DISTRIBUTION OF ZEROS AND EIGENVALUES

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LECTURE 1: NON-TAME DISTRIBUTION OF ZEROS OF ZETAFUNCTIONS.

LECTURE 2: SPECTRA OF SURFACES AND REGULAR GRAPHS.

PENN-STATE OCT 2025.

- WE REVIEW DEVELOPMENTS AROUND THE DISTRIBUTIONS OF ZEROS OF ZETA FUNCTIONS OVER NUMBER FIELDS, FUNCTION FIELDS AND CLOSELY RELATED PROBLEMS FOR EIGENVALUES OF REGULAR GRAPHS AND RIEMANNIAN SURFACES.

THE BOOK

"ZETA AND L-FUNCTIONS IN NUMBER THEORY AND COMBINATORICS"

WINNIE LI

CBMS 129 (2014)

GIVES AN EXCELLENT INTRODUCTION AND ACCOUNT OF THESE TOPICS.

GRAPHS

- X A CONNECTED GRAPH WITH n VERTICES $v \in V = V(X)$.
- ADJACENCY MATRIX $A : \ell^2(X) \to \ell^2(X)$

$$Af(v) = \sum_{w \sim v} f(w)$$

SYMMETRIC AND <u>INTEGRAL</u> IN THIS BASIS.

- $\Delta = D - A$; $D = \text{DIAG}(d_v)$, d_v DEG OF v

"LAPLACIAN"

$$\Delta f(v) = \cancel{\sum} d_v f(v) - \sum_{w \sim v} f(w)$$

INTEGRAL SYMMETRIC

- $\Delta f = 0$ IFF f IS CONSTANT

SPECTRUM OF Δ ; $0 = \mu_0 < \mu_1 \leq \mu_2 \ldots \leq \mu_{n-1}$

IF $L : \mathbb{Z}^n \to \mathbb{Z}$ IS THE LINEAR FORM $\sum_{j=1}^{n} x_j$

THEN $\mathrm{IM}(\Delta) \subset \ker(L)$

<u>DEF^N</u> (LORENZINI) $\mathrm{JAC}(X) = \ker(L) / \mathrm{Im}(\Delta)$

IS A <u>FINITE</u> ABELIAN GROUP

IT ORDER IS DENOTED $h(X)$.

MATRIX TREE THEOREM (~~KIRCH~~ KIRCHOFF)

$$\det{}^*(\Delta_X) = \prod_{j=1}^{n-1} \mu_j = h(X).n$$

AND $h(X)$ IS THE NUMBER OF SPANNING TREES ON X (ALSO DENOTED $\kappa(X)$ CALLED THE COMPLEXITY).

- WE RESTRICT TO GRAPHS X WHICH ARE k-REGULAR $(k \geq 3)$, IE $d_v = k$ FOR ALL v. DENOTE THESE BY

$$\mathcal{X}_k.$$

- FOR $X \in \mathcal{X}_k$ THE SPECTRUM OF A_X AND Δ_X ARE RELATED

$$\sigma(A) = \{ \lambda_0 = k > \lambda_1 \geq \dots \geq \lambda_{n-1} \geq -k \}$$

AND $\mu_j = k - \lambda_j$.

KEMENY'S "CONSTANT":

THE EXPECTED TIME FOR THE RANDOM WALK ON X STARTING AT SOME POINT TO HIT A RANDOM OTHER POINT, IS INDEPENDENT OF THE STARTING POINT AND IS CALLED KEMENY'S CONSTANT $KEM(X)$.

FOR $X \in \mathcal{X}_k$ $\quad KEM(X) = (n-1)k + I(X)$

WHERE

$$I(X) = \sum_{j=1}^{n-1} \frac{1}{1-\lambda_j/k}.$$

FOR $X \in \mathcal{X}_k$ THERE IS A SIMPLE POSITIVITY INEQUALITY THAT RESTRICTS THE POSSIBLE DISTRIBUTION OF THE EIGENVALUES AS $n \to \infty$.

$$\#\left\{\begin{array}{l}\text{PATHS OF LENGTH } m \text{ ON } X \\ \text{STARTING AT A VERTEX } v \\ \text{AND ENDING AT } v\end{array}\right\} \geq \left\{\begin{array}{l}\text{THE SAME WITH } X \\ \text{REPLACED BY } T_k \\ \text{THE } k\text{-REGULAR TREE}\end{array}\right\}$$

<u>PLANCHAREL MEASURE</u> (KESTEN, SALLY-SHALIKA, McKAY)

$$\mu_k = \frac{k\sqrt{4(k-1) - x^2}}{2\pi(k^2 - x^2)} \quad \text{FOR } |x| \leq 2\sqrt{k-1}$$
AND 0 FOR $|x| > 2\sqrt{k-1}$.

SO SUPPORTED IN $[-2\sqrt{k-1}, 2\sqrt{k-1}] \subsetneqq [-k, k]$.

(IT IS THE "DENSITY DISTRIBUTION" FOR THE SPECTRUM OF Δ ON $\ell^2(T_k)$)

<u>DEFINITION</u>:

X IS <u>RAMANUJAN</u> IF

$\lambda_j \in [-2\sqrt{k-1}, 2\sqrt{k-1}]$, FOR $j \neq 0$ OR $n-1$ IF X IS BIPARTITE.

THE POSITIVITY IMPLIES:

IF $f(x)$ ON $[-1,1)$ HAS UNIFORMLY CONVERGENT TAYLOR SERIES ON $[-1,\tau)$ FOR ANY $\tau<1$ AND IS OF THE FORM

$$f(x)=\sum_{n=0}^{\infty} a_n x^n, \quad a_n \geqslant 0$$

THEN

$$\varliminf_{\substack{X\in\mathcal{X}_k \\ X\to\infty}} \frac{1}{n}\sum_{j=1}^{n-1} f\left(\frac{\lambda_j}{k}\right) \geqslant \int_{-k}^{k} f\left(\frac{t}{k}\right) d\mu_k(t).$$

WITH EQUALITY IF X IS RANDOM (OR RAMANUJAN).

(ALL BEING ACHIEVED WITH RANDOM!)

APPLIED WITH

(a) $f(x) = -\log(1-x)$ GIVES

$$\varlimsup_{X\in\mathcal{X}_k} \frac{\log h(X)}{|X|} \leqslant c(k) = \frac{(k-1)^{k-1}}{(k^2-2k)^{(k/2-1)}}$$

(McKAY)

(b). $f(x) = \dfrac{1}{1-x}$ GIVES

$$\varliminf_{X\in\mathcal{X}_k} \frac{\mathrm{KEM}(X)}{|X|} \geqslant k + \int_{-k}^{k} \frac{k}{k-t}\, d\mu_k(t).$$

(c) $f(x) = (1-x)^{-m}$ FOR LARGE m

$$\varliminf_{X\in\mathcal{X}_k} \lambda_1(X) \geqslant 2\sqrt{k-1}$$

ALON-BOPPANA

DEFINE THE GONALITY OF X FOR $X \in \mathcal{X}_k$ TO BE THE LEAST GENUS SUCH THAT X EMBEDS WITHOUT EDGES CROSSING. SO

$$\mathrm{gon}(X) = 0 \quad \text{IFF} \quad X \text{ IS PLANAR.}$$

- TAME SEQUENCES ARE ONES FOR WHICH

$$\frac{\mathrm{gon}(X)}{|X|} \to 0 .$$

FOR THESE:

$$\lim_{\substack{X \to \infty \\ X \text{ TAME}}} \frac{\mathrm{KEM}(X)}{|X|} = \infty$$

$$\lim_{\substack{X \to \infty \\ X \text{ TAME}}} \lambda_1(X) = k \qquad (\text{LIPTON-TARJAN})$$

ONE CAN ASK ABOUT <u>LOCAL STATISTICS</u> FOR RANDOM X.

