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A Note on Median Eigenvalues of Bipartite Graphs

Yezhou Wu[1], Yujun Yang[2], Dong Ye[3]

[1]*Key Laboratory of Ocean Observation-Imaging Testbed of Zhejiang Province Ocean Colleage, Zhejiang University, Zhoushan, Zhejiang 316021, China*
yezhouwu@zju.edu.cn

[2]*School of Mathematics and Information Science, Yantai University Yantai, Shandong 264005, China*
yangyj@yahoo.com

[3]*Department of Mathematical Sciences and Center for Computational Sciences Middle Tennessee State University, Murfreesboro, TN 37132, USA*
dong.ye@mtsu.edu

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Abstract

Let G be a connected simple graph with n vertices. The eigenvalues of G can be ordered as $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$. The two eigenvalues $\lambda_H(G)$ and $\lambda_L(G)$ with $H = \lfloor (n+1)/2 \rfloor$ and $L = \lceil (n+1)/2 \rceil$ are called median eigenvalues of G. The HOMO-LUMO gap of a graph G is defined as $\Delta_{\mathrm{HL}}(G) = \lambda_H(G) - \lambda_L(G)$, which has physical meaning in chemistry. In this note, we show that all bipartite graphs with at most one perfect matching have median eigenvalues in $[-1, 1]$. A corollary of our result is that all trees have median eigenvalues in $[-1, 1]$.

1 Introduction

A great deal of attention has been focused on the HOMO-LUMO gap of molecules (see [8, 9, 11]), the difference between the energies of the highest occupied molecular orbital and lowest unoccupied molecular orbital in conjugated-carbon structures. Many physico-chemical parameters of molecules are determined by or are dependent upon their HOMO-LUMO gaps [3, 11]. In 1950s, Günthard and Primas [6] discovered that the HMO π-electron energy levels of a molecule are in a simple linear manner related to the eigenvalues of the skeleton graph of the molecule, in which vertices correspond to atoms of the molecule and edges represent the bonds between two atoms. Many physical properties of a molecule can be interpreted by topological indices of its skeleton graph [10].

Let G be a graph with n vertices. The adjacency matrix of G is an $n \times n$-matrix $A = [a_{ij}]$ such that $a_{ij} = 1$ if $ij \in E(G)$, and $a_{ij} = 0$ if $ij \notin E(G)$. The eigenvalues of A are also called the eigenvalues of G. Denote these eigenvalues of G in decreasing order by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \lambda_H(G) \geq \lambda_L(G) \cdots \geq \lambda_n(G)$, where $H = \lfloor (n+1)/2 \rfloor$ and $L = \lceil (n+1)/2 \rceil$. The eigenvalues $\lambda_H(G)$ and $\lambda_L(G)$ are called median eigenvalues of G. The difference $\lambda_H(G) - \lambda_L(G)$ is called the HOMO-LUMO gap of graph G, denoted by $\Delta_{\mathrm{HL}}(G)$. Note that, if $n \equiv 1 \pmod 2$, then $H = L$ and hence $\lambda_H(G) = \lambda_L(G)$. So $\Delta_{\mathrm{HL}}(G) = \lambda_H(G) - \lambda_L(G) = 0$ if G has an odd number of vertices. For bounding HOMO-LUMO gap, only graphs with an even number of vertices are interesting.

By the HMO model [2, 6], the π-electron energy levels E_i $(i = 1, 2, \ldots, n)$ of a molecule obey a linear relation $E_i = \alpha + \beta\lambda_i(G)$ where G is the skeleton graph of the molecule and, α and $\beta < 0$ are constants. Then the HOMO-LUMO gap of a molecule is equal to $\beta\Delta_{\mathrm{HL}}(G)$.

The computational results of Fowler and Pisanski [3, 4] suggest that most subcubic graphs (also called chemical graphs), graphs with maximum degree at most 3, have their median eigenvalues belonging to the interval $[-1, 1]$. The only known exceptional graph is the Heawood graph which has median eigenvalues $\lambda_H(G) = \sqrt{2}$ and $\lambda_L(G) = -\sqrt{2}$. Fowler and Pisanski [3] conjectured that there are finitely many subcubic graphs with median eigenvalues beyond the interval $[-1, 1]$. Based on a result of Zhang and Chang [25] on eigenvalues of trees, Fowler and Pisanski obtained the following result.

Theorem 1.1 (Fowler and Pisanski [3]) *Let G be a tree with maximum degree at most 3. Then $\lambda_H(G), \lambda_L(G) \in [-1, 1]$.*

The above result was generalized to all subcubic bipartite graphs by Mohar [19, 21] as follows.

