

# My conjectures in spectral graph theory

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# Spectral notation

- $n$  - number of vertices;  $m$  - number of edges
- $\overline{G}$  - complement of  $G$
- $A$  - adjacency matrix
- $\mu = \mu_1 \geq \dots \geq \mu_n$  eigenvalues of  $A$  ( $\sum_i \mu_i = \text{tr}(A) = 0$ )

$$s^+ = \sum_{+ve} \mu_i^2 \text{ and } s^- = \sum_{-ve} \mu_i^2 \text{ so } s^+ + s^- = \sum_i \mu_i^2 = \text{tr}(A^2) = 2m$$

$s^+$  and  $s^-$  called *positive and negative square energies*

- $\omega(G)$  - clique number;  $\alpha(G) = \omega(\overline{G})$  - independence number
- $\chi(G)$  - chromatic number
- $\chi_v(G) = \vartheta'(\overline{G})$  - vector chromatic number = Schrijver variant of Lovász theta function of complement
- $\chi_f(G) = \lim_{b \rightarrow \infty} \frac{\chi_b(G)}{b}$  - fractional chromatic number
- $\omega(G) \leq \chi_v(G) \leq \vartheta(\overline{G}) \leq \chi_f(G) \leq \chi(G)$
- $(n^+, n^-, n^0)$  - numbers of positive, negative and zero eigenvalues (known as inertia)

# Some applications of spectral graph theory

- Spectral proofs of non-spectral results eg characterisation of Moore graphs with diameter 2 (Hoffman, Singleton) and proof of Sensitivity Conjecture in computer science (Hao Huang)
- Spectral bounds for non-spectral (often NP-hard) parameters, eg

$$1 + \frac{\mu_1}{|\mu_n|} \leq \chi(G) \leq 1 + \mu$$

- Non-spectral bounds for spectral parameters eg

$$\mu \geq \frac{2m}{n} = d \text{ with equality only for regular graphs}$$

# Proven conjecture 1 - lower bound for $\omega(G)$

- $\frac{2m}{2m-\mu^2} \leq \chi(G)$  - Elphick PhD (1981)
- $\frac{2m}{2m-\mu^2} \leq \omega(G)$  - Conjecture in Edwards and Elphick (1983)
- $\frac{2m}{2m-\mu^2} \leq \omega(G)$  - Proved by Nikiforov (2002) and cited 200x
- This provides a spectral proof of the concise version of Turán's Theorem (1941) since:

$$\frac{4m^2}{n^2} \leq \mu^2 \leq \frac{2m(\omega-1)}{\omega} \Rightarrow \frac{2m}{n} = d \leq \frac{n(\omega-1)}{\omega}$$

- Proof tools of Nikiforov: 1/3 page using Motzkin-Straus inequality (1965), which states that for any  $n$ -vector with  $\sum_{i=1}^n x_i = 1$  and  $x_i \geq 0$ :

$$\sum_{ij \in E} x_i x_j \leq \frac{\omega-1}{2\omega}.$$

Also use Rayleigh quotient, normalized principal eigenvector and Cauchy-Schwarz.

## Proven conjecture 2 - Introducing $s^+$ and $s^-$

- $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \leq \chi(G)$  - Conj. by Wocjan/Elphick (2013)
- $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \leq \chi_v(G)$  - Conjecture by Wocjan, Elphick, Anekstein (2023)
- $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \not\leq \omega(G)$  eg 5-cycle
- $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \leq \chi(G)$  - Proved by Ando/Lin (2015)
- $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \leq \chi_v(G)$  - Proved by Coutinho/Spier (2023)
- $\frac{2m}{2m-\mu^2} \leq \frac{2m}{2m-s^+} = 1 + \frac{s^+}{s^-}$  - my inspiration for the conjecture
- Proof tools of Coutinho/Spier: spectral decomposition, semidefinite programs, positive semidefinite matrices, Cauchy-Schwarz (4 pages)

