

Est.
1841

YORK
ST JOHN
UNIVERSITY

Dechant, Pierre-Philippe ORCID

logoORCID: <https://orcid.org/0000-0002-4694-4010> (2014) Recent developments in affine symmetry principles for non-crystallographic systems. In: Open Statistical Physics Annual Meeting, 26th March 2014, Open University, Milton Keynes. (Unpublished)

Downloaded from: <https://ray.yorks.ac.uk/id/eprint/4021/>

Research at York St John (RaY) is an institutional repository. It supports the principles of open access by making the research outputs of the University available in digital form. Copyright of the items stored in RaY reside with the authors and/or other copyright owners. Users may access full text items free of charge, and may download a copy for private study or non-commercial research. For further reuse terms, see licence terms governing individual outputs. [Institutional Repository Policy Statement](#)

RaY

Research at the University of York St John

For more information please contact RaY at ray@yorks.ac.uk



Recent developments in affine symmetry principles for non-crystallographic systems

Pierre-Philippe Dechant

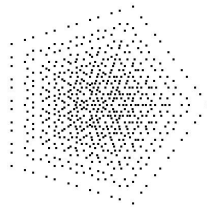
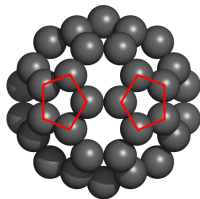
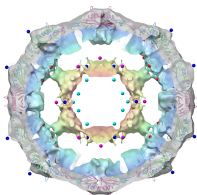
Mathematics Department, Durham University

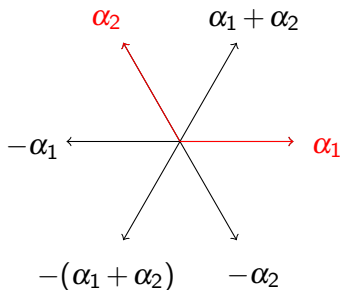
Open Statistical Physics Annual Meeting – March 26, 2014

- 1 Affine extensions
 - Direct extensions
 - Induced extensions
- 2 Applications
 - Virus Structure
 - Fullerenes and Carbon onions
- 3 Conclusions

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**



Root systems – A_2 

Root system Φ : set of vectors α such that

$$\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \quad \forall \alpha \in \Phi$$

and $s_\alpha \Phi = \Phi \quad \forall \alpha \in \Phi$

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_i s is $A_{ij} = 2 \frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2 \frac{|\alpha_j|}{|\alpha_i|} \cos \theta_{ij}$

Cartan Matrices

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

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

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

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

Cartan Matrices

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

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

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

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

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

$$A_2 \circ \text{---} \circ \quad H_2 \circ \overset{5}{\text{---}} \circ \quad I_2(n) \circ \overset{n}{\text{---}} \circ$$

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 $(s_i s_j)^{m_{ij}} = 1$ with $m_{ij} = m_{ji} \geq 2$ for $i \neq j$.

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 \mathcal{E} . In particular, let $(\cdot|\cdot)$ denote the inner product in \mathcal{E} , and $v, \alpha \in \mathcal{E}$.

The **generator** s_α corresponds to the **reflection**

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

at a hyperplane perpendicular to the **root vector** α .

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

Affine extensions

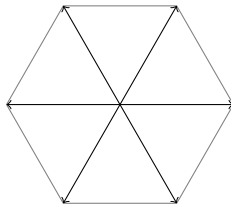
An **affine Coxeter group** is the extension of a Coxeter group by an **affine reflection in a hyperplane not containing the origin** $s_{\alpha_0}^{aff}$ whose geometric action is given by

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

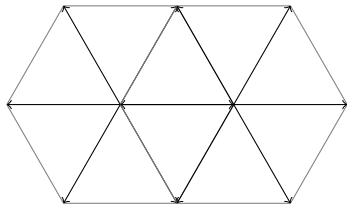
Non-distance preserving: includes the **translation generator**

