# LECTURE 2

## PRESCRIBING THE SPECTRA OF CUBIC GRAPHS

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- **CUBIC**: CONNECTED FINITE 3-REGULAR GRAPHS.

INSTEAD OF $\Delta$ WE USE THE ADJACENCY MATRIX $A$ AND ITS SPECTRUM, FOR $X \in$ CUBIC

$$Af(x) = \sum_{y \sim x} f(y) \quad ; \quad f : V(X) \to \mathbb{C}$$

$\sigma(X)$ IS THE SPECTRUM OF $A$ CONTAINED IN $[-3, 3]$

3 IS A SIMPLE EIGENVALUE

$-3$ IS AN EIGENVALUE IFF $X$ IS BIPARTITE.

- $\Delta = 3I - A$

QUESTION: WHAT GAPS CAN BE CREATED IN $\sigma(X)$ FOR LARGE $X$.

- THE GAP AT THE TOP (IE 3) IS OUR BASE NOTE SPECTRUM AND IS THE NOTION OF "EXPANDER".
- TIGHT BINDING HAMILTONIANS IN PHYSICS AS FOR A GAP AT $-3$
- IN THE CHEMISTRY OF LARGE CARBON CLUSTERS (EG FULLERENES) THE GAP NEAR 0 IS DECISIVE (HUCKELL ORBITAL STABILITY).

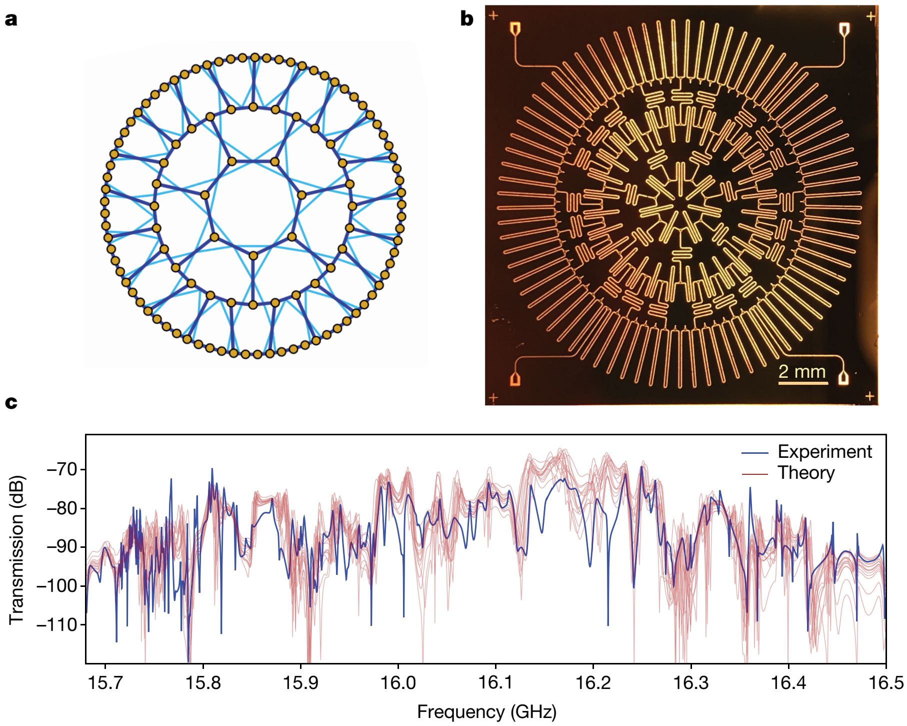



**Fig. 6 | The heptagon-kagome device. a**, Resonator layout (dark blue) and effective lattice (light blue) for a circuit that realizes two shells of the heptagon-kagome lattice. Orange circles indicate three-way capacitive couplers. **b**, Photograph of a physical device that realizes the layout and effective graphs in **a**. The device consists of 140 CPW resonators with fundamental resonance frequencies of 8 GHz, second harmonic frequencies of 16 GHz and a hopping rate of −136.2 MHz at the second harmonic. Four additional CPW lines at each corner of the device couple microwaves into and out of the device for transmission measurements. Short stubs protruding inward from the outermost three-way couplers are high-frequency $\lambda/4$ resonators, which maintain a consistent loading of the sites in the outer ring, ensuring uniform on-site energies. **c**, Experimental transmission ($S_{21}$) for the device in **b** is shown in dark blue. The red curves show theoretical transmission for an ensemble of theoretical models including small systematic offsets in the on-site energies and realistic disorder levels, demonstrating reasonable agreement between theory and experiment.