FOR $\mathrm{JAC}(X)$, $X \in \mathcal{X}_k$ RANDOM THERE IS A COMPLETE ANSWER

<u>THEOREM</u> (WOOD; MESZAROS): $\mathrm{JAC}(X)$ SATISFIES A SUITABLE FORM OF A COHEN-LENSTA DISTRIBUTION FOR RANDOM $X \in \mathcal{X}_k$!

<u>UNSOLVED:</u> FOR RANDOM $X \in \mathcal{X}_k$, THE LOCAL SCALED SPACING STATISTICS FOLLOWS GOE.

(CONJECTURED BY JAKOBSON, RIVIN, MILLER, RUDNICK WHO EXPERIMENTED NUMERICALLY)

ARCHIMEDIAN McKAY LAW

FOR X A RIEMANNIAN SURFACE (OF GENUS $g(X)$) DEFINE

$$\det{}^*(X) = \det{}^*(\Delta_X) = \prod_{j=1}^{\infty} \mu_j \quad \text{(REGULARIZED)}.$$

ONE CAN STUDY ITS EXTREMAL:

(OSGOOD-PHILLIPS-S): $A(X) = \text{AREA}(X)$.

(i) $$\max_{\substack{g(X)=0 \\ A(X)=4\pi}} \det{}^* X = \exp\left(\tfrac{1}{2} - 4\zeta'(-1)\right)$$

WITH EQUALITY IFF X IS THE ROUND SPHERE.

(ii) $$\max_{\substack{g(X)=1 \\ A(X)=1}} \det{}^* X = \frac{\sqrt{3}}{2}\left|\eta\left(\frac{1}{2} + \frac{i\sqrt{3}}{2}\right)\right|^4$$

WITH EQUALITY IFF X IS THE HEXAGONAL TORUS.

(iii) FOR $g \geq 2$ FIXED

$$\max_{\substack{g(X)=g \\ A(X)=4\pi(g-1)}} \frac{\log \det{}^* X}{A(X)} = \eta(g) < \infty$$

ACHIEVED BY A HYPERBOLIC SURFACE!

USING THE LAST ONE CAN SHOW USING THE TRACE FORMULA THAT

$$\overline{\lim_{\substack{X \text{ HYPERBOLIC} \\ g(X)\to\infty}}} \frac{\log \det^* X}{A(X)} \leq E := 4\zeta'(-1) - \frac{1}{2} + \log 2\pi$$

AND NAUD HAS RECENTLY SHOWN THAT THE RANDOM (WEIL-PETERSON USING MIRZAKANI'S WORK)

ACHIEVES THE ABOVE LIMSUP.

HENCE

$$\overline{\lim_{\substack{g(X)\to\infty \\ A(X)=4\pi(g-1)}}} \frac{\log \det^*(X)}{A(X)} = E$$

WITH EQUALITY IF X IS HYPERBOLIC AND RANDOM!

$\boxed{\text{ARCHIMEDIAN McKAY}}$

BACK TO GRAPHS:

HOW ABOUT GAPS IN THE SPECTRUM AS $n \to \infty$?

WE RESTRICT TO $\mathcal{X}_3$ THAT IS CUBIC GRAPHS DENOTED CUBIC.

$$\sigma(X) \subset [-3,3]$$

SUPPORT OF PLANCHEREL IS $[-2\sqrt{2}, 2\sqrt{2}]$

NB: $-3 \in \sigma(X)$ IFF X IS BIPARTITE.

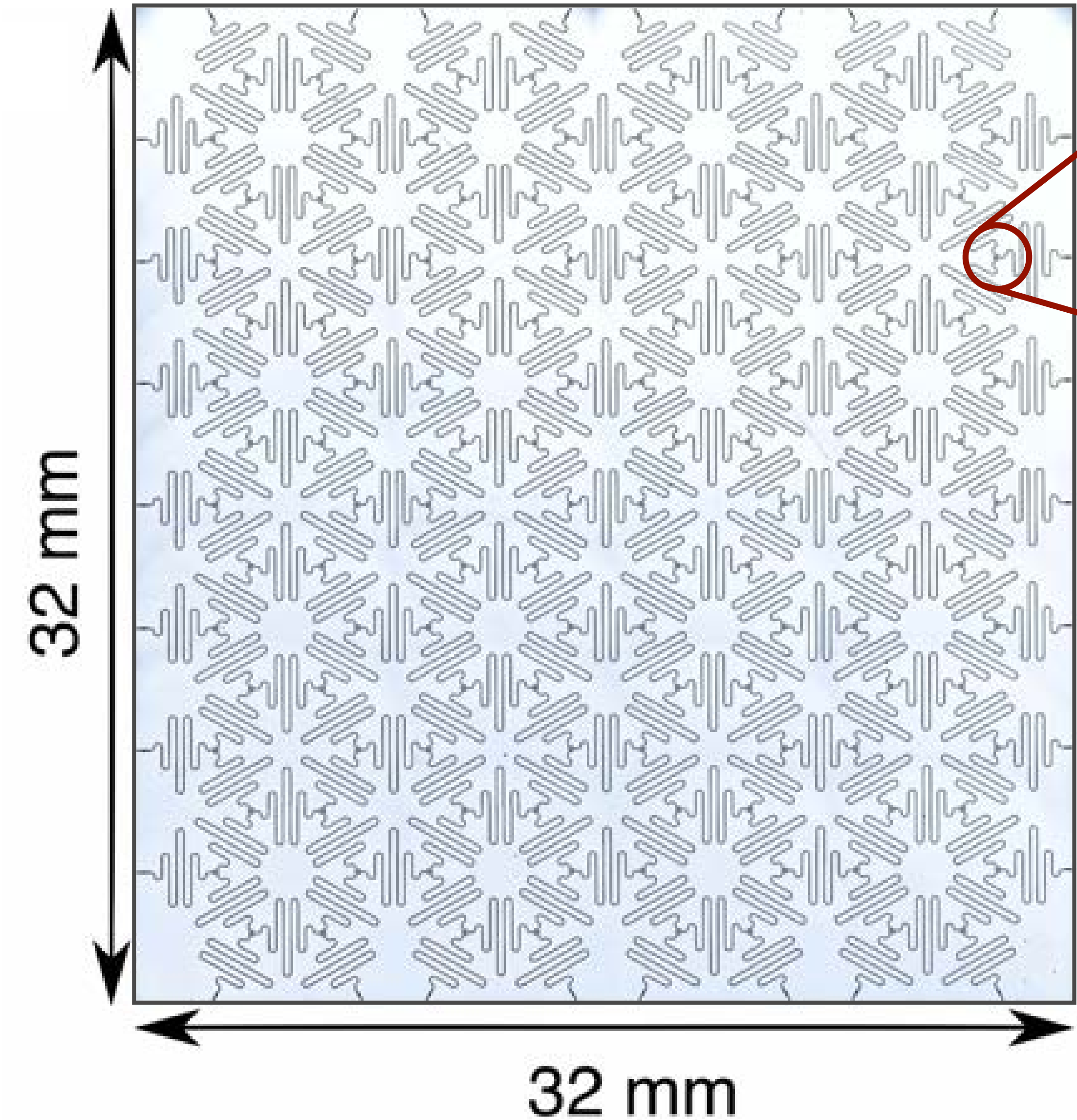
QUESTION: GAPS IN THE SPECTRUM?

