

Median Eigenvalues of Subcubic Graphs

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Subcubic graphs: max deg ≤ 3 .

Eigenvalues of adjacency matrix: $\lambda_1 \geq \dots \geq \lambda_n$

Median eigenvalues: $\lambda_H = \lambda_{\lfloor \frac{n+1}{2} \rfloor}$, $\lambda_L = \lambda_{\lceil \frac{n+1}{2} \rceil}$.

Hückel Model Theory

Chemistry

Organic molecules

π -electron energy levels

Highest occupied molecule orbital energy

Lowest un — — — — —

Molecule's kinetic stability

Maths

Chemical graphs
(connected + subcubic)

Eigenvalues

λ_H

λ_L

$\lambda_H - \lambda_L$

Fowler & Pisanski 2010

Computational experiments: most chemical graphs have med. eigenvals in

Single exception: Heawood graph (3-reg. 14 vertices)

Incidence graph of Fano plane

Eigenvals: $-3, (-\sqrt{2})^6, (\sqrt{2})^6, 3$.

$[-1, 1]$

Conjecture: All but finitely many chemical graphs, $\lambda_H, \lambda_L \in [-1, 1]$.

Optimality of $[-1, 1]$: Guo and Mohar constructed infinitely many bipartite chemical graphs with median eigenvalues ± 1 .

Known results

Fowler & Pisanski 2010: subcubic trees.

Mohar 2013: planar bipartite.

2016: bipartite except Heawood.

Wang & Zhang 2024 ..., Benediktovich 2014.

Tray (Acharya, Jeter, J, 2025) All chemical but Heawood.

For simplicity, only focus on $\lambda_H \leq 1$.

Proof of 99% of the cases:

(1) Take maximum cut of subcubic G . say (A, B)

(2). Assume in addition $|A| > |B|$

(3). Note max deg of $G[A] \leq 1 \Rightarrow \lambda_1(G[A]) \leq 1$

Cauchy interlace $\Rightarrow \lambda_H(G) \leq \lambda_1 + |B| (G) \leq 1$.

□

99% of the proof for the rest 1% of the cases

Key ideas:

① Tail reducer: move k vertices, say C , from A to B s.t.

$$\lambda_k(h[B \cup C]) \leq 1. \quad (\text{then Cauchy interlace implies } \lambda_1 \leq 1).$$

② Cut enhancer: find C s.t. $(A \oplus C, B \oplus C)$ is larger cut, which is a contradiction.

③ Underlying graph (multigraph) M

vertices of M are edges of $G[A] \cup G[B]$. and

$$\begin{array}{ccc} \text{if} & \begin{array}{c} \xrightarrow{\alpha \in G[A]} \\ \xleftarrow{\beta \in G[B]} \end{array} & \text{then} \end{array} \quad \begin{array}{c} \alpha \\ \vdots \\ \parallel \\ \vdots \\ \beta \end{array} \leftarrow k \text{ edges in } M.$$