

## Eigenvalues of (3, 6)-Fullerenes

Luis Goddyn

joint work with:

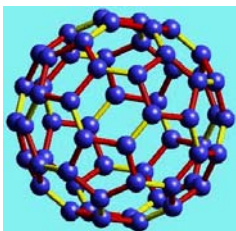
Matt DeVos, Bojan Mohar, Robert Šámal

Simon Fraser University, Burnaby, BC

Coast-to-coast Seminar: 2007-09-25



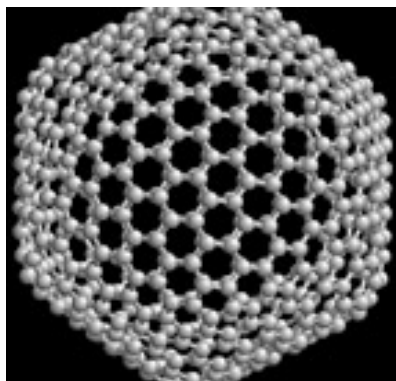
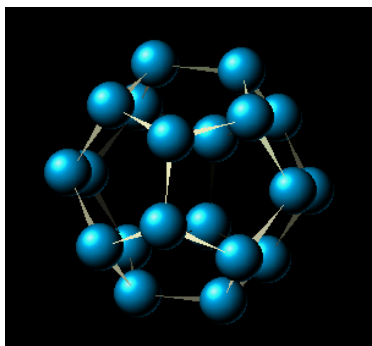
Richard Buckminster Fuller  
1895 - 1983



Buckyball - C<sub>60</sub> molecule  
1985

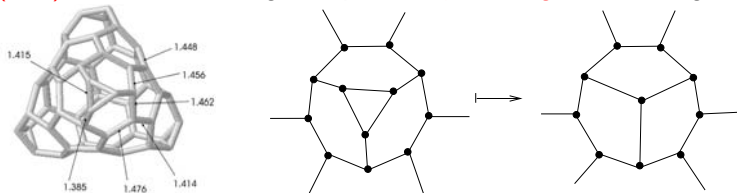
## Definition: Fullerene

**(5,6)-Fullerene:** 3-regular, planar, (12) pentagons & hexagons



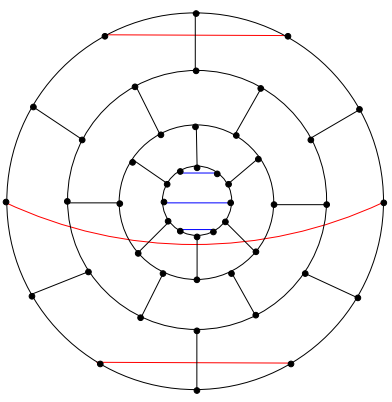
## Definition: (3,6)-Fullerene

- **(3,6)-Fullerene:** 3-regular, planar, (4) triangles & hexagons

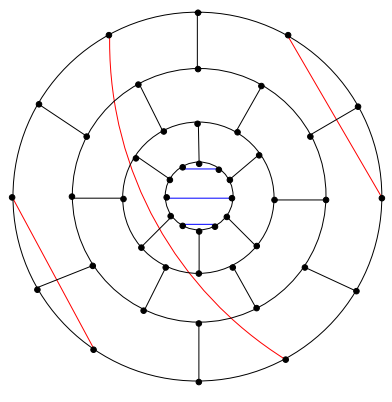


- Chemistry/Physics Interest:
  - They modify to “tetrahedral” (5,6)-Fullerenes
  - Can model “nanotubes”
  - Easier to characterize
  - **Critical Question:** Find “Energy Spectrum” = eigenvalues of adjacency matrix

## Tube Construction of all (3,6)-Fullerenes



(4, 6, 0) – tube



(4, 6, 1) – tube

(length, girth, twist)

Specification is 3-to-1.

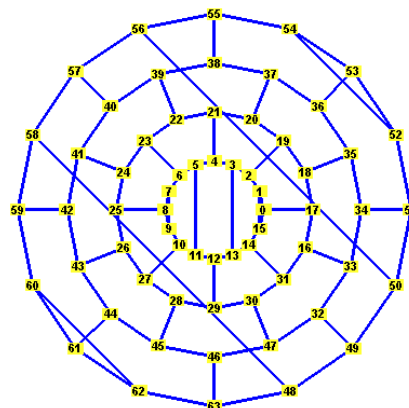
# Maple Tests – GraphTheory package

```

> cylinder := proc( n::posint, ell::posint )
local v;
if irem(n, 4) <> 0 then error "1st argument must be a multiple of 4";
fi;
v := (i,j) -> i*n+j;
Graph( seq(Trail( seq(v(i,j), j=0..n-1), v(i,0) ), i=0..ell-1),
      { seq(seq(v(i,2*j), v(i+1,2*j+1)), j=0..n/2-1), i=0..ell-2 }
);
end;
> poly36 := proc( n, ell, shift)
local v, G;
v := (i,j) -> i*n+j;
G := AddEdge( cylinder(n,ell), { seq((v(0,2*i+1), v(0,n-(2*i+1))), i=
0..n/4-1), seq((v(ell-1,irem(2*shift+2*i,n)), v(ell-1,irem(2*shift+n-2*
i-2, n))), i=0..n/4-1) } );
SetVertexPositions(G, [seq(seq(evalf((i+1)*cos(2*Pi*(j-1)/n), sin(2*
Pi*(j-1)/n))), j=0..n-1), i=0..ell-1]);
G
end;

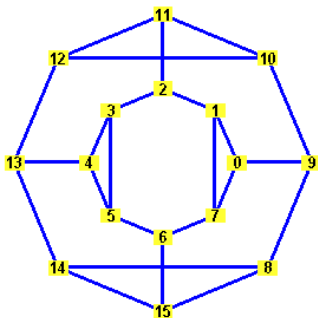
```

```
> DrawGraph(poly36(16,4,3));
```



## Maple Tests – Adjacency Matrix

> DrawGraph(poly36(8,2,0));



> AdjacencyMatrix(poly36(8,2,0));

0	1	0	0	0	0	1	0	1	0	0	0	0	0	0
1	0	1	0	0	0	1	0	0	0	0	0	0	0	0
0	1	0	1	0	0	0	0	0	0	1	0	0	0	0
0	0	1	0	1	1	0	0	0	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0	0	0	0	0	1	0
0	0	1	1	0	1	0	0	0	0	0	0	0	0	0
0	0	0	1	0	1	0	0	0	0	0	0	0	0	1
1	1	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	1	1
1	0	0	0	0	0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
0	0	1	0	0	0	0	0	0	1	0	1	0	0	0
0	0	0	0	0	0	0	0	0	1	1	0	1	0	0
0	0	0	1	0	0	0	0	0	0	1	0	1	0	0
0	0	0	0	0	0	0	1	0	0	0	0	1	0	1
0	0	0	0	0	1	0	1	0	0	0	0	1	0	0

(9)



## Fowler conjecture

### Conjecture (Fowler, 1995)

*The spectrum of every (3, 6)-Fullerene takes the form*

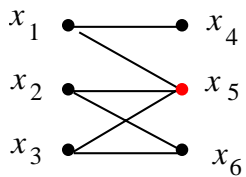
$$\{3, -1, -1, -1\} \cup \Lambda \cup -\Lambda.$$

*where  $\Lambda$  is a multiset of reals.*

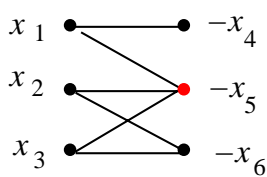
(3,6)-Fullerenes are “spectrally almost bipartite”?