Theorem 1.2 (Mohar [21]) *Let G be a subcubic bipartite graph. Then $\lambda_H(G), \lambda_L(G) \in [-1, 1]$.*

Using a graph partition method, Mohar [20] proved that all subcubic graphs have median eigenvalues in $[-\sqrt{2}, \sqrt{2}]$, which is the smallest interval for subcubic graphs because of the Heawood graph, and he further conjectured that every plane subcubic graph has median eigenvalues in $[-1, 1]$. Gao and Mohar [7] constructed infinitely many regular bipartite graphs with median eigenvalue 1. Without the degree condition, Jaklič, Fowler and Pisanski [13] show that for any constant K, there is a graph with median eigenvalues beyond $[-K, K]$.

Besides graph partition, there are several other methods have been developed to bound median eigenvalues of graphs, such as graph inverse [14, 24] and graph square [15], etc. By using graph inverse, it has been shown that the median eigenvalues of all stellated trees and so-called corona graphs belong to $[-1, 1]$. By using graph square, it has been shown that the median eigenvalues of benzenoid systems and nanotubes are bounded by the fraction of total number of degree two vertices over total number of vertices [15], which shows that, in most of cases, the HOMO-LUMO gaps of benzenoid systems approach to zero as their sizes grow. Li et. al. [17] show that almost all trees have median eigenvalues zero. In this paper, we show the following result.

Theorem 1.3 *Let G be a bipartite graph with at most one perfect matching. Then $\lambda_H(G), \lambda_L(G) \in [-1, 1]$.*

A tree is a bipartite graph with at most one perfect matching. The following result is a direct corollary of Theorem 1.3, which generalizes Theorem 1.1.

Corollary 1.4 *Every tree has median eigenvalues in $[-1, 1]$.*

In the next section, we introduce some definitions and preliminary results for graph inverse. In Section 3, we prove our main result, Theorem 1.3.

2 Graph inverse

A graph G is *invertible* if its adjacency matrix A is invertible. The *inverse* of a graph G is a weighted graph (G^{-1}, w) such that $V(G^{-1}) = V(G)$ and for $i, j \in V(G^{-1})$, the weight function $w(ij) = [A^{-1}]_{ij}$, the ij-entry in the inverse of A.

A *2-matching* S is a subgraph of G such that each component of S is either a cycle or K_2. A 2-matching is *perfect* if S is spanning. For convenience, a perfect 2-matching is denoted by $S = \mathcal{C} \cup M$ where $\mathcal{C}$ consists of the cycles of S (including loops), and M consists of all components of S isomorphic to K_2. A 2-matching is a perfect matching if it has no cycle component, and a 2-matching is a 2-factor if it has no K_2 component. Let M be a perfect matching of G, and let x and y be two vertices of G. Then an (x, y)-path P is M-alternating if $M \cap P$ is a perfect matching of P. The following result shows how to compute the determinant of the adjacency matrix of a graph.

Theorem 2.1 (Harary, [12]) *Let G be a graph and A be the adjacency matrix of G. Then*

$$\det(A) = \sum_{S} 2^{|\mathcal{C}|}(-1)^{|\mathcal{C}|+|E(S)|},$$

where $S = \mathcal{C} \cup M$ is a perfect 2-matching.

By Theorem 2.1, an invertible bipartite graph always has a perfect 2-matching. Note that, a cycle in a bipartite graph always has even length and can be decomposed into two disjoint matchings. So an invertible bipartite graph always has a perfect matching. If the determinant of an adjacency matrix A of a graph G is not zero, then G has an inverse (G^{-1}, w). The following result characterizes the weight function of the inverse of bipartite graphs G with a unique perfect matching.

Theorem 2.2 ([23]) *Let G be a bipartite graph with a unique perfect matching M. Then G has an inverse (G^{-1}, w) such that*

$$w(ij) = \begin{cases} \sum\limits_{P \in \mathcal{P}_{ij}} (-1)^{|E(P) \setminus M|} & \text{if } i \neq j; \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathcal{P}_{ij}$ is the set of all M-alternating (i, j)-paths.

If G is a bipartite graph, the set of eigenvalues of G is symmetric with respect to the origin. It follows that $\lambda_H(G) = -\lambda_L(G)$ and hence $\Delta_{\mathrm{HL}}(G) = 2\lambda_H(G)$. If a bipartite graph G is not invertible, then $\lambda_H(G) = 0$ and $\Delta_{\mathrm{HL}}(G) = 0$. In order to bound the median eigenvalues of bipartite graph, we need only pay attention to invertible bipartite graphs.

