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

Pierre-Philippe Dechant

Mathematics Department, Durham University Work with Reidun Twarock (York) and Céline Bœhm (Durham)

30th International Colloquium on Group Theoretical Methods in Physics, Ghent – July 17, 2014

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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



Direct extensions Induced extensions

Root systems – A_2



Root system Φ : set of vectors α such that $\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \ \forall \ \alpha \in \Phi$ and $s_{\alpha}\Phi = \Phi \ \forall \ \alpha \in \Phi$

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

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Direct extensions Induced extensions

Cartan Matrices

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

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Cartan Matrices

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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 $I_j^2 = \frac{A_{ij}}{A_{ji}}I_i^2$
 $A_{ii} = 2$ $A_{ij} \in \mathbb{Z}^{\leq 0}$ $A_{ij} = 0 \Leftrightarrow A_{ji} = 0$.
 A_2 : $A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$

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Cartan Matrices

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 $\overline{A_{ii} = 2}$ $A_{ij} \in \mathbb{Z}^{\leq 0}$ $\overline{A_{ij} = 0 \Leftrightarrow A_{ji} = 0}$.
 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 $\frac{\pi}{m}$.

 $A_2 \sim H_2 \sim H_2 \sim I_2(n) \sim n$

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Direct extensions Induced extensions

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 $m_{ij} = m_{ji} \ge 2$ for $i \ne j$.

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 \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

$$s_{lpha}: v
ightarrow s_{lpha}(v) = v - 2 rac{(v|lpha)}{(lpha|lpha)} lpha$$

at a hyperplane perpendicular to the root vector α . The action of the Coxeter group is to permute these root vectors.



Direct extensions Induced extensions

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

$$s^{aff}_{lpha_0} v = lpha_0 + v - rac{2(lpha_0|v)}{(lpha_0|lpha_0)} lpha_0$$

Non-distance preserving: includes the translation generator

$$Tv = v + lpha_0 = s_{lpha_0}^{aff} s_{lpha_0} v$$

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Affine extensions – A_2



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Affine extensions Applications Conclusions Direct extensions Induced extensions

Affine extensions – A_2

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

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Direct extensions Induced extensions

Affine extensions of crystallographic groups A_4 , D_6 and E_8



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Direct extensions Induced extensions

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







 $H_2 \subset H_3 \subset H_4$: 10, 120, 14,400 elements, the only Coxeter groups that generate rotational symmetries of order 5 linear combinations now in the extended integer ring

$$\mathbb{Z}[\tau] = \{a + \tau b | a, b \in \mathbb{Z}\} \text{ golden ratio} \quad \tau = \frac{1}{2}(1 + \sqrt{5}) = 2\cos\frac{\pi}{5}$$
$$x^2 = x + 1 \quad \tau' = \sigma = \frac{1}{2}(1 - \sqrt{5}) = 2\cos\frac{2\pi}{5} \quad \tau + \sigma = 1, \tau \sigma = -1$$

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Direct extensions Induced extensions

Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



Direct extensions Induced extension

Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



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Direct extensions Induced extensions

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'.

Direct extensions Induced extension

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

Direct extensions Induced extensions

More Blueprints



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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.



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Direct extensions Induced extension

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

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Direct extensions Induced extensions

Road Map



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Road Map



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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:

$$A^{aff} = \begin{pmatrix} 2 & \underline{v}^{T} \\ \underline{w} & A \end{pmatrix} \quad \boxed{A^{aff}_{ii} = 2} \quad \boxed{A^{aff}_{ij} \in \mathbb{Z}[\cdot]}$$
$$\boxed{A^{aff}_{ij} \leq 0} \text{ moreover, } \boxed{A^{aff}_{ij} = 0 \Leftrightarrow A^{aff}_{ji} = 0}$$
$$\boxed{\text{determinant constraint } \det A^{aff} = 0}$$

Direct extensions Induced extensions

Kac-Moody approach to $H_2 \circ 5_{--}$



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

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$$A = egin{pmatrix} 2 & \cdot & \cdot \ \cdot & 2 & - au \ \cdot & - au & 2 \end{pmatrix}$$

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Direct extensions Induced extensions

Extension along the highest root







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).- 4 回 ト 4 ヨ ト 4 ヨ ト

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Fibonacci scaling

The (non-trivial) units in $\mathbb{Z}[\tau]$ are $\tau^k, k \in \mathbb{Z}$ Can generate all solutions to the determinant constraint $|xy = \sigma^2|$ by scaling $x \to \tau^{-k}x, y \to \tau^{k}y$: 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

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Direct extensions Induced extensions

Extension along a bisector



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3 Conclusions

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Conclusions

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Projection and Diagram Foldings



 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

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Direct extensions Induced extensions

Recap: Affine extensions of crystallographic groups



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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.