## Proven conjecture 3 - lower bound for $\chi_v(G)$

- $\delta_1 =$  largest eigenvalue of signless Laplacian  $Q = D + A$
- $\lambda_1 =$  largest eigenvalue of Laplacian  $L = D - A$
- $1 + \frac{\mu_1}{\mu_1 - \delta_1 + \lambda_1} \leq \chi(G)$  - proved by Kolotilina (2010)
- $\chi_v(G) \leq \chi(G)$  for all graphs;  $\chi_v(G) \ll \chi(G)$  for some graphs
- $1 + \frac{\mu_1}{\mu_1 - \delta_1 + \lambda_1} \leq \chi_v(G)$  - conjecture by Elphick, experimental evidence by Anekstein, proof by Wocjan (2023)
- Exact for example for strongly regular, distance regular and symmetric graphs
- Inspiration: Galtman proved that  $1 + \frac{\mu_1}{|\mu_n|} \leq \chi_v(G)$  and  $|\mu_n| = \mu_1 - \delta_1 + \lambda_1$  for regular graphs
- Proof tools: Majorization, Gram matrices, Perron-Frobenius theorem, spectral decomposition, Schur products, stochastic matrices, correlation matrices (3 pages)

# Proven conjecture 4 - an inertial bound

- $1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) \leq \chi_f(G) \leq \chi(G)$  - Conjecture by Elphick/Wocjan (2017)
- $1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) \leq \chi(G)$  - Proven by Elphick/Wocjan (2017)
- Inspiration was that  $\chi_f(G) \geq n/\alpha(G)$  and  $\alpha(G) \leq \min(n^+ + n^0, n^- + n^0)$ . Also complete  $q$ -partite graphs have  $n^+ = 1$  and  $n^- = q - 1$ .
- Interesting that  $n^0$  is required in upper bound for  $\alpha(G)$  but not required in lower bound for  $\chi(G)$ .
- Proof tools: Hermitian matrices, unitary matrices, rank of positive semidefinite matrices, orthogonal projectors, matrix algebra (2 pages)



# Unproven conjecture 1 - a Nordhaus-Gaddum bound

- $n - 1 \leq \mu(G) + \mu(\overline{G}) < \sqrt{2}n$  - proof by Nosal (1970)
- $\mu(G) + \mu(\overline{G}) \leq 4n/3 - 1$  - conjecture by Nikiforov (2007) and best possible
- $\mu(G) + \mu(\overline{G}) \leq 1.3660n - 1$  - proof by Csikvári (2009)
- $\mu(G) + \mu(\overline{G}) \leq 4n/3 - 1$  - proof by Terpai (2011), using graphons and analysis
- $\sqrt{s^+(G)} + \sqrt{s^+(\overline{G})} < \sqrt{2}n$  - proof by Elphick and Aouchiche (2017)
- $\sqrt{s^+(G)} + \sqrt{s^+(\overline{G})} \leq 4n/3 - 1$  - conjecture by Elphick and Aouchiche (2017) and best possible
- No counter-examples found using AGX software or in Wolfram Mathematica database of graphs with up to 40 vertices
- Very hard to prove so perhaps search for a counter-example using AI

# Unproven conjecture 2 - an inertial bound for $\chi_f(G)$

- $1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) \leq \chi_f(G)$  - Conj. by Elphick/Wocjan (2017)
- $1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) \not\leq \chi_v(G)$  - Noted by Elphick/Wocjan (2017)
- This bound is exact for Kneser graphs, and  $\chi_f(G)$  can be defined in terms of homomorphisms from  $G$  to Kneser graphs
- Very surprised if false
- Combine proof for  $\chi(G)$  due to Elphick and Wocjan with proof that  $1 + \max\left(\frac{s^+}{s^-}, \frac{s^-}{s^+}\right) \leq \chi_f(G)$  due to Guo and Spiro (2023)

# Unproven conjecture 3 - lower bound for $\omega(G)$

- For  $G \neq K_n$ ,  $\mu_1^2 + \mu_2^2 \leq \frac{2m(\omega-1)}{\omega}$  - Conjecture by Bollobás and Nikiforov (2007)
- Proved for triangle-free graphs by Lin, Ning and Wu (2021) and for regular graphs by Zhang (2024)
- In 2023, Elphick, Linz and Wocjan conjectured that for all  $G$

$$\sum_{i=1}^{\ell} \mu_i^2 \leq \frac{2m(\omega-1)}{\omega} \text{ where } \ell = \min(n^+, \omega)$$

They proved this conjecture for triangle-free, weakly perfect and Kneser graphs and Kumar and Pragada (2024) proved for graphs with at most  $O(m^{1.5-\epsilon})$  triangles.

