Affine symmetry principles for non-crystallographic systems & applications to viruses/carbon onions

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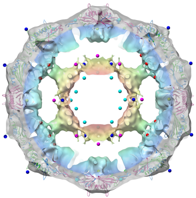
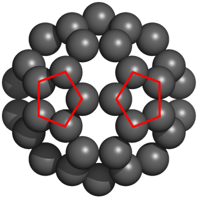
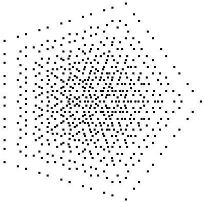
Doppler Institute, Technical University, Prague – December 16, 2014

Motivation: Viruses

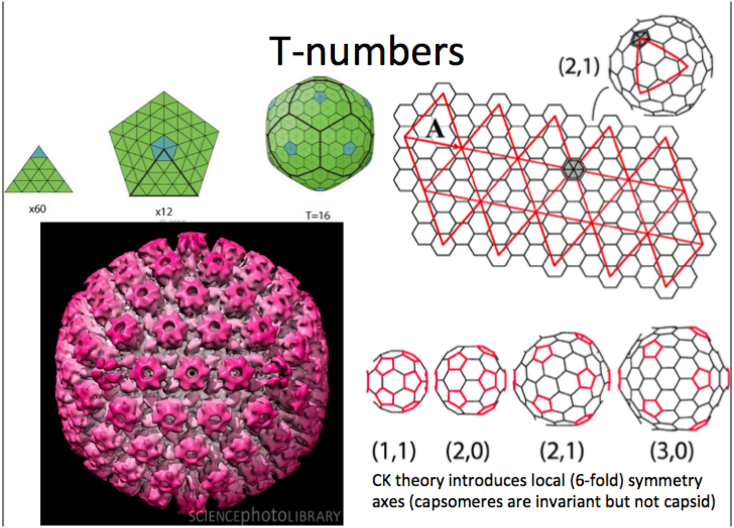
- Geometry of polyhedra described by Coxeter groups
- Viruses have to be 'economical' with their genes
- Encode structure modulo symmetry
- Largest discrete symmetry of space is the icosahedral group
- Many other 'maximally symmetric' objects in nature are also icosahedral: Fullerenes & Quasicrystals
- But: viruses are not just polyhedral – they have radial structure. Affine extensions give translations



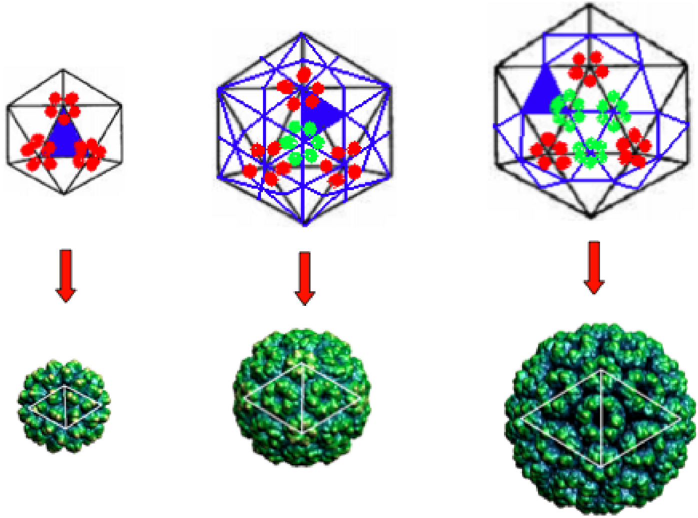




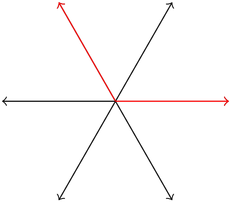
Viruses: Caspar-Klug triangulations



Viruses: Caspar-Klug triangulations



Root systems – A_2

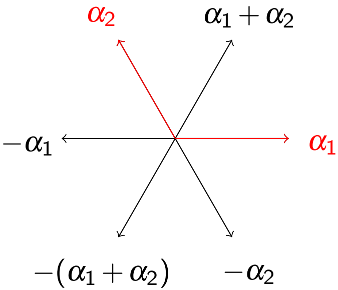


Root system Φ: set of vectors α such that

1. $\boxed{\Phi\cap\mathbb{R}\alpha=\{-\alpha,\alpha\}\ \forall\,\alpha\in\Phi}$

2. $\boxed{s_\alpha\Phi=\Phi\ \forall\,\alpha\in\Phi}$

Root systems – A_2



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2. $\boxed{s_\alpha \Phi = \Phi \ \forall \ \alpha \in \Phi}$

Simple roots: express every element of Φ via a $\mathbb{Z}$-linear combination (with coefficients of the same sign).

Cartan Matrices

Cartan matrix of α_is is $\boxed{A_{ij} = 2\frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2\frac{|\alpha_j|}{|\alpha_i|}\cos\theta_{ij}}$

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angles $\boxed{\cos^2\theta_{ij} = \frac{1}{4}A_{ij}A_{ji}}$ lengths $\boxed{l_j^2 = \frac{A_{ij}}{A_{ji}}l_i^2}$

$\boxed{A_{ii} = 2}$ $\boxed{A_{ij} \in \mathbb{Z}^{\leq 0}}$ $\boxed{A_{ij} = 0 \Leftrightarrow A_{ji} = 0}$.

$$A_2\colon\; A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

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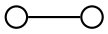
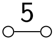
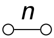
Coxeter-Dynkin diagrams: node = simple root, no link = roots orthogonal, simple link = roots at $\frac{\pi}{3}$, link with label m = angle $\frac{\pi}{m}$.

A_2  H_2 

$I_2(n)$ 

Coxeter groups

A Coxeter group is a group generated by some involutive generators $s_i, s_j \in S$ subject to relations of the form $\boxed{(s_i s_j)^{m_{ij}} = 1}$ with $m_{ij} = m_{ji} \geq 2$ for $i \neq j$.

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The finite Coxeter groups have a geometric representation where the involutions are realised as reflections at hyperplanes through the origin in a Euclidean vector space $\mathscr{E}$. In particular, let $(\cdot|\cdot)$ denote the inner product in $\mathscr{E}$, and v, $\alpha \in \mathscr{E}$.

The generator s_α corresponds to the reflection

$$\boxed{s_\alpha : v \rightarrow s_\alpha(v) = v - 2\frac{(v|\alpha)}{(\alpha|\alpha)}\alpha}$$

at a hyperplane perpendicular to the root vector α.

The action of the Coxeter group is to permute these root vectors.

