SOME PROPERTIES OF THE ENERGY & SPECTRUM OF PLANAR HONEYCOMB GRAPHS

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ABSTRACT

- The planar honeycomb graphs consist of equal regular

  hexagons. Using the concept of He-matrix corresponding to characteristic/dual graph of honeycomb graph, we present various properties of spectrum which include lower and upper bounds.

- Main focus of the presentation is to highlight the relationship between the eigenvalues and energy of a honeycomb graph and its structure such as the number of triangles, pairs of pendant vertices, concatenation, coalescence, etc.

- Some open problem will also be discussed.

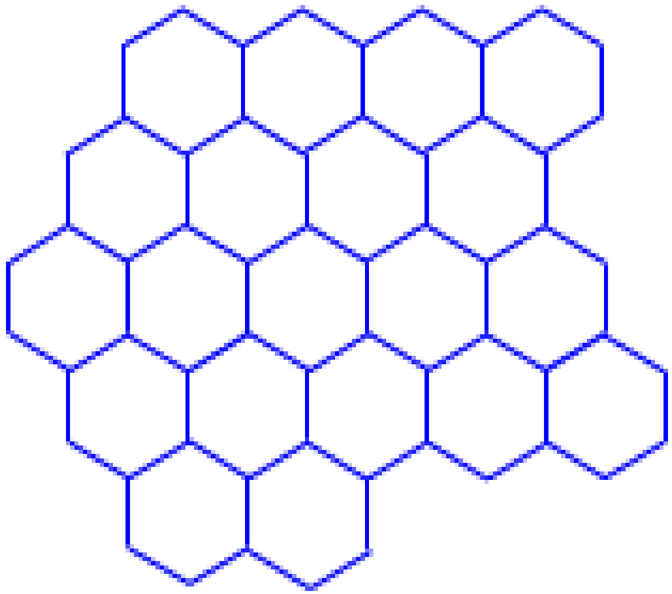
MY Talk

My talk consists of:

- Types of honeycomb graphs
- Inner dualist graph
- Representing graphs using He matrix
- Rotations and Reflections
- Graph eigenvalues
- Isomorphisms
- Relation between eigenvalues and structure
  - Edges, Triangles, Pendant vertices
- Adjacency energy and He energy of graphs
- Energy bounds
- Concatenation and Coalescence

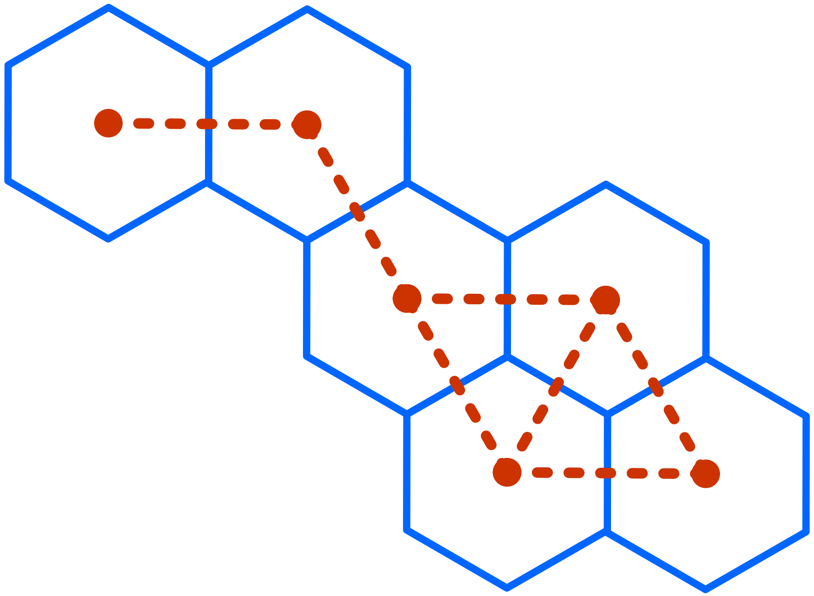
PLANAR HONEYCOMB GRAPH

- **Planar honeycomb graph** is obtained by connecting some equal regular hexagons such that any two adjacent hexagons have one edge in common.



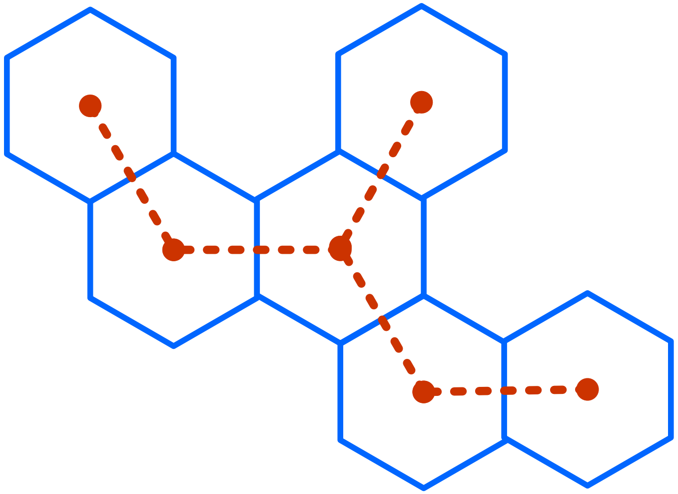
INNER DUALIST GRAPH

- The **inner dualist graph** of a planar honeycomb graph is obtained by placing a vertex in the center of each hexagon and connecting the vertices of adjacent hexagons.



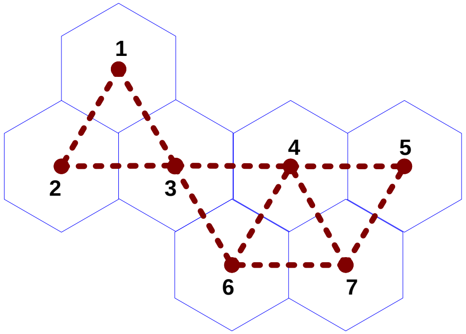
TYPES OF HONEYCOMBGRAPHS

- **Benzoid:** **The planar honeycomb lattice is also called benzoid.**
- **Cata Condensed: Benzoid is called Cata Condensed if the resulting characteristic/dual graph is non cyclic.**

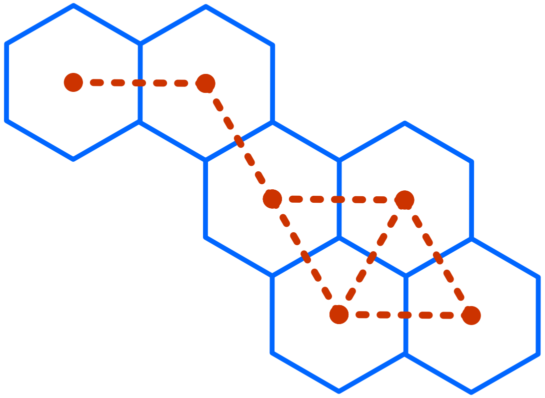


Peri-condensed Benzoid

- **Two Types of Peri-condensed Benzoids**
  - i) **A graph where all edges are part of some cycle. Such a graph is always a triangular lattice.**



ii) A graph in which there is at least one edge that is not the part of any cycle.