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

Affine extensions – A_2

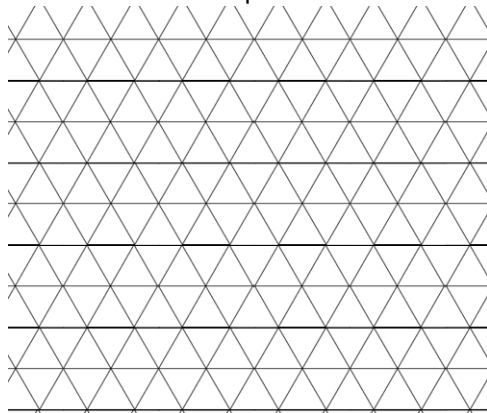


Affine extensions – A_2

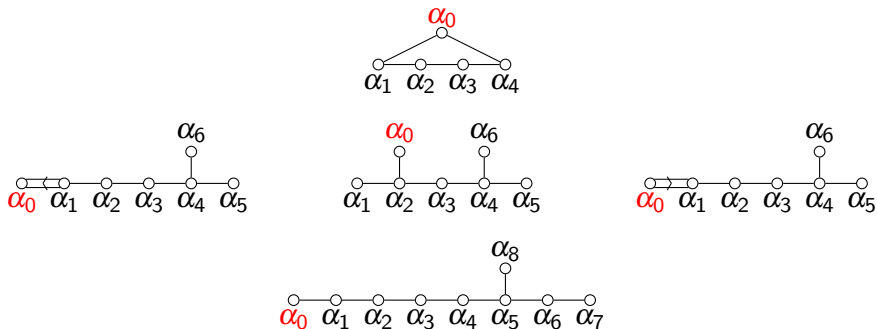


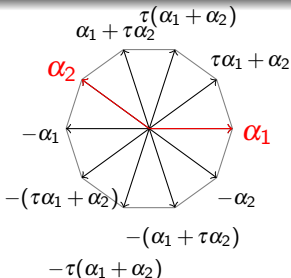
Affine extensions – A_2

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

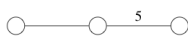


Affine extensions of crystallographic groups A_4 , D_6 and E_8



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**

$$\mathbb{Z}[\tau] = \{a + \tau b \mid a, b \in \mathbb{Z}\} \quad \text{golden ratio}$$

$$\tau = \frac{1}{2}(1 + \sqrt{5}) = 2 \cos \frac{\pi}{5}$$

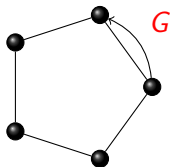
$$x^2 = x + 1$$

$$\tau' = \sigma = \frac{1}{2}(1 - \sqrt{5}) = 2 \cos \frac{2\pi}{5}$$

$$\tau + \sigma = 1, \tau\sigma = -1$$

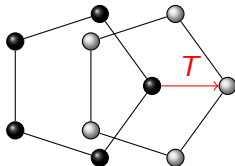
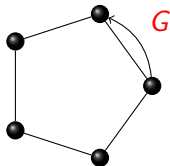
Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



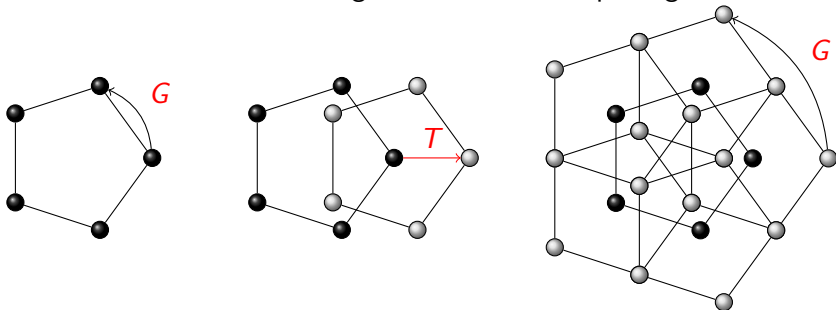
Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