Affine extensions

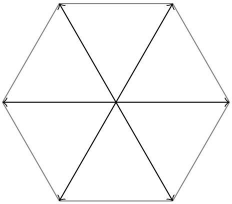
An affine Coxeter group is the extension of a Coxeter group by an affine reflection in a hyperplane not containing the origin $s_{\alpha_0}^{aff}$ whose geometric action is given by

$$\boxed{s_{\alpha_0}^{aff}v = \alpha_0 + v - \frac{2(\alpha_0|v)}{(\alpha_0|\alpha_0)}\alpha_0}$$

Non-distance preserving: includes the translation generator

$$\boxed{Tv = v + \alpha_0 = s_{\alpha_0}^{aff}s_{\alpha_0}v}$$

Affine extensions – A_2



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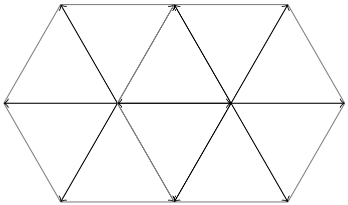
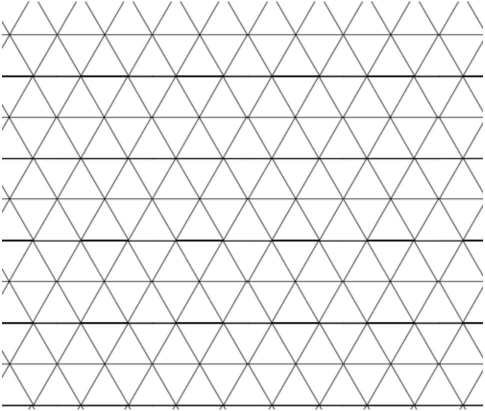
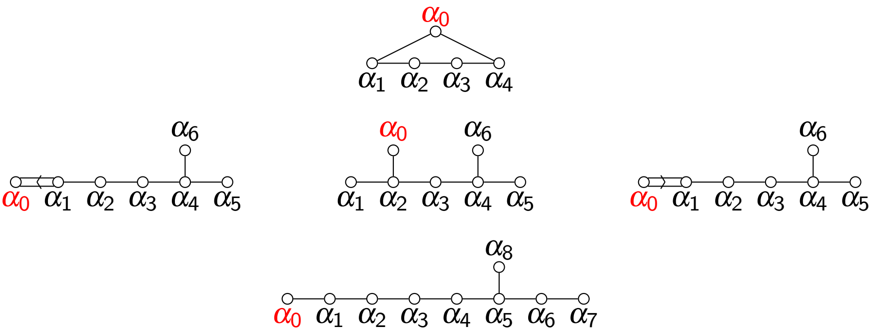


Affine extensions – A_2

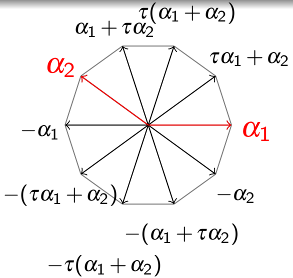
Affine extensions of crystallographic Coxeter groups lead to a tessellation of the plane and a lattice.

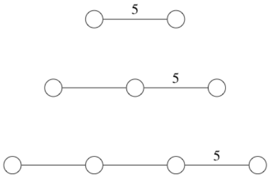


Affine extensions of crystallographic groups A_4, D_6 and E_8



Non-crystallographic Coxeter groups $H_2 \subset H_3 \subset H_4$





$$A=\begin{pmatrix}2 & -\tau\\ -\tau & 2\end{pmatrix}$$

$$A=\begin{pmatrix}2 & -1 & 0\\ -1 & 2 & -\tau\\ 0 & -\tau & 2\end{pmatrix}$$

$$A=\begin{pmatrix}2 & -1 & 0 & 0\\ -1 & 2 & -1 & 0\\ 0 & -1 & 2 & -\tau\\ 0 & 0 & -\tau & 2\end{pmatrix}$$

$H_2 \subset H_3 \subset H_4$: 10, 120, 14,400 elements, the only Coxeter groups that generate rotational symmetries of order 5

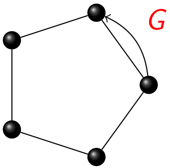
linear combinations now in the extended integer ring

$\boxed{\mathbb{Z}[\tau]=\{a+\tau b|a,b\in\mathbb{Z}\}}$ golden ratio $\boxed{\tau=\frac{1}{2}(1+\sqrt{5})=2\cos\frac{\pi}{5}}$

$\boxed{x^2=x+1}$ $\boxed{\tau'=\sigma=\frac{1}{2}(1-\sqrt{5})=2\cos\frac{2\pi}{5}}$ $\boxed{\tau+\sigma=1,\tau\sigma=-1}$

Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



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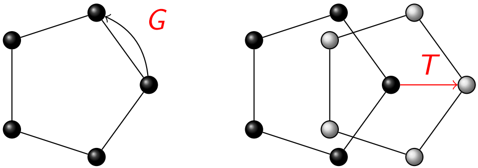

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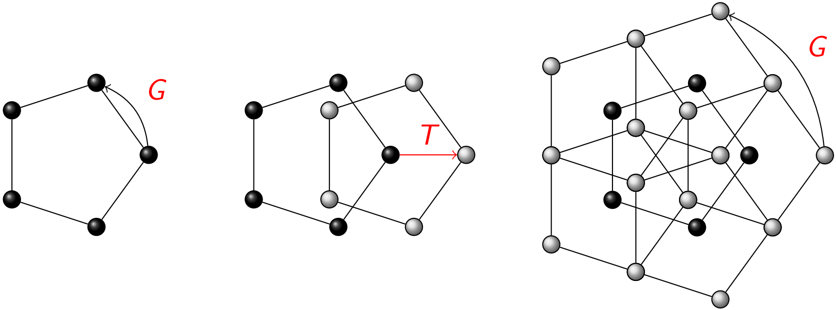
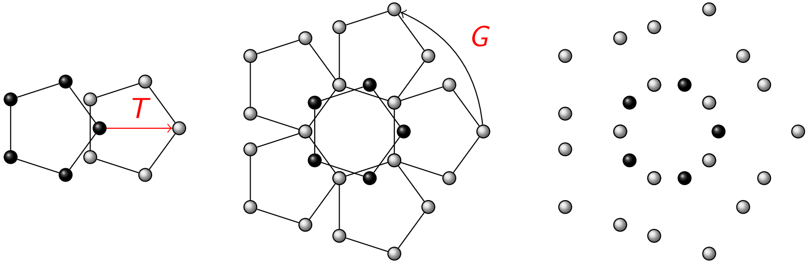


A random translation would give 5 secondary pentagons, i.e. 25 points. Here we have degeneracies due to 'coinciding points'.

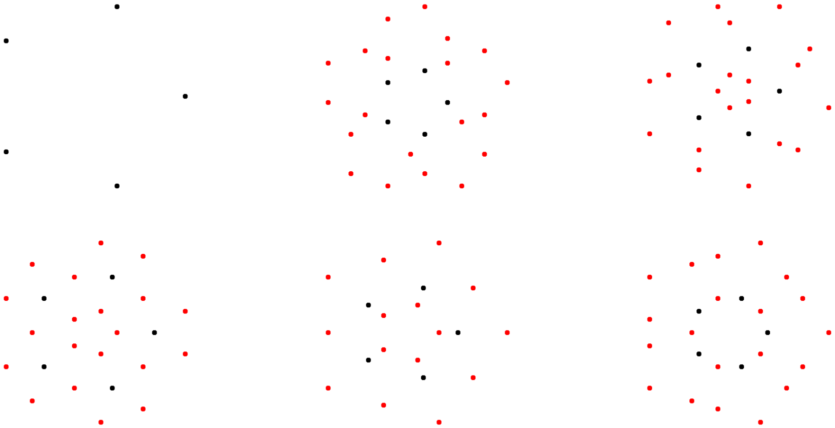
Affine extensions of non-crystallographic root systems

Translation of length $\tau = \frac{1}{2}(1+\sqrt{5}) \approx 1.618$ (golden ratio)



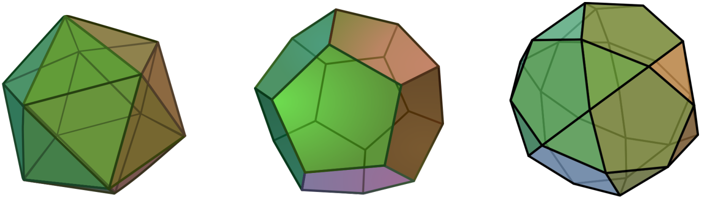
Looks like a virus or carbon onion

More Blueprints

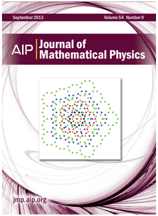


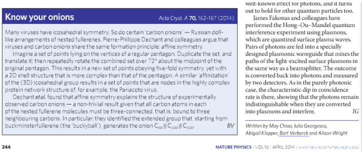
Extend icosahedral group with distinguished translations

- Radial layers are simultaneously constrained by affine symmetry
- Affine extensions of the icosahedral group (giving translations) and their classification.