ALGEBRAIC REPRESENTATIONS OF GRAPHS

Adjacency Matrix:

$$a_{ij} = \begin{cases} 0 & \text{if } i = j \text{ or } V_i \text{ isn't adjacent to } V_j \\ 1 & \text{if } V_i \text{ is adjacent to } V_j \end{cases}$$

$$\mathbf{a} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

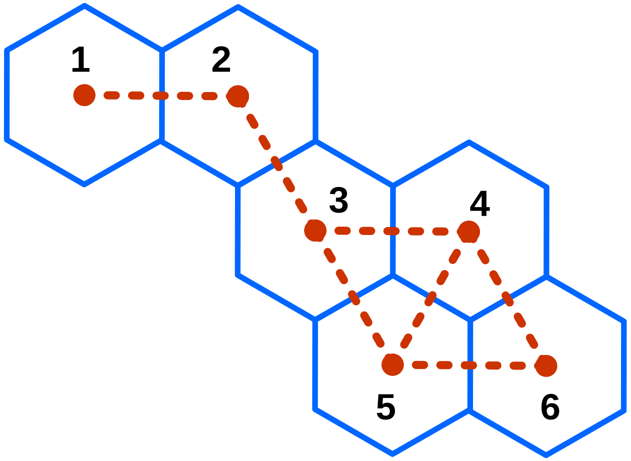


Fig.1

ALGEBRAIC REPRESENTATIONS OF GRAPHS

Laplacian Matrix(Normalized version)

$$L(u,v)=\begin{cases}1 & \text{if } u=v\\ -\dfrac{1}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ are adjacent } (u_u \approx v_v)\\ 0 & \text{otherwise}\end{cases}$$

$$\begin{bmatrix}1 & \frac{-1}{\sqrt{2}} & 0 & 0 & 0 & 0\\ \frac{-1}{\sqrt{2}} & 1 & \frac{-1}{\sqrt{6}} & 0 & 0 & 0\\ 0 & \frac{-1}{\sqrt{6}} & 1 & \frac{-1}{3} & \frac{-1}{3} & 0\\ 0 & 0 & \frac{-1}{3} & 1 & \frac{-1}{3} & \frac{-1}{\sqrt{6}}\\ 0 & 0 & \frac{-1}{3} & \frac{-1}{3} & 1 & \frac{-1}{\sqrt{6}}\\ 0 & 0 & 0 & \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{6}} & 1\end{bmatrix}$$

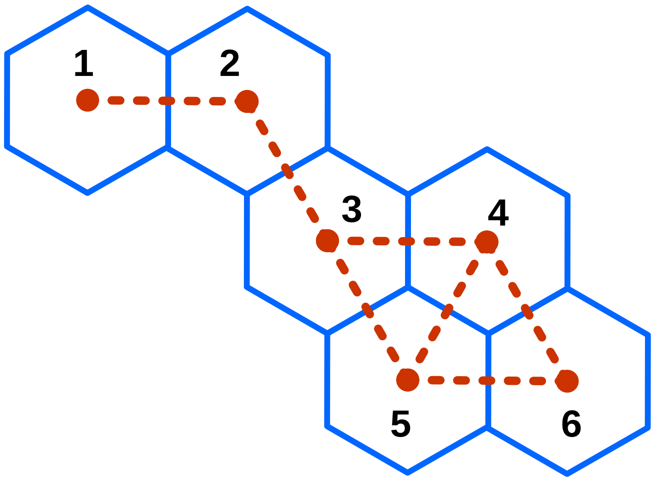


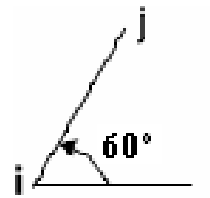
Fig. 2

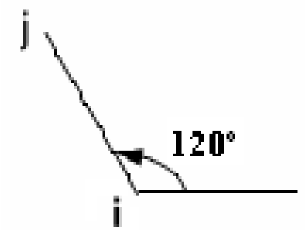
The concept of He - Matrix

Throughout this talk, we will use **He-matrix** representation.

It is given below.

$$h_{ij}\begin{cases} 0, & \text{if } i=j, \text{or } V_i \text{ isn't adjacent to } V_j\text{ ;} \\ 1, & \text{if } V_i \text{ is adjacent to } V_j \text{ and the angle between } \overline{V_iV_j} \text{ and the} \\ & \text{positive horizontal direction is } k\pi; \\ 2, & \text{if } V_i \text{ is adjacent to } V_j \text{ and the angle previously stated is } k\pi+\pi/3; \\ 3, & \text{if } V_i \text{ is adjacent to } V_j \text{ and the angle previously stated is } k\pi+2\pi/3. \end{cases}$$





HE-MATRIX REPRESENTATION

$$H = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 1 & 3 & 0 \\ 0 & 0 & 1 & 0 & 2 & 3 \\ 0 & 0 & 3 & 2 & 0 & 1 \\ 0 & 0 & 0 & 3 & 1 & 0 \end{bmatrix}$$

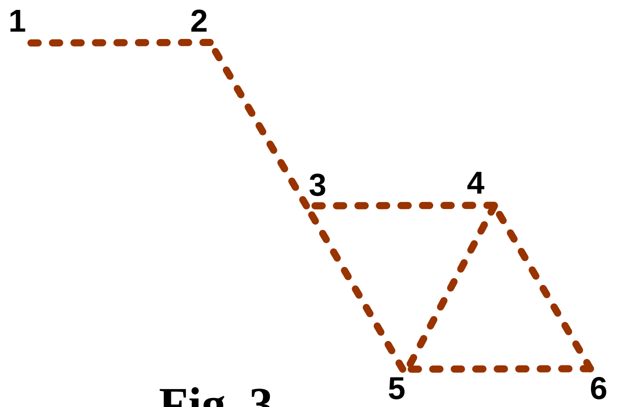


Fig. 3

Characteristic polynomial:

$\mathrm{Det}(H - \lambda I)$

$= \lambda^6 - 34\lambda^4 - 24\lambda^3 + 214\lambda^2 + 132\lambda - 64$

Eigenvalues are the roots of Characteristic Polynomial

ALGEBRAIC REPRESENTATIONS OF GRAPHS

$$H = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 1 & 3 & 0 \\ 0 & 0 & 1 & 0 & 2 & 3 \\ 0 & 0 & 3 & 2 & 0 & 1 \\ 0 & 0 & 0 & 3 & 1 & 0 \end{bmatrix}$$

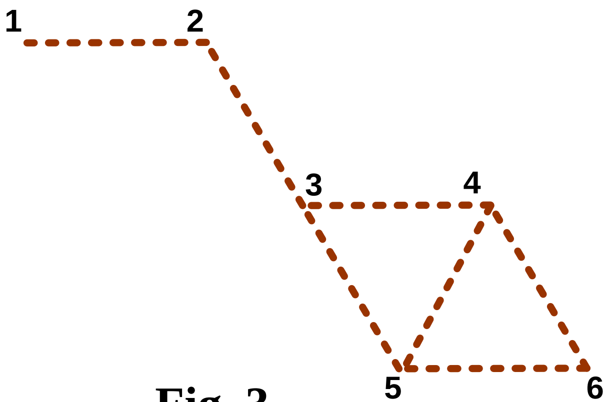


Fig. 3

Since H is real and symmetric, the eigenvalues of H will be real.

Eigenvalues

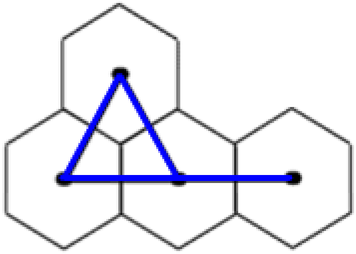
$$\begin{bmatrix} 5.53549 \\ -4.35946 \\ -3.19995 \\ 2.66164 \\ -0.961561 \\ 0.323833 \end{bmatrix}$$

Eigenvectors

$$\begin{bmatrix} 0.152384 & 0.843522 & 1.50564 & 1.35032 & 1.48452 & 1 \\ 0.915239 & -3.98995 & 5.49292 & -0.137756 & -3.94619 & 1 \\ 0.0133383 & -0.042682 & 0.0410806 & -1.19955 & 0.398715 & 1 \\ -0.416813 & -1.10941 & -0.845346 & 0.86334 & 0.0716251 & 1 \\ -1.60148 & 1.53992 & 0.0402508 & 0.221721 & -1.62672 & 1 \\ 2.52008 & 0.816086 & -0.751935 & 0.457908 & -1.04989 & 1 \end{bmatrix}$$

Rotation and Reflection

- Any honeycomb graph can be rotated and reflected in at most 12 positions
- Consider the following graph