A graph has a *split spectrum* if the half number of eigenvalues of G are positive and the other half number of eigenvalues are negative. A molecular system with a split spectrum is a proper closed shell. For further discussions, readers may refer to [3, 4]. All non-singular bipartite graphs have split spectra. It is interesting but may be very challenging to characterize all non-bipartite graphs with split spectra. Manolopoulos, Woodall and Fowler [18] show that all leapfrog fullerenes have split spectra (see also Section 9.9 in [11]). The following proposition is given in [24], which is the key idea to use graph inverse to bound the median eigenvalues.

Proposition 2.3 ([24]) *Let G be an invertible graph and let (G^{-1}, w) be its inverse. If G has a split spectrum, so does its inverse (G^{-1}, w) and $\lambda_H(G) = 1/\lambda_1(G^{-1}, w)$ and $\lambda_L(G) = 1/\lambda_n(G^{-1}, w)$.*

By Proposition 2.3, a lower bound for $\lambda_1(G^{-1}, w)$ will give an upper bound of $\lambda_H(G)$, and a upper bound for $\lambda_n(G^{-1}, w)$ will give a lower bound for $\lambda_L(G)$. The following result generalizes a result in [24] for signed graphs, which gives rough bounds for the largest eigenvalue and the smallest eigenvalue of weighted graphs with weights being rational numbers.

Theorem 2.4 *Let (G, w) be a weighted graph such that $w : E(G) \to \mathbb{R}\backslash\{0\}$. Let G_+ and G_- be spanning subgraphs of G in which every component is a vertex-induced subgraph with only positive edges and negative edges respectively. Then*

$$\lambda_1(G, w) \geq \frac{2w(G_+)}{|V(G)|} \text{ and } \lambda_n(G, w) \leq \frac{2w(G_-)}{|V(G)|},$$

where $w(G_+) = \sum_{e \in E(G_+)} w(e)$ and $w(G_-) = \sum_{e \in E(G_-)} w(e)$.

Proof. Let G^+ be the spanning subgraph of (G, w) such that every component of G^+ is a vertex-induced subgraph with only positive edges. Such spanning subgraphs exist, as the spanning subgraph without edges is a trivial example. Let $Q_1, ..., Q_k$ be all components of the spanning subgraph G_+ of (G, w). Let (Q, w) be the weighted multi-graph obtained from (G, w) by contracting all edges in G_+, and let $q_1, ..., q_k$ be all vertices of Q and define $w(q_\gamma q_\alpha) = \sum_{ij \in E(Q_\gamma, Q_\alpha)} w(ij)$ where $E(Q_\gamma, Q_\alpha)$ is the set of all edges of G joining a vertex in Q_γ and a vertex in Q_α. For each vertex q_i, let $E(q_\alpha) := \{q_\gamma q_\alpha | q_\gamma q_\alpha \in E(Q) \text{ and } \gamma < \alpha\}$. Assign $x(q_\alpha) \in \{-1, 1\}$ to each vertex q_α such that

$$\sum_{q_\gamma q_\alpha \in E(q_\alpha)} x(q_\gamma) w(q_\gamma q_\alpha) x(q_\alpha) \geq 0.$$

The weight-function $x : V(Q) \to \{-1, 1\}$ does exist because the sign of $x(q_\alpha)$ can always be adjusted to maintain the above inequality. So (Q, w) has a weight-function $x : V(Q) \to \{-1, 1\}$ such that

$$\sum_{q_\gamma q_\alpha \in E(Q)} x(q_\gamma) w(q_\gamma q_\alpha) x(q_\alpha) \geq 0.$$

Let $i, j \in V(G)$ and $ij \in E(G_+)$. Assume that ij is contracted to a vertex q_α of Q. Now, extend the weight-function x to $V(G)$ such that $x(i) = x(j) = x(q_\alpha)$, and define the vector $\mathbf{x} : V(G) \to \{-1, 1\}^n$ such that $x_i = x(i)$. Let $\mathbb{A}$ be the adjacency matrix of (G, w). Note that $E(G) = E(G_+) \cup E(Q)$. Then it follows that

$$\begin{aligned}
\langle \mathbb{A}\mathbf{x}, \mathbf{x} \rangle = 2 \sum_{ij \in E(G)} (\mathbb{A})_{ij} x_i x_j &= 2 \sum_{ij \in E(Q)} (\mathbb{A})_{ij} x_i x_j + 2 \sum_{ij \in E(G_+)} (\mathbb{A})_{ij} x_i x_j \\
&= 2 \sum_{ij \in E(Q)} x_i w(ij) x_j + 2 \sum_{ij \in E(G_+)} x_i w(ij) x_j \\
&\geq 2 \sum_{ij \in E(G_+)} w(ij).
\end{aligned}$$

Further,

$$\lambda_1(G, w) \geq \frac{2 \sum_{ij \in E(G)} (\mathbb{A})_{ij} x_i x_j}{\| \mathbf{x} \|} \geq \frac{2 \sum_{ij \in E(G_+)} w(ij)}{|V(G)|} = \frac{2w(G_+)}{|V(G)|}.$$