Applications of affine extensions of non-crystallographic root systems





Know your onions *Acta Cryst. A* **70**, 162–167 (2014)

Many viruses have icosahedral symmetry. So do certain 'carbon onions' — Russian doll-like arrangements of nested fullerenes. Pierre-Philippe Dechant and colleagues argue that viruses and carbon onions share the same formation principle: affine symmetry.

Imagine a set of points lying on the vertices of a regular pentagon. Duplicate the set, and translate it; then repeatedly rotate the combined set over 72° about the midpoint of the original pentagon. This results in a new set of points obeying five-fold symmetry, yet with a 2D shell structure that is more complex than that of the pentagon. A similar 'affinization' of the (3D) icosahedral group results in a set of points that are nodes in the highly complex protein network structure of, for example, the Pariacoto virus.

Dechant *et al.* found that affine symmetry explains the structure of experimentally observed carbon onions — a non-trivial result given that all carbon atoms in each of the nested fullerene molecules must be three-connected, that is, bound to three neighbouring carbons. In particular, they identified the extended group that, starting from buckminsterfullerene (the 'buckyball'), generates the onion $C_{60}@C_{240}@C_{540}$. *BV*

well-known effect for photons, and it turns out to hold for other quantum particles too.

James Fakonas and colleagues have performed the Hong–Ou–Mandel quantum interference experiment using plasmons, which are quantized surface plasma waves. Pairs of photons are fed into a specially designed plasmonic waveguide that mixes the paths of the light-excited surface plasmons in the same way as a beamsplitter. The outcome is converted back into photons and measured by two detectors. As in the purely photonic case, the characteristic dip in coincidence rate is there, showing that the photons remain indistinguishable when they are converted into plasmons and interfere. *IG*

Written by May Chiao, Iulia Georgescu, Abigail Klopper, Bart Verberck and Alison Wright

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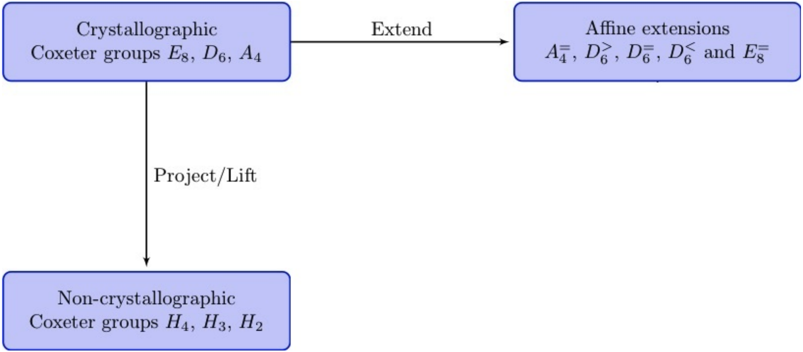
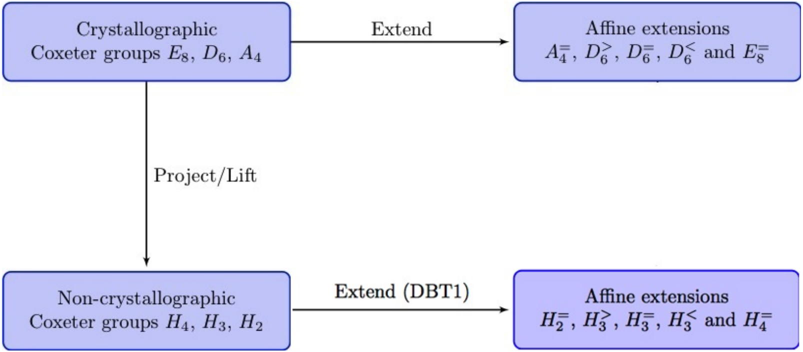
There are interesting applications to quasicrystals, viruses or carbon onions later, concentrate on the mathematical aspects for now

Road Map


Crystallographic
Coxeter groups E_8, D_6, A_4
Extend
Affine extensions
$A_4^=$, $D_6^>$, $D_6^=$, $D_6^<$ and $E_8^=$
Project/Lift
Non-crystallographic
Coxeter groups H_4, H_3, H_2

Road Map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Extend (DBT1)
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Road Map

$$\begin{tikzcd}
\boxed{\begin{array}{c}\text{Crystallographic}\\ \text{Coxeter groups } E_8,\ D_6,\ A_4\end{array}} \arrow[r, "\text{Extend}"] \arrow[d, "\text{Project/Lift}"] & \boxed{\begin{array}{c}\text{Affine extensions}\\ A_4^=,\ D_6^>,\ D_6^=,\ D_6^< \text{ and } E_8^=\end{array}} \arrow[d, dashed, "\text{Induce (DBT2)}"] \\
\boxed{\begin{array}{c}\text{Non-crystallographic}\\ \text{Coxeter groups } H_4,\ H_3,\ H_2\end{array}} \arrow[r, "\text{Extend (DBT1)}"] & \boxed{\begin{array}{c}\text{Affine extensions}\\ H_2^=,\ H_3^>,\ H_3^=,\ H_3^< \text{ and } H_4^=\end{array}}
\end{tikzcd}$$

Overview

1. Affine extensions
   - Direct extensions
   - Induced extensions
2. Applications
   - Virus Structure
   - Fullerenes and Carbon onions
3. A 3D spinorial view of 4D exceptional phenomena
4. Conclusions

Kac-Moody approach

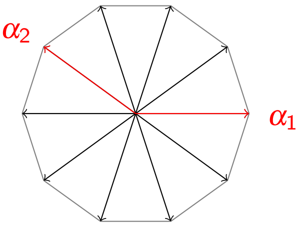
Can recover these directly at the Cartan matrix level:
Kac-Moody-type affine extension A^{aff} of a Cartan matrix is an extension of the Cartan matrix A of a Coxeter group by further rows $\underline{v}$ and columns $\underline{w}$ such that:

$$A^{aff} = \begin{pmatrix} 2 & \underline{v}^T \\ \underline{w} & A \end{pmatrix} \quad \boxed{A_{ii}^{aff} = 2} \boxed{A_{ij}^{aff} \in \mathbb{Z}[\cdot]}$$

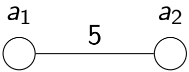
$$\boxed{A_{ij}^{aff} \leq 0} \text{ moreover, } \boxed{A_{ij}^{aff} = 0 \Leftrightarrow A_{ji}^{aff} = 0}$$

determinant constraint $\boxed{\det A^{aff} = 0}$

Kac-Moody approach to H_2

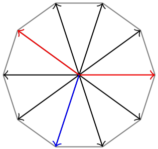


$$\boxed{\alpha_1 = (1,0),\ \alpha_2 = \frac{1}{2}(-\tau, \sqrt{3-\tau})}$$



$$A = \begin{pmatrix} 2 & \cdot & \cdot \\ \cdot & 2 & -\tau \\ \cdot & -\tau & 2 \end{pmatrix}$$