## Device measurements

We have constructed a device to realize a finite section of the heptagon-kagome lattice. It consists of one central heptagon and two shells of neighbouring tiles, and is shown schematically in Fig. 6a, where each resonator has been approximated by a single line, and the lengths have not been held fixed. The resonators are 7.5 mm long with a fundamental resonance frequency of 8 GHz and a second harmonic of 16 GHz. The second harmonic of this device realizes the heptagon-kagome lattice with a hopping rate of −136.2 MHz. (The fundamental modes of the device obey a different tight-binding model owing to the asymmetry of the mode function within each resonator[22]. See the Methods for details.)

To minimize parasitic systematic frequency differences between resonator geometries, each resonator type was fabricated individually, and the corresponding resonant frequencies were measured. Commercial microwave simulation packages were unable to achieve the required level of absolute or relative accuracy, so the resonator lengths were then fine-tuned empirically to remove the residual offsets at the level of 30 MHz. For the device shown in Fig. 6b, the average difference between the fundamental frequencies of resonators with different shapes is approximately 0.13% (10 MHz), limited by intrinsic reproducibility within a fabrication run[23] and wire-bonding or parasitic capacitances sensitive to variations between fabrication runs. Each individual shape has a fabrication-induced reproducibility of 0.036% (2.9 MHz), consistent with previous work[23]. In addition to the lattice itself, the circuit contains four measurement ports, visible in each corner, which are used to interrogate the lattice.

Theoretical transmission curves for 15 different disorder realizations are shown in Fig. 6c, along with a plot of the experimental transmitted power near the second harmonic frequency of the device. These theoretical curves reproduce most of the qualitative features of the data, including the onset of peaks, the location and Fano-like lineshapes of the highest-frequency peaks, and the markedly larger linewidth of the modes near 16.2 GHz which have the largest overlap with the coupling ports. This device therefore demonstrates that hyperbolic lattices can be produced on chip by using CPW resonators, and it paves the way to the study of interactions in hyperbolic space and to simulation of new models with non-constant curvature.

Because of the combination of systematic and random disorder, in practice the flat band will no longer be completely degenerate and will hybridize slightly with the rest of the spectrum. For this heptagon-kagome device, the systematic shape-dependent disorder causes the largest effects: about $0.12|t|$ for the worst shapes and about $0.07|t|$ for typical ones. Random disorder contributes at about the $0.04|t|$ level. Using graph-theoretic studies beyond the scope of the discussion here, we have have shown that the bulk gap for the heptagon-kagome lattice is about $0.4|t|$ and that the lower-lying eigenvalues seen in finite-size numerics are whispering-gallery-like edge modes which are very strongly confined to the boundary[46]. Therefore, the gapped flat band of the heptagon-kagome lattice is noticeably broadened, but is able to survive in the experimental realization. These graph-theoretic studies also revealed the existence of closely related and readily realizable lattices with gaps as large as $|t|$ for which the hierarchy of energy scales is favourable.

## Conclusion

We have shown that lattices of CPW resonators can be used to produce artificial photonic materials in an effective curved space, including hyperbolic lattices which are typically prohibited as they cannot be isometrically embedded, even in three dimensions. In particular, we conducted numerical tight-binding simulations of hyperbolic analogs of the kagome lattice and demonstrated that they display a flat band

FOR $X \in$ CUBIC DENOTE ITS ADJACENCY EIGENVALUES

$$3 = \lambda_0(X) > \lambda_1(X) \geq \lambda_2(X) \cdots \geq \lambda_{n-1}(X) = \lambda_{min}(X) \quad \boxed{n = |X|}.$$

<u>NB</u>: THE EIGENVALUES ARE TOTALLY REAL ALGEBRAIC INTEGERS.