Affine extensions of non-crystallographic root systems

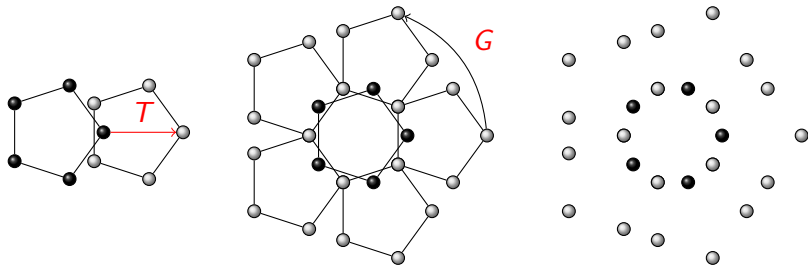
Unit translation along a vertex of a unit pentagon



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

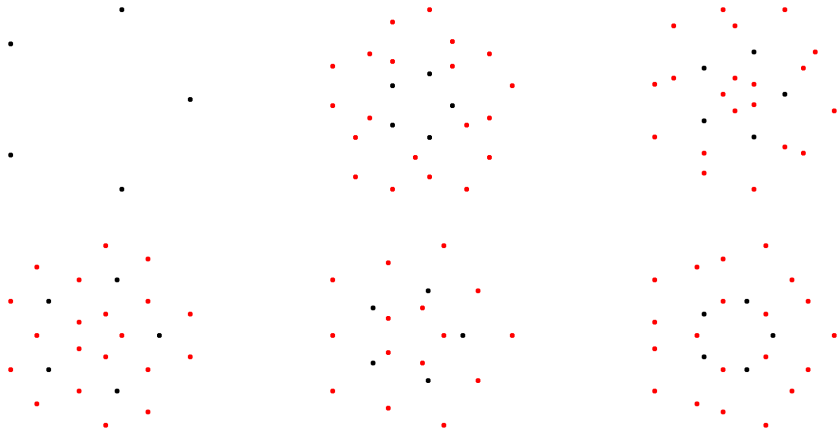
Affine extensions of non-crystallographic root systems

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



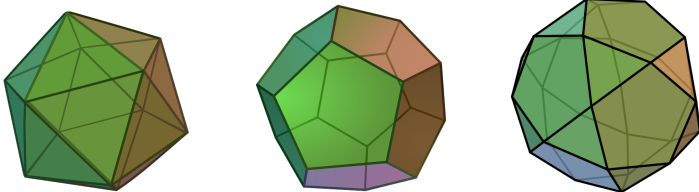
Looks like a **virus** or **carbon onion**

More Blueprints

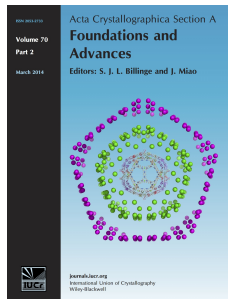
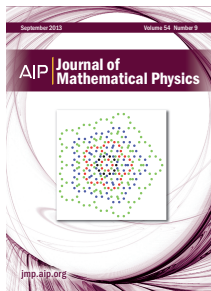