Extension along the highest root

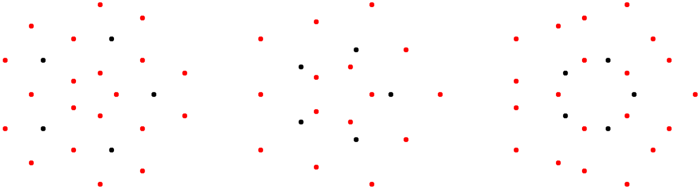


$$A = \begin{pmatrix} 2 & x & x \\ y & 2 & -\tau \\ y & -\tau & 2 \end{pmatrix}$$

$\boxed{xy = 2 - \tau = \sigma^2}$

symmetric $\boxed{x = y = \sigma = 1 - \tau}$ recovers H_2^{aff} from Twarock et al

new asymmetric e.g. $\boxed{(x,y) = (\tau - 2, -1)}$ or $\boxed{(x,y) = (-1, \tau - 2)}$



Write $x = (a + \tau b)$ and $y = (c + \tau d)$ with $a, b, c, d \in \mathbb{Z}$, i.e. H_2^{aff} is $(a, b; c, d) = (1, -1; 1, -1)$.

Fibonacci scaling

The (non-trivial) units in $\mathbb{Z}[\tau]$ are τ^k, $k \in \mathbb{Z}$

Can generate all solutions to the determinant constraint $\boxed{xy = \sigma^2}$ by

scaling $\boxed{x \to \tau^{-k}x, y \to \tau^k y}$: xy invariant (giving the angle),

but different lengths $\sqrt{\frac{x}{y}} \to \sqrt{\frac{x}{y}}\tau^{-k}$

Fibonacci scaling

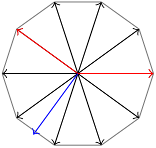
$(a, b; c, d) \to (b, a+b; d-c, c)$ for multiplication by (τ, τ^{-1}) and

$(a, b; c, d) \to (b-a, a; d, c+d)$ for multiplication by (τ^{-1}, τ)

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

Swapping $\boxed{x \leftrightarrow y}$ generates another solution, but here symmetric

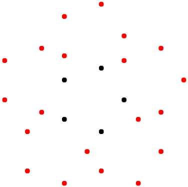
Extension along a bisector

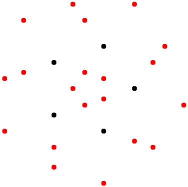


$$A = \begin{pmatrix} 2 & x & 0 \\ y & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$

$$\boxed{xy = 3 - \tau}$$

$$\boxed{(x, y) = (\tau - 3, -1)} \text{ or } \boxed{(x, y) = (-1, \tau - 3)}$$





Extension along the highest root – two-fold axis T_2

$$\boxed{\alpha_1 = (0,1,0),\ \alpha_2 = -\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3 = (0,0,1)}$$

$$\boxed{T_2 = (1,0,0)} \qquad A = \begin{pmatrix} 2 & 0 & x & 0 \\ 0 & 2 & -1 & 0 \\ y & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix} \qquad \boxed{xy = \sigma^2 = 2 - \tau}$$

Same solution as in the previous case of H_2.

Extension along a three-fold axis T_3

$$\boxed{\alpha_1 = (0,1,0),\ \alpha_2 = -\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3 = (0,0,1)}$$

$$\boxed{T_3 = (\tau,0,\sigma)} \qquad A = \begin{pmatrix} 2 & 0 & 0 & x \\ 0 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ y & 0 & -\tau & 2 \end{pmatrix} \qquad \boxed{xy = \frac{4}{3}\sigma^2}$$

No longer $\mathbb{Z}[\tau]$-valued, and hence solutions do not exist in $\mathbb{Z}[\tau]$. What now? Allow $\mathbb{Q}[\tau]$? Write $x = \gamma(a+\tau b)$ and $y = \delta(c+\tau d)$ with $a,b,c,d \in \mathbb{Z}$ and $\gamma,\delta \in \mathbb{Q}$. Need $\boxed{\gamma\delta = \frac{4}{3}}$, then can recycle integer solution

Extension along a five-fold axis T_5

$$\boxed{\alpha_1 = (0,1,0),\ \alpha_2 = -\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3 = (0,0,1)}$$

$$\boxed{T_5 = (\tau,-1,0)} \qquad A = \begin{pmatrix} 2 & x & 0 & 0 \\ y & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix} \qquad \boxed{xy = \frac{4}{5}(3-\tau)}$$

Same solution (two series) as before in the case of H_2, but this time with the additional degree of freedom.

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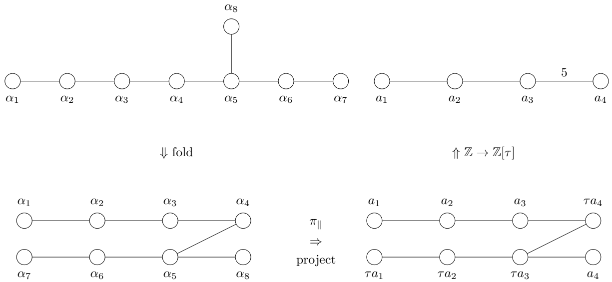
Projection and Diagram Foldings



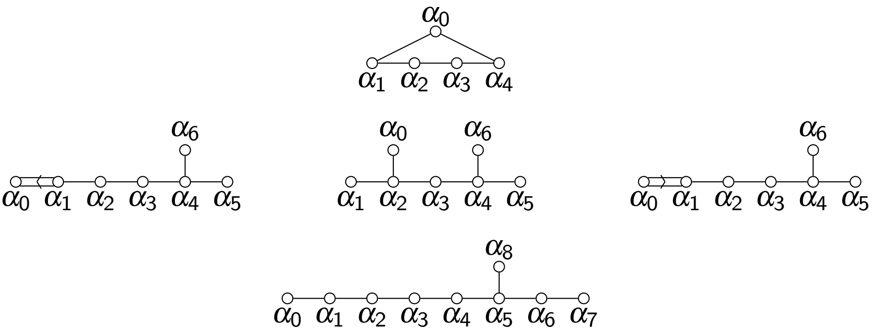
$$\boxed{s_{\beta_1} = s_{\alpha_1} s_{\alpha_7},\ s_{\beta_2} = s_{\alpha_2} s_{\alpha_6},\ s_{\beta_3} = s_{\alpha_3} s_{\alpha_5},\ s_{\beta_4} = s_{\alpha_4} s_{\alpha_8} \Rightarrow H_4}$$

E_8 has two H_4-invariant subspaces – blockdiagonal form

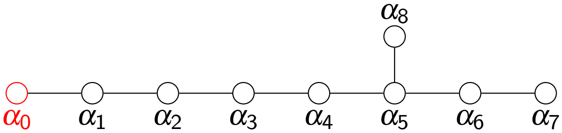
D_6 has two H_3-invariant subspaces

A_4 has two H_2-invariant subspaces

Recap: Affine extensions of crystallographic groups



Affine extensions – $E_8^{=}$

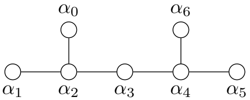


$$\boxed{-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8}$$

AKA E_8^{+} and along with E_8^{++} and E_8^{+++} thought to be the underlying symmetry of String and M-theory

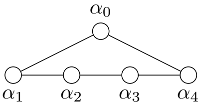
Also interesting from a pure mathematics point of view: E_8 lattice, McKay correspondence and Monstrous Moonshine.