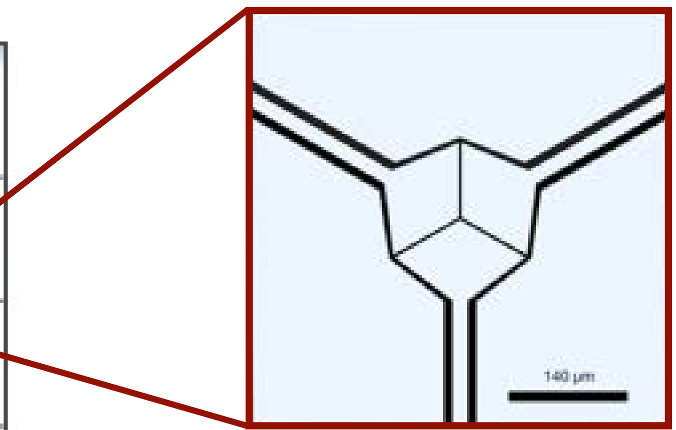
- THE GAP AT THE TOP (IE 3) IS RELATED TO X BEING AN EXPANDER.

- TIGHT BINDING HAMILTONIANS FOR COPLANAR WAVE GUIDE RESONATORS ASK FOR A GAP AT -3.

- IN CHEMISTRY OF LARGE CARBON CLUSTERS (EG FULLERENES) THE GAP IN THE MIDDLE (NEAR 0) IS THE HUCKELL ORBITAL STABILITY HOMO / LUMO.

CPW Lattices





- Capacitive coupling of resonators
- Photonic material
- t < 0, constant function at high energy

$$\mathbf{H_{TB}} = \omega_0 \sum_{\mathbf{i}} \mathbf{a_i^\dagger a_i} - \mathbf{t} \sum_{\mathbf{<i,j>}} (\mathbf{a_i^\dagger a_j} + \mathbf{a_j^\dagger a_i})$$

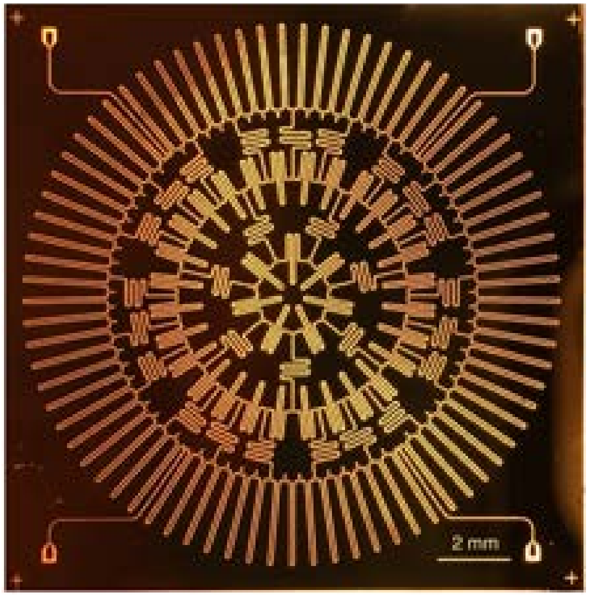
multiple of the identity

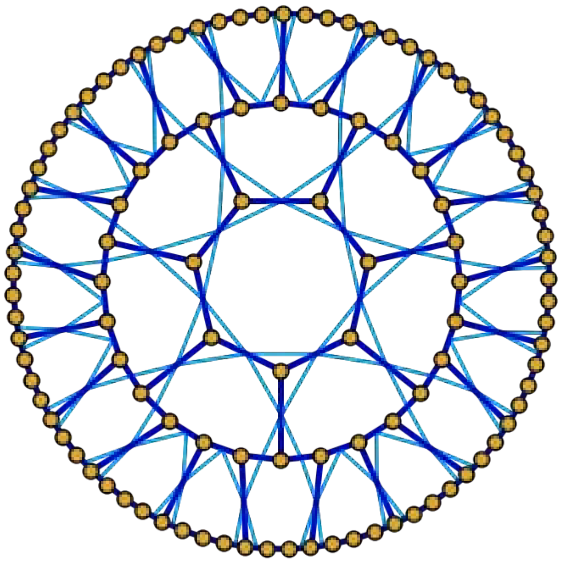
graph adjacency matrix

Houck *et al*. Nat Phys **8**, (2012)

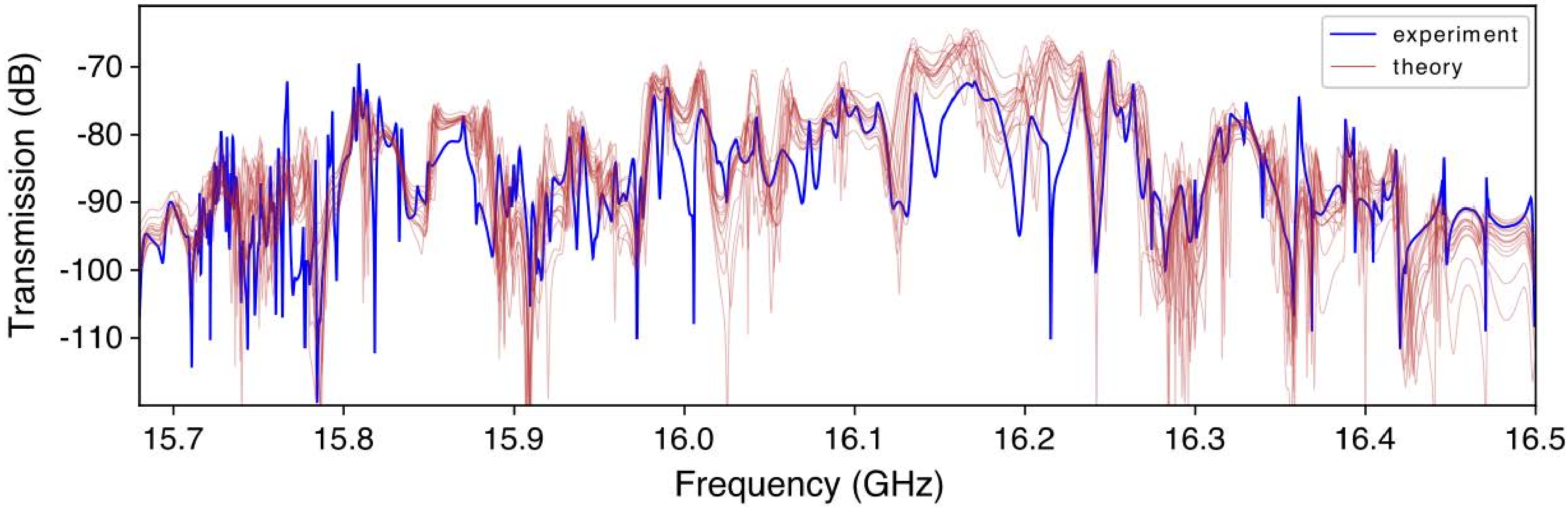
Underwood *et al*. PRA **86**, 023837 (2012)