Extend icosahedral group with distinguished translations

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

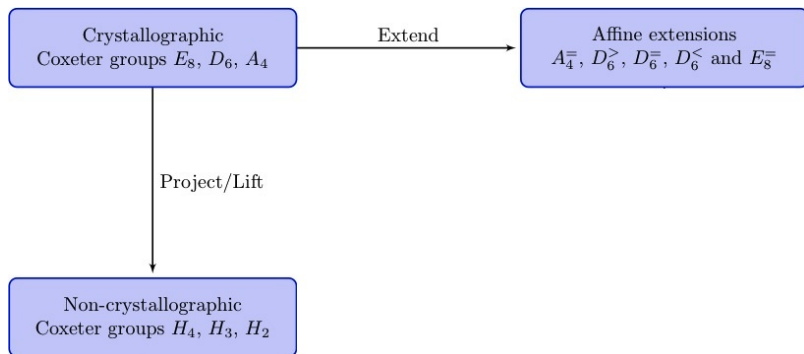


Applications of affine extensions of non-crystallographic root systems

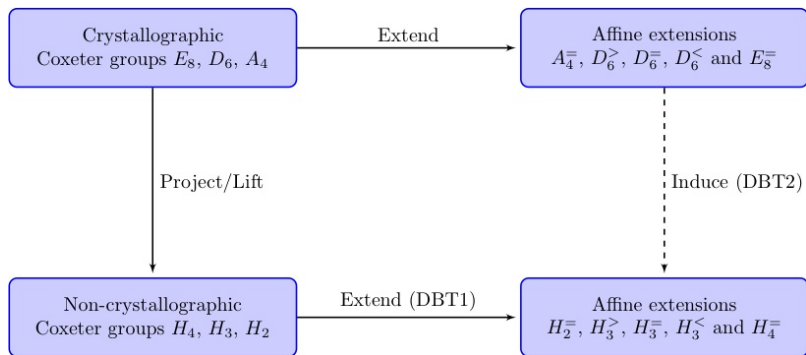


There are interesting applications to **quasicrystals**, **viruses** or **carbon onions** later, concentrate on the **mathematical** aspects for now

Road Map



Road Map



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:

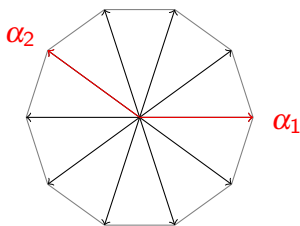
$$A^{aff} = \begin{pmatrix} 2 & \underline{v}^T \\ \underline{w} & A \end{pmatrix} \quad \boxed{A_{ii}^{aff} = 2} \quad \boxed{A_{ij}^{aff} \in \mathbb{Z}[\cdot]}$$

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

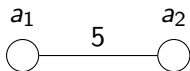
$$\text{determinant constraint } \boxed{\det A^{aff} = 0}$$

Kac-Moody approach to H_2

5

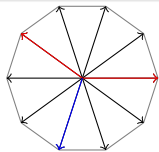


$$\alpha_1 = (1, 0), \quad \alpha_2 = \frac{1}{2}(-\tau, \sqrt{3-\tau})$$



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

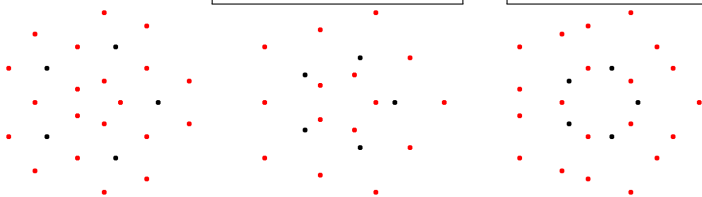
Extension along the highest root



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

$$xy = 2 - \tau = \sigma^2$$

symmetric $x = y = \sigma = 1 - \tau$ recovers H_2^{aff} from Twarock et al
 new asymmetric e.g. $(x, y) = (\tau - 2, -1)$ or $(x, y) = (-1, \tau - 2)$



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 $xy = \sigma^2$
by

scaling $x \rightarrow \tau^{-k}x, y \rightarrow \tau^k y$: xy invariant (giving the **angle**),
but different **lengths** $\sqrt{\frac{x}{y}} \rightarrow \sqrt{\frac{x}{y}}\tau^{-k}$

Fibonacci scaling

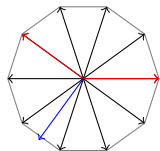
$(a, b; c, d) \rightarrow (b, a + b; d - c, c)$ for multiplication by (τ, τ^{-1}) and

$(a, b; c, d) \rightarrow (b - a, a; d, c + d)$ 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 $x \leftrightarrow y$ generates another solution, but here symmetric