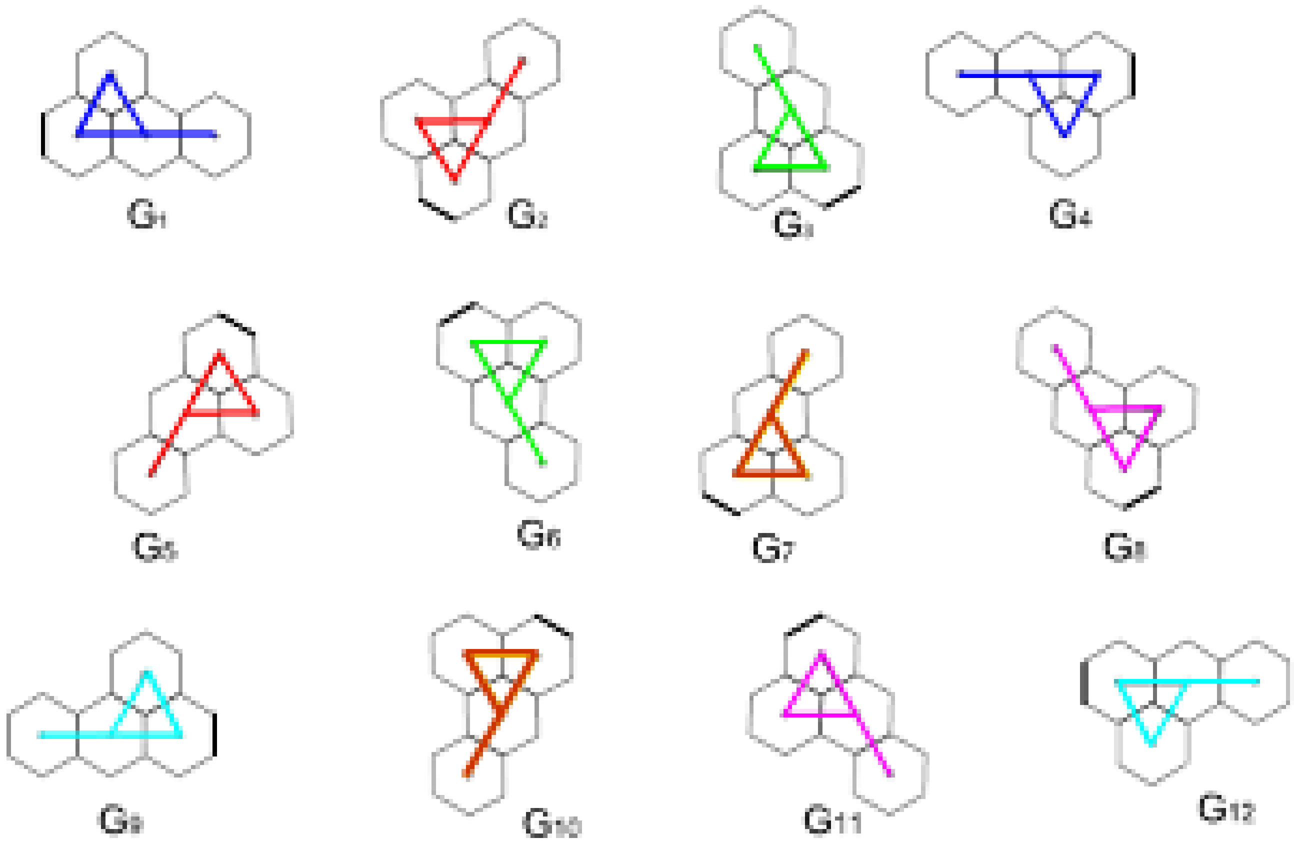
G_1

$$\mathbf{H(G1)} = \begin{bmatrix} 0 & 2 & 3 & 0 \\ 2 & 0 & 1 & 0 \\ 3 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- Eigenvalues = {4.1999, 0.2534, -1.1323, -3.3201}

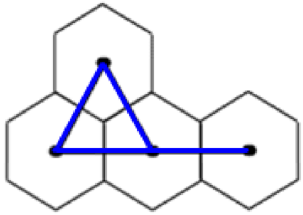
ROTATION AND REFLECTION

- Its 12 transformations result are as



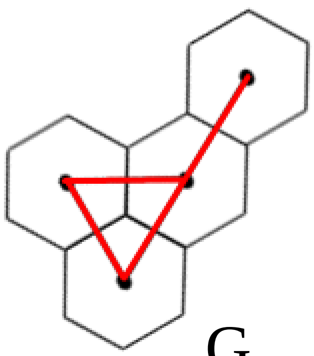
ROTATION AND REFLECTION

ROTATION BY 60^O



G_1

$$H(G2) = \begin{bmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 3 \\ 2 & 1 & 0 & 2 \\ 0 & 3 & 2 & 0 \end{bmatrix}$$

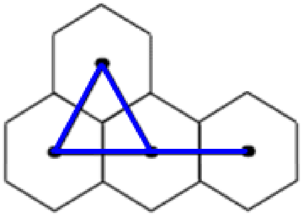


G_2

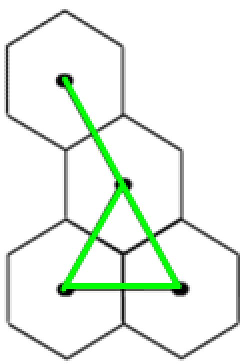
Eigenvalues = {4.3422, 1.1530, -2.1485, -3.3467}

ROTATION AND REFLECTION

ROTATION BY 120^O



G_1



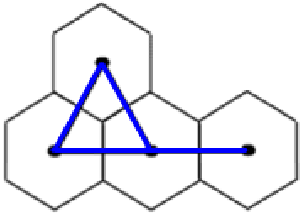
G3

$$H(G3) = \begin{bmatrix} 0 & 3 & 0 & 0 \\ 3 & 0 & 2 & 3 \\ 0 & 2 & 0 & 1 \\ 0 & 3 & 1 & 0 \end{bmatrix}$$

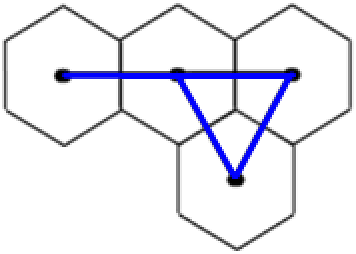
Eigenvalues = {5.0039, 0.4179, -0.9660, -4.4557}

ROTATION AND REFLECTION

ROTATION BY 180^{O}



G_1



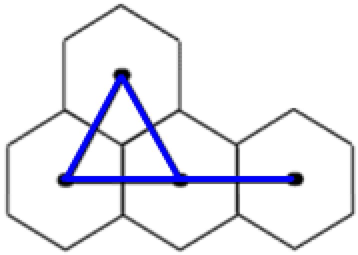
G_4

$$\mathbf{H(G4)} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 3 \\ 0 & 1 & 0 & 2 \\ 0 & 3 & 2 & 0 \end{bmatrix}$$

Eigenvalues = {4.1989, 0.2534, -1.1323, -3.3201}

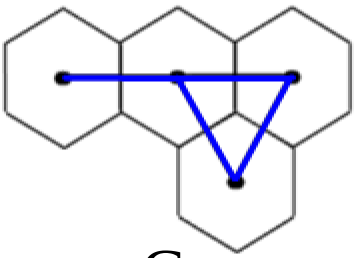
ROTATION AND REFLECTION

ROTATION BY 180^{O}



G_1

- Same eigenvalues as G1
- Matrix has flipped across the antidiagonal



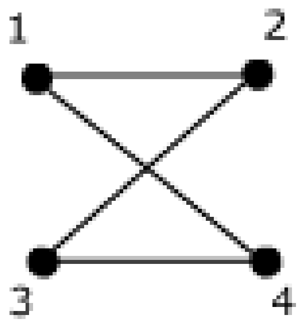
G_4

- $H(G4) = P\ H(G1)\ P^{-1}$

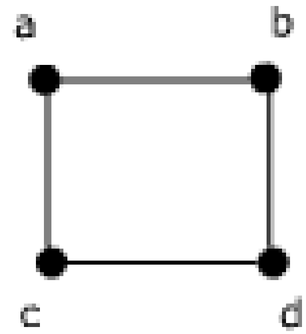
  where $P = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$