**Lemma**  
*G has spectrum  $\Lambda \cup -\Lambda$  iff G is bipartite.*

Eigenvector  $x : V \rightarrow \mathbb{C}$     $\sum_{uv \in E} x(u) = \lambda x(v)$



$$x_1 + x_2 + x_3 = \lambda x_5$$

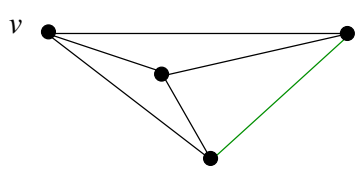
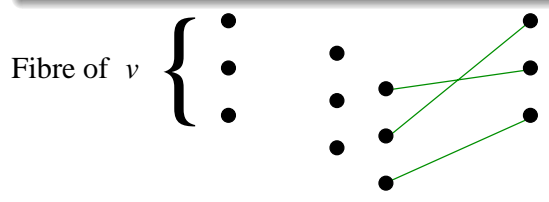


$$= (-\lambda)(-x_5)$$

Why  $\{3, -1, -1, -1\}$ ?

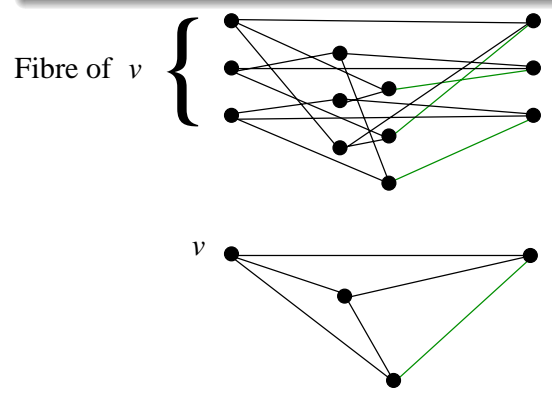
**Lemma**

*Every (3,6)-Fullerene is a cover of  $K_4$ .*



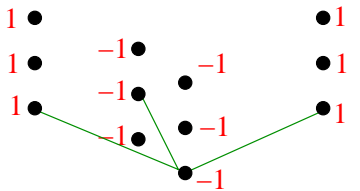
# Why $\{3, -1, -1, -1\}$ ?

**Lemma**  
*Every (3,6)-Fullerene is a cover of  $K_4$ .*

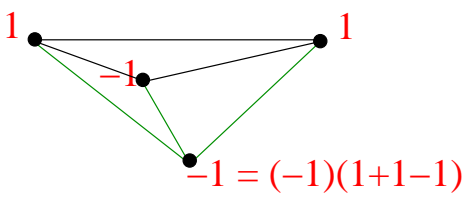


Why  $\{3, -1, -1, -1\}$ ?

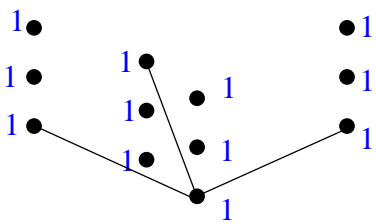
Eigenvector lift to covers



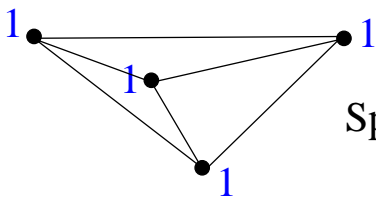
Eigenvalue = -1



# Why $\{3, -1, -1, -1\}$ ?



Eigenvalue = 3



$$\text{Spec}(K_4) = \{3, -1, -1, -1\}$$

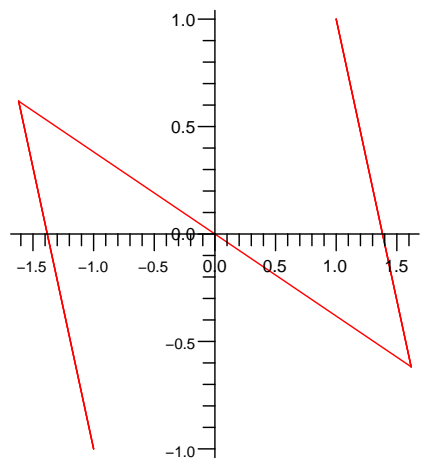
## Experimenting...



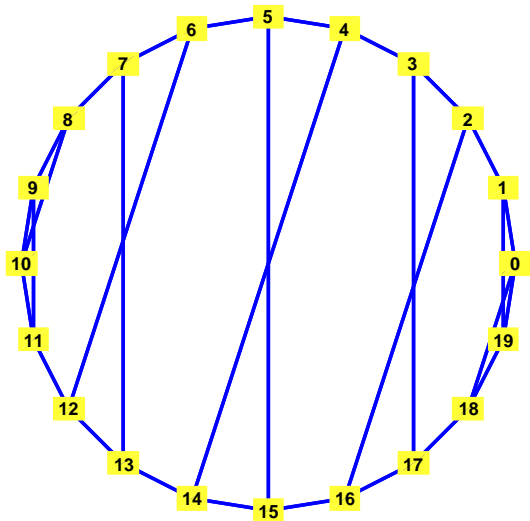
### Idea

Where  $x, x'$  are eigenvectors for  $\lambda, -\lambda$ , plot vertex  $v$  at coordinates  $(x_v, x'_v)$ .

```
> lambda,X := Eigenvectors(AdjacencyMatrix(poly36(4, 2, 0))):  
Transpose(lambda);  
[ 1 sqrt(5) -sqrt(5) 3 -1 -1 -1 -1 ]  
(15)  
> plot(convert(SubMatrix(X,1..-1,[2,3]),listlist));
```



```
> G:=poly36(20,1,0): DrawGraph(G);
```

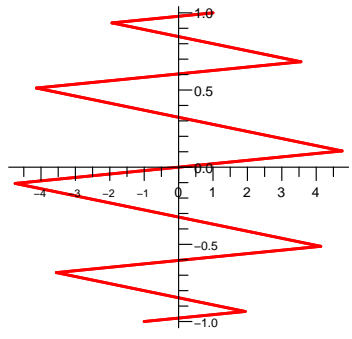


```
> lambda, X := Eigenvectors(AdjacencyMatrix(G));
Transpose(lambda);

$$\left[ \sqrt{6+\sqrt{5}}, \sqrt{6+\sqrt{5}}, \sqrt{6-\sqrt{5}}, \sqrt{6-\sqrt{5}}, -1, -1, -1, -1, -1, -1, -1, -1, 1, 1, 1, 1, 1, 1, \sqrt{4+\sqrt{5}}, \right. \quad (17)$$


$$\left. \sqrt{4+\sqrt{5}}, \sqrt{4-\sqrt{5}}, \sqrt{4-\sqrt{5}}, 3 \right]$$

> plot(convert(SubMatrix(X, 1..-1, [1,2]), listlist));
```

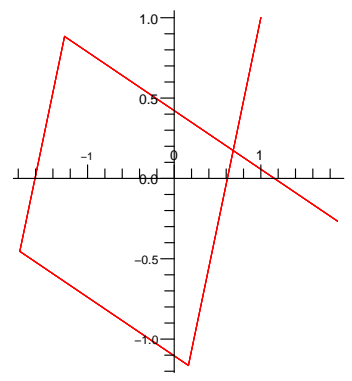


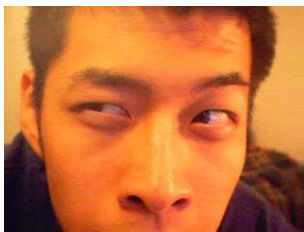


```
> lambda, X := Eigenvectors(AdjacencyMatrix(G)) :
Transpose(lambda) ;

$$\left[ \sqrt{6+\sqrt{5}}, \sqrt{6+\sqrt{5}}, -\sqrt{6-\sqrt{5}}, \sqrt{6-\sqrt{5}}, 3, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1, -1, -1, -1, -1, -1, \sqrt{4+\sqrt{5}}, \sqrt{4+\sqrt{5}}, -\sqrt{4-\sqrt{5}}, \sqrt{4-\sqrt{5}} \right] \quad (15)$$

> plot(convert(SubMatrix(X, 1..-1, [-1, -2]), listlist)) :
```