Affine extensions – simply-laced $D_6^{=}$, $A_4^{=}$



$$A\left(D_6^{=}\right) = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

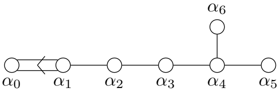
$$\boxed{-\alpha_0 = \alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6}$$



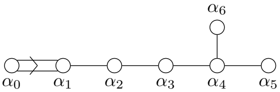
$$A\left(A_4^{=}\right) = \begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

$$\boxed{-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4}$$

Affine extensions – $D_6^<$ and $D_6^>$



$$A(D_6^<) = \begin{pmatrix} 2 & -2 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$



$$A(D_6^>) = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ -2 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

$$\boxed{-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \frac{1}{2}\alpha_5 + \frac{1}{2}\alpha_6}$$

$$\boxed{-\alpha_0 = 2\alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6}$$

Induced affine roots: $H_4^=$ from $E_8^=$

$$\boxed{-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8}$$

$$\boxed{-a_0 = \pi_{\parallel}(-\alpha_0) = 2(1+\tau)a_1 + (3+4\tau)a_2 + 2(2+3\tau)a_3 + (3+5\tau)a_4}$$

$$\boxed{(a_1|a_2) = -\frac{1}{2},\ (a_2|a_3) = -\frac{1}{2},\ (a_3|a_4) = -\frac{\tau}{2}},$$

$$A(H_4^=) := \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix}$$

induced affine root of lengths τ and $1/\tau$ along the highest root $\alpha_H = (1,0,0,0)$ of H_4

Induced affine extensions: $H_i^=$ from $A_4^=$, $D_6^=$ and $E_8^=$

affine extensions of lengths τ and $1/\tau$ along the highest root α_H of H_i

$$A(H_4^=) := \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^=) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_2^=) := \begin{pmatrix} 2 & \tau-2 & \tau-2 \\ -1 & 2 & -\tau \\ -1 & -\tau & 2 \end{pmatrix}$$

Induced affine extensions: three H_3^+ from D_6^+

$$A(H_3^=) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

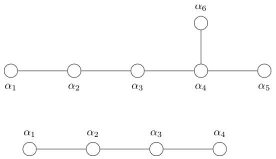
$$A(H_3^<) := \begin{pmatrix} 2 & \frac{4}{5}(\tau-3) & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

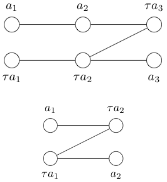
$$A(H_3^>) := \begin{pmatrix} 2 & \frac{2}{5}(\tau-3) & 0 & 0 \\ -2 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

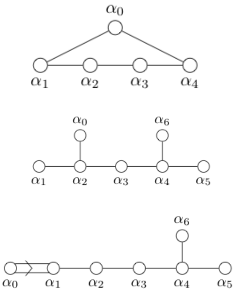
Comparison with DBT1

- H_i^{aff} was the symmetric special case of the Fibonacci 'family' of solutions
- $H_i^{=}$ induced by projection of the affine extensions $E_8^{=}$, $D_6^{=}$, $A_4^{=}$ is the 'first asymmetric case'
- Achieved by scaling the symmetric solution of H_i^{aff} by (τ, τ^{-1})
- Projection from $D_6^{<}$ and $D_6^{>}$ give extensions along 5-fold axes of icosahedral symmetry, from $D_6^{=}$ along 2-fold axes
- These are exactly what we were looking for for icosahedral applications!

Invariance under Dynkin diagram automorphisms







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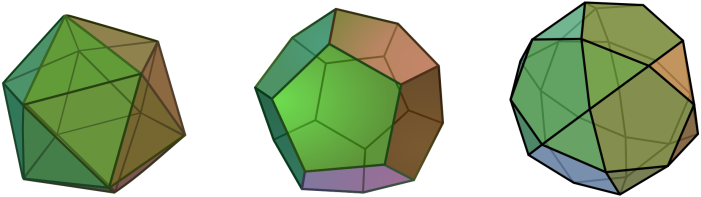
Overview

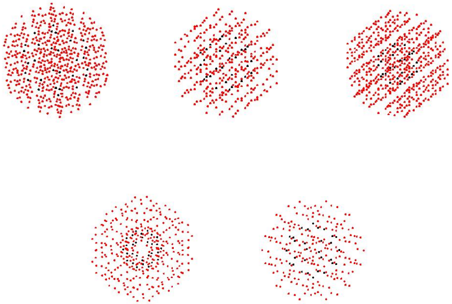
Extend icosahedral group with distinguished translations

- Radial layers are simultaneously constrained by affine symmetry
- Works very well in practice: finite library of blueprints
- Select blueprint from the outer shape (capsid)
- Can predict inner structure (nucleic acid distribution) of the virus from the point array



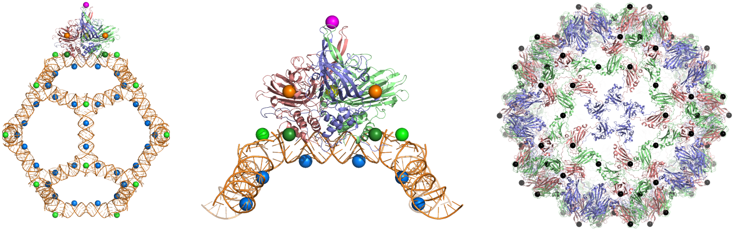
Affine extensions of the icosahedral group (giving translations) and their classification.

What’s the point?



Use in Mathematical Virology

- Suffice to say point arrays work very exceedingly well in practice. Two papers on the mathematical (Coxeter) aspects.
- Implemented computational problem in Clifford – some very interesting mathematics comes out as well (see paper 'Platonic solids generate their 4-dimensional analogues').



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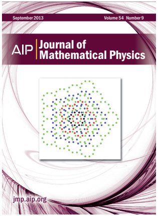

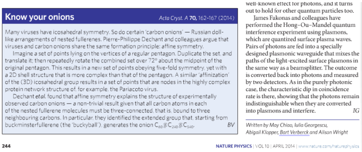

Know your onions *Acta Cryst. A* **70,** 162-167 (2014)

Many viruses have icosahedral symmetry. So do certain 'carbon onions' — Russian doll-like arrangements of nested fullerenes. Pierre-Philippe Dechant and colleagues argue that viruses and carbon onions share the same formation principle: affine symmetry.

Imagine a set of points lying on the vertices of a regular pentagon. Duplicate the set, and translate it; then repeatedly rotate the combined set over 72° about the midpoint of the original pentagon. This results in a new set of points obeying five-fold symmetry, yet with a 2D shell structure that is more complex than that of the pentagon. A similar 'affinization' of the (3D) icosahedral group results in a set of points that are nodes in the highly complex protein network structure of, for example, the Pariacoto virus.

Dechant *et al.* found that affine symmetry explains the structure of experimentally observed carbon onions — a non-trivial result given that all carbon atoms in each of the nested fullerene molecules must be three-connected, that is, bound to three neighbouring carbons. In particular, they identified the extended group that, starting from buckminsterfullerene (the 'buckyball'), generates the onion $C_{60}@C_{240}@C_{540}$. *BV*

well-known effect for photons, and it turns out to hold for other quantum particles too.