ISOMORPHISM

- The following graphs are isomorphic



G1



G2

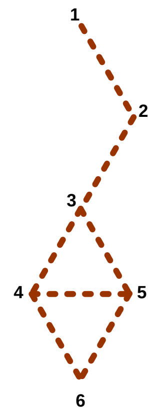
Let f:V(G1) -> V(G2), s.t. uv ϵ E(G1) $\Leftrightarrow$ f(v)f(v) ϵ E(G2)

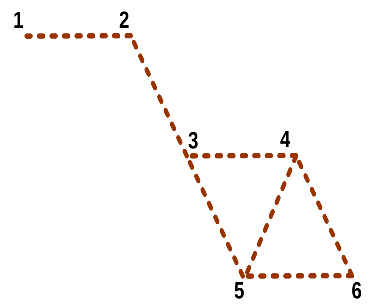
f(1) = a f(2) = b

f(3) = d f(4) = c

ISOMORPHISM

- The following graphs are isomorphic:



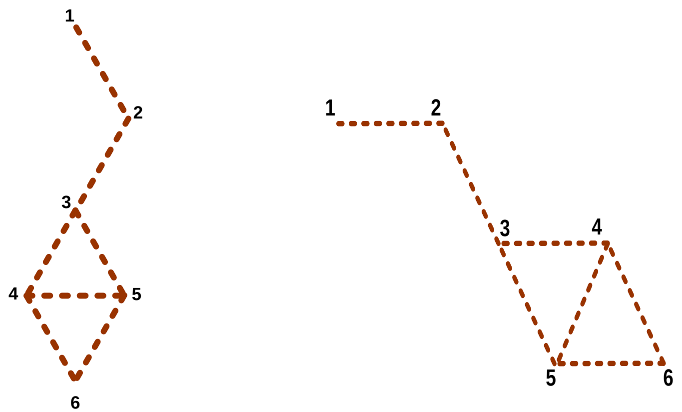


- But these graphs should not be isomorphic when using He matrix
- Reason: Different edge weights, different eigenvalues and different angles.
- Problem with Adjacency matrix representation and loss of orientation!

ORIENTATION-ISOMORPHISM

- Have to add another condition

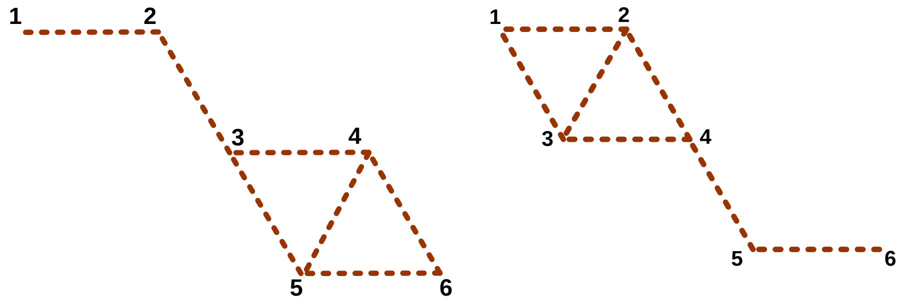
- Let f:V(G1) -> V(G2), s.t.
  1. uv ϵ E(G1) ⇔ f(v)f(v) ϵ E(G2)
  2. w(uv) = w(f(u)f(v)) (where w means weight)



- These 2 graphs are not orientation-isomorphic

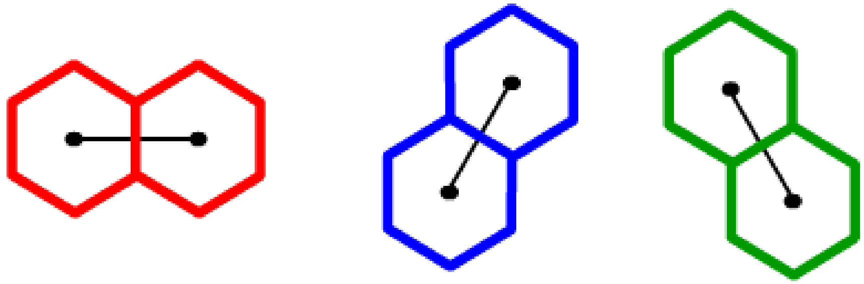
ORIENTATION-ISOMORPHISM

- These graphs are orientation isomorphic



- A rotation of **180^{o}** produces the same edge orientation (and thus same edge weights)
- The 2 graphs behave in the same manner

A VERY SIMPLE GRAPH



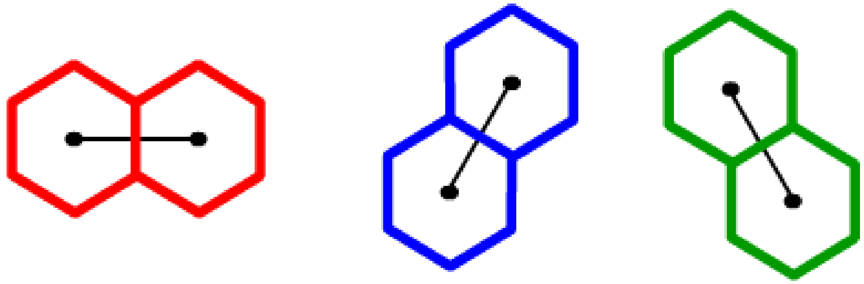
H_{2a} H_{2b} H_{2c}

Eigenvalues of H_{2a} : {-1, 1}

Eigenvalues of H_{2b} : {-2, 2}

Eigenvalues of H_{2c} : {-3, 3}

A VERY SIMPLE GRAPH



H_{2a} H_{2b} H_{2c}

Conjecture:

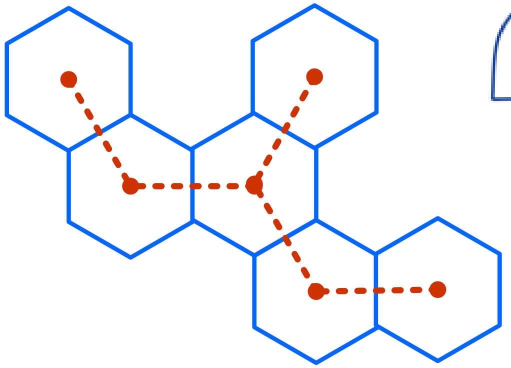
H_{2a}, H_{2b} and H_{2c} are the only honeycomb graphs with integer spectrum with He-matrix.

More Notations and Definitions

- m_1 = number of edges at 0^o
- m_2 = number of edges at 60^o
- m_3 = number of edges at 120^o
- Δ = number of triangles

EIGENVALUE BOUNDS

- $-12 < \lambda_i < 12 \qquad i=1,2,\ldots,n$
- If the honeycomb graph is a catacondensed system, then
  $$-6 < \lambda_i < 6$$
- $\lambda_1 < \max_i \left\{ \frac{1}{d_i} \sum_{j:j\sim i} a_{ij} d_j \right\}$
- $\lambda_1 \geq \frac{2(m_1 + 2m_2 + 3m_3)}{n}$



Catacondensed graph G1

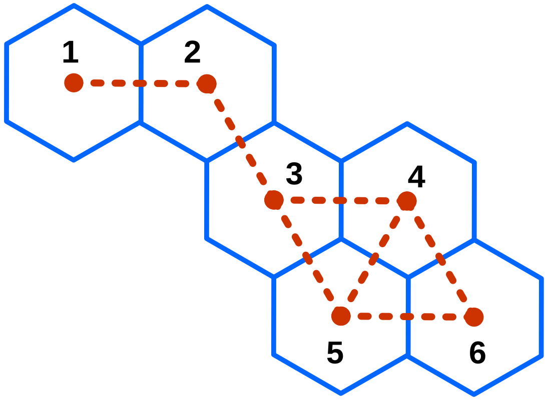
Eigenvalues of G1 =
$$\begin{Bmatrix} 3.9883 \\ 2.7934 \\ 0.53855 \\ -0.53855 \\ -2.7934 \\ -3.9883 \end{Bmatrix}$$

$$\begin{aligned} \lambda_1 &= 3.9883 \\ &\geq 2(2 + 2*1 + 3*2)/6 \\ &= 3.33 \end{aligned}$$

$\Sigma \lambda^2$ AND THE NUMBER OF EDGES

- $$\sum_{i=1}^{n} \lambda_i^2(H) = 2(m_1 + 4m_2 + 9m_3)$$
- We know from Frobenius norm that $\Sigma\lambda^2$ is equal to the sum of the squares of the entries of a matrix
- Since there are only 3 types of edges, we can group them together after squaring

FORMULA FOR THE NUMBER OF TRIANGLES



- $$\sum_{i=1}^{n} \lambda_i^3 = 36 \times \Delta$$
- 6 ways to traverse a triangle abc:
  - abc, acb, bac, bca, cab, cba
- If A is the adjacency matrix, then entries A^3 depict the number of paths of length 3 from vertex i to j
- In H is the He matrix (which is weighted) each entry in H^3 represents the total weight of a path of length 3 from vertex i to j.