### Suspicion

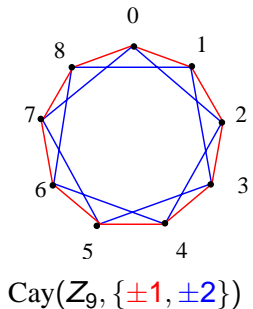
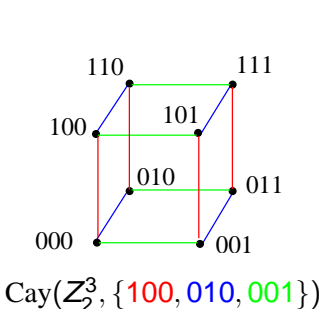
*Where  $x, x'$  are (appropriately scaled) eigenvectors for  $\lambda, -\lambda$ , the complex numbers  $x(v) + ix'(v)$  are (phase shifted) roots of unity.*



# Cayley Graph

$\Gamma =$  additive abelian group.    $S \subseteq \Gamma$ , the *symbol set*.    $S = -S$

$\text{Cay}(\Gamma, S) : \quad V = \Gamma, \quad E = \{uv \mid u - v \in S\}$

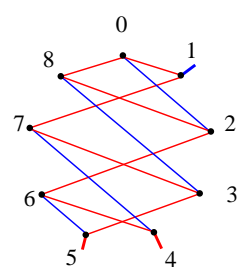
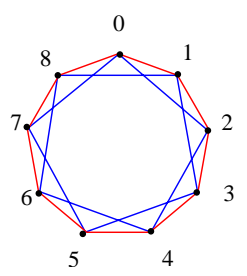
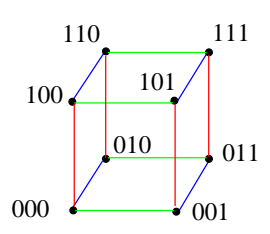


# Cayley Sum Graph

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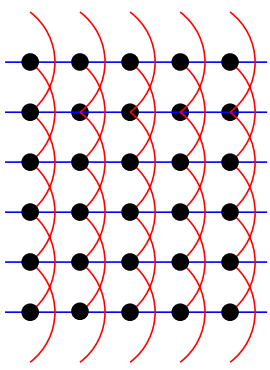
$\text{CaySum}(\Gamma, S) : V = \Gamma \quad E = \{uv \mid u + v \in S\}$



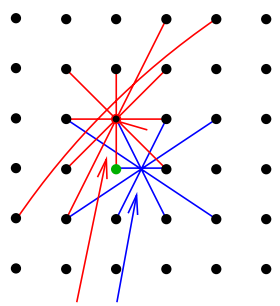
$\text{Cay}(\mathbb{Z}_2^3, \{100, 010, 001\})$     $\text{Cay}(\mathbb{Z}_9, \{\pm 1, \pm 2\})$     $\text{CaySum}(\mathbb{Z}_9, \{\pm 1, 2\})$

$\text{CaySum}(\mathbb{Z}_2^3, \{100, 010, 001\})$

# Geometric Cayley Sum Graphs



$Cay(\mathbb{Z}^2, \{(\pm 1, 0), (0, \pm 2)\})$



Concurrence of edges

$CaySum(\mathbb{Z}^2, \{(1, 0), (0, 2)\})$

## Cayley Sum Graphs - Facts

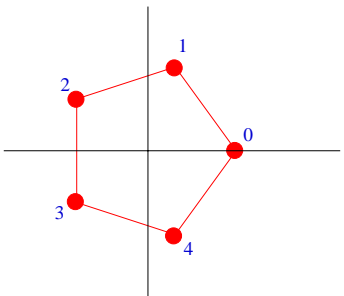
- $\text{CaySum}(\Gamma, S)$  is  $|S|$ -regular (counting loops once)
- $\text{CaySum}(\Gamma, S) \simeq \text{CaySum}(\Gamma, S + 2t)$  (via  $x \mapsto x + t$ )
- $\text{CaySum}(\Gamma, S)^{(2)} = \text{Cay}(\Gamma, S - S)$
- (F. Chung, 1989) Good expansion
- (B. Green, 2003) Pseudorandom clique size
- (D. Grynkiewicz et al, 2007) Connectivity
- (N. Alon, 2007+) Independence Number
- (B. Cheyne et al 2003; V. Lev, 2008+) Hamiltonicity

# Abelian Group Characters

$\chi : \Gamma \rightarrow \mathbb{C}$  is a homomorphism.

eg.  $\Gamma = \mathbb{Z}_5$

- $\chi_1 : x \mapsto e^{2i\pi \frac{x}{5}}$
- $\chi_2 : x \mapsto e^{2i\pi \frac{2x}{5}}$
- $\chi_0 : x \mapsto 1$

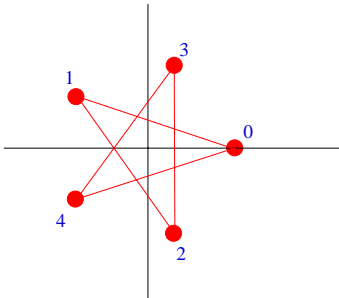


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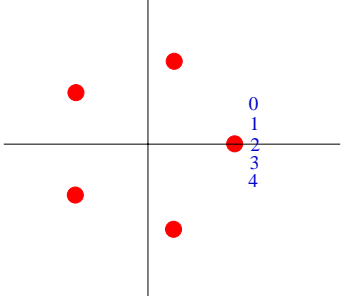
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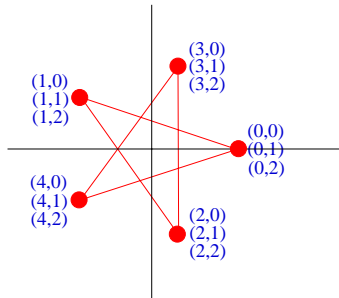
- $\chi_1 : x \mapsto e^{2i\pi \frac{x}{5}}$
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- $\chi_0 : x \mapsto 1$

For  $a \in Z_n$ ,  $\chi_a(x) = e^{2i\pi \frac{ax}{n}}$

# Abelian Group Characters

eg.  $\Gamma = \mathbb{Z}_5 \times \mathbb{Z}_3$

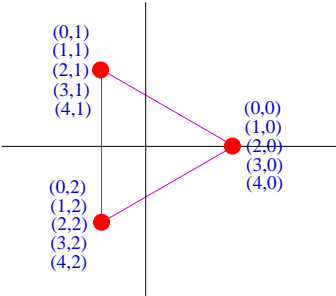
- $\chi(2,0) : (x_1, x_2) \mapsto e^{2i\pi \frac{2x_1}{5}}$
- $\chi(0,1) : (x_1, x_2) \mapsto e^{2i\pi \frac{x_2}{3}}$
- $\chi(3,2) : (x_1, x_2) \mapsto e^{2i\pi(\frac{3x_1}{5} + \frac{2x_2}{3})}$