James Fakonas and colleagues have performed the Hong–Ou–Mandel quantum interference experiment using plasmons, which are quantized surface plasma waves. Pairs of photons are fed into a specially designed plasmonic waveguide that mixes the paths of the light-excited surface plasmons in the same way as a beamsplitter. The outcome is converted back into photons and measured by two detectors. As in the purely photonic case, the characteristic dip in coincidence rate is there, showing that the photons remain indistinguishable when they are converted into plasmons and interfere. *IG*

Written by May Chiao, Iulia Georgescu, Abigail Klopper, Bart Verberck and Alison Wright

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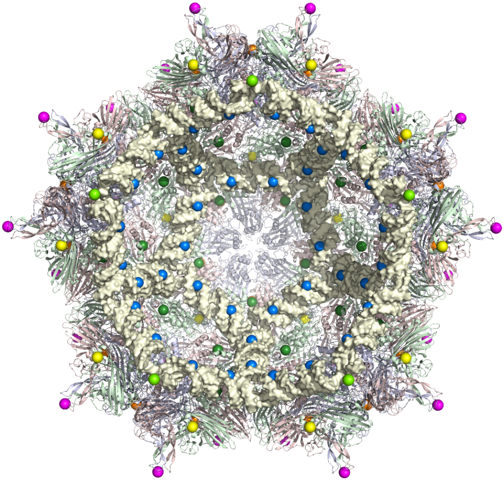
Use in Mathematical Virology

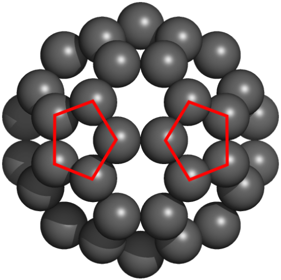


Overview

1. Affine extensions
   - Direct extensions
   - Induced extensions
2. Applications
   - Virus Structure
   - Fullerenes and Carbon onions
3. A 3D spinorial view of 4D exceptional phenomena
4. Conclusions

Constraints of carbon chemistry

- Relevant carbon bonding here is trivalent
- Bond lengths and angles need to be pretty uniform
- For example, the well-known football-shaped Buckyball C_{60}

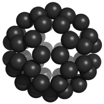


Strategy

- Extend icosahedral shapes with a translation and take orbit under the compact group
- Select outer shells that are three-coordinated and uniform enough
- For the usual icosahedron, dodecahedron, icosidodecahedron find few not very interesting possibilities
- For C_{60} and C_{80} start, get a unique extension that exactly give the known carbon onions $C_{60} - C_{240} - C_{540}$ and $C_{80} - C_{180} - C_{320}$

Fullerene cages derived from C_{60}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{60}: carbon onion $(C_{60} - C_{240} - C_{540})$



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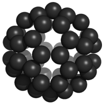

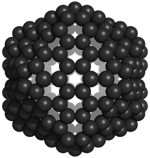

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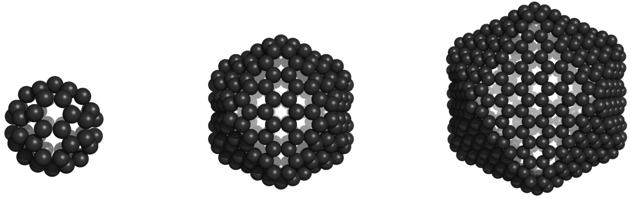
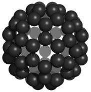


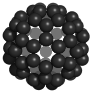
Fullerene cages derived from C_{80}

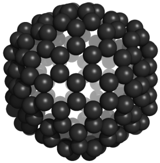
- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{80}: carbon onion $(C_{80} - C_{180} - C_{320})$



Fullerene cages derived from C_{80}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{80}: carbon onion $(C_{80} - C_{180} - C_{320})$





Fullerene cages derived from C_{80}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
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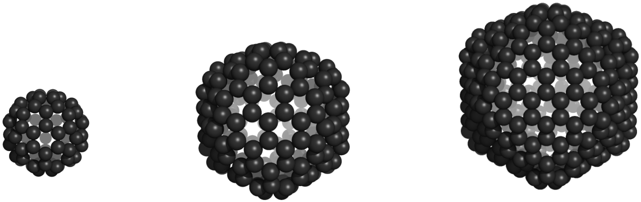
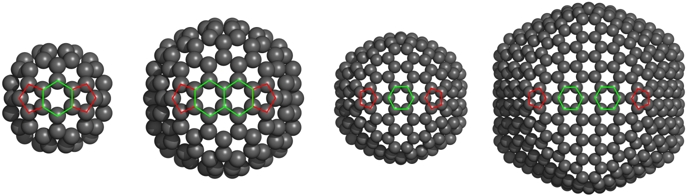


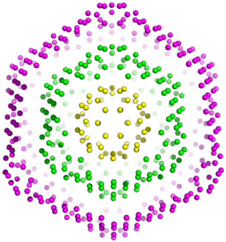
Growth of shells by a hexamer at a time

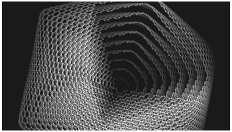
- Hence, for C_{60} and C_{80} start, get a unique extension that exactly give the known carbon onions $C_{60} - C_{240} - C_{540}$ and $C_{80} - C_{180} - C_{320}$ by inserting an additional hexamer at each step



Viruses and fullerenes – symmetry as a common thread?

- Get nested arrangements like Russian dolls: carbon onions (e.g. June: Nature 510, 250253)
- Potential to extend to other known carbon onions with different start configuration, chirality etc





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- Affine extensions of non-crystallographic Coxeter groups induced by projection with Twarock/Bœhm Journal of Mathematical Physics 54 093508 (2013), Cover article September
- Viruses and Fullerenes – Symmetry as a Common Thread? with Twarock/Wardman/Keef Acta Crystallographica A 70 (2). pp. 162-167 (2014), Cover article March, Nature Physics Research Highlight

References (single-author)

- Clifford algebra unveils a surprising geometric significance of quaternionic root systems of Coxeter groups
  Advances in Applied Clifford Algebras 23 (2). pp. 301-321 (2013)
- A Clifford algebraic framework for Coxeter group theoretic computations (Conference Prize at AGACSE 2012)
  Advances in Applied Clifford Algebras 24 (1). pp. 89-108 (2014)
- Rank-3 root systems induce root systems of rank 4 via a new Clifford spinor construction Journal of Physics (2015) – accepted today!
- Platonic Solids generate their 4-dimensional analogues
  Acta Cryst. A69 (2013)

3D vs 4D

- Have A_n, B_n and D_n families of root systems in any dimension
- In 3D, have H_3 as an accident (icosahedron and dodecahedron)
- In 4D, have F_4 and H_4 (and in some sense D_4) as accidents
- These 4D accidents have unusual automorphism groups
- Can induce all of these from the 3D cases, show they are root systems and explain their automorphism groups

Clifford Algebra and orthogonal transformations

- Form an algebra using the Geometric Product for two vectors

$$\boxed{ab \equiv a \cdot b + a \wedge b}$$

- Inner product is symmetric $a \cdot b = \frac{1}{2}(ab + ba)$
- Reflecting a in b is given by $\boxed{a' = a - 2(a \cdot b)b = -bab}$ (b and $-b$ doubly cover the same reflection)
- Via Cartan-Dieudonné theorem any orthogonal transformation can be written as successive reflections

$$\boxed{x' = \pm n_1 n_2 \ldots n_k x n_k \ldots n_2 n_1} = \pm A x \tilde{A}$$

Clifford Algebra of 3D

- E.g. Pauli algebra in 3D (likewise for Dirac algebra in 4D) is

$$\underbrace{\{1\}}_{\text{1 scalar}} \quad \underbrace{\{e_1, e_2, e_3\}}_{\text{3 vectors}} \quad \underbrace{\{e_1e_2, e_2e_3, e_3e_1\}}_{\text{3 bivectors}} \quad \underbrace{\{I \equiv e_1e_2e_3\}}_{\text{1 trivector}}$$

- We can form the elements of the Coxeter groups by multiplying together root vectors in this algebra $\alpha_i\alpha_j\dots$
- In general get something with 8 components, here restrict to even products (rotations/spinors) with four components:

$$\boxed{R = a_0 + a_1e_2e_3 + a_2e_3e_1 + a_3e_1e_2 \Rightarrow R\tilde{R} = a_0^2 + a_1^2 + a_2^2 + a_3^2}$$

- So behaves as a 4D Euclidean object – norm $(R_1, R_2) = \frac{1}{2}(R_2\tilde{R}_1 + R_1\tilde{R}_2)$

Induction Theorem – root systems

- Theorem: 3D spinor groups give 4D root systems.