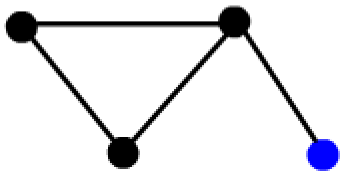
Eigenvalues $\mathbf{5.53549, -4.35946, -3.19995, 2.66164, -0.961561, 0.323833}$

$$\sum_{i=1}^{n} \lambda_i^3 = \mathbf{169.616 - 82.824 - 32.737 + 18.855 - 0.889 + 0.0339}$$

$$\mathbf{= 72 = 36 \text{ x } 2}$$

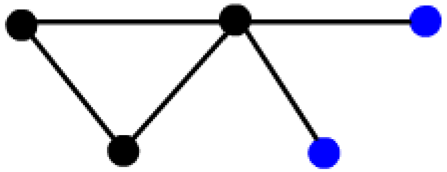
PAIRS OF PENDANT VERTICES

- A Pendant Vertex is one which has only one neighbor. Eg:



- The blue vertex is a pendant vertex

- We call two pendant vertices a *pair* if their single neighbor is common. Eg (pair in blue)

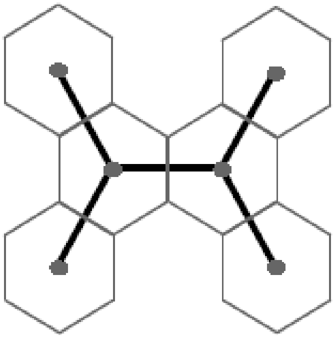


PAIRS OF PENDANT VERTICES

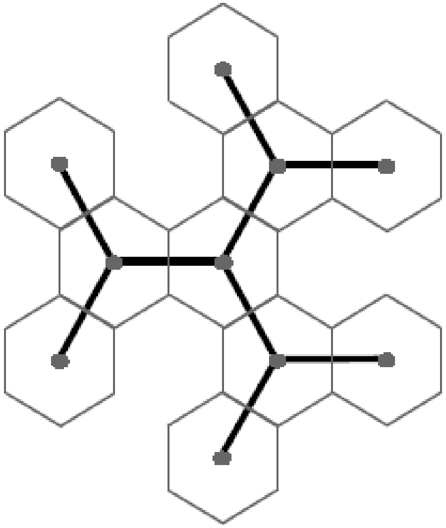
- For each pair of pendant vertices, there is atleast one eigenvalue equal to zero
- Can have more eigenvalues equal to zero

PAIRS OF PENDANT VERTICES

- Example:



(a) Graph G_1



(b) Graph G_2

- Graph G1 has two eigenvalues equal to zero
- Graph G2 has four eigenvalues equal to zero

GRAPH ENERGY

- Graph Energy is defined as the sum of the absolute values of eigenvalues.

$$E(G) = \sum_{i=1}^{n} |\lambda'_i|$$

- Where λ'_i is an eigenvalue of the adjacency matrix of graph G

APPLICATIONS IN CHEMISTRY

- First results obtained as early as 1940
- π-electron energy is the energy of the corresponding molecular graph

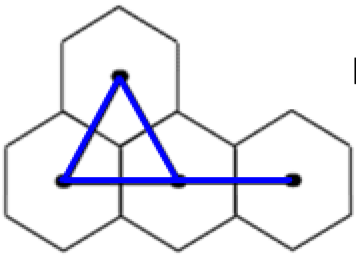
GRAPH HE-ENERGY

- We define He Energy, *HEE(G)*, as the sum of the absolute values of the eigenvalues of the He matrix of a honeycomb graph

$$HEE(G) = \sum_{i=1}^{n} |\lambda_i|$$ Where λ_i is an eigenvalue of G

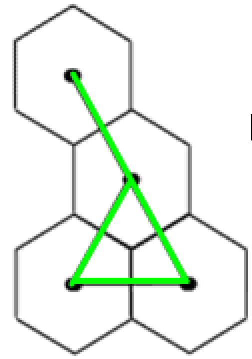
- This has its advantages because different orientations of honeycomb graphs result in different energies (except for 180^o rotations)

