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Median Eigenvalues of Bipartite Planar Graphs

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Abstract

Motivated by the problem about HOMO-LUMO separation that arises in mathematical chemistry, Fowler and Pisanski [2, 3] introduced the notion of the HL-index which measures how large in absolute value may be the median eigenvalues of a graph. In this note we prove that the median eigenvalues of every bipartite planar graph of maximum degree at most three belong to the interval $[-1, 1]$. This proves the bipartite case of a conjecture of the author that was proposed in [6].

1 Introduction

In a recent work, Fowler and Pisanski [2, 3] introduced the notion of the *HL-index* of a graph that is related to the HOMO-LUMO separation studied in theoretical chemistry (see also Jaklič et al. [4]). This is the gap between the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO). In the Hückel model [1], the energies of these orbitals are in linear relationship with eigenvalues of the corresponding molecular graph and can be expressed as follows. Let G be a (molecular) graph of order n, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of its adjacency matrix. The eigenvalues occurring in the HOMO-LUMO separation are λ_H and λ_L, where

$$H = \lfloor \tfrac{n+1}{2} \rfloor \qquad \text{and} \qquad L = \lceil \tfrac{n+1}{2} \rceil.$$

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The *HL-index* $R(G)$ of the graph G is then defined as

$$R(G) = \max\{|\lambda_H|, |\lambda_L|\}.$$

Let us recall that a simple unweighted graph G is said to be *subcubic* if its maximum degree is at most 3. In chemical literature (cf. [2, 4]) connected subcubic graphs are sometimes termed as *chemical graphs.* In [2, 3] it is proved that every subcubic graph G satisfies $0 \le R(G) \le 3$ and that if G is bipartite, then $R(G) \le \sqrt{3}$. The following is the main result from [6].

Theorem 1.1. *The median eigenvalues $\lambda_H(G)$ and $\lambda_L(G)$ of every subcubic graph G are contained in the interval $[-\sqrt{2}, \sqrt{2}\,]$, i.e., $R(G) \le \sqrt{2}$.*

This result is best possible since the Heawood graph (the bipartite incidence graph of points and lines of the Fano plane) has $\lambda_H = -\lambda_L = \sqrt{2}$ as it has been observed in [4].

The following conjecture was proposed in [6]. Let us recall that a graph is *planar* if it can be drawn in the plane such that different edges intersect only at common endvertices.

Conjecture 1.2. *If G is a planar subcubic graph, then $R(G) \le 1$.*

In this paper we prove the conjecture for bipartite graphs.

2 Bipartite planar graphs

Theorem 2.1. *The median eigenvalues λ_H and λ_L of every subcubic planar bipartite graph G are contained in the interval $[-1, 1]$, i.e., $R(G) \le 1$.*

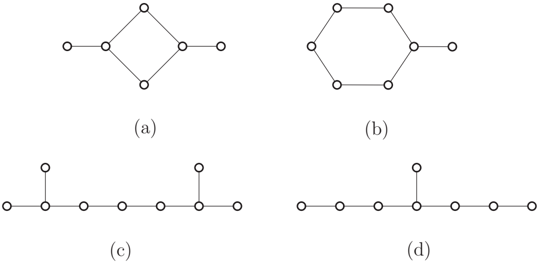
In order to prove the theorem, we need some preparation. Let us first mention that eigenvalues of bipartite graphs are symmetric with respect to 0, i.e., if λ is an eigenvalue, then $-\lambda$ is an eigenvalue as well and has the same multiplicity as λ. This in particular implies that $\lambda_H \ge 0$ and that $\lambda_L = -\lambda_H$. Therefore, it suffices to prove that $\lambda_H \le 1$.

Let us next recall the eigenvalue interlacing theorem (cf., e.g., [5]) that will be our main tool in the sequel. For a graph G, we let $\lambda_i(G)$ be the ith largest eigenvalue of G (counting multiplicities).

Theorem 2.2. *Let $A \subset V(G)$ be a vertex set of cardinality k, and let $K = G - A$. Then for every $i = 1, \ldots, n-k$, we have*

$$\lambda_i(G) \ge \lambda_i(K) \ge \lambda_{i+k}(G).$$

In estimating the eigenvalues, we shall also use the following lemma, which is easy to verify by computer.