- Proof by Zhang uses that  $\mu_2 > 0$ , so may be possible to generalise his proof for regular graphs
- Liu and Ning (2023) placed these conjectures 3rd and 4th in their review of "Unsolved Problems in spectral graph theory"

# Unproven conjecture 4 - bound for $s^+$ and $s^-$

- $\mu^2 \leq 2m - n + 1$  - Proved by Hong (1988)
- For any *connected* graph, Elphick, Farber, Goldberg and Wocjan (2016) conjectured that

$$\max(s^+, s^-) \leq 2m - n + 1 \text{ equivalent to: } \min(s^+, s^-) \geq n - 1$$

They proved this for bipartite, barbell and regular graphs and for almost all graphs. For regular graphs, using Ando/Lin and Brooks theorem:

$$\min(s^+, s^-) \geq \frac{2m}{\chi(G)} \geq \frac{2m}{\Delta} = \frac{2m}{d} = n$$

with separate treatment for complete graphs and odd cycles.

- In general, if  $G$  has  $\kappa$  components, then  $\min(s^+, s^-) \geq n - \kappa$
- $s^+ = s^- = n - 1$  for trees and  $s^- = n - 1$  for complete graphs
- Liu and Ning (2023) placed this conjecture 1st in their review of over 20 "Unsolved Problems in spectral graph theory"

# Unproven conjecture 4 - bound for $s^+$ and $s^-$ continued

- I regard as my best conjecture to date because simple to state and straightforward to prove for regular graphs and almost all graphs. Easy counter-examples for disconnected graphs. I would be very surprised if false and conjecture does not "look" hard at first sight.
- Abiad, de Lima, Desai, Guo, Hogben, Madrid (2023) gave the name positive and negative square energies to  $s^+$  and  $s^-$  and developed new tools, but made modest progress in proving for new graph classes
- $s^+ \gg s^-$  for almost all graphs so could treat as 2 conjectures
- $s^+(G) \not\geq s^+(G - e)$  and  $s^-(G) \not\leq s^-(G - e)$  - otherwise fairly trivial proof using spanning trees
- I think hard because  $A$  is an irreducible matrix for connected graphs and little is known, apart from Perron-Frobenius theorem, about spectrum of irreducible matrices.

# Unproven conjecture 5 - a weaker conjecture for $s^+$ and $s^-$

- Elphick and Linz (2024), conjectured that for *all* graphs

$$\min(s^+, s^-) \geq \max(n^+, n^-).$$

- This conjecture is weaker than Unproven Conjecture 4 and there is no counter-example in Wolfram Mathematica database of graphs with  $n \leq 100$
- Let  $E(G) = \sum_{i=1}^n |\mu_i|$  denote the energy of  $G$ . Simple, using Cauchy-Schwarz, that  $s^+ \geq E^2/4n^+$  and  $s^- \geq E^2/4n^-$ .
- Aouchiche and Hansen conjectured in 2010 that:

$$\frac{E(G)}{2} = \sum_{\mu_i > 0} \mu_i = \sum_{\mu_i < 0} |\mu_i| \geq \max(n^+, n^-). \quad (1)$$

- Akbari *et al* (2009) proved that  $E(G) \geq n^+ + n^-$  using AM-GM inequality and that  $\prod_{\mu_i \neq 0} |\mu_i| \geq 1$ .
- However  $\prod_{\mu_i > 0} \mu_i \not\geq 1$  and  $\prod_{\mu_i < 0} |\mu_i| \not\geq 1$ , so need a new approach to prove (1).

# A final thought

- In 1940, Coulson proved that

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n - x \frac{d}{dx} \ln \phi(G; ix) \right] dx \quad (2)$$

where  $\phi(G; x) = \det(xI_n - A(G))$  is the characteristic polynomial of  $G$  and  $i = \sqrt{-1}$ .