G2, G3 and G4 are 60°, 120° and 180° rotations of G1 respectively



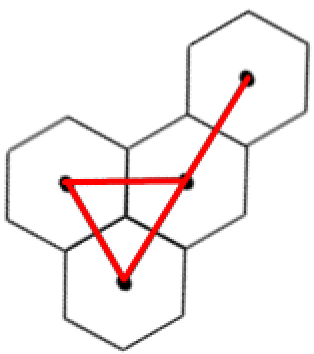
G_1

He-Energy(G1) = 8.90467



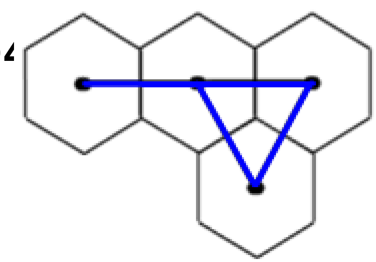
G_3

He-Energy(G3) = 10.8435



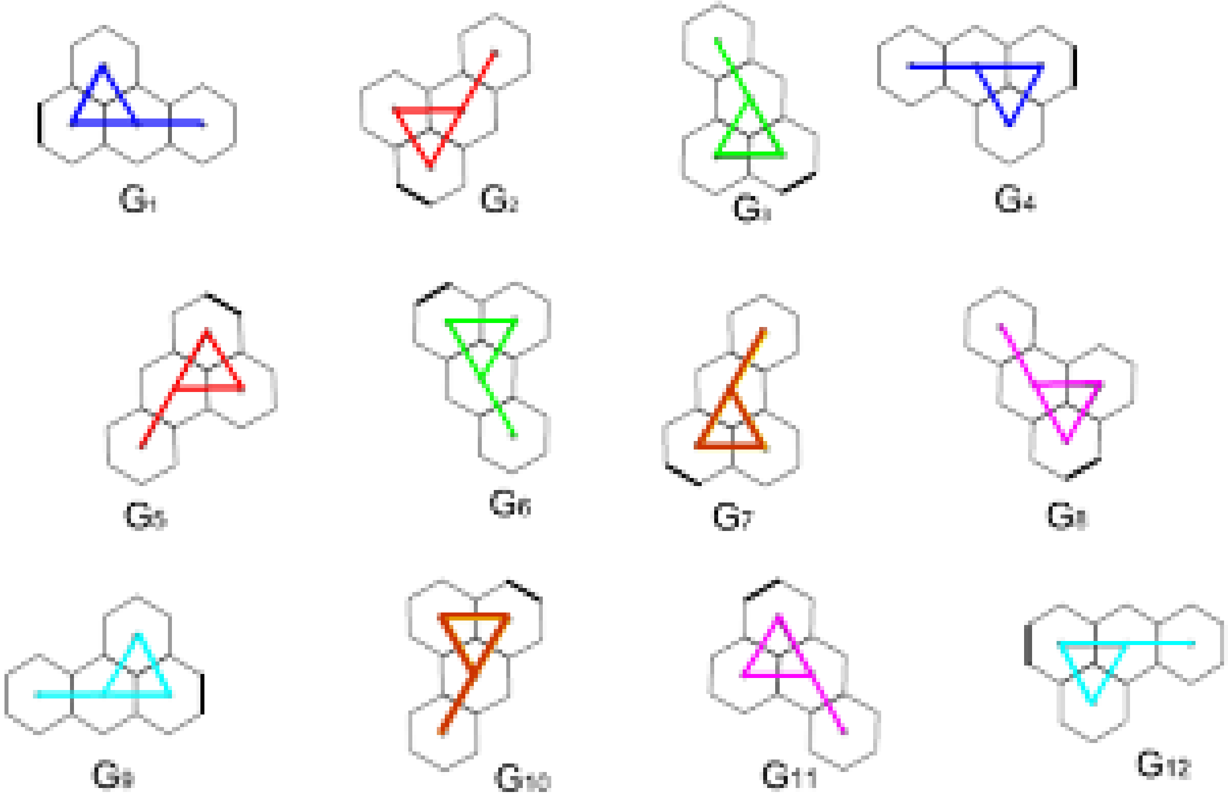
G_2

He-Energy(G2) = 10.990



G_4

He-Energy(G4) = 8.90467



Adjacency Energy:
4.96239

He-Matrix Energy

Graph	Energy	Graph	Energy
G_1	8.90467	G_7	9.53439
G_2	10.9904	G_8	11.8608
G_3	10.8435	G_9	9.28085
G_4	8.90467	G_{10}	9.53439
G_5	10.9904	G_{11}	11.8608
G_6	10.8435	G_{12}	9.28085

ENERGY BOUNDS FOR HE-MATRIX

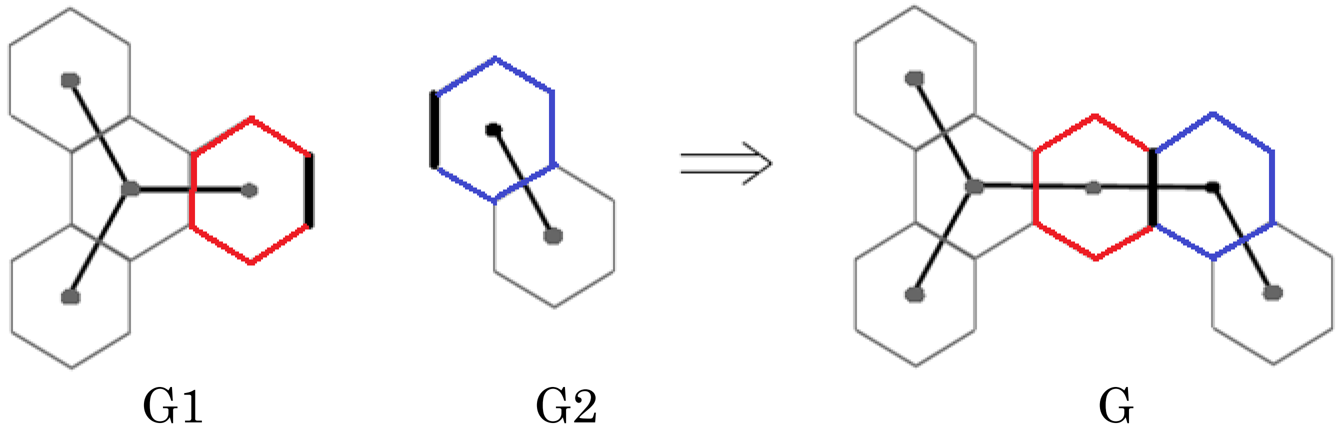
1. $$\frac{4M}{n} \le HEE(G) \le \frac{2M}{n} + \sqrt{(n-1)\left(W - \frac{4M^2}{n^2}\right)}$$

Where $W = 2(m_1 + 4m_2 + 9m_3)$

And $M = 2(m_1 + 2m_2 + 3m_3)$

2. $$HEE(G) \le \sqrt{2n(m_1 + 4m_2 + 9m_3)}$$

CONCATENATION



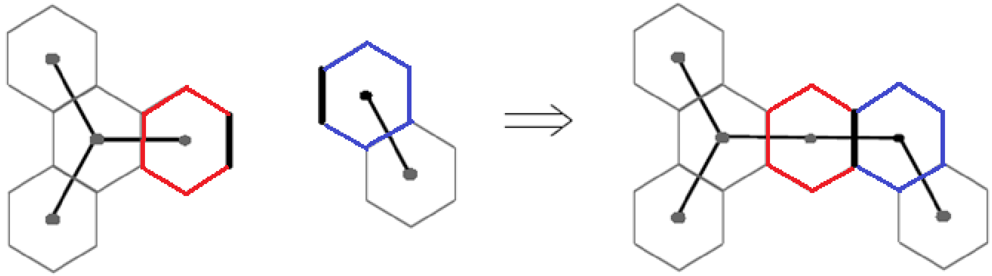
Concatenation: Identify an edge from G1 and an edge from G2, to obtain G

Notice the extra edge in the inner dualist of G

CONCATENATION

If $\lambda_1(G_1)$, $\lambda_1(G_2)$ and λ_1 (G) are the largest eigenvalues of G_1, G_2 and G respectively, then

$$\lambda_1(G) \geq \lambda_1(G_1)$$
$$\lambda_1(G) \geq \lambda_1(G_2)$$

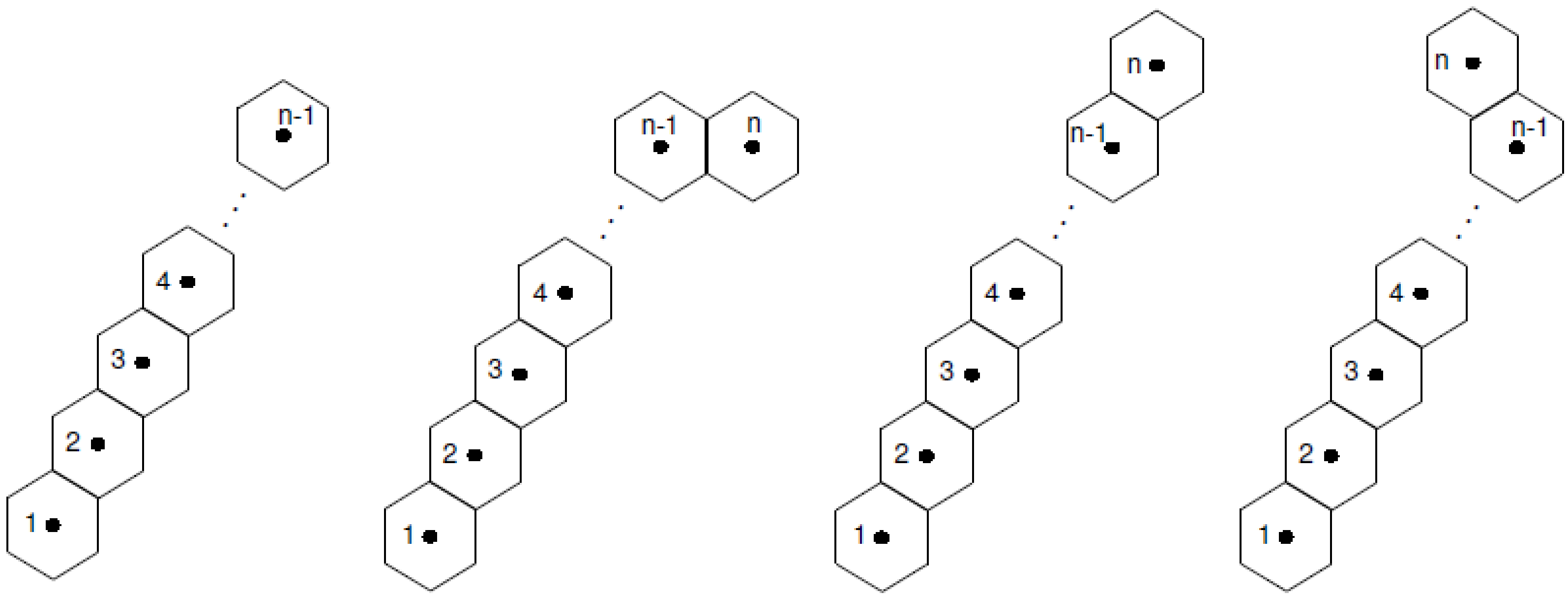


From example,

$$\lambda_1(G_1) = 3.74166$$
$$\lambda_1(G_2) = 3$$
$$\lambda_1(G) = 3.77307$$

RECURSIVE CONCATENATION

- Recursively attach a single hexagon to the honeycomb graph



- Example: the nth hexagon can be attached in 3 places (actually 5, but that would cause cycles)