(a) (b) (c) (d)

Figure 1: The graphs in Lemma 2.3

Lemma 2.3. (a) *Let G be the graph depicted in Fig. 1(a). Then* $\lambda_2(G) = 1$.

(b) *Let G be any of the graphs depicted in Fig. 1(b)–(d). Then* $\lambda_3(G) = 1$.

A partition $\{A, B\}$ of vertices of G is called *unfriendly* if every vertex in A has at least as many neighbors in B as in A, and every vertex in B has at least as many neighbors in A as in B. A partition $\{A, B\}$ of $V(G)$ is *unbalanced* if $|A| \neq |B|$.

Lemma 2.4. *If G is a subcubic graph with an unbalanced unfriendly partition, then* $R(G) \leq 1$.

Proof. Let $\{A, B\}$ be an unfriendly partition with $|B| > |A|$. Since G is subcubic, the maximum degree in $G(B)$ is at most 1, i.e., all components of $G(B)$ are isomorphic to either K_1 or K_2. In particular, every eigenvalue of $G(B)$ is equal to either 0, 1, or -1. Thus, $\lambda_1(G(B)) = |\lambda_{|B|}(G(B))| \leq 1$. Since $G(B) = G - A$ is obtained from G by deleting $|A|$ vertices and $|A| < H$, the eigenvalue interlacing theorem shows that $\lambda_H(G) \leq \lambda_{|A|+1}(G) \leq \lambda_1(G(B)) \leq 1$. Similarly, interlacing of smallest eigenvalues gives $\lambda_L(G) \geq \lambda_{n-|A|}(G) \geq \lambda_{|B|}(G(B)) \geq -1$. This implies that $-1 \leq \lambda_L(G) \leq \lambda_H(G) \leq 1$ and thus $R(G) \leq 1$. □

Every multigraph has an unfriendly partition, and they are easy to find. Unfortunately, some graphs have no unbalanced unfriendly partition. A planar and bipartite example of such a graph is the graph of the cube. A more general class of examples are subcubic graphs that contain a spanning subgraph consisting of 4-cycles. Since every 4-cycle needs to have two of its vertices in one part and the other two in another, every unfriendly partition is balanced.

Let $\{A, B\}$ be an unfriendly partition of $V(G)$. Suppose that $C \subset V(G)$ is a vertex set. If $C \cap A \neq \emptyset$ and $\{A \setminus C, B \cup C\}$ is also an unfriendly partition (or the same holds with the roles of A and B interchanged), then we say that C is *unstable* (with respect to the partition $\{A, B\}$).

Lemma 2.5. *If $\{A, B\}$ is an unfriendly partition of a subcubic graph G and $C \subset V(G)$ is an unstable vertex set, then $R(G) \leq 1$.*

Proof. One of the unfriendly partitions $\{A, B\}$ or $\{A \setminus C, B \cup C\}$ is unbalanced. We are done by Lemma 2.4. □

We say that a partition $\{A, B\}$ of $V(G)$ with $|A| < |B|$ is *k-unbalanced* if $|B| \geq |A| + 2k - 1$. Let us recall that $G(B) = G - A$ denotes the subgraph of G induced on B.

Lemma 2.6. *Suppose that $\{A, B\}$ is a vertex partition of a subcubic bipartite graph G, where $|A| < |B|$. Suppose that precisely one component Q of $G(B)$ has more than two vertices. If the partition is k-unbalanced for some $k \geq 1$ and $\lambda_k(Q) \leq 1$, then $R(G) \leq 1$.*

Proof. The proof is essentially the same as the proof of Lemma 2.4. Conditions of the lemma imply that $\lambda_k(G(B)) \leq 1$. Since $G(B) = G - A$ is obtained from G by deleting $|A|$ vertices and $|A| + k \leq H$, the eigenvalue interlacing theorem shows that $\lambda_H(G) \leq \lambda_{|A|+k}(G) \leq \lambda_k(G(B)) \leq 1$. Since G is bipartite, this implies that $R(G) \leq 1$. □

We are ready for the proof of our main theorem.