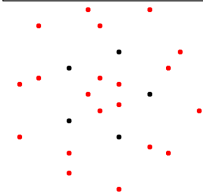
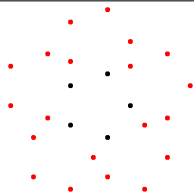
Extension along a bisector



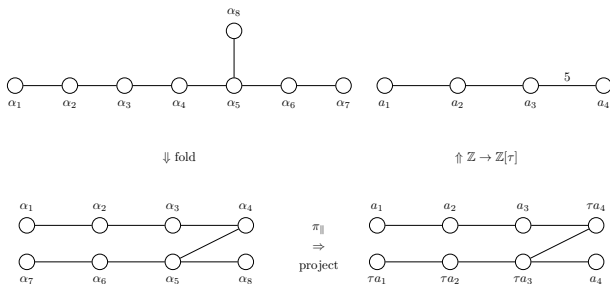
$$A = \begin{pmatrix} 2 & x & 0 \\ y & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$

$$xy = 3 - \tau$$

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



Projection and Diagram Foldings



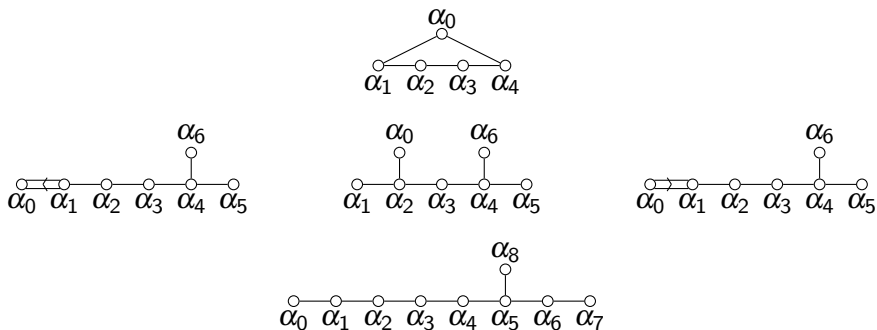
$$s_{\beta_1} = s_{\alpha_1} s_{\alpha_7}, \quad s_{\beta_2} = s_{\alpha_2} s_{\alpha_6}, \quad s_{\beta_3} = s_{\alpha_3} s_{\alpha_5}, \quad s_{\beta_4} = s_{\alpha_4} s_{\alpha_8} \Rightarrow H_4$$

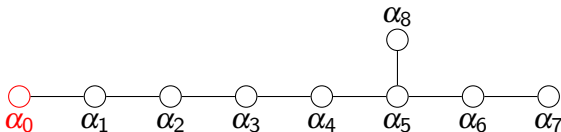
E_8 has two H_4 -invariant subspaces – blockdiagonal form

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^- 

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

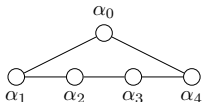
AKA E_8^+ and along with E_8^{++} and E_8^{+++} thought to be the underlying symmetry of **String and M-theory**

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

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

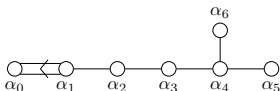
$$A(D_6^=) = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

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

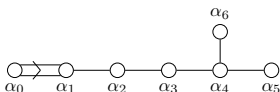


$$A(A_4^=) = \begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

$$-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$$

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

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



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

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

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

Induced affine roots: H_4^- from E_8^-

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

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

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

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

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

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

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

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

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

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

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

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

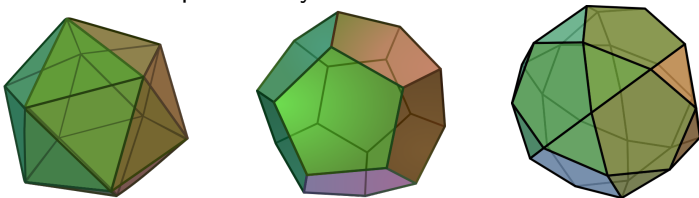
Comparison with DBT1

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

- 1 Affine extensions
 - Direct extensions
 - Induced extensions
- 2 Applications
 - Virus Structure
 - Fullerenes and Carbon onions
- 3 Conclusions