THE A-BASS NOTE IS $\lambda_1(X)$ AND FOR $\mathcal{F} \subset X$

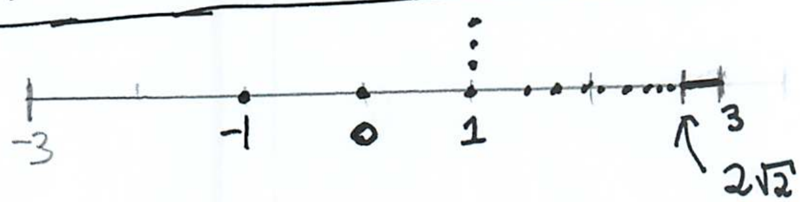
$$BASS_A(\mathcal{F}) = \overline{\{\lambda_1(X) : X \in \mathcal{F}\}}.$$

<u>RECALL</u>: THE $L^2$ SPECTRUM OF $A$ ON $T_3$ 3-REGULAR TREE IS

$$\sigma_A(T_3) = [-2\sqrt{2}, 2\sqrt{2}]. \quad 2\sqrt{2} = 2.8284\ldots$$

<u>THEOREM (....) BASS NOTE SPECTRUM FOR CUBIC</u>

$BASS_A(\text{CUBIC}) =$




$BASS_A^D(\text{CUBIC}) = \{-1, 0, 1, 1, 1, 1, 1.56, \cdots\}$ DISCRETE AND INFINITE IN $[-1, 2\sqrt{2})$

$BASS_A^L(\text{CUBIC}) = [2\sqrt{2}, 3]$

$BASS_A(\text{PLANAR})$ IS RIGID

$BASS_A^D(\text{PLANAR}) = \{-1, 1, 1, \cdots\} \subset [-1, 3)$ DISCRETE

$BASS_A^L(\text{PLANAR}) = \{3\}.$

## COMMENTS

(a) FOR PLANAR ; $\lambda_1(X) \to 3$ AS $|X| \to \infty$

(E.G. LIPTON-TARJAN) "PLANAR GRAPHS CANNOT BE EXPANDERS."

(b) FOR $X \in$ CUBIC J. FRIEDMAN SHOWS THAT

$$\lambda_1(X) \geq 2\sqrt{2} - \frac{100}{(\log X)^2} \Rightarrow$$ $\mathrm{BASS}_A(\text{CUBIC})$ IS DISCRETE IN $[-1, 2\sqrt{2})$.

(c) SPECIAL RAMANUJAN GRAPHS CONSTRUCTED FROM MODULAR FORMS ENSURE THAT

$$|\mathrm{BASS}_A^D(\text{CUBIC})| = \infty.$$

- N. ZUBRILINA ; USING WORK OF COLEMAN AND EDIXHOVEN SHOWS THAT FOR CERTAIN OF THE ABOVE

$$\lambda_1(X) \leq 2\sqrt{2} - (1.3)^{-|X|}$$

- MARCUS-SPIELMAN-SRIVASTAVA'S METHOD FOR CONSTRUCTING RAMANUJAN GRAPHS GIVES X'S WITH

$$\lambda_1(x) \leq 2\sqrt{2} - \frac{100}{|X|}.$$

(d) USING THAT THE RANDOM X IN CUBIC IS ALMOST RAMANUJAN (FRIEDMAN) AND THAT ITS EIGENVALUES ARE DELOCALIZED (H.T. YAU / HUANG / ..).