RECURSIVE CONCATENATION

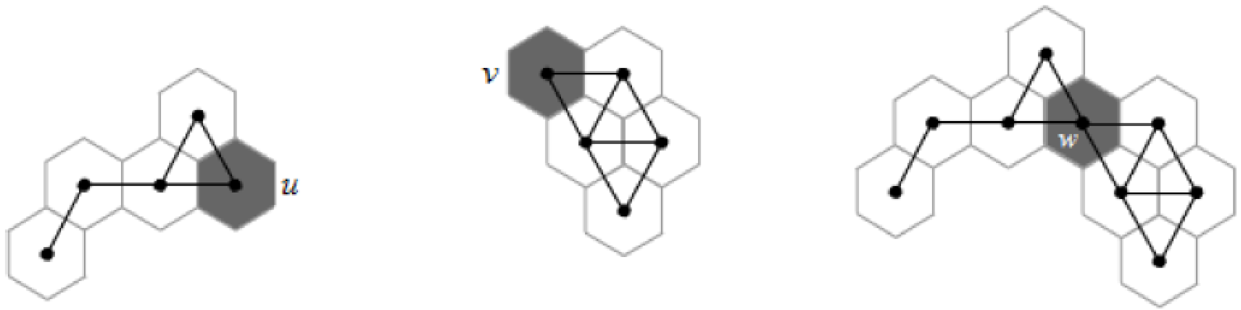
- Use Energy to predict orientation and positioning

n	Energy		
	n^{th} at 0°	n^{th} at 60°	n^{th} at 120°
3	4.472	5.657	7.211
4	7.211	8.944	10.77
5	9.549	10.93	12.61
⋮	⋮	⋮	⋮
21	50.37	51.93	53.69
22	53.03	54.61	56.38
23	55.47	57.03	58.79
24	58.12	59.70	61.47
⋮	⋮	⋮	⋮

The chain is growing at 60°.

The table shows the energy for various positions of the nth hexagon

COALESCENCE

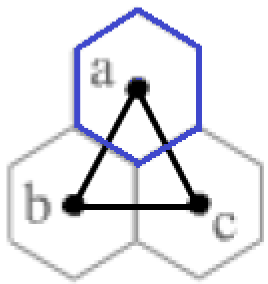


(a) Graph H_1 (b) Graph H_2 (c) Graph H

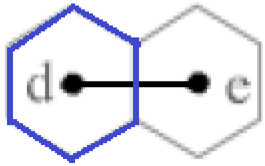
- Coalescence: Merge hexagons from 2 graphs to create a new graph.

- In the example above, the gray hexagons in H1 and H2 are merged are to create H

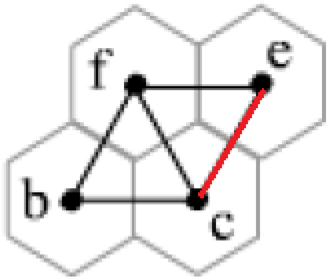
COALESCENCE: INDUCED EDGES



(a) H_1



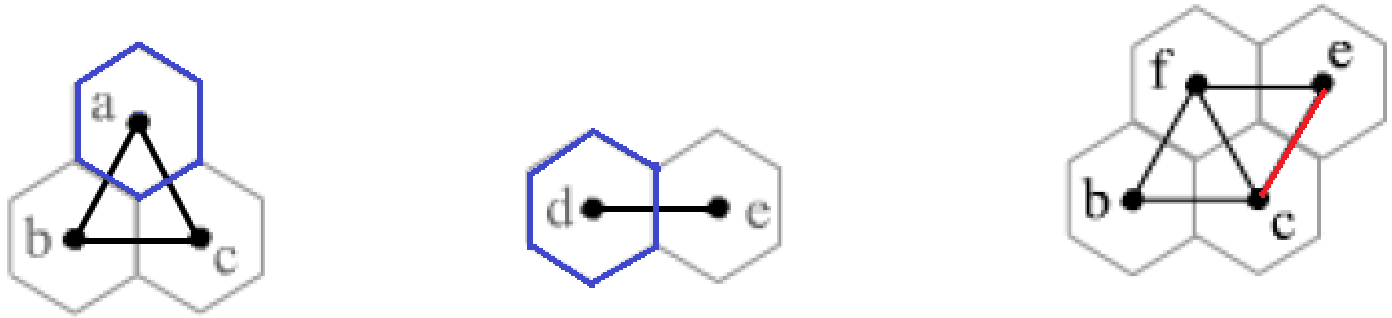
(b) H_2



(c) H

- Merging a and d gives rise to graph H
- However, the inner dualist of H has a new edge, which was not present in the inner dualists of either H1 or H2

COALESCENCE: INDUCED EDGES



(a) H_1 (b) H_2 (c) H

- Energy bound:

$$E(H) \leq E(H_1) + E(H_2) + E(I)$$

Where *E(I)* is the energy of induced edges.

When there are no induced edges, *E(I)* = 0

Energy of Catacondensed Hexagonal Systems

Let H be some Catacondensed hexagonal system with n - 1 hexagons, with inner dual graph G. Then obviously G is a bipartite graph. Now concatenate a hexagon to some hexagon of H such that the new system is also Catacondensed. The new hexagon can be attached to another hexagon in the system in at most three different angles. This can result in systems H_1 if it is attached at 0°, H_2 if it is attached at 60°, and H_3 if it is attached at 120°. Let the inner dual graphs of these systems be $G1$, $G2$ and $G3$ respectively.

Lemma:

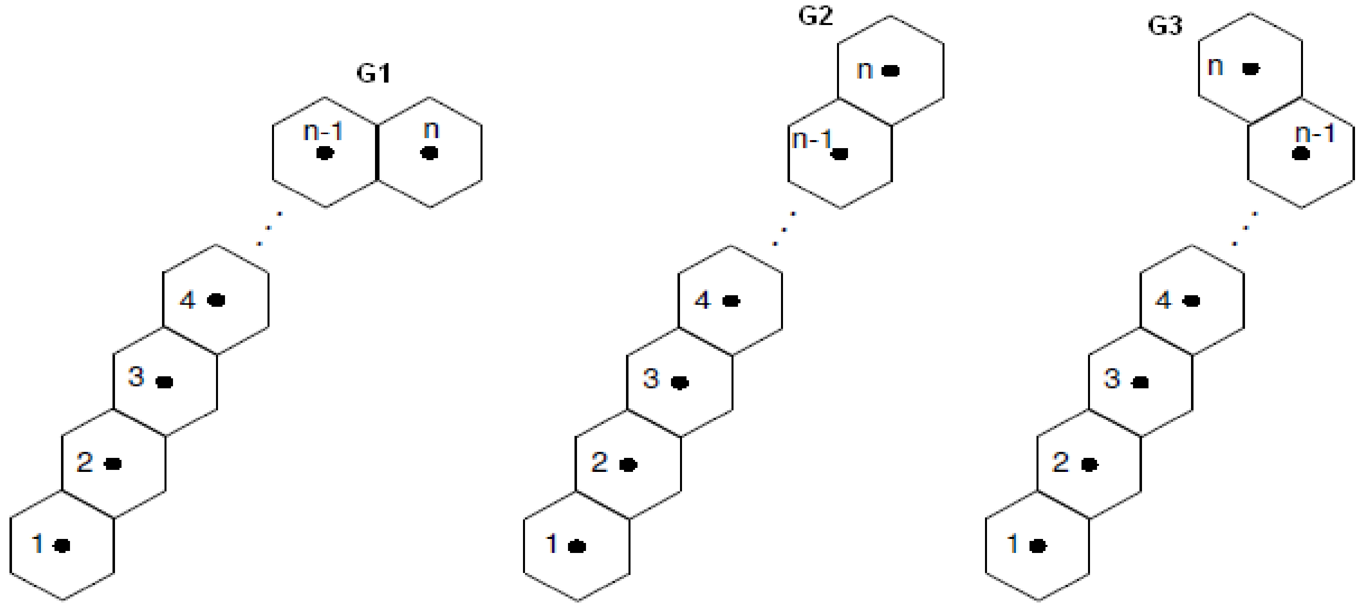
Let G_e *be an arbitrary inner dualist graph of one of types G1, G2 and G3 as defined above. If the matching polynomial (and hence the characteristic polynomial) of a hexagonal system is given by*