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- Check axioms:
  1. $\boxed{\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \ \forall\, \alpha \in \Phi}$
  2. $\boxed{s_\alpha \Phi = \Phi \ \forall\, \alpha \in \Phi}$

Induction Theorem – root systems

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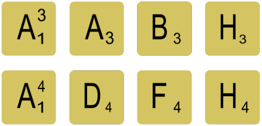
  1. $\boxed{\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \ \forall \alpha \in \Phi}$
  2. $\boxed{s_\alpha \Phi = \Phi \ \forall \alpha \in \Phi}$
- Proof: 1. R and $-R$ are in a spinor group by construction (double cover of orthogonal transformations), 2. closure under reflections is guaranteed by the closure property of the spinor group (with a twist: $-R_1\tilde{R}_2R_1$)
- Induction Theorem: Every rank-3 root system induces a rank-4 root system (and thereby Coxeter groups)
- Counterexample: not every rank-4 root system is induced in this way

Spinors from reflections

- The 3D Coxeter groups that are symmetry groups of the Platonic Solids:
- The 6 reflections in $A_1 \times A_1 \times A_1$ generate 8 spinors.
- $\pm e_1$, $\pm e_2$, $\pm e_3$ give the 8 spinors $\pm 1, \pm e_1 e_2, \pm e_2 e_3, \pm e_3 e_1$
- The discrete spinor group is isomorphic to the quaternion group Q.

Spinors from reflections

- The 3D Coxeter groups that are symmetry groups of the Platonic Solids:
- The 6/12/18/30 reflections in $A_1 \times A_1 \times A_1/A_3/B_3/H_3$ generate 8/24/48/120 spinors.
- E.g. $\pm e_1$, $\pm e_2$, $\pm e_3$ give the 8 spinors $\pm 1, \pm e_1 e_2, \pm e_2 e_3, \pm e_3 e_1$
- The discrete spinor group is isomorphic to the quaternion group Q / binary tetrahedral group $2T$/ binary octahedral group $2O$/ binary icosahedral group $2I$).

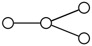


Exceptional Root Systems

- The 16-cell, 24-cell, 24-cell and dual 24-cell and the 600-cell are in fact the root systems of $A_1 \times A_1 \times A_1 \times A_1$, D_4, F_4 and H_4
- Exceptional phenomena: D_4 (triality, important in string theory), F_4 (largest lattice symmetry in 4D), H_4 (largest non-crystallographic symmetry)
- Exceptional D_4 and F_4 arise from series A_3 and B_3
- In fact, as we have seen one can strengthen this statement on inducing polytopes to a statement on inducing root systems

Root systems in three and four dimensions

The spinors generated from the reflections contained in the respective rank-3 Coxeter group via the geometric product are realisations of the binary polyhedral groups Q, $2T$, $2O$ and $2I$, which were known to generate (mostly exceptional) rank-4 groups, but not known why, and why the 'mysterious symmetries'.

rank-3 group	diagram	binary	rank-4 group	diagram
$A_1 \times A_1 \times A_1$	$\circ \quad \circ \quad \circ$	Q	$A_1 \times A_1 \times A_1 \times A_1$	$\circ \quad \circ \quad \circ \quad \circ$
A_3	$\circ - \circ - \circ$	$2T$	D_4	
B_3	$\circ - \circ \overset{4}{-} \circ$	$2O$	F_4	$\circ - \circ \overset{4}{-} \circ - \circ$
H_3	$\circ - \circ \overset{5}{-} \circ$	$2I$	H_4	$\circ - \circ - \circ \overset{5}{-} \circ$

Induction Theorem – automorphism

- So induced 4D polytopes are actually root systems.
- Clear why the number of roots $|\Phi|$ is equal to $|G|$, the order of the spinor group
- Spinor group is trivially closed under conjugation, left and right multiplication. Results in non-trivial symmetries when viewed as a polytope/root system.
- Now explains symmetry of the polytopes/root system and thus the order of the rank-4 Coxeter group
- Theorem: The automorphism group of the induced root system contains two factors of the respective spinor group acting from the left and the right.

Spinorial Symmetries of 4D Polytopes

Spinorial symmetries

rank 3	$\|\Phi\|$	$\|W\|$	rank 4	$\|\Phi\|$	Symmetry
A_3	12	24	D_4 24-cell	24	$2 \cdot 24^2 = 576$
B_3	18	48	F_4 lattice	48	$48^2 = 2304$
H_3	30	120	H_4 600-cell	120	$120^2 = 14400$
A_1^3	6	8	A_1^4 16-cell	8	$3! \cdot 8^2 = 384$
$A_1 \oplus A_2$	8	12	$A_2 \oplus A_2$ prism	12	$12^2 = 144$
$A_1 \oplus H_2$	12	20	$H_2 \oplus H_2$ prism	20	$20^2 = 400$
$A_1 \oplus I_2(n)$	$n+2$	$2n$	$I_2(n) \oplus I_2(n)$	$2n$	$(2n)^2$

Similar for Grand Antiprism (H_4 without $H_2 \oplus H_2$) and Snub 24-cell ($2I$ without $2T$). Additional factors in the automorphism group come from 3D Dynkin diagram symmetries!

Some non-Platonic examples of spinorial symmetries

- Grand Antiprism: the 100 vertices achieved by subtracting 20 vertices of $H_2 \oplus H_2$ from the 120 vertices of the H_4 root system 600-cell – two separate orbits of $H_2 \oplus H_2$
- This is a semi-regular polytope with automorphism symmetry $\mathrm{Aut}(H_2 \oplus H_2)$ of order $400 = 20^2$
- Think of the $H_2 \oplus H_2$ as coming from the doubling procedure? (Likewise for $\mathrm{Aut}(A_2 \oplus A_2)$ subgroup)
- Snub 24-cell: $2T$ is a subgroup of $2I$ so subtracting the 24 corresponding vertices of the 24-cell from the 600-cell, one gets a semiregular polytope with 96 vertices and automorphism group $2T \times 2T$ of order $576 = 24^2$.

Arnold's Trinities

Arnold's observation that many areas of real mathematics can be complexified and quaternionified resulting in theories with a similar structure.