F. WEI AND N. ALON SHOW THAT EVERY POINT IN $[2\sqrt{2}, 3]$ IS A LIMIT POINT OF $\lambda_1(X)$'S.

# 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 $\Longrightarrow$

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

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 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 $T(X) := L(S(X)) \in \text{CUBIC}.$

$$|\cancel{X}\, T(X)| = 3|X|.$$

(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> (ALICIA 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.

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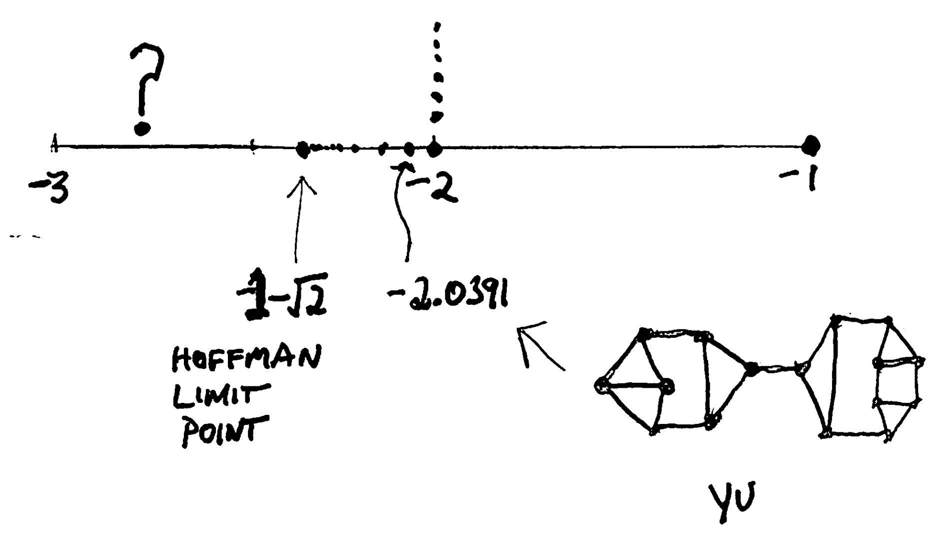
DEFINE THE HOFFMAN SPECTRUM OF CUBIC GRAPHS TO BE THE VALUES OF $\lambda_{min}$:

$$\mathrm{HOFF}_A(\mathrm{CUBIC}) := \overline{\{\lambda_{min}(Y) : Y \in \mathrm{CUBIC}\}}$$

IT IS KNOWN (HOFFMAN, .., YU) THAT

$\mathrm{HOFF}_A(\mathrm{CUBIC}) =$



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 $\xi$ HAS A NBH $U$ WHICH IS AN $\mathcal{Y}$-GAP SET.

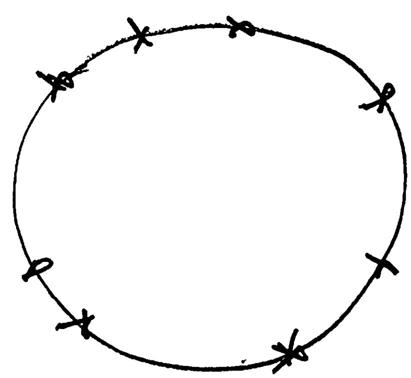
THE PREVIOUS PROPOSITION SHOWS THAT $[-3,2)$ IS A MAXIMAL CUBIC GAP ~~SET~~ INTERVAL AND WE SAW THAT $(2\sqrt{2},3)$ IS AS WELL.

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

SIMILAR QUESTIONS IN ANOTHER SETTING:

- ZEROS OF ZETA FUNCTIONS (OR EIGENVALUES OF FROBENIUS ON COHOMOLOGY) OF CURVES AND ABELIAN VARIETIES $A$ OVER A FIXED FINITE FIELD $\mathbb{F}_q$. (TFASMAN–VLADUT, DRINFELD, SERRE) IN CONNECTION WITH GOPPA CODES.

$C_q =$
$|\lambda| = \sqrt{q}$



$A$ - DIMENSION $g$.
$2g$ EIGENVALUES
SYMMETRIC
(CONJ INVARIANCE)

- WHAT KIND ~~OF GAPS~~ SPECTRAL SETS $K$ CAN BE ACHIEVED AS $g \to \infty$?

