.3, $\beta_T = x^T Ax$, $\beta_S = y^T Ay$ and $\alpha_{T,S} = x^T Ay$ and the result is clear. □

Remark 4.12. *In Theorem 4.11, if $\mathbf{G}$ is a regular graph, Theorem 4.3 and 4.11 are identical and if $w_i = 1$ for each $1 \leqslant i \leqslant n$, then the results of Theorem 4.3 will be obtained. We can replace by d_i, $t_i = \sum_{j\sim i} d_j$(called 2-degree of vertex v_i), $N_i = \sum_{j\sim i} t_j$ or $M_i = \sum_{j\sim i} N_j$ where $j \sim i$ means v_j is adjacent to v_i. If $\mathbf{G}$ and $\mathbf{H}$ are the graphs Mentioned in Example 4.5 and T is the set of all vertices whose degrees are $\Delta(\mathbf{G})$ and $S = \mathbf{V}(\mathbf{G}) - T$, then we have the followig results:*
i) *Taking $w_i = d_i$, we have $\lambda_1(\mathbf{G}) \geqslant 2.16935$ and $\lambda_1(\mathbf{H}) \geqslant 2.24536$.*
ii) *Taking $w_i = t_i$, we have $\lambda_1(\mathbf{G}) \geqslant 2.16842$ and $\lambda_1(\mathbf{H}) \geqslant 2.24600$.*
iii) *Taking $w_i = N_i$, we have $\lambda_1(\mathbf{G}) \geqslant 2.16935$ and $\lambda_1(\mathbf{H}) \geqslant 2.24693$.*
iv) *Taking $w_i = M_i$, we have $\lambda_1(\mathbf{G}) \geqslant 2.16977$ and $\lambda_1(\mathbf{H}) \geqslant 2.24696$.*

Remark 4.13. Note that Theorem 4.11 is more general than what was mentioned in Remark 4.12. In fact, for a fixed pair of disjoint subsets of $\mathbf{V}(\mathbf{G})$, the list of weights provides a list of bounds for λ_1 and λ_n.

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