- The fundamental trinity is thus $(\mathbb{R}, \mathbb{C}, \mathbb{H})$
- The projective spaces $(\mathbb{R}P^n, \mathbb{C}P^n, \mathbb{H}P^n)$
- The spheres $(\mathbb{R}P^1 = S^1, \mathbb{C}P^2 = S^2, \mathbb{H}P^1 = S^4)$
- The Möbius/Hopf bundles $(S^1 \rightarrow S^1, S^4 \rightarrow S^2, S^7 \rightarrow S^4)$
- The Lie Algebras (E_6, E_7, E_8)
- The symmetries of the Platonic Solids (A_3, B_3, H_3)
- The 4D groups (D_4, F_4, H_4)
- New connections via my Clifford spinor construction (see McKay correspondence)

Platonic Trinities

- Arnold's connection between (A_3, B_3, H_3) and (D_4, F_4, H_4) is very convoluted and involves numerous other trinities at intermediate steps:
- Decomposition of the projective plane into Weyl chambers and Springer cones
- The number of Weyl chambers in each segment is $24 = 2(1+3+3+5), 48 = 2(1+5+7+11), 120 = 2(1+11+19+29)$
- Notice this miraculously matches the quasihomogeneous weights $((2,4,4,6),(2,6,8,12),(2,12,20,30))$ of the Coxeter groups (D_4, F_4, H_4)
- Believe the Clifford connection is more direct

A unified framework for polyhedral groups

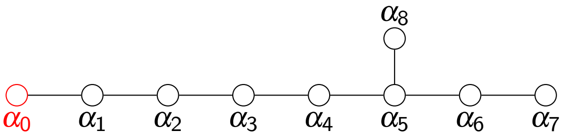
Group	Discrete subgroup	Action Mechanism
$SO(3)$	rotational (chiral)	$x \to \tilde{R}xR$
$O(3)$	reflection (full/Coxeter)	$x \to \pm\tilde{A}xA$
$\mathrm{Spin}(3)$	binary	$(R_1, R_2) \to R_1R_2$
$\mathrm{Pin}(3)$	pinor	$(A_1, A_2) \to A_1A_2$

- e.g. the chiral icosahedral group has 60 elements, encoded in Clifford by 120 spinors, which form the binary icosahedral group
- together with the inversion/pseudoscalar I this gives 60 rotations and 60 rotoinversions, i.e. the full icosahedral group H_3 in 120 elements (with 240 pinors)
- all three are interesting groups, e.g. in neutrino and flavour physics for family symmetry model building

Some Group Theory: chiral, full, binary, pin

- Easy enough to calculate conjugacy classes etc of pinors in Clifford algebra
- Chiral (binary) polyhedral groups have irreps
- tetrahedral (12/24): 1, $1'$, $1''$, 2_s, $2_s'$, $2_s''$, 3
- octahedral (24/48): 1, $1'$, 2, 2_s, $2_s'$, 3, $3'$, 4_s
- icosahedral (60/120): 1, 2_s, $2_s'$, 3, $\bar{3}$, 4, 4_s, 5, 6_s
- Binary groups are discrete subgroups of $SU(2)$ and all thus have a 2_s spinor irrep
- Connection with the McKay correspondence!

Affine extensions – $E_8^{=}$

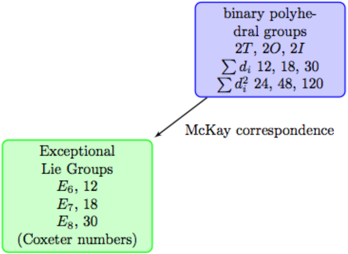


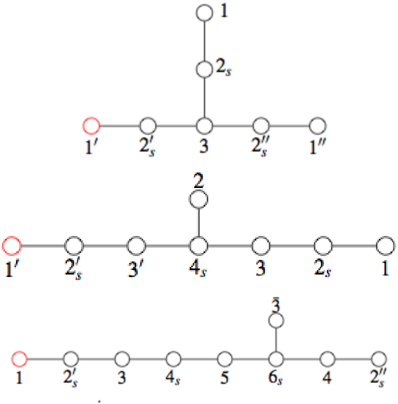
$$\boxed{-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8}$$

AKA E_8^{+} and along with E_8^{++} and E_8^{+++} thought to be the underlying symmetry of String and M-theory

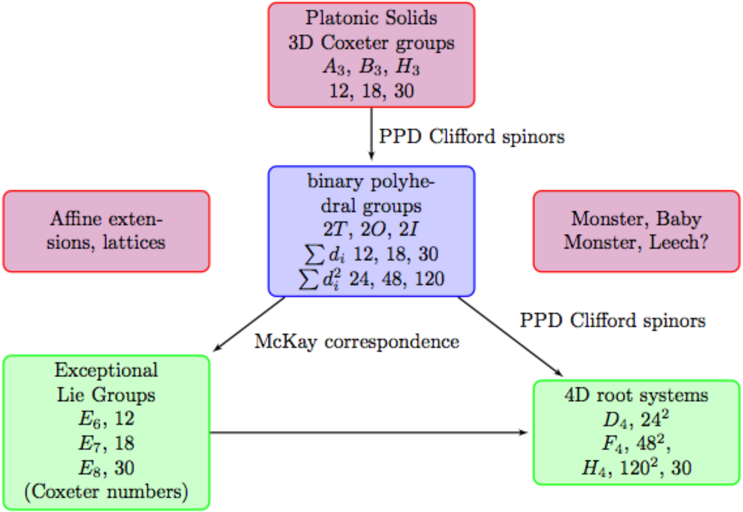
Also interesting from a pure mathematics point of view: E_8 lattice, McKay correspondence and Monstrous Moonshine.

The McKay Correspondence





The McKay Correspondence



The McKay Correspondence

More than E-type groups: the infinite family of 2D groups, the cyclic and dicyclic groups are in correspondence with A_n and D_n, e.g. the quaternion group Q and D_4^+. So McKay correspondence not just a trinity but ADE-classification. We also have $I_2(n)$ on top of the trinity (A_3, B_3, H_3)

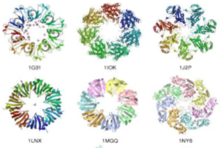
rank-3 group	diagram	binary	rank-4 group	diagram	Lie algebra	diagram
$A_1 \times A_1 \times A_1$		Q	$A_1 \times A_1 \times A_1 \times A_1$		D_4^+	
A_3		$2T$	D_4		E_6^+	
B_3	4	$2O$	F_4	4	E_7^+	
H_3	5	$2I$	H_4	5	E_8^+	

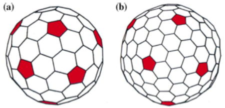
4D geometry is surprisingly important for HEP

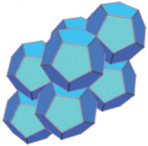
- 4D root systems are surprisingly relevant to HEP
- A_4 is $SU(5)$ and comes up in Grand Unification
- D_4 is $SO(8)$ and is the little group of String theory
- In particular, its triality symmetry is crucial for showing the equivalence of RNS and GS strings
- B_4 is $SO(9)$ and is the little group of M-Theory
- F_4 is the largest crystallographic symmetry in 4D and H_4 is the largest non-crystallographic group
- The above are subgroups of the latter two
- Spinorial nature of the root systems could have surprising consequences for HEP

Conclusions

- Novel mathematical structures – Interesting in their own right
- Numerous applications to real systems: Viruses, Proteins, Fullerenes, Quasicrystals, Tilings, Packings etc.
- Potential applications to engineering and medicine: nanotechnology and drug delivery
- Novel connection between geometry of 3D and 4D
- In fact, 3D seems more fundamental – contrary to the usual perspective of 3D subgroups of 4D groups
- Clear why spinor group gives a root system and why two factors of the same group reappear in the automorphism group







Thank you!