Heptagon-Kagome Device





- 2 shells
- Operating frequency: 16 GHz
- 4 input-output ports

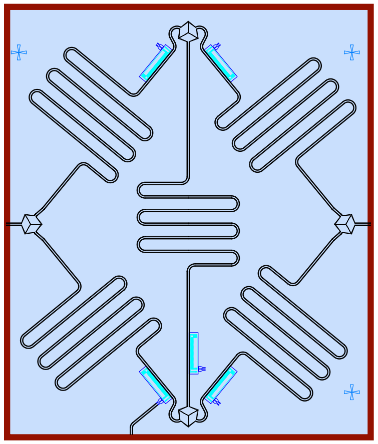


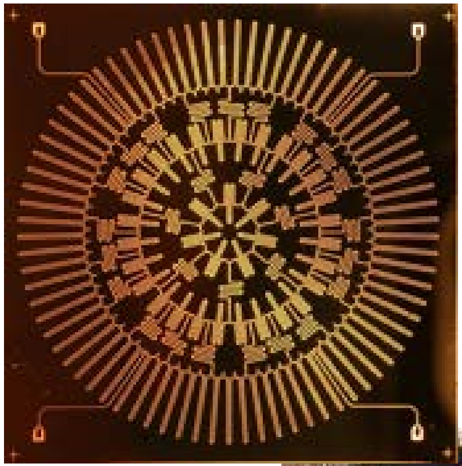
Kollár *et al*. Nature **571** (2019)

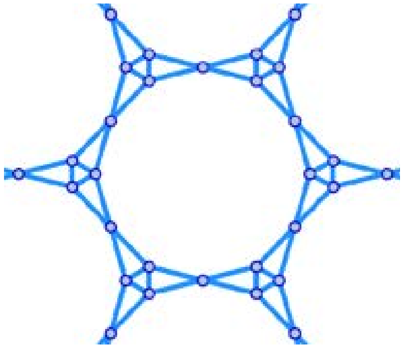
Conclusion and Outlook

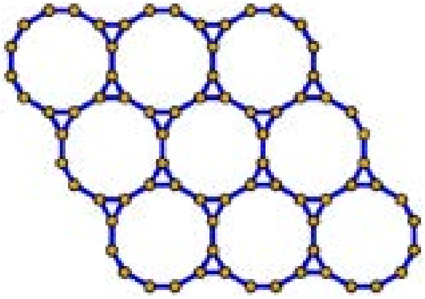
- Circuit QED lattices
  - Artificial photonic materials
  - Interacting photons
- Hyperbolic lattices
  - On-chip fabrication
- Flat-band lattices
  - Optimal gaps
- Mathematical Connections
  - Graph spectra
  - Quantum error correction

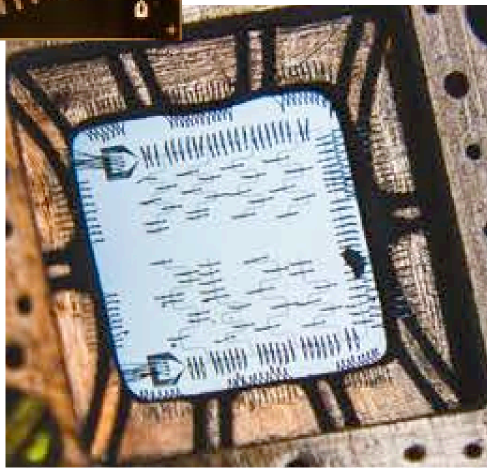
- Outlook
  - Synthetic graph systems
  - Fullerene spectra

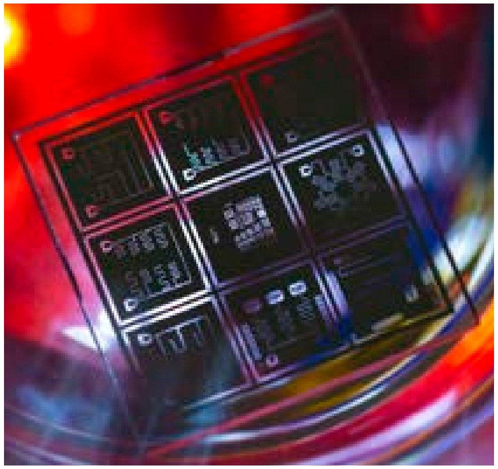












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Boettcher *et al*. arXiv:2105.0187 (2021)
Bienias *et al*. Phys. Rev. Lett. **128**, 013601 (2022)
Chapman, Flammia, AJK, PRX Quantum **3**, 03021 (2022)
Long, AJK *et al*. Phys. Rev. Lett. **128**, 183602 (2022)

GAP AT THE TOP:

THIS HAS BEEN INTENSIVELY STUDIED BECAUSE IT YIELDS OPTIMAL "EXPANDERS".

NO EIGENVALUES IN $(2\sqrt{2}, 3)$
(AND $[-3, -2\sqrt{2})$)

RAMANUJAN GRAPHS.

THESE EXIST:

- FIRST CONSTRUCTED USING NUMBER THEORY AND ARE EXPLICIT (LUBOTZKY-PHILLIPS-S, MARGULIS)! A KEY INPUT IS WEIL'S RIEMANN HYPOTHESIS FOR CURVES OVER FINITE FIELDS.

- MARCUS-SPIELMAN-SRIVASTAVA, GIVE A CONSTRUCTION USING AMONG OTHER THINGS THE LEE-YANG (HELLMAN-LIEB) THEOREM ABOUT ZERO OF MATCHING POLYNOMIALS.

- HUANG-McKENZIE-H.T. YAU RECENTLY PROVED THAT THE RANDOM GRAPH IN $\mathcal{X}_3$ IS RAMANUJAN WITH PROBABILITY 69%!

GAP AT THE BOTTOM -3 ; HOFFMAN SPECTRUM

IF Z IS ANY CONNECTED GRAPH

$L(Z)$ ITS LINE GRAPH:

VERTICES OF $L(Z)$ ARE EDGES OF Z

AND JOIN TWO IF THEY SHARE A VERTEX.

- FACTORIZATION VIA THE INCIDENCE MATRIX $\Rightarrow$

$$\sigma_A(L(Z)) = \{-2\}^{m-n} \cup \sigma(-2I + A_Z + D_Z)$$

D_Z: DIAGONAL WITH VALENCE

$$\subset [-2, \infty)$$

$m = \#$ OF EDGES OF Z

$n = \#$ OF VERTICES

"HOFFMAN GRAPH"

SO $\lambda_{min}(L(Z)) \geq -2$.

FROM $\lambda_{min}(Z) = \min\limits_{v \neq 0} \dfrac{\langle v, A_Z v\rangle}{\langle v, v\rangle}$

IT FOLLOWS THAT FOR ANY INDUCED SUBGRAPH B OF Z

$$\lambda_{min}(Z) \leq \lambda_{min}(B).$$

SO IF Z IS A HOFFMAN GRAPH THEN 5
IT CANNOT CONTAIN A HOST OF SMALL INDUCED MINORS.

$\Longrightarrow$ CLASSIFICATION OF HOFFMAN GRAPHS USING CARTAN MATRICES

CAMERON-GOETHELS-SEIDEL-SHULT (1975)
"LINE GRAPHS, ROOT SYSTEMS AND ELLIPTIC GEOMETRY"

EXCEPT FOR A FINITE LIST OF SPORADIC GRAPHS ALL HOFFMAN GRAPHS ARE GENERALIZED LINE GRAPHS.

- TO CONSTRUCT LINE GRAPHS IN CUBIC DEFINE

$$T : \text{CUBIC} \to \text{CUBIC}$$

FIRST $X \to S(X)$ BY SUBDIVIDING X ADDING VERTICES AT THE MIDPOINTS OF EDGES

THIS GIVES A 2-3 REGULAR GRAPH

LET $T(X) := L(S(X)) \in$ CUBIC.

$$|T(X)| = 3|X|.$$

(EQUIVALENT TO SEWING IN A TRIANGLE AT EACH VERTEX OF X)

FROM THE CLASSIFICATION OF GRAPHS WITH $\lambda_{MIN} \geq -2$ ONE DEDUCES

<u>PROPOSITION</u> (A. KOLLAR, FITZPATRICK, HOUCK, S ..)