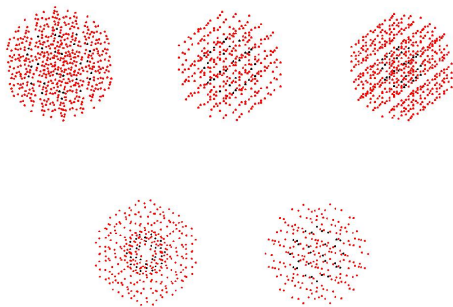
Extend icosahedral group with distinguished translations

- 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



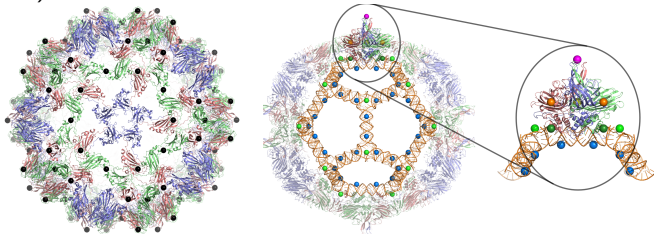
Affine extensions of the icosahedral group (giving translations) and their **classification**.

What's the point?



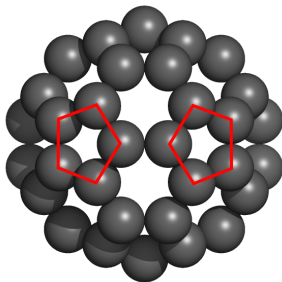
Use in Mathematical Virology

- Suffice to say **point arrays work very exceedingly well** in practice.
- **Implemented computational problem in Clifford algebra** – some **very interesting mathematics** comes out as well (see later).



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 $C_{80} - C_{180} - C_{320}$

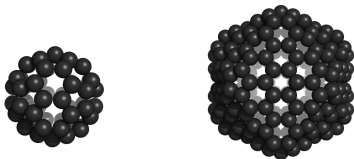
Fullerene cages derived from C_{60}

- 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** ($C_{60} - C_{240} - C_{540}$)



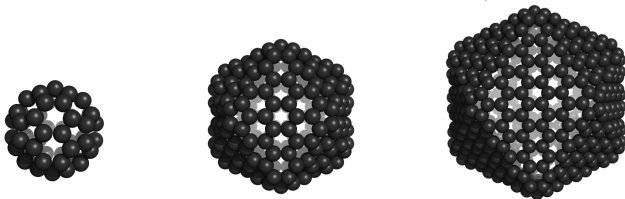
Fullerene cages derived from C_{60}

- 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** ($C_{60} - C_{240} - C_{540}$)



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** ($C_{60} - C_{240} - C_{540}$)



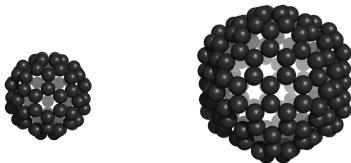
Fullerene cages derived from C_{80}

- 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** ($C_{80} - C_{180} - C_{320}$)



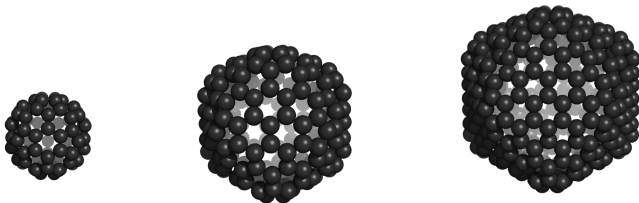
Fullerene cages derived from C_{80}

- 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** ($C_{80} - C_{180} - C_{320}$)