# Abelian Group Characters

eg.  $\Gamma = Z_5 \times Z_3$

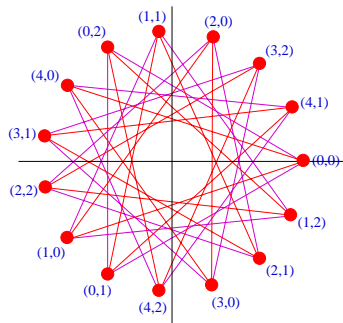
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For  $(a_1, a_2) \in \mathbb{Z}_5 \times \mathbb{Z}_3$ ,  $\chi_{(a_1, a_2)}(x_1, x_2) = e^{2i\pi(\frac{a_1 x_1}{5} + \frac{a_2 x_2}{3})}$

## Abelian Group Characters

eg.  $\Gamma = \mathbb{Z}_5 \times \mathbb{Z}_3$

- $\chi_{(2,0)} : (x_1, x_2) \mapsto e^{2i\pi \frac{2x_1}{5}}$
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- $\chi_{(3,2)} : (x_1, x_2) \mapsto e^{2i\pi (\frac{3x_1}{5} + \frac{2x_2}{3})}$

For  $\mathbf{a} \in \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \cdots \times \mathbb{Z}_{n_k}$ ,  $\chi_{\mathbf{a}}(\mathbf{x}) = e^{2i\pi (\frac{a_1 x_1}{n_1} + \cdots + \frac{a_k x_k}{n_k})}$

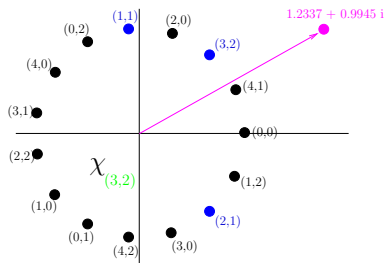
## Spectra of Cayley Graphs

### Theorem (Classic)

$$\text{Spec}(\text{Cay}(\Gamma, \{s_1, \dots, s_k\})) = \left\{ \sum_i \chi_a(s_i) \mid a \in \Gamma \right\}$$

$\text{Cay}(\mathbb{Z}_5 \times \mathbb{Z}_3, \{(1, 1), (2, 1), (3, 2)\})$

$\lambda_{(3,2)} = 1.2337 + 0.9945i$



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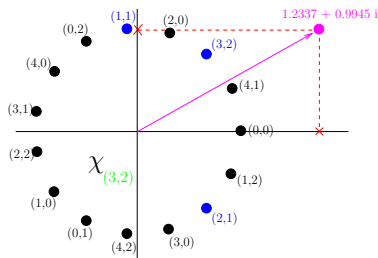
$\text{Cay}(\mathbb{Z}_5 \times \mathbb{Z}_3, \{(1, 1), (2, 1), (3, 2)\})$

$\lambda_{(3,2)} = 1.2337 + 0.9945i$

$\Re(\lambda_{(3,2)}) = 1.2337$

$\Im(\lambda_{(3,2)}) = 0.9945$

2-to-2 (unless  $\chi_a$  is real-valued)



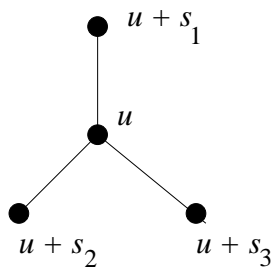
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**Proof:**

$$\begin{aligned} (A \chi_a)(u) &= \sum_{v \in N(u)} \chi_a(v) \\ &= \sum_i \chi_a(u + s_i) \\ &= \chi_a(u) \sum_i \chi_a(s_i) \end{aligned}$$



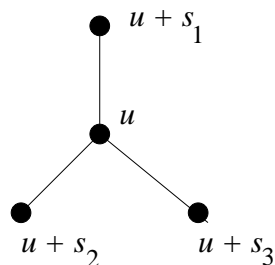
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### Theorem (Classic)

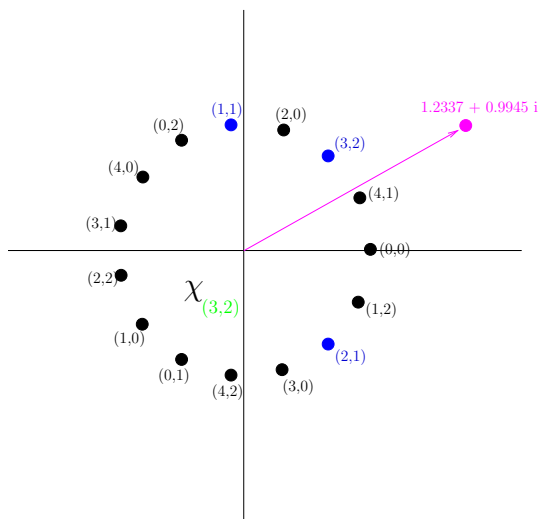
$$\text{Spec}(\text{Cay}(\Gamma, \{\overset{\mathbf{S}}{s_1, \dots, s_k}\})) = \left\{ \underbrace{\sum_i \chi_a(s_i)}_{\chi_a(\mathbf{S})} \mid \mathbf{a} \in \Gamma \right\}$$

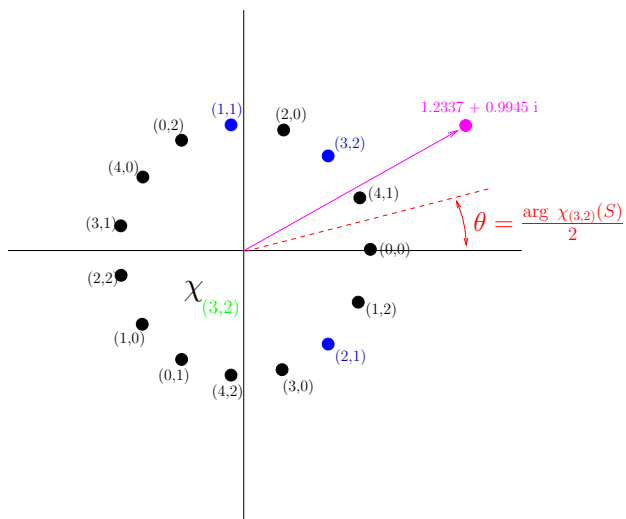
**Proof:**

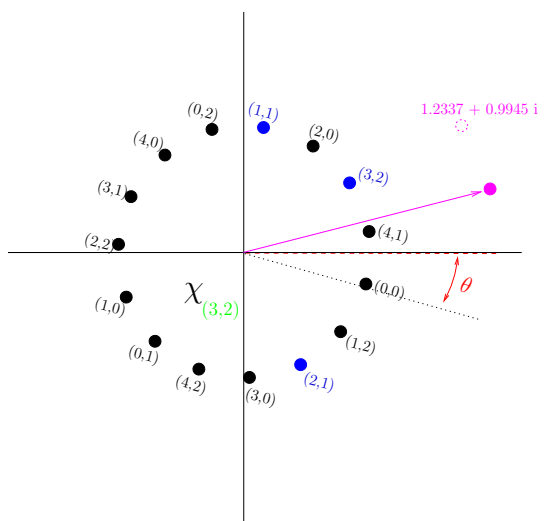
$$\begin{aligned} (A \chi_a)(u) &= \sum_{v \in N(u)} \chi_a(v) \\ &= \sum_i \chi_a(u + s_i) \\ &= \chi_a(u) \underbrace{\sum_i \chi_a(s_i)}_{\chi_a(\mathbf{S})} \end{aligned}$$