For second inequality, consider the weighted graph $(G, -w)$. Then $\lambda_1(G, -w) = -\lambda_n(G, w)$. Therefore,

$$\lambda_n(G, w) = -\lambda_1(G, -w) \leq \frac{2w(G_-)}{|V(G)|}$$

since G_- is a spanning subgraph of $(G, -w)$ in which every component is vertex-induced subgraph with only positive edges. This completes the proof. $\square$

The above theorem is very useful to bound median eigenvalues. A special case of above result has been used in [24] to bound median eigenvalues of stellated trees and corona graphs. In the next section, we use it to prove that all bipartite graphs with at most one perfect matching have median eigenvalues in $[-1, 1]$.

3 Bipartite graphs

Let G be a bipartite graph. If G has at most one perfect matching, then the determinant of its adjacency matrix is -1, 0 or 1 by Theorem 2.1. So such bipartite graphs are unimodular (cf. [1]). Bipartite graphs with a unique perfect matching have other combinatorial interest (see [23]) and include all acyclic graphs [8, 14]. The HOMO-LUMO gap of acyclic graphs has been studied in [14, 22, 25].

Let (G, w) be a weighted graph with n vertices. A weight-function w' is *equivalent* to w if there exists an edge cut S such that w' is obtained from w by switching the signs of edges in S, i.e., $w'(e) = -w(e)$ if $e \in S$ and $w'(e) = w(e)$ otherwise. Two weighted graphs (G, w) and (G', w') are *equivalent* if $G = G'$ and w is equivalent to w'.

Proposition 3.1 ([24]) *Let (G, w) be a weighted graph and w' be an equivalent weight-function of w. Then $\lambda_i(G, w) = \lambda_i(G, w')$.*

Now, we are going to prove our main result, Theorem 1.3.

Proof of Theorem 1.3. Let G be a bipartite graph with at most one perfect matching. If G has no perfect matching, then G is not invertible by Theorem 2.1. Therefore, $\lambda_H(G) = \lambda_L(G) = 0$ and the theorem holds.

So in the following, assume that G is a bipartite graph with a unique perfect matching M. By Theorem 2.2, G has an inverse (G^{-1}, w) such that $w : E(G) \to \mathbb{Z}\backslash\{0\}$. For any edge $ij \in M$, there is exactly one M-alternating path joining i and j which is the edge ij. So $w(ij) = 1$ by Theorem 2.2. Hence all edges of M are positive edges of (G^{-1}, w).

In (G^{-1}, w), let G_+^{-1} be the spanning subgraph induced by edges in M. Then it follows from Theorem 2.4 that

$$\lambda_1(G^{-1}, w) \geq \frac{2w(G_+^{-1})}{|V(G)|} = \frac{2|M|}{|V(G)|} = 1.$$

So $\lambda_H(G) = 1/\lambda_1(G^{-1}, w) \leq 1$ by Proposition 2.3.

On the other hand, let (G^{-1}, w') be a weighted graph obtained from (G^{-1}, w) by switching operation along the edge-cut $E(A, B)$, where (A, B) is a bipartition of G and $E(A, B)$ is the set of all edges with end-vertices from two different partitions of G. Then, $\lambda_n(G^{-1}, w') = \lambda_n(G^{-1}, w)$ by Proposition 3.1. In the (G^{-1}, w'), all edges in M have negative weight, and let G_-^{-1} be the spanning subgraph induced by edges in M. Then it follows from Theorem 2.4 that

$$\lambda_1(G^{-1}, w') \leq 2\frac{w'(G_-^{-1})}{|V(G)|} = -\frac{2|M|}{|V(G)|} = -1.$$

So $\lambda_L(G) = 1/\lambda_n(G^{-1}, w) = 1/\lambda_n(G^{-1}, w') \geq -1$ by Proposition 2.3. This completes the proof. $\square$

Remark. Note that, a bipartite graph with a unique perfect matching always has a cut edge [16]. A result of [24] characterizes all graphs with a unique perfect 2-matching and the characterization provides a linear time algorithm to recognize such graphs, including bipartite graphs with a unique perfect matching.

Shao and Hong [22] characterized all trees with the largest HOMO-LUMO gap, which are so-called combs obtained by attaching a pendant edge to each vertex of a path. Gutman [8] proved that among all trees with fixed number of vertices, paths maximize the energy which is defined as the sum of absolute eigenvalues. Among all trees with an even number of vertices, K_2 and P_4 are the only graphs maximizing both energy and HOMO-LUMO gap. We conclude by mentioning a specific open question: which bipartite graphs with a unique perfect matching maximize the HOMO-LUMO gap?

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