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Direct extensions Induced extensions

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



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Direct extensions Induced extensions

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



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Direct extensions Induced extensions

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

$$\begin{split} \hline -\alpha_0 &= 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8 \\ \hline -a_0 &= \pi_{\parallel}(-\alpha_0) = 2(1+\tau)a_1 + (3+4\tau)a_2 + 2(2+3\tau)a_3 + (3+5\tau)a_4 \\ \hline (a_1|a_2) &= -\frac{1}{2}, \ (a_2|a_3) = -\frac{1}{2}, \ (a_3|a_4) = -\frac{\tau}{2} \\ A(H_4^{=}) &:= \begin{pmatrix} 2 & \tau - 2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix} \\ \hline \text{induced affine root of lengths } \tau \text{ and } 1/\tau \text{ along the highest root} \\ \alpha_H &= (1,0,0,0) \text{ of } H_4 \end{split}$$

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affine extensions of lengths au and 1/ au along the highest root $lpha_H$ of

$$\begin{array}{l}
H_{i} \\
A(H_{4}^{=}) := \begin{pmatrix} 2 & \tau - 2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix} \\
A(H_{3}^{=}) := \begin{pmatrix} 2 & 0 & \tau - 2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix} \\
A(H_{2}^{=}) := \begin{pmatrix} 2 & \tau - 2 & \tau - 2 \\ -1 & 2 & -\tau \\ -1 & -\tau & 2 \end{pmatrix}$$

Direct extensions Induced extensions

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

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

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Direct extensions Induced extensions

Comparison with DBT1

- *H*^{aff}_i 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!

1 Affine extensions

- Direct extensions
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2 Applications

- Virus Structure
- Fullerenes and Carbon onions

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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.

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Virus Structure Fullerenes and Carbon onions

What's the point?



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Virus Structure Fullerenes and Carbon onions

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 poster 'Platonic solids generate their 4-dimensional analogues').



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Virus Structure Fullerenes and Carbon onions

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 poster 'Platonic solids generate their 4-dimensional analogues').



Know your onions

New visces the cost-body known to, Socie cost-at "calcion origin" — houses calminate and action originate of motion because there which be constrained and actions and the set of the set

breved carbon prices — a non-trivial result given that all carbon abons in each the needed fullement relacules must be three-connected, that is bound to three eightbouring controls. In particular, they identified the extended group that, starting from ucliminsterfullement (the "bodyball") generates the onion $C_{\rm BR} S_{\rm Lino} = 8$

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

Jurne Haloma and colleagues have performed the Halom-Co-Mindel quantum interference experiment using plasmons, which are quantified participations, which are quantified participations, designed plasmonic weregolde that image the designed plasmonic weregolde that image the sourcest ob back in the photons and neosured by two detectors. As in the party photonic case, the characteristic dig to considere case, the characteristic dig to considere indistinguishable when they are convention indistinguishable when they are convention to plasmons and instreter. [7]

Written by May Chias, Iulia Georgesce, Abigal Klapper, <u>Bart Writersk</u> and Alison Wright

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Pierre-Philippe Dechant

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Virus Structure Fullerenes and Carbon onions

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}



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

Virus Structure Fullerenes and Carbon onions

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



Virus Structure Fullerenes and Carbon onions

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







Virus Structure Fullerenes and Carbon onions

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



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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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Virus Structure Fullerenes and Carbon onions

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- 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 arXiv:1207.7339 (2012)
- Platonic Solids generate their 4-dimensional analogues Acta Cryst. A69 (2013)

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



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Thank you!

(For a construction that induces from every rank 3 root system a rank 4 root system via Clifford spinors, see my poster)

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Extension along the highest root – two-fold axis T_2

$$\alpha_{1} = (0,1,0), \ \alpha_{2} = -\frac{1}{2}(-\sigma,1,\tau), \ \alpha_{3} = (0,0,1)$$

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

Same solution as in the previous case of H_2 .

Extension along a three-fold axis T_3

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

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

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

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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

$$\alpha_{1} = (0,1,0), \ \alpha_{2} = -\frac{1}{2}(-\sigma,1,\tau), \ \alpha_{3} = (0,0,1)$$

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

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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Invariance under Dynkin diagram automorphisms



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

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