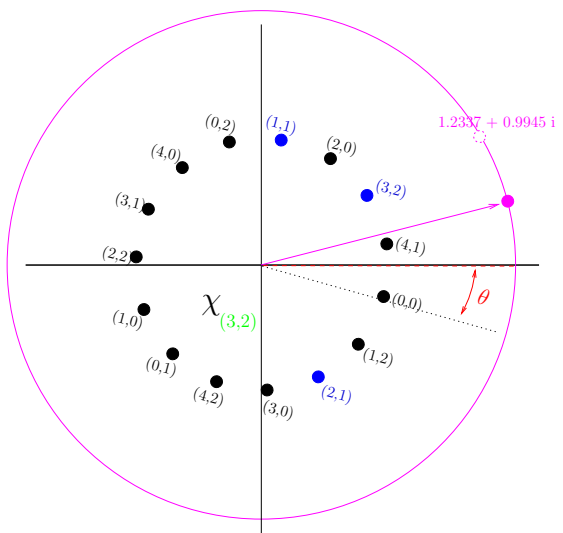












Eigenvalues:  $\pm|1.2337 + 0.9945i| = \pm 2.4423$   
 2-to-2

**Proof:**

$$\begin{aligned}
 (A \chi_a)(u) &= \sum_{v \in N(u)} \chi_a(v) = \sum_{s \in S} \chi_a(s - u) \\
 &= \sum_{s \in S} \chi_a(s) \chi_a(u)^{-1} = \chi_a(S) \overline{\chi_a(u)} \quad \text{Not quite!}
 \end{aligned}$$

**Proof:** Phase change:  $\rho := e^{-\frac{\arg \chi_a(S)}{2}}$ . So  $\chi_a(S)\rho^2 = |\chi_a(S)|$ .

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**Proof:** Phase change:  $\rho := e^{-\frac{\arg \chi_a(S)}{2}}$ . So  $\rho^2 \chi_a(S) = |\chi_a(S)|$ .

$$\begin{aligned} (A \rho \chi_a)(u) &= \sum_{v \in N(u)} \rho \chi_a(v) = \sum_{s \in S} \rho \chi_a(s - u) \\ &= \sum_{s \in S} \rho^2 \chi_a(s) (\rho \chi_a(u))^{-1} = |\chi_a(S)| \overline{\rho \chi_a(u)} \end{aligned}$$

So

$\Re(\rho \chi_a)$  has eigenvalue  $+ |\chi_a(S)|$

$\Im(\rho \chi_a)$  has eigenvalue  $- |\chi_a(S)|$

2 to 2 (unless  $a$  is an involution).

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So

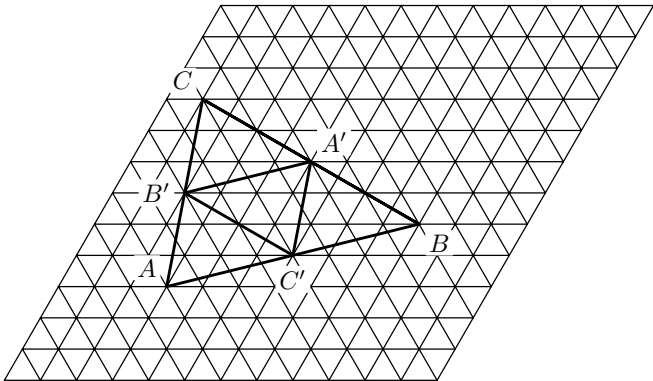
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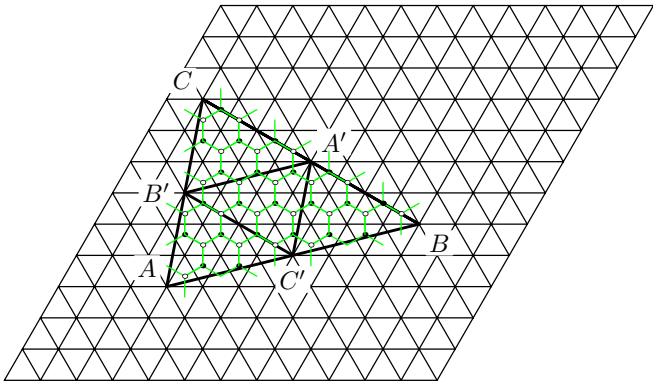


## Grid Construction of (3, 6)-Fullerenes



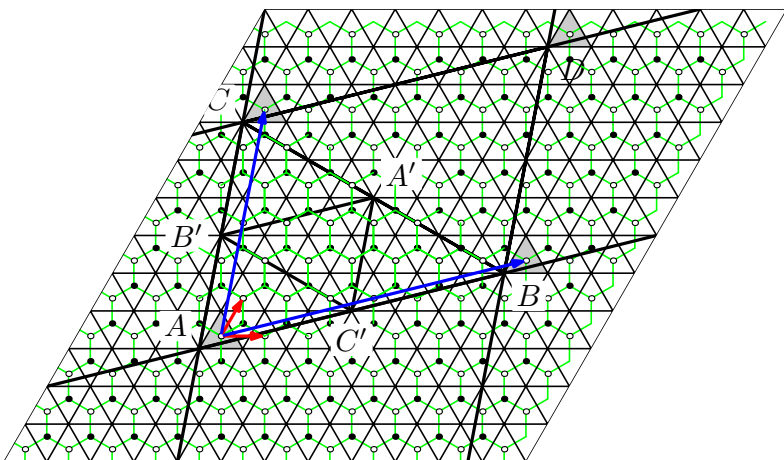
- $ABC$  any acute triangle on Eisenstein grid
- Midpoints  $A'$ ,  $B'$ ,  $C'$  are grid points
- Fold tetrahedron
- Take the dual graph

## Grid Construction of (3, 6)-Fullerenes

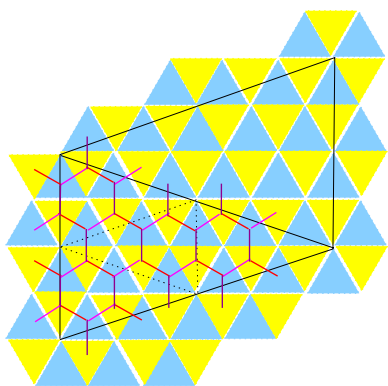


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# Proof Setup

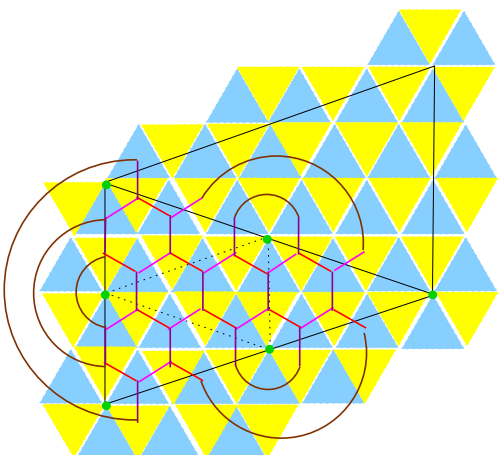


# Proof Setup



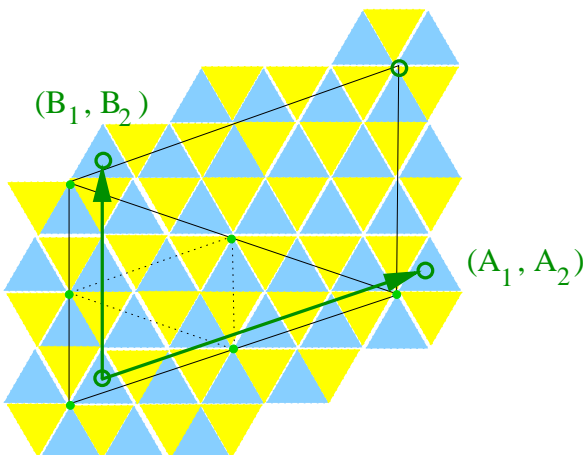
Vertices are Up-triangles and Down-triangles