- FOR CURVES TFASMAN–VLADUT SHOW THAT NO GAPS CAN BE CREATED — RIGID!

- FOR ABELIAN VARIETIES $A/\mathbb{F}_q$, SERRE 2018 SHOWS USING HONDA TATE THEORY THAT THE ONLY CONSTRAINT ON SYMMETRIC SPECTRAL SETS $K \subset C_q$ IS THAT THEIR TRANFINITE DIAMETER OR CAPACITY BE AT LEAST $q^{1/4}$ $\left( \mathrm{CAP}(C_q) = q^{1/2} \right)$.

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

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

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

<u>THEOREM</u> (FEKETE 1930)
FOR $K \subset \mathbb{C}$ COMPACT; IF $\mathrm{CAP}(K) < 1$ THEN $\left\{ \alpha : \alpha \text{ AN ALGEBRAIC INTEGER ALL OF WHOSE CONJ ARE IN } K \right\}$ IS FINITE!

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- RAPHAEL ROBINSON PROVED AN ESSENTIAL CONVERSE FOR SETS $K \subset \mathbb{R}$, THAT IF $\mathrm{CAP}(K) \geq 1$ THEN $K$ CONTAINS INFINITELY MANY SUCH TOTALLY REAL ALGEBRAIC INTEGERS!

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

- VERY RECENTLY ALEX SMITH RESOLVED A QUANTITATIVE VERSION OF ROBINSON CONCERNING THE POSSIBLE LIMIT MEASURES ASSOCIATED TO THE DISTRIBUTION OF THE GALOIS ORBITS CONDENSING ONTO $K$.

BACK TO SPECTRAL GAPS FOR CUBIC:

THEOREM (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

THE SPECTRUM OF $T(X)$ IS RELATED TO $X$

VIA

$$\sigma(T(X)) = f^{-1}(\sigma(X)) \cup \{0\}^{n/2} \cup \{-2\}^{n/2}$$

WHERE

$$f(x) = x^2 - x - 3$$

SO THE DYNAMICS OF $f$ ON $\mathbb{R}$ AND $[-3,3]$ IS CRITICAL.

$$f^{-1}([-3,3]) = [-2,0] \sqcup [1,3]$$

$$[-3,3] \supset f^{-1}([-3,3]) \supset f^{(-2)}[-3,3] \supset \cdots$$

$$\Lambda = \bigcap_{m=0}^{\infty} f^{-m}([-3,3])$$ IS A CANTOR SET (THE JULIA SET OF $f$)