IF $Y \in$ CUBIC AND $\lambda_{MIN}(Y) \geq -2$ THEN EITHER $Y = K_4$ (WHEN $\lambda_{MIN}(Y) = -1$) OR $\lambda_{MIN}(Y) = -2$, AND IF Y IS LARGE THEN $Y = T(Z)$ FOR SOME $Z \in$ CUBIC.

DEFINITIONS: $\mathcal{Y}$ A SUBSET OF CUBIC.

- AN OPEN $U \subset [-3,3]$ IS A GAP SET FOR $\mathcal{Y}$ IF THERE ARE INFINITELY MANY $X \in \mathcal{Y}$ WITH
$$\sigma(X) \cap U = \phi .$$

- A CLOSED $K \subset [-3,3]$ IS $\mathcal{Y}$-SPECTRAL IF THERE ARE INFINITELY MANY $X \in \mathcal{Y}$ WITH
$$\sigma(X) \subset K .$$

- $\xi \in [0,3)$ IS $\mathcal{Y}$-GAPPED IF ξ HAS A NBH U WHICH IS AN $\mathcal{Y}$-GAP SET.

THE PREVIOUS PROPOSITION SHOWS THAT $[-3,2)$ IS A MAXIMAL CUBIC GAP ~~SET~~ INTERVAL AND WE SAW THAT $(2\sqrt{2},3)$ IS AS WELL.

WE SEEK MAXIMAL GAP SETS OR MINIMAL SPECTRAL SETS AND THEIR DEPENDENCE ON $\mathcal{Y}$.

- FOR $K \subset \mathbb{C}$ COMPACT; ITS TRANSFINITE DIAMETER OR CAPACITY IS DEFINED BY

$$n \geq 1 \quad ; \quad d_n(K) = \max_{z_1, \ldots, z_n} \Big(\prod_{i<j} |z_i - z_j| \Big)^{2/n(n-1)}$$

GEOMETRIC MEAN

$d_n(K)$ IS DECREASING AND $\mathrm{CAP}(K) = \lim_{n\to\infty} d_n(K)$.

THEOREM (FEKETE 1930)

FOR $K \subset \mathbb{C}$ COMPACT, IF $\mathrm{CAP}(K) < 1$

THEN $\{\alpha : \alpha$ AN ALGEBRAIC INTEGER ALL OF WHOSE CONJUGATES ARE IN $K\}$ IS FINITE!

CONVERSES TO FEKETE!

- RAPHAEL ROBINSON PROVED AN ESSENTIAL CONVERSE FOR SETS $K \subset \mathbb{R}$, THAT IF $\mathrm{CAP}(K) > 1$ THEN K CONTAINS INFINITELY MANY SUCH TOTALLY REAL ALGEBRAIC INTEGERS. (USES CHEBYSHEV POLYNOMIALS)
- FOR SYMMETRIC ABOUT THE REAL AXIS K's FEKETE AND SZEGO PROVE A SIMILAR CONVERSE.

- SERRE REDUCES THE "WEIL NUMBER" OR EIGENVALUES OF FROBENIUS FOR ABELIAN VARIETIES TO ROBINSON'S CONSTRUCTION.

BACK TO SPECTRAL GAPS FOR CUBIC:

<u>THEOREM</u> (A. KOLLAR, S 2021):

(a) ANY CUBIC SPECTRAL SET K HAS CAPACITY AT LEAST 1.

(b) A CUBIC GAP INTERVAL CAN HAVE LENGTH AT MOST 2.

(c) EVERY POINT $\xi \in [-3,3)$ CAN BE GAPPED WITH PLANAR GRAPHS.

(d). THERE ARE PLANAR CUBIC SPECTRAL SETS OF CAPACITY 1.

(e) $(-1,1)$ AND $(-2,0)$ ARE MAXIMAL GAP INTERVALS AND THE FIRST CAN BE GAPPED WITH PLANAR GRAPHS.

COMMENTS ABOUT PROOFS:

(a) THE LOWER BOUND ON THE CAPACITY OF SPECTRAL SETS HAS ITS ROOTS IN FEKETE.

(b) THE UPPER BOUND OF 2 ON THE LENGTH OF A GAP INTERVAL IS PROVED COMBINATORIALLY : ONE SHOWS THAT ONE CAN CONSTRUCT AN APPROXIMATE EIGENFUNCTION WITH EIGENVALUE IN A LARGER INTERVAL BY BUILDING ONE IN THE NBH OF A LONG GEODESIC .

(C) THE PROOF THAT THE GAPPABLE SET OF PLANAR GRAPHS IS ALL OF $[-3,3)$ INVOLVES VARIOUS STEPS:

(i) USING ABELIAN COVERS OVER (IN FACT SPECIAL LARGE CYCLIC COVERS) OF SMALL MEMBERS OF CUBIC, ONE ANALYZES INFINITE SUCH TOWERS USING BLOCH WAVE THEORY (GENERALIZATION OF FLOQUET THEORY) AND CREAT SOME GAPS.

(ii) THESE ROOT EXAMPLES ARE USED TOGETHER WITH THE MAP

$$T : \text{CUBIC} \to \text{CUBIC}$$

TO MOVE THE GAPS AROUND DYNAMICALLY. THE MOST DIFFICULT REGION TO GAP IS NEAR 3 SINCE WE ARE PLANAR GAPPING AND 3 ITSELF CANNOT BE GAPPED.

THE DYNAMICS ARE USED AS FOLLOWS

- A IS A MINIMAL SPECTRAL SET, IT HAS CAPACITY 1 AND $\{X \in \text{CUBIC} : \sigma(X) \subset A\}$ CONSISTS OF FINITELY MANY Γ-ORBITS (AND X's ARE PLANAR!).

- THE MAXIMAL GAP INTERVALS $(-1,1)$ AND $(-2,0)$ WERE FOUND BY ENGINEERING SOME ABELIAN COVERS AND "FLAT BANDS".

- ANOTHER MINIMAL CUBIC SPECTRAL SET IS $[-2\sqrt{2}, 2\sqrt{2}] \cup \{3\}$.

THAT THIS SET IS SPECTRAL FOLLOWS FROM THE EXISTENCE OF RAMANUJAN GRAPHS

THAT IT IS MINIMAL FOLLOWS FROM A THEOREM OF ABERT-GLASNER-VIRAG

ANY SEQUENCE OF RAMANUJAN GRAPHS MUST B-S CONVERGE TO T_3.

$\bar{W}_\alpha$ is contained in $\sigma(\bar{W}_\alpha)$. This follows from G_α being amenable. If Γ_α acts freely on the vertices of $\bar{W}_\alpha$, i.e. any element $\gamma \neq 1$ in Γ_α fixes none of the vertices of $\bar{W}_\alpha$, then the quotient $\bar{W}_\alpha/\Gamma_\alpha$ is a multigraph whose spectrum is contained in $\sigma(\bar{W}_\alpha)$. If Γ_α acts without fixing any edges, then the quotient is a graph. We examine each case $\alpha = a, b$ in turn.