# Proof Setup



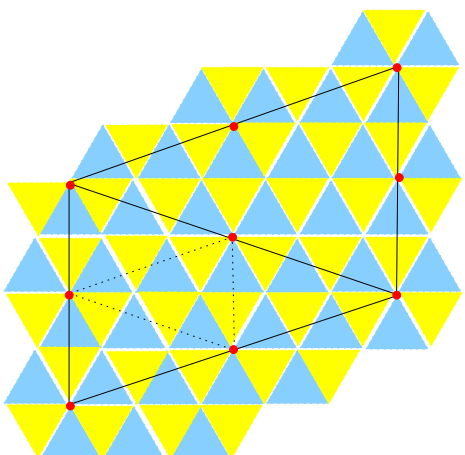
Folding identifies vertices and connects edges

# Proof Setup



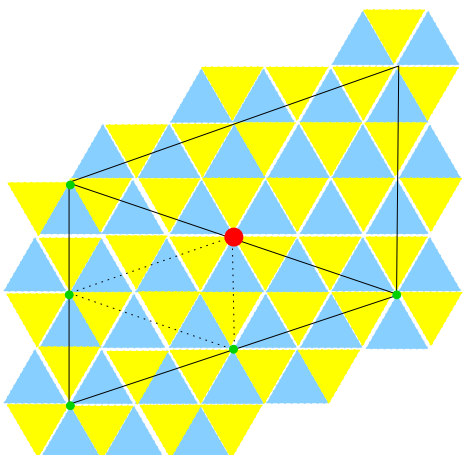
$A = (A_1, A_2)$  and  $B = (B_1, B_2)$  generate lattice  $\mathcal{L}$

# Proof Setup



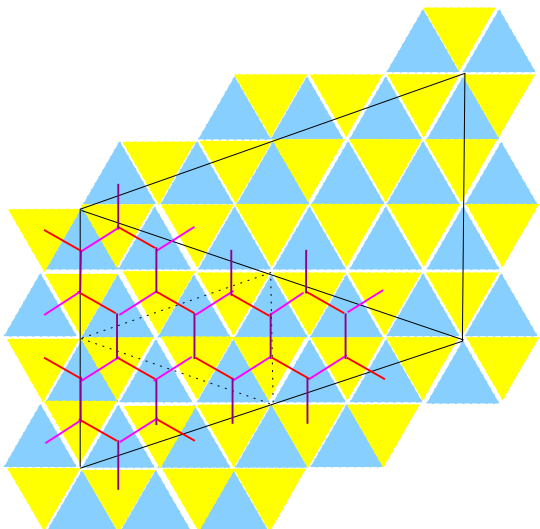
Translated lattice of pivot points

# Proof Setup

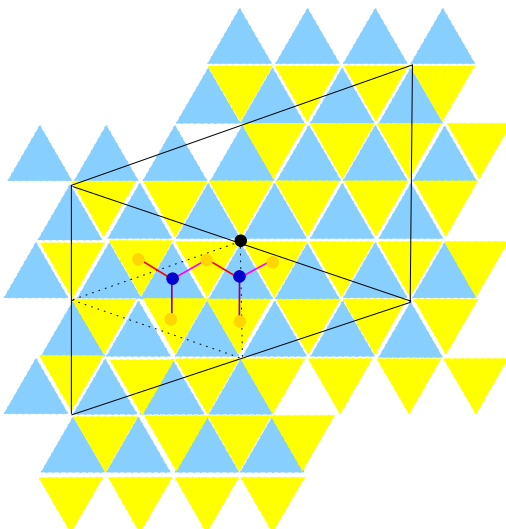


Reflect (rotate) down-triangles about any **pivot point**

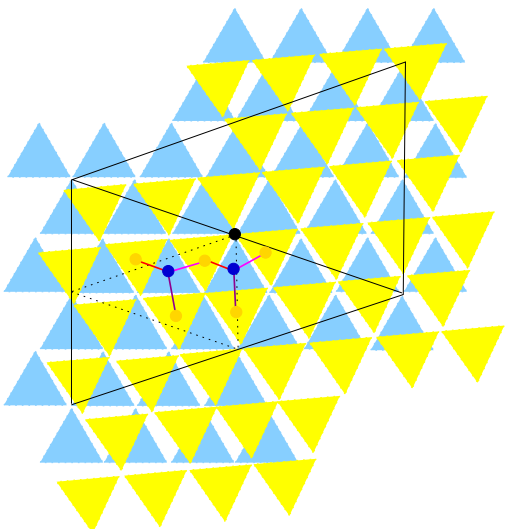
# Universal Cover is an Eisenstein Cayley Sum Graph