Proof of Theorem 2.1. Let G be a subcubic planar bipartite graph of order $n \geq 3$. Our goal is to find an unfriendly partition and apply Lemma 2.4, 2.5, or 2.6. We start by taking the bipartition $\{A, B\}$ of G, which is obviously an unfriendly partition. If $|A| \neq |B|$ (and in particular if n is odd), we have an unbalanced unfriendly partition, and we are done. Similarly, if there is an unstable vertex set with respect to this partition, one of the two partitions is unbalanced, and we are done. Thus we assume henceforth that $|A| = |B|$ and that there are no unstable vertex sets.

If v is a vertex of degree at most 1, then $\{v\}$ is unstable with respect to the bipartition. So, we may assume that every vertex of G has degree two or three.

Suppose that G contains a 4-cycle $C = v_1v_2v_3v_4$. We will assume that C is selected in such a way that the number of vertices of G inside the disk D bounded by C (in an embedding of G in the plane) is minimum. For $i = 1, \ldots, 4$, let u_i be the neighbor of v_i that is not on C (if $\deg(v_i) = 2$, then we set $u_i = v_i$). If $u_1 = u_3$ and $u_2 = u_4$, then one of the vertices u_1 or u_2 (say u_1) lies inside D. But then replacing C with the 4-cycle $v_1u_1v_3v_4$ contradicts our choice of C having minimum number of vertices in its interior. Thus we may assume that $u_1 \neq u_3$. Recall that the bipartition $\{A, B\}$ of G is balanced. We may assume that $v_1, v_3 \in A$. The partition $\{A \setminus V(C), B \cup V(C)\}$ is 2-unbalanced, and $G(B)$ consists of isolated vertices plus one component Q containing C that is isomorphic to the graph depicted in Figure 1(a) (or to an induced subgraph of that one if $u_1 = v_1$ or $u_3 = v_3$). Lemma 2.3(a) shows that $\lambda_2(Q) \leq 1$ and thus Lemma 2.6 implies that $R(G) \leq 1$.

From now on, we may assume that G has no 4-cycles and that it is connected. Suppose that G has two vertices, x and y, both of degree 2, that belong to the same bipartite class, say $x, y \in A$. Let P be a shortest path connecting x and y in G. Let $A' = A + V(P)$ and $B' = B + V(P)$, where $+$ denotes the symmetric difference. Clearly, $|V(P) \cap A| = |V(P) \cap B| + 1$, since x and y both belong to A. Therefore, the partition $\{A', B'\}$ is unbalanced. Each vertex in $V(G) \setminus V(P)$ has at most one neighbor on the path P – having two would either create a 4-cycle or contradict our choice of P as a shortest path from x to y. It is also obvious that every vertex in $A' \cap V(P) = B \cap V(P)$ has at most one neighbor in A' since such a neighbor must be in $A \setminus V(P)$. The same holds for $B' \cap V(P)$. Therefore, the partition $\{A', B'\}$ is an unbalanced unfriendly partition of G, and the proof is complete by Lemma 2.4.

For the rest of the proof, we may assume that each of A and B contains at most one vertex of degree 2. Thus, G has at most two vertices of degree 2. A well-known consequence of Euler's formula (see, e.g., [7]) is that every plane graph of minimum degree at least 2 satisfies the following condition:

$$\sum_{i \geq 1} f_i(i - 6) \geq 12 - 2n_2 \tag{1}$$

where f_i denotes the number of faces of G of length i and n_2 denotes the number of vertices of degree 2 in G. (This formula is usually formulated for the case when the minimum degree is at least 3, i.e. $n_2 = 0$. But adding a vertex of degree 2 is like subdividing an edge by inserting the degree-2 vertex in the middle of an edge. Since such an operation either increases the lengths of two faces by 1, or increases the length of one face by 2, it preserves the inequality (1).) Since we have $n_2 \leq 2$, the right hand side of (1) is positive. This contradicts the fact that G has no cycles and hence no faces of length less than 6 (which implies that the left hand side of (1) cannot be positive). This contradiction completes the proof. □

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