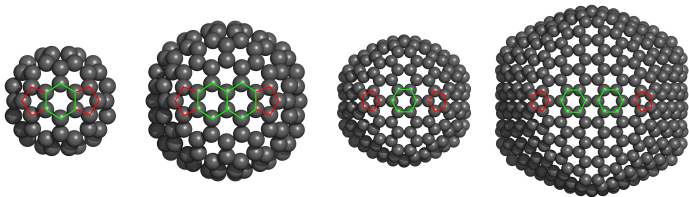
Fullerene cages derived from C_{80}

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



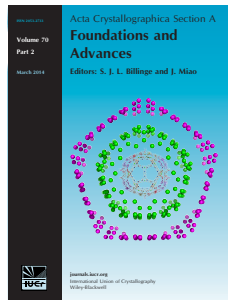
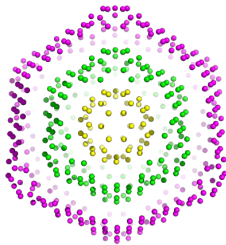
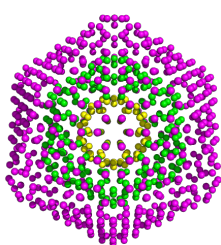
Growth of shells by a hexamer at a time

- 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: **fullerene carbon onions**
- Potential to extend to **other known carbon onions** with different start configuration, chirality etc



References (collaborations)

- **Novel Kac-Moody-type affine extensions of non-crystallographic Coxeter groups** with Twarock/Bøehm
J. Phys. A: Math. Theor. 45 285202 (2012)
- **Affine extensions of non-crystallographic Coxeter groups induced by projection** with Twarock/Bøehm
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](#)

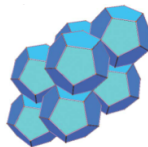
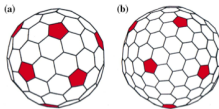
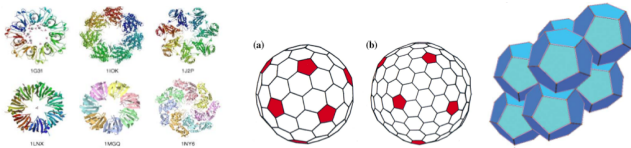
References (single-author)

- 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)
- Nomination for W.K. Clifford Prize (2014)
- 6 month invitation to Arizona State University
- Rank-3 root systems induce root systems of rank 4 via a new Clifford spinor construction arXiv:1207.7339 (2012)
- Platonic Solids generate their 4-dimensional analogues
Acta Cryst. A69 (2013)

- 1 Affine extensions
 - Direct extensions
 - Induced extensions
- 2 Applications
 - Virus Structure
 - Fullerenes and Carbon onions
- 3 Conclusions

Conclusions

- **Novel mathematical structures**
- **Interesting in their own right**
- **Numerous applications to real systems:** Viruses, Proteins, Fullerenes, Quasicrystals, Tilings, Packings etc.



Thank you!

Extension along the highest root – two-fold axis T_2

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

$$T_2 = (1, 0, 0)$$

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

$$xy = \sigma^2 = 2 - \tau$$

Same solution as in the previous case of H_2 .

Extension along a three-fold axis T_3

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

$$T_3 = (\tau, 0, \sigma)$$

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

$$xy = \frac{4}{3}\sigma^2$$

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 $\gamma\delta = \frac{4}{3}$, then can recycle
integer solution

Extension along a five-fold axis T_5

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

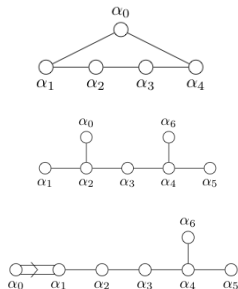
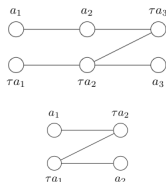
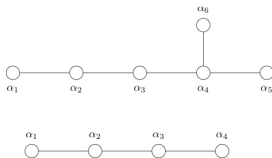
$$T_5 = (\tau, -1, 0)$$

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

$$xy = \frac{4}{5}(3 - \tau)$$

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

Invariance under Dynkin diagram automorphisms



$$-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$$

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

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