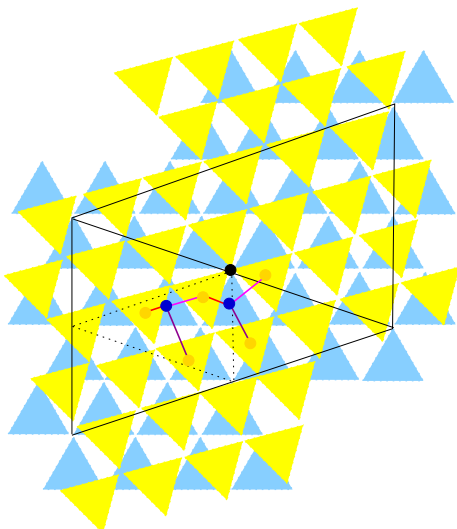
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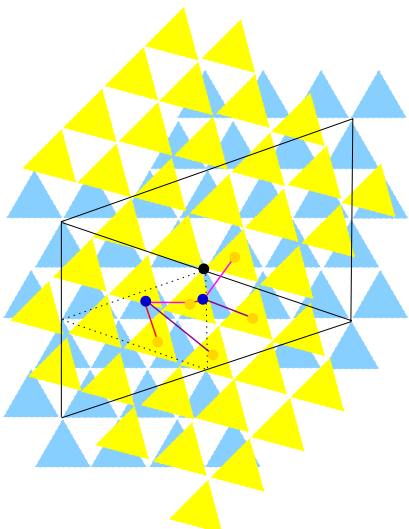
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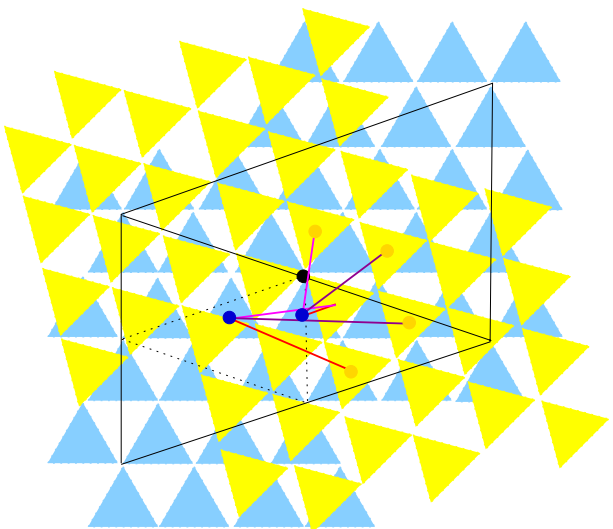
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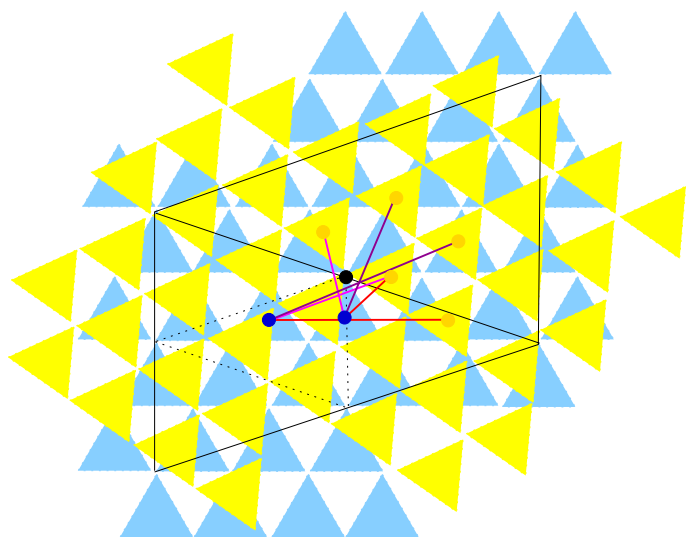
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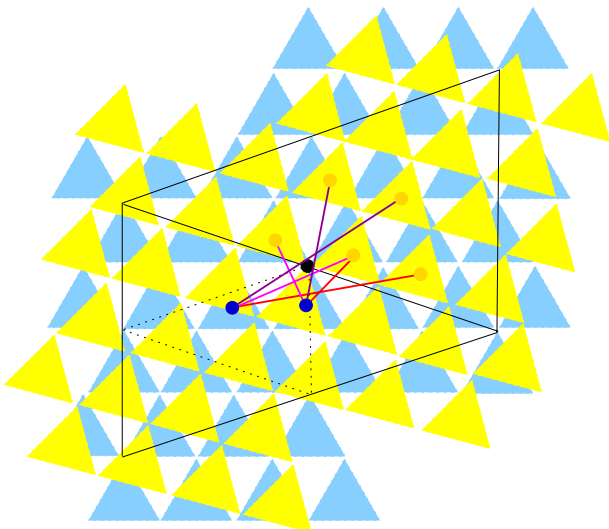
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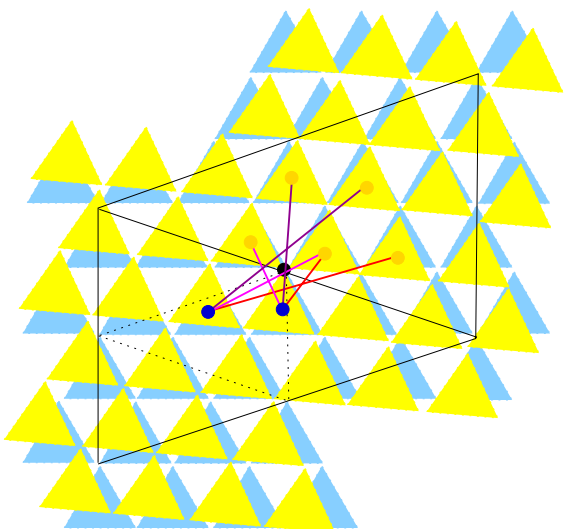
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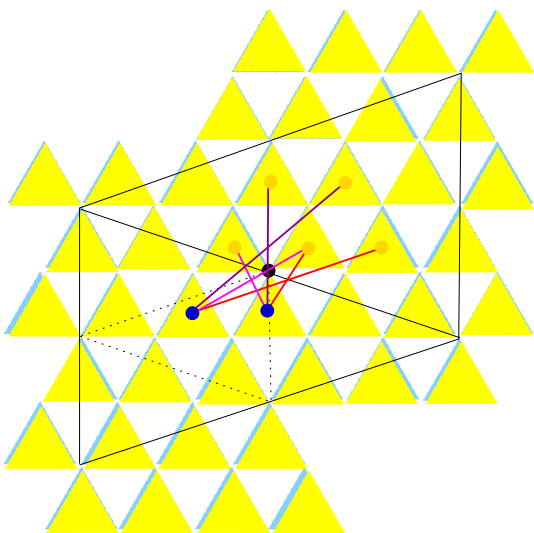
# Universal Cover is an Eisenstein Cayley Sum Graph



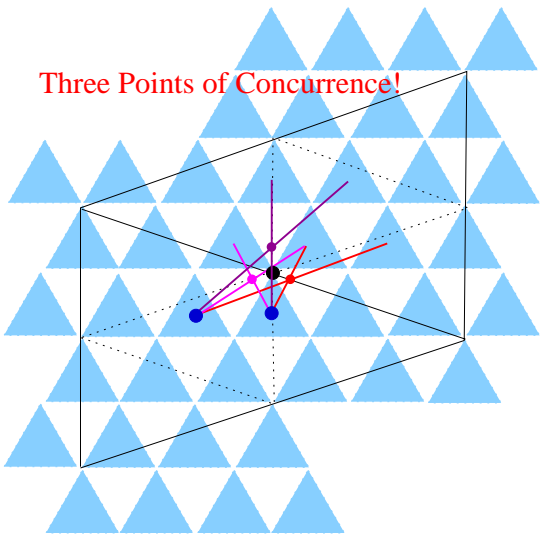
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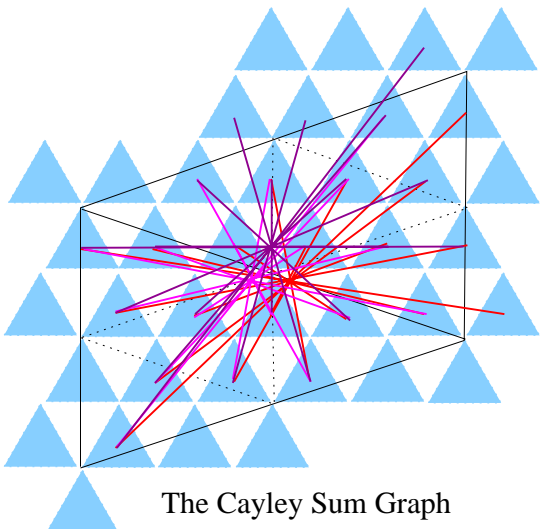
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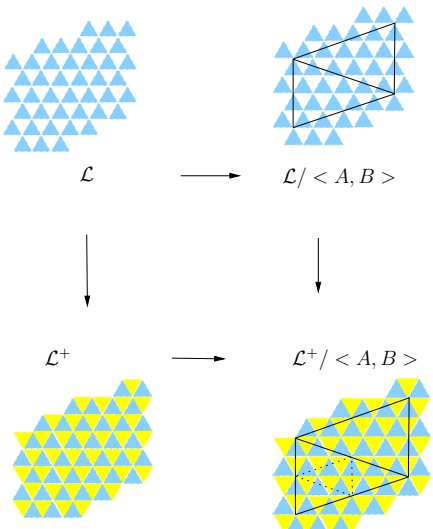


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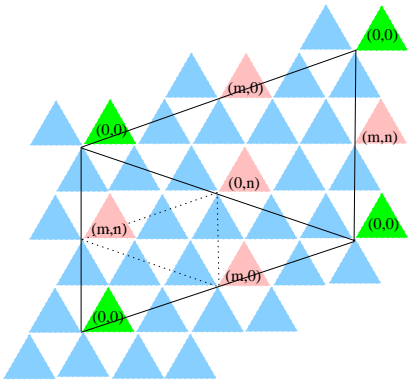