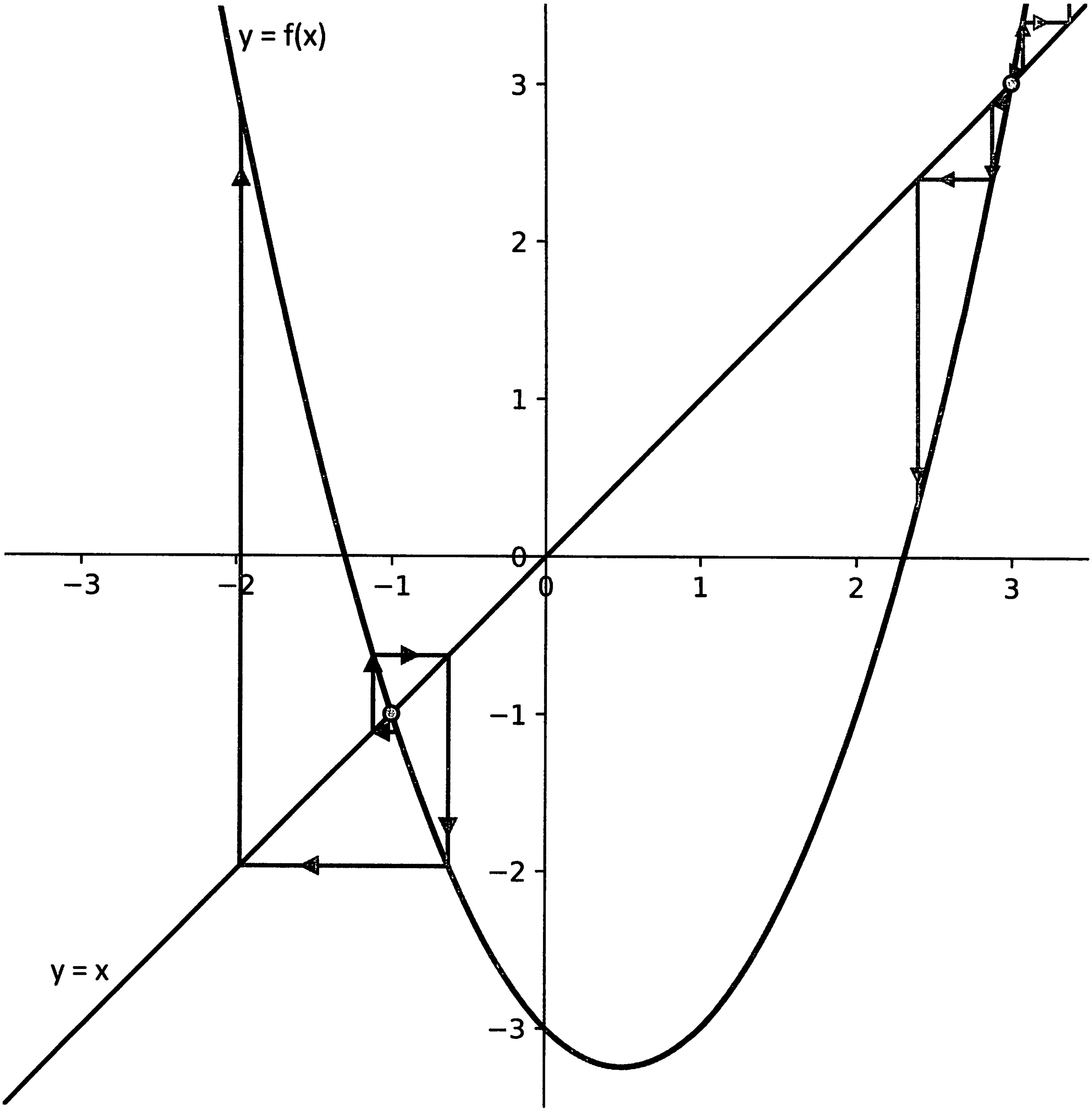
$f^m(x) \to \infty$ AS $m \to \infty$ IF $x \notin \Lambda$.

$f|_\Lambda$ IS TOPOLOGICALLY EQUIVALENT TO THE SHIFT ON $\{0,1\}^{\mathbb{N}}$.

LET $$A = \Lambda \cup \bigcup_{m=0}^{\infty} f^{-m}(\{0\}.)$$

$A$ IS CLOSED AND CONSISTS OF THE CANTOR SET $\Lambda$ TOGETHER WITH ISOLATED POINTS THAT ACCUMULATE ON $\Lambda$.

13



- $A$ IS A MINIMAL SPECTRAL SET, IT HAS CAPACITY 1 AND $\{X \in \text{CUBIC} : \sigma(X) \subset A\}$ CONSISTS OF FINITELY MANY T-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 $G_\alpha$ being amenable. If $\Gamma_\alpha$ acts freely on the vertices of $\bar{W}_\alpha$, i.e. any element $\gamma \neq 1$ in $\Gamma_\alpha$ 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 $\Gamma_\alpha$ acts without fixing any edges, then the quotient is a graph. We examine each case $\alpha = a, b$ in turn.