$$\phi G_e(x) = x^n + \sum_{k=1}^{\lfloor n/2 \rfloor} (-1)^k m_k (G_e) x^{n-2k}$$

then m_k *is of the form*

$$a_k + w(e)^2 b_k$$

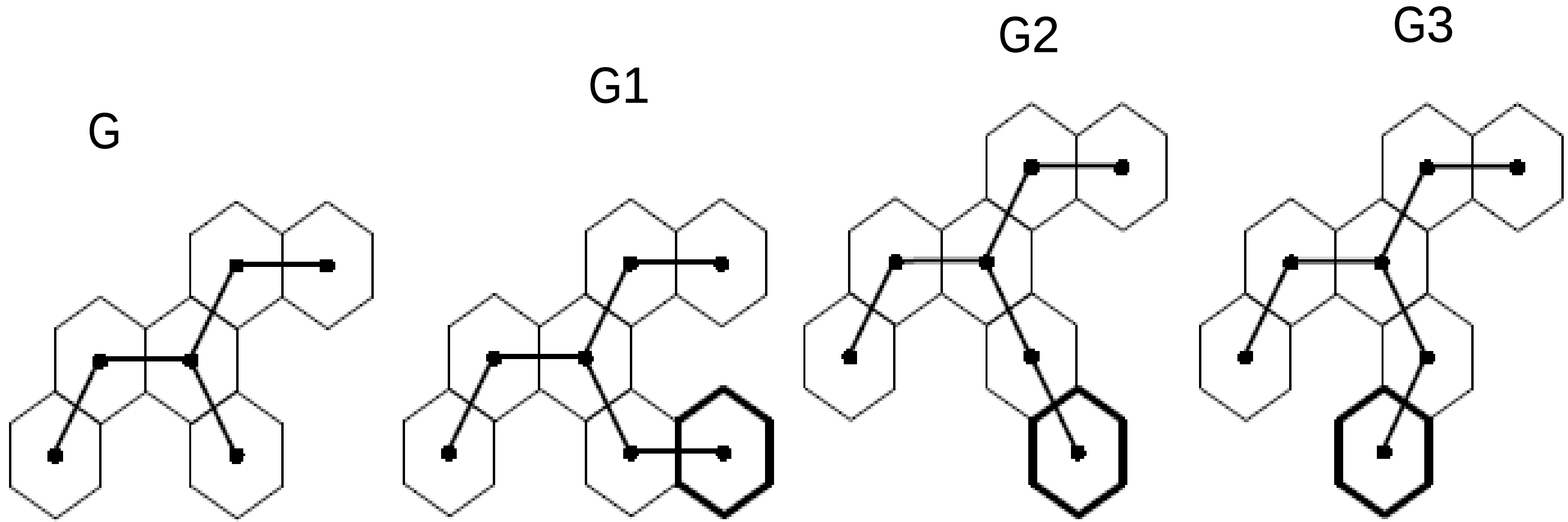
where $w(e)$ *is the weight of the edge* $(n, n - 1)$.



Theorem:

If G1, G2 and G3 are the 3 types of graphs defined above, and the energy of a graph G is written E(G), then the energies of G1, G2 and G3 satisfy:

$$E(G1) < E(G2) < E(G3)$$



(a) The original graph, T, growing at 60° (b) T_1. nth hexagon attached at 0° (c) T_2. nth hexagon attached at 60° (d) T_3. nth hexagon attached at 120°

An Integral formula for the energy of a graph was introduced by Coulson (1940) [11]. An adjusted formula only for bipartite graphs is given by

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x^2} \log \left(1 + \sum_{k=1}^{\lfloor n/2 \rfloor} (-1)^k m_k(G) x^{2k} \right)$$

It is clear that the energy of a bipartite graph is a strictly increasing function of each of the

parameters $m_k(G)$. Since $m_k(G1) < m_k(G2) < m_k(G3)$, we can infer that

$$E(G1) < E(G2) < E(G3).$$

For the figure above, we have

$$E(T1)=13.679$$

$$E(T2)=14.946$$

$$E(T3)=16.515$$

Which therefore satisfy

$$E(G1)<E(G2)<E(G3)$$

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- **W. C. He, W. B. He (1985)**, *A novel nomenclature of polycyclic aromatic hydrocarbons without using graph centre*, Theoretica Chimica Acta **68** 301-313.

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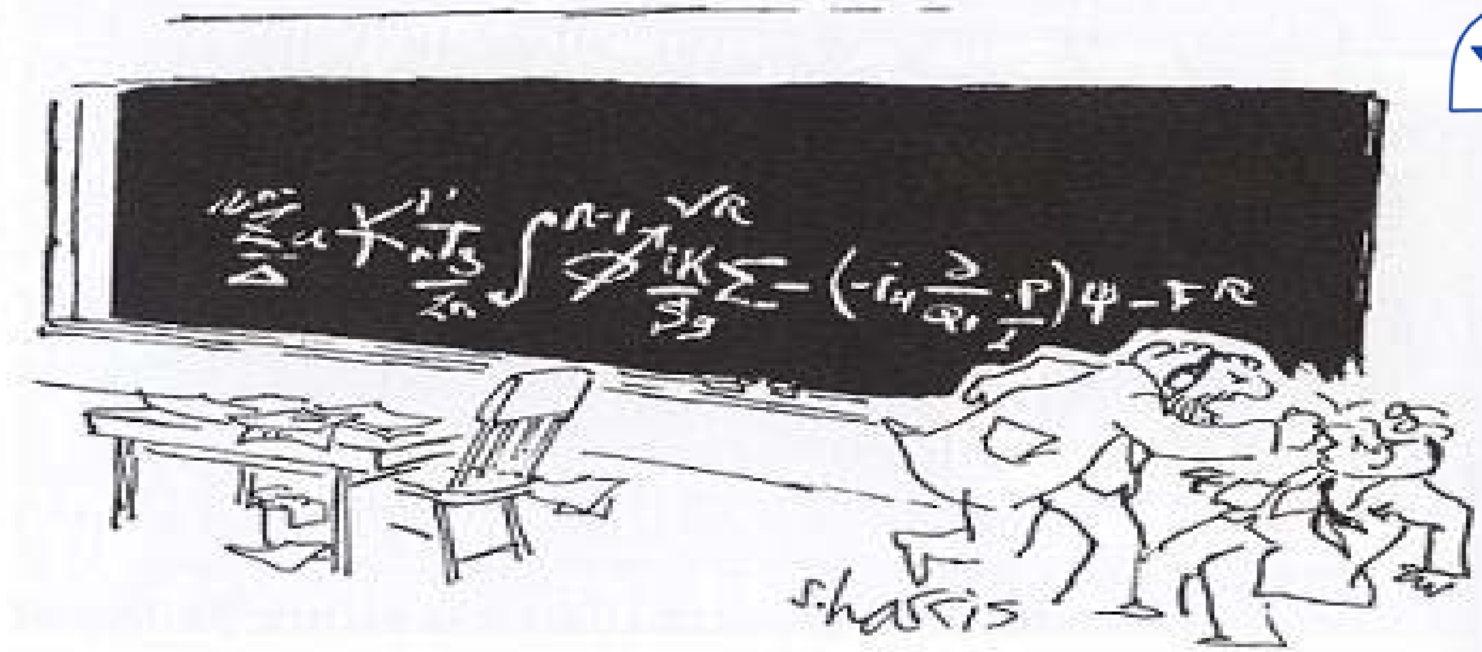

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THANK YOU

Questions & Answers