The Cayley Sum Graph

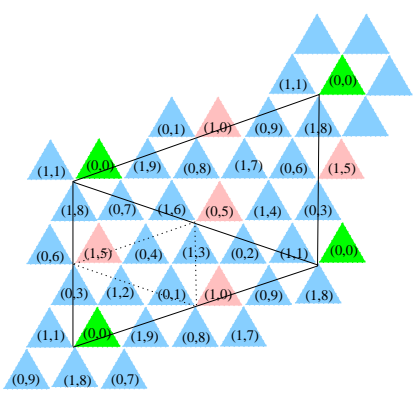
## General Procedure



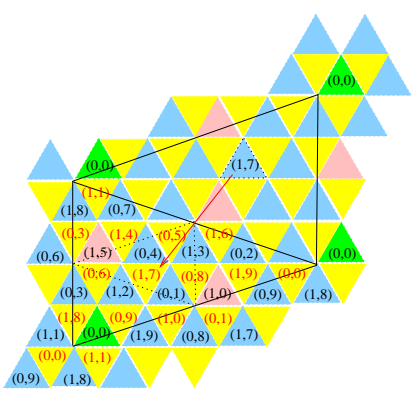
# Finding the Homomorphism $\mathbb{E} \rightarrow \mathcal{L} \rightarrow \mathbb{Z}_{2m} \times \mathbb{Z}_{2n}$



## Finding the Homomorphism $\mathbb{E} \rightarrow \mathcal{L} \rightarrow \mathbb{Z}_{2m} \times \mathbb{Z}_{2n}$

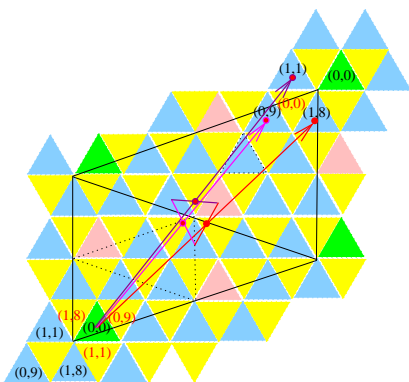


Finding the Homomorphism  $\mathbb{E} \rightarrow \mathcal{L} \rightarrow \mathbb{Z}_{2m} \times \mathbb{Z}_{2n}$



Rotate

Finding the Homomorphism  $\mathbb{E} \rightarrow \mathcal{L} \rightarrow \mathbb{Z}_{2m} \times \mathbb{Z}_{2n}$



Generators are  $\Gamma$ -coords of Eisenstein  $[-1, 0], [0, -1], [-1, -1]$

## Computing It: Lattice Basis Change

- $\mathbb{E} = [a, b] \begin{pmatrix} \mathbb{Z} \\ \mathbb{Z} \end{pmatrix} \quad AB = 4a + 2b \quad AC = -2a + 4b$
- Put  $M = \begin{pmatrix} 4 & -2 \\ 2 & 4 \end{pmatrix}$
- SNF:  $UMV = D$ , (for some  $U, V$  unimodular,  $D$  diagonal)

$$\begin{pmatrix} 1 & 1 \\ 2 & -1 \end{pmatrix} \cdot \begin{pmatrix} 4 & -2 \\ 2 & 4 \end{pmatrix} \cdot \begin{pmatrix} -1 & -2 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 10 \end{pmatrix}$$

- Hence  $\Gamma = \mathbb{Z}_2 \times \mathbb{Z}_{10}$ .
- If  $U = (u_1 \ u_2)$ , then

$$S = \{-u_1, -u_2, -u_1 - u_2\} = \{(1, 8), (1, 1), (0, 9)\}$$

## Computing an eigenvalue

Let  $a = (1, 3) \notin \text{Inv}(\mathbb{Z}_2 \times \mathbb{Z}_{10})$ , say.

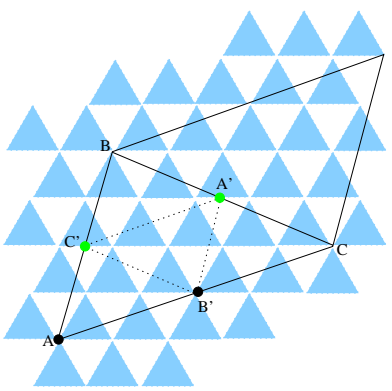
$$S = \{(1, 8), (1, 1), (0, 9)\}$$

$$\begin{aligned}\chi_{(1,3)}(S) &= e^{\frac{2i\pi 1(1)}{2} + \frac{2i\pi 3(8)}{10}} + e^{\frac{2i\pi 1(1)}{2} + \frac{2i\pi 3(1)}{10}} + e^{\frac{2i\pi 1(0)}{2} + \frac{2i\pi 3(9)}{10}} \\ &= (2 \cos(\pi/5) - \cos 2\pi/5) - i \sin 2\pi/5 \\ &= 1.618033989 e^{-\pi/5}\end{aligned}$$

Corresponding eigenvalues:  $\pm |\chi_{(1,3)}(S)| = \pm 1.618033989$

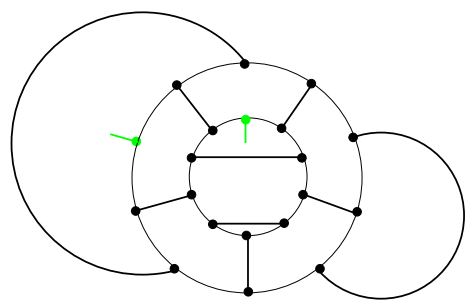
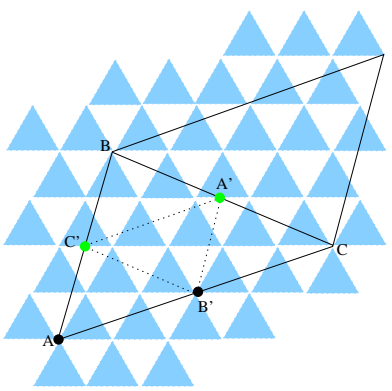
Phase shift for eigenvectors:  $\frac{-1}{2} \arg(\chi_{(1,3)}(S)) = -\pi/10$ .

# What if $A'$ , $B'$ , $C'$ are not gridpoints?



Semiloops!  
(0, 3, 6)-Fullerene: 3-regular, planar, hexagons & triangles & (up to 4) semiloops

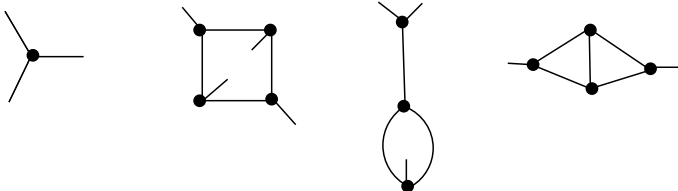
What if  $A'$ ,  $B'$ ,  $C'$  are not gridpoints?



(5, 2, 1)

**Semiloops!**  
**(0, 3, 6)-Fullerene:** 3-regular, planar, hexagons & triangles & (up to 4) semiloops

## Some (0, 3, 6)-Fullerenes



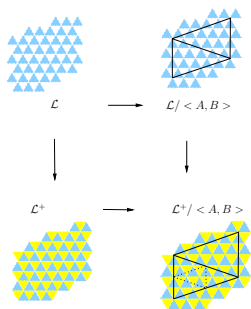
$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}$$

Eigenvalues = {3, 1, -1, -1}.





## Other Possibilities



- $\mathcal{L} = A_2$      $\mathcal{L}^+ = A_2^+$  : triangular grid ( (3,6)-Fullerenes )
- $\mathcal{L} = D_2$      $\mathcal{L}^+ = Z^2$  : checkerboard ( requires 4 semiloops )
- $\mathcal{L} = D_3$      $\mathcal{L}^+ = D_3^+$  : diamond packing ( 8 unpaired eigenvalues )

## Summary

- We proved Fowler's conjecture and described precisely eigenvalues and eigenvectors of  $(0, 3, 6)$ -polyhedra.
- Other lattices yield families with  $A \cup \Lambda \cup -\Lambda$
- Other natural families of spectrally nearly bipartite graphs?
- Much Harder:  $(5, 6)$ -Fullerenes. One problem: When are there more negative than positive eigenvalues?