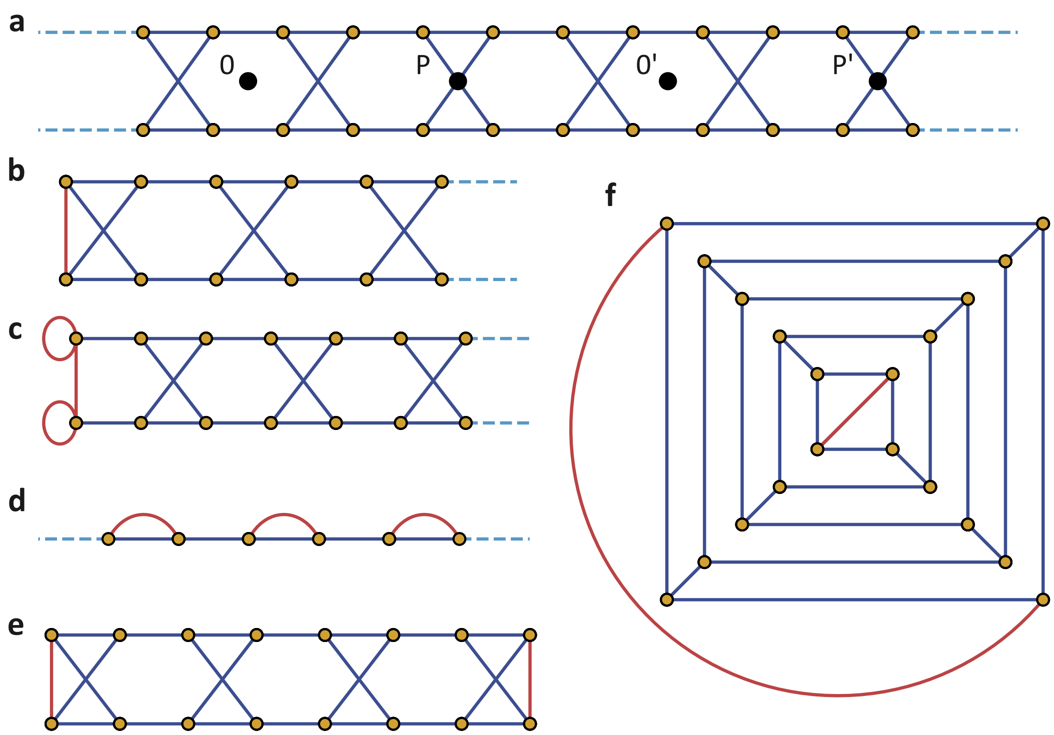


FIGURE 13. **Finite planar quotients of $\bar{W}_b$. a**: The infinite graph $\bar{W}_b$. Four sample involution symmetry points are indicated by black dots. **b**: The quotient obtained with respect to the automorphism σ_0: rotation about O or O' by π. New edges induced by the quotient are indicated in red. In this case, no loops or multiple edges appear. **c**: The quotient with respect to σ_P. In this case, two loops appear. **d**: The quotient with respect to reflection about the central axis. Infinitely many multiple edges appear. **e**, **f**: The quotient with respect to σ_O and $\sigma_{O'}$, when O and O' are four unit cells apart. This quotient is a planar graph which is $(-1, 1)$ gapped.

Consider first $\bar{W}_b$. Its automorphism group is generated by four types of elements.

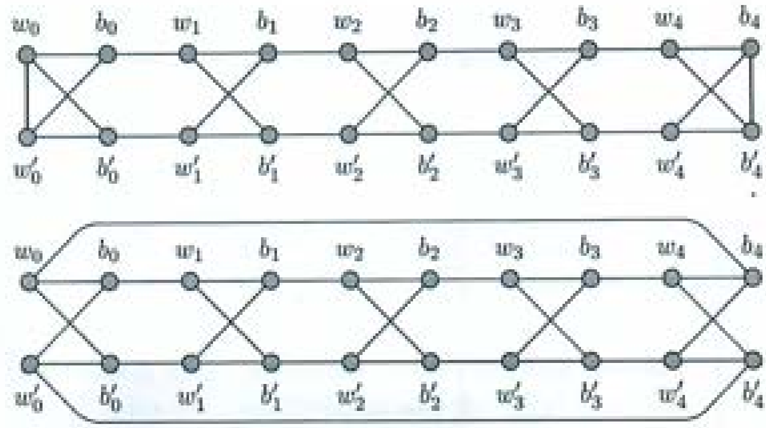
(i) Translations $t(n)$ by n unit cells. The quotients $\bar{W}_b/\langle t(n)\rangle$ for $n \geq 2$ are the hamburger graphs $W_b(n)$ shown in Fig. 14**b**.

(ii) The involution σ_O rotating about a central point O by π. Two example points O and O' are shown in Fig. 13**a**. The quotient $\bar{W}_b/\langle\sigma_O\rangle$ is the graph shown in Fig. 13**b**.

(iii) The involution σ_P rotating about a central point P by π. Two example points P and P' are shown in Fig. 13**a**. The quotient $\bar{W}_b/\langle\sigma_P\rangle$ is a multigraph, shown in Fig. 13**c**.

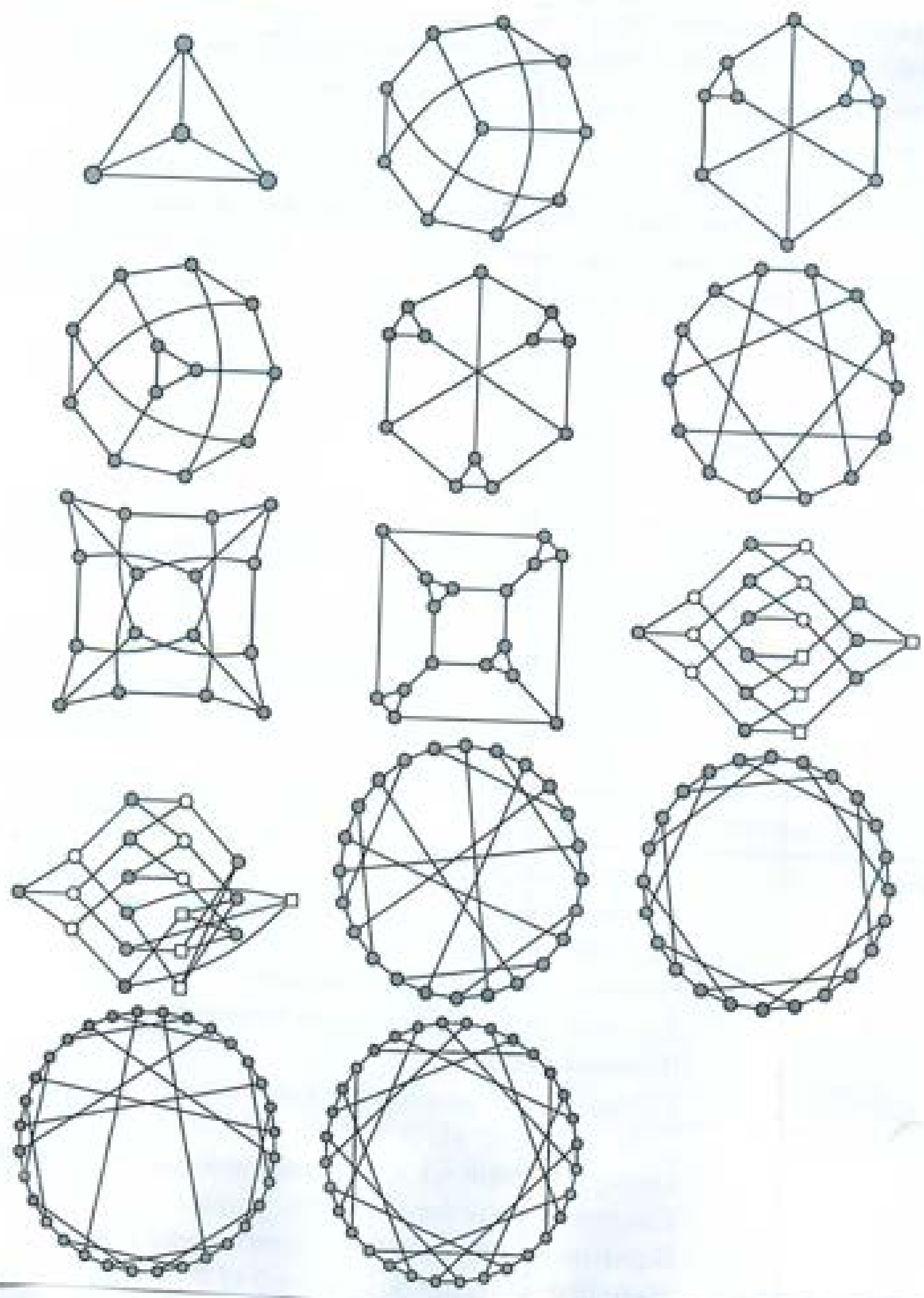
K. GUO AND F. ROYLE (2024)

