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5. Classification scheme

A hierarchy of the classification

Dimensions

Symmetry class

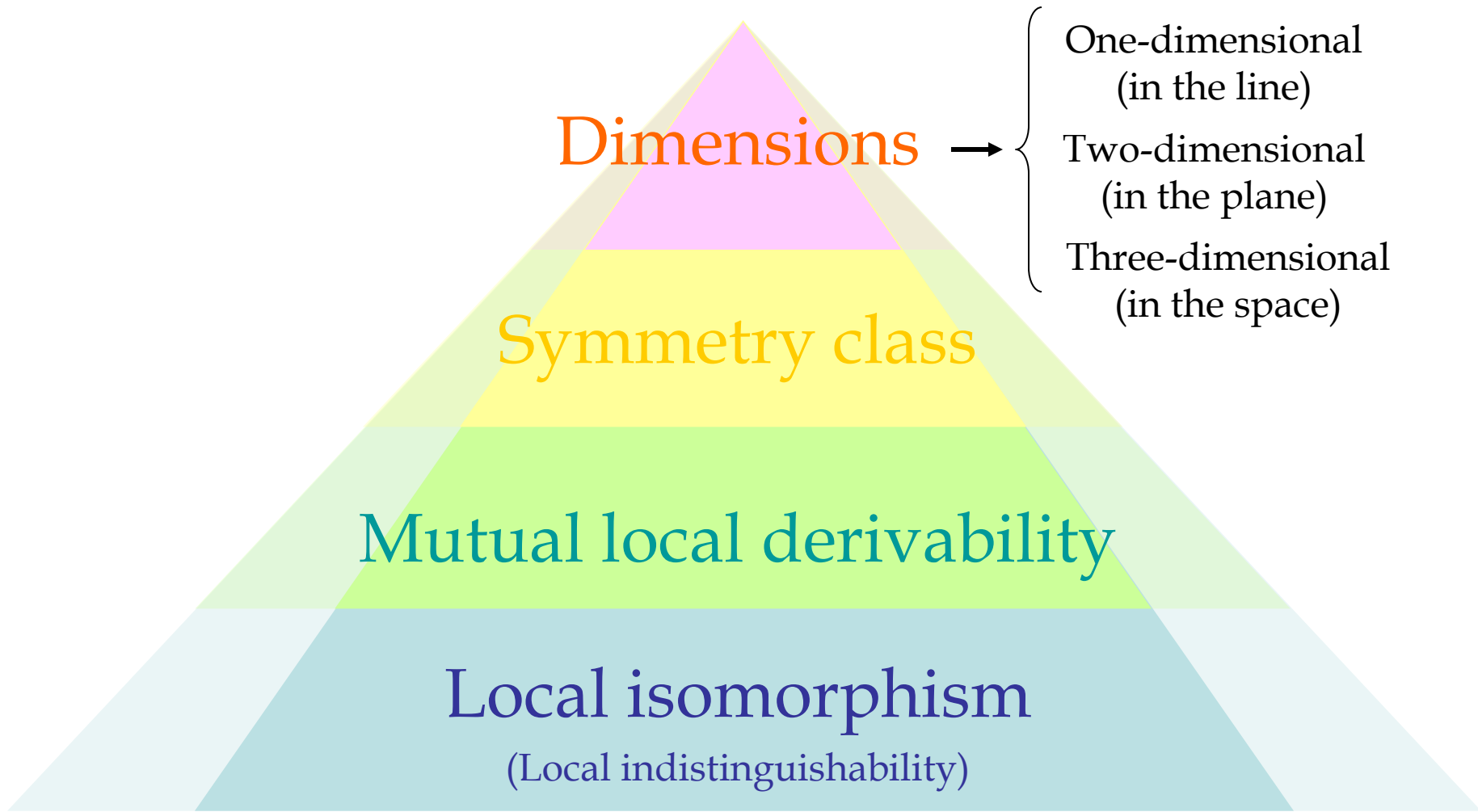
Mutual local derivability

Local isomorphism

(Local indistinguishability)

A class in a higher layer is subdivided in a lower layer.

A hierarchy of the classification



A class in a higher layer is subdivided in a lower layer.

A hierarchy of the classification

Dimensions

Symmetry class → Bravais classes

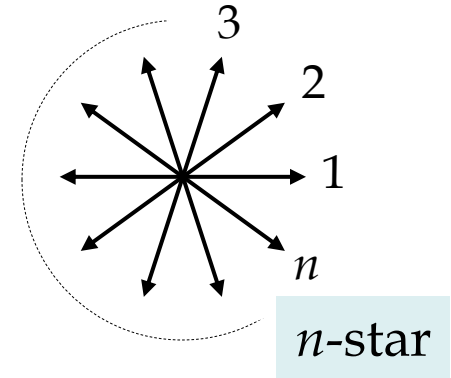
Mutual local derivability

Local isomorphism
(Local indistinguishability)

A class in a higher layer is subdivided in a lower layer.

2-dimensional case

	n -fold symmetry C_n (in Schönflies)	module rank $r = \phi(n)$
Bravais classes	2	1
	3	2
	4	2
	(5)	4
	6	2
	(7)	6
	8	4
	(9)	6
	10	4
	(11)	10
	12	4



Within conventional crystallography

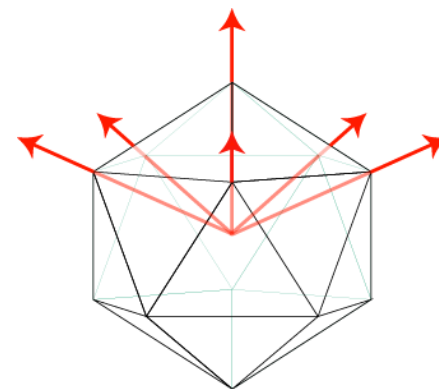
Quasi-crystallography (standard)

Quasi-crystallography (for experts)

$\phi(n)$ (the Euler function): the number of positive integer $m(<n)$ coprime with n .

3-dimensional case

	Icosahedral symmetry I_h (in Schönflies)	module rank r
Bravais classes	P-type	} 6
	F-type	
	I-type	



6 independent basis vectors in the physical space

$$\Lambda_P := \{n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 + n_4 \mathbf{a}_4 + n_5 \mathbf{a}_5 + n_6 \mathbf{a}_6 \mid n_j \in \mathbb{Z}\}$$

$$\Lambda_F := \{n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 + n_4 \mathbf{a}_4 + n_5 \mathbf{a}_5 + n_6 \mathbf{a}_6 \mid \sum_j n_j = 0 \pmod{2}, n_j \in \mathbb{Z}\}$$

$$\Lambda_I := \{n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 + n_4 \mathbf{a}_4 + n_5 \mathbf{a}_5 + n_6 \mathbf{a}_6 \mid (n_j) = (000000) \text{ or } (111111) \pmod{2}, n_j \in \mathbb{Z}\}$$

A hierarchy of the classification

Dimensions

Symmetry class