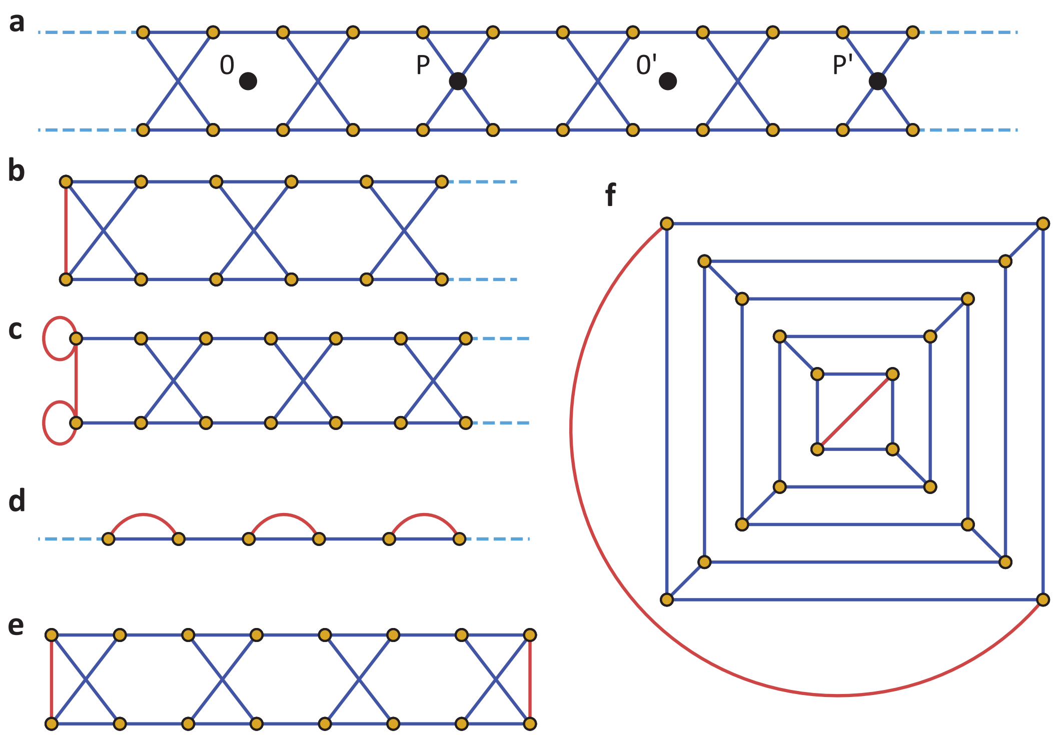



FIGURE 13. **Finite planar quotients of $\bar{W}_b$. a**: The infinite graph $\bar{W}_b$. Four sample involution symmetry points are indicated by black dots. **b**: The quotient obtained with respect to the automorphism $\sigma_0$: rotation about $O$ or $O'$ by $\pi$. New edges induced by the quotient are indicated in red. In this case, no loops or multiple edges appear. **c**: The quotient with respect to $\sigma_P$. 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 $\sigma_O$ 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 $\sigma_O$ rotating about a central point $O$ by $\pi$. 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 $\sigma_P$ rotating about a central point $P$ by $\pi$. 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**.