ALL CUBICS WITH NO EIGENVALUES IN $(-1,1)$



TWO INFINITE FAMILIES

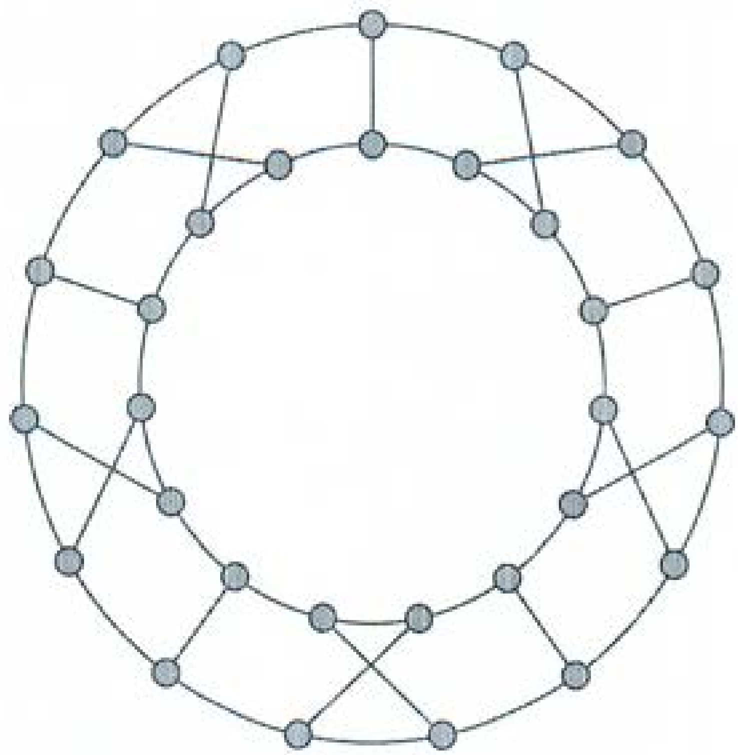
Figure 2: The Kollár-Sarnak graph (top) and Guo-Mohar graph (bottom)



SPORADIC

GRAPHS WITH NO EIGENVALUES IN (−2, 0)
(K. GUO AND G. ROYLE 2025)

ONE INFINITE FAMILY :



FIVE SPORADIC X'S
3-PRISM, K(3,3), PETERSON GRAPH, DODECAHEDRON AND TUTTE'S 8-CAGE (30 VERTICES)

RIGIDITY:

WE RESTRICT TO PLANAR GRAPHS IN CUBIC. FOR k AN INTEGER LET $\mathcal{F}(k)$ DENOTE THE PLANAR SUCH GRAPHS WITH AT MOST k EDGES PER FACE. EQUIVALENTLY THEIR DUALS ARE TRIANGULATIONS OF S^2 FOR WHICH THE VERTICES HAVE DEGREE AT MOST k.

- $F(k)$ IS FINITE FOR $k<6$ (EULER'S FORMULA)
- $F(6)$ IS ALREADY QUITE RICH AND CORRESPOND TO WHAT THURSTON CALLS TRIANGULATIONS OF "NON-NEGATIVE CURVATURE". HE PARAMERIZES THEM IN TERMS OF THE ORBITS OF INTEGER POINTS UNDER THE LINEAR ACTION OF AN ARITHMETIC SUBGROUP OF $SU(9,1)$.
- $F(k)$, $k \geq 7$ ARE ALREADY VERY RICH.

. THE SUBSET OF $\mathcal{F}(6)$ CONSISTING OF PLANAR CUBIC GRAPHS WITH 6 OR 5 FACES (HEXAGONS AND PENTAGONS - THERE BEING EXACTLY 12 PENTAGONS) ARE CALLED <u>FULLERENES</u>.

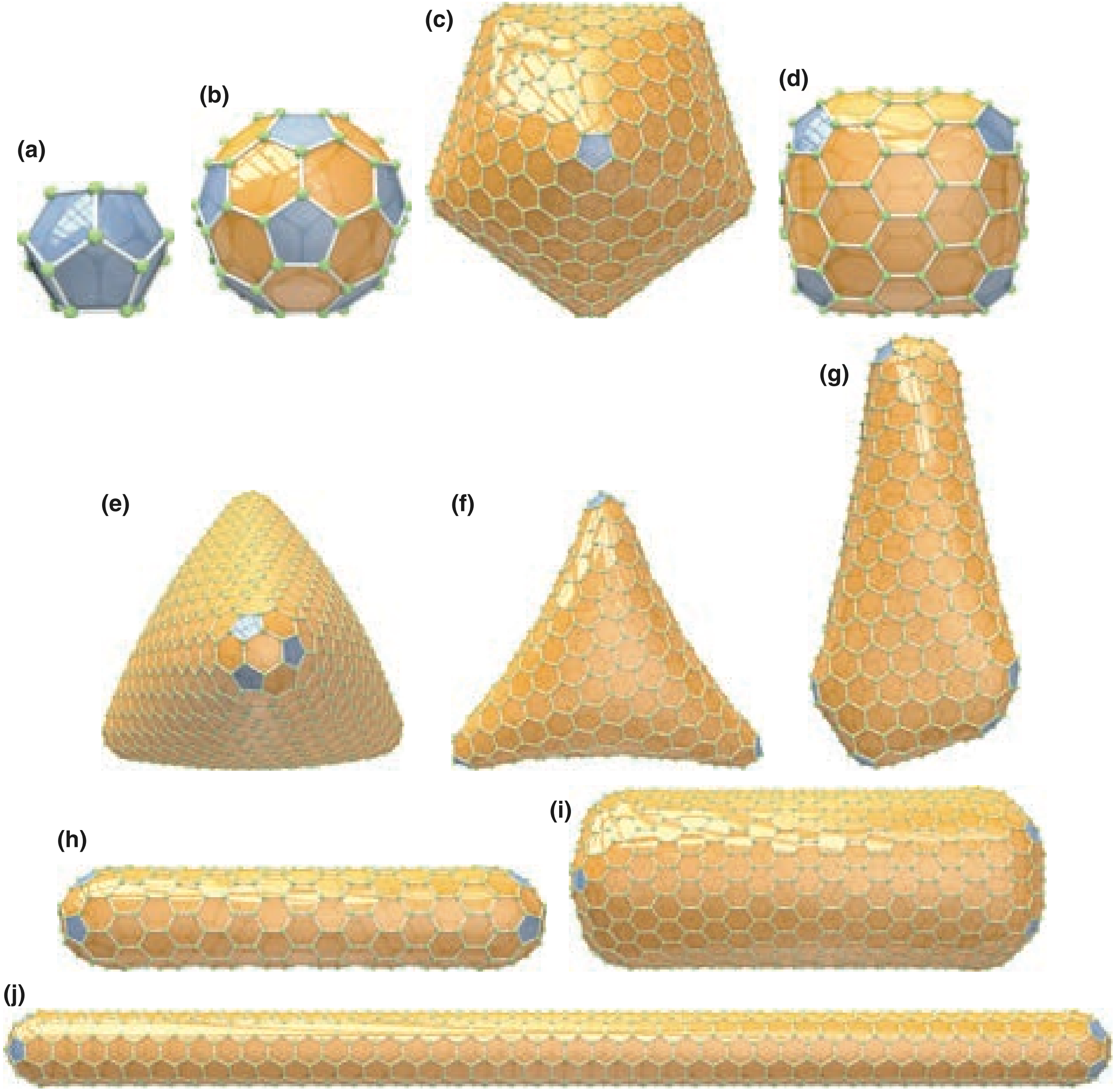


FIGURE 2 | A selection of different 3D shapes for regular fullerenes (distribution of the pentagons D_P are set in parentheses). 'Spherically' shaped (icosahedral), for example, (a) C_{20}-I_h, (b) C_{60}-I_h, and (c) C_{960}-I_h ($D_P = 12 \times 1$); barrel shaped, for example, (d) C_{140}-D_{3h} ($D_P = 6 \times 2$); trigonal pyramidally shaped (tetrahedral structures), for example, (e) C_{1140}-T_d ($D_P = 4 \times 3$); (f) trihedrally shaped C_{440}-D_3 ($D_P = 3 \times 4$); (g) nano-cone or menhir C_{524}-C_1 ($D_P = 5 + 7 \times 1$); cylindrically shaped (nanotubes), for example, (h) C_{360}-D_{5h}, (i) C_{1152}-D_{6d}, (j) C_{840}-D_{5d} ($D_P = 2 \times 6$). The fullerenes shown in this figure and throughout the paper have been generated automatically using the *Fullerene* program.[35]

properties, not least of which is their deep connections to algebraic geometry.[19]

Fullerenes have the neat property that the graphs formed by their bond structure are both cubic, planar, and three-connected, for which all faces are either pentagons or hexagons. Because of this, the mathematics describing them is in many cases both rich, simple, and elegant. We are able to derive many properties about their topologies, spatial shapes, surface, as well as indicators of their chemical behaviors, directly from their graphs.

Planar connected graphs fulfil *Euler's polyhedron formula*,

$$N - E + F = 2 \tag{1}$$

with $N = |\mathcal{V}|$ being the number of vertices (called the *order* of the graph), $E = |\mathcal{E}|$ the number of edges, and $F = |\mathcal{F}|$ the number of faces (for fullerenes these are

THURSTON'S PARAMTRIZATION OF MEMBERS OF F(6) IN TERMS OF THE ORBIT ON INTEGRAL POINTS UNDER THE LINEAR ACTION OF ~~AN~~ ARITHMETIC LATTICE IN SU(9,1) ALLOWS ONE TO APPLY THE SIEGEL–WEIL FORMULA FOR THESE HERMITIAN FORMS TO GET EXPLICIT COUNTS.

IN A REMARKABLE PAPER ENGEL AND SMILLIE (WITH AN APPENDIX BY GOEDGEBEUR) GIVE AN EXACT FORMULA FOR THE NUMBER OF FULLERENES WITH $2n$ CARBON ATOMS.

FOR EXAMPLE IF $n \equiv 1(3)$ AND IS NOT DIVISIBLE BY 2 OR 5 THEN THIS NUMBER IS

$$\sum_{d \mid n} \chi_3(d)\, p(\chi_3(d) \cdot d), \text{ WHERE}$$

$$p(d) = \frac{1}{2^{15} 3^{13} 5^{-2}} \big(809 d^9 - 29529 d^8 - 4126380 d^6 + 38500902 d^5 - 421442982 d^4 + 3622325100 d^3 - 1804262382 0 d^2 + 38826517889 d - 2401158589\big)$$

AND

$$\chi_3(m) = \begin{cases} 0 & \text{IF } 3 \mid m \\ 1 & \text{IF } m \equiv 1(3) \\ -1 & \text{IF } m \equiv 2(3) \end{cases}.$$

- THE FORMULA FOR GENERAL n IS SIMILAR BUT A BIT MORE COMPLICATED.

IT IS PERHAPS NOT SURPRISING THAT NO CHEMIST GUESSED OR ANY MACHINE PREDICTED THIS LONG SOUGHT FORMULA!

THEOREM (ALICIA KOLLAR/FAN WEI/S 2022):

(a) FOR $k \geq 64$ EVERY $\xi \in [-3,3)$ CAN BE $\mathcal{Y}(k)$ GAPPED. WE CONJECTURE THAT THIS CONTINUES TO HOLD FOR $k \geq 7$.

(b) RIGIDITY: THE ONLY POINTS THAT CAN BE $\mathcal{Y}(6)$ GAPPED ARE IN $(-1,1)$ AND THIS INTERVAL IS THE UNIQUE MAXIMAL $\mathcal{Y}(6)$ GAP SET.

(c) THE ONLY POINTS THAT CAN BE FULLERENE GAPPED ARE IN

$$J = (-a, b) \cup (b, a)$$

WHERE $a = 0.382\cdots$, $b = 0.288\ldots$

(a AND b ARE EXPLICIT ALGEBRAIC INTEGERS).

MOREOVER J IS ESSENTIALLY THE UNIQUE MAXIMAL FULLERENE GAP SET.

COMMENTS ON PROOFS

• $k \geq 64$. IN ORDER TO LIMIT THE NUMBER OF FACES IN AN ITERATIVE PROCESS OF CONSTRUCTING X's IN $\mathcal{Y}(k)$ WITH GAPS (ESPECIALLY NEAR 3) WE SEW IN SOME CAREFULLY CRAFTED SEED GRAPHS IN THE EDGES OF AN INITIAL GRAPH. THE FORMULAE FOR THE NEW SPECTRA OF THE SEWEN IN GRAPHS INVOLVE RATIONAL FUNCTIONS OF λ AND THEIR INTERATED DYNAMICS ARE STUDIED THROUGH CONTINUED FRACTIONS.

• FOR THE $\mathcal{Y}(6)$ RIGIDITY, WE NEED A DETAILED STUDY OF THE B-S LIMITS OF $\mathcal{Y}(6)$'s. THESE CORRESPOND TO INFINITE QUOTIENTS OF THE HEXAGONAL LATTICE, KNOWN AS NANO-TUBES + AN EXPLICIT DETERMINATION OF THEIR SPECTRA AND CONVERGENCE OF SPECTRA.

- FOR FULLERENES THERE IS THE ISSUE OF CAPPING NANO-TUBES WITH PENTAGONS (AND HEXAGONS). THIS LEADS TO THE STUDY OF THE SPECTRA OF INFINITE ONE SIDED NANO-TUBES AND IN PARTICULAR THEIR BOUND STATES.

- THE SPECTRALLY EXTREMAL NANO-TUBE THAT CAN BE FULLERENE CAPPED HAS A UNIQUE ONE SIDED SUCH CAPPING AND THE SINGULAR POINT b IN J THAT CANNOT BE FULLERENE CAPPED CORRESPONDS TO A BOUND STATE.

<u>OPEN QUESTION:</u> WHILE THE THEOREM GIVES A COMPLETE DESCRIPTION OF GAP SETS FOR FULLERENES IT DOES NOT ANSWER THE QUESTION OF WHETHER THE GAP BETWEEN THE TWO MIDDLE EIGENVALUES OF A FULLERENE X ; THE <u>HOMO-LUMO GAP</u> IN HUCKEL THEORY, MUST CLOSE AS $|X| \to \infty$? (CARBON CLUSTER STABILITY)