- The book *Graph Energy* by Li, Shi and Gutman provides a fairly straightforward proof of (2).
- This formula can be used to calculate graph energy without knowing a graph's eigenvalues.
- Could this approach help to prove  $E(G) \geq 2 \max(n^+, n^-)$ ?
- Are there Coulson-type equalities for square energies?
- Could such equalities help to prove Unproven Conjectures 4 or 5?

# Selected References

- A. Abiad *et al*, *Positive and negative square energies of graphs*, Elec. J. Linear Algebra, 39, 307 - 326, 2023.
- S. Akbari, E. Ghorbani and S. Zare, *Some relations between rank, chromatic number and energy of graphs*, Discrete Math., 309, (2009), 601 - 605.
- M Aouchiche and P Hansen, *A survey of automated conjectures in spectral graph theory*, Lin. Alg. Appl., 432, (2010), 2293 - 2322.
- T. Ando and M. Lin, *Proof of a conjectured lower bound on the chromatic number of a graph*, Lin. Alg. Appl., 485, 480-484, 2015.
- B. Bollobás and V. Nikiforov, *Cliques and the spectral radius*, J. Comb. Theory Ser. B, 97, 859 - 865, 2007.
- C. A. Coulson, *On the calculation of the energy in unsaturated hydrocarbon molecules*, Proc. Cambridge Phil. Soc., 36, 201203, (1940).
- G. Coutinho and T. Spier, *Sums of squares of eigenvalues and the vector chromatic number*, math arxiv:2308.04475, (2023).
- C. Edwards and C. Elphick, *Lower bounds for the clique and chromatic number of a graph*, Discrete Appl. Math., 5, 51 - 64, 1983.
- C. Elphick *et al*, *Conjectured bounds for the sum of squares of positive eigenvalues of a graph*, Discrete Math., 339, 2215 - 2223, 2016.
- C. Elphick and P. Wocjan, *An inertial lower bound for the chromatic number of a graph*, Elec. J. Combinatorics, 24(1), 2017.
- C. Elphick and M. Aouchiche, *Nordhaus-Gaddum and other bounds for the sum of squares of the positive eigenvalues of a graph*, Lin. Alg. Appl. 530, (2017), 150 - 159.



# Selected References

- C. Elphick, W. Linz and P. Wocjan, *Two conjectured strengthenings of Turán's theorem*, Lin. Alg. Appl. 684, 23 - 36, 2024.
- C. Elphick and W. Linz, *Symmetry and asymmetry between positive and negative square energies of graphs*, Elec. J. Lin. Alg., 40, 418 - 432, 2024.
- K. Guo and S. Spiro, *New eigenvalue bound for the fractional chromatic number*, J. Graph Theory, 2023.
- H. Kumar and S. Pragada, *Bollobás-Nikiforov conjecture for graphs with not so many triangles*, math arXiv:2407.19341.
- L. Liu and B. Ning, *Unsolved problems in spectral graph theory*, Oper. Res. Trans., 27(4), 33 - 60, 2023.
- V. Nikiforov, *Some inequalities for the largest eigenvalue of a graph*, Combin. Probab. Comput., 11, 179 - 189, 2002.
- V. Nikiforov, *Eigenvalue problems of Nordhaus-Gaddum type*, Discrete math., 307, 774 - 780, 2007.
- T. Terpai, *Proof of a conjecture due to V. Nikiforov*, Combinatorica, 31, 739 - 754, (2011).
- P. Wocjan and C. Elphick, *New spectral bounds on the chromatic number encompassing all eigenvalues of the adjacency matrix*, Elec. J. Combinatorics, 20(3), (2013).
- P. Wocjan, C. Elphick and D. Anekstein, *More Tales of Hoffman: Bounds for the vector chromatic number of a graph*, Discusiones Mathematicae Graph Theory, 43, 159 - 169, (2023).
- S. Zhang, *On the first two eigenvalues of regular graphs*, Lin. Alg. Appl. 686(15), 2024.