# 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>.

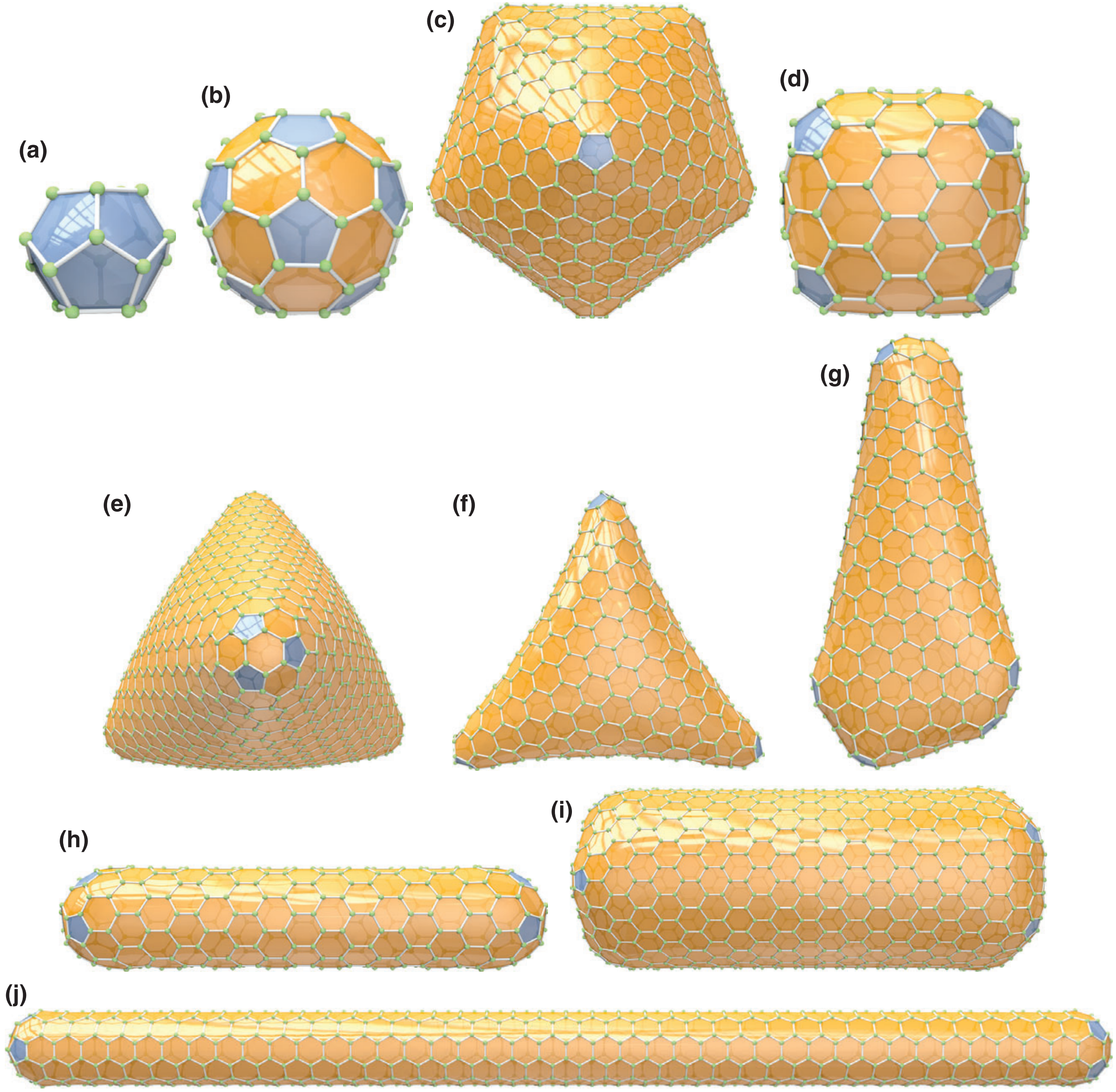



**FIGURE 2 |** A selection of different 3D shapes for regular fullerenes (distribution of the pentagons $D_P$ are set in parentheses). 'Spherically' shaped (icosahedral), for example, (a) $C_{20}$-$I_h$, (b) $C_{60}$-$I_h$, and (c) $C_{960}$-$I_h$ ($D_P = 12 \times 1$); barrel shaped, for example, (d) $C_{140}$-$D_{3h}$ ($D_P = 6 \times 2$); 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 A~~N~~ 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

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

$$p(d) = \frac{1}{2^{15}3^{13}5^{2}}\big(809d^9 - 29529d^8 - 4126380d^6 + 38500902d^5 - 421442982d^4 + 3622325100d^3 - 18042623820d^2 + 3882651789d - 2401958589\big)$$

AND

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

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

(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 $a = 0.382\ldots$, $b = 0.288\ldots$

($a$ 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 $\lambda$ 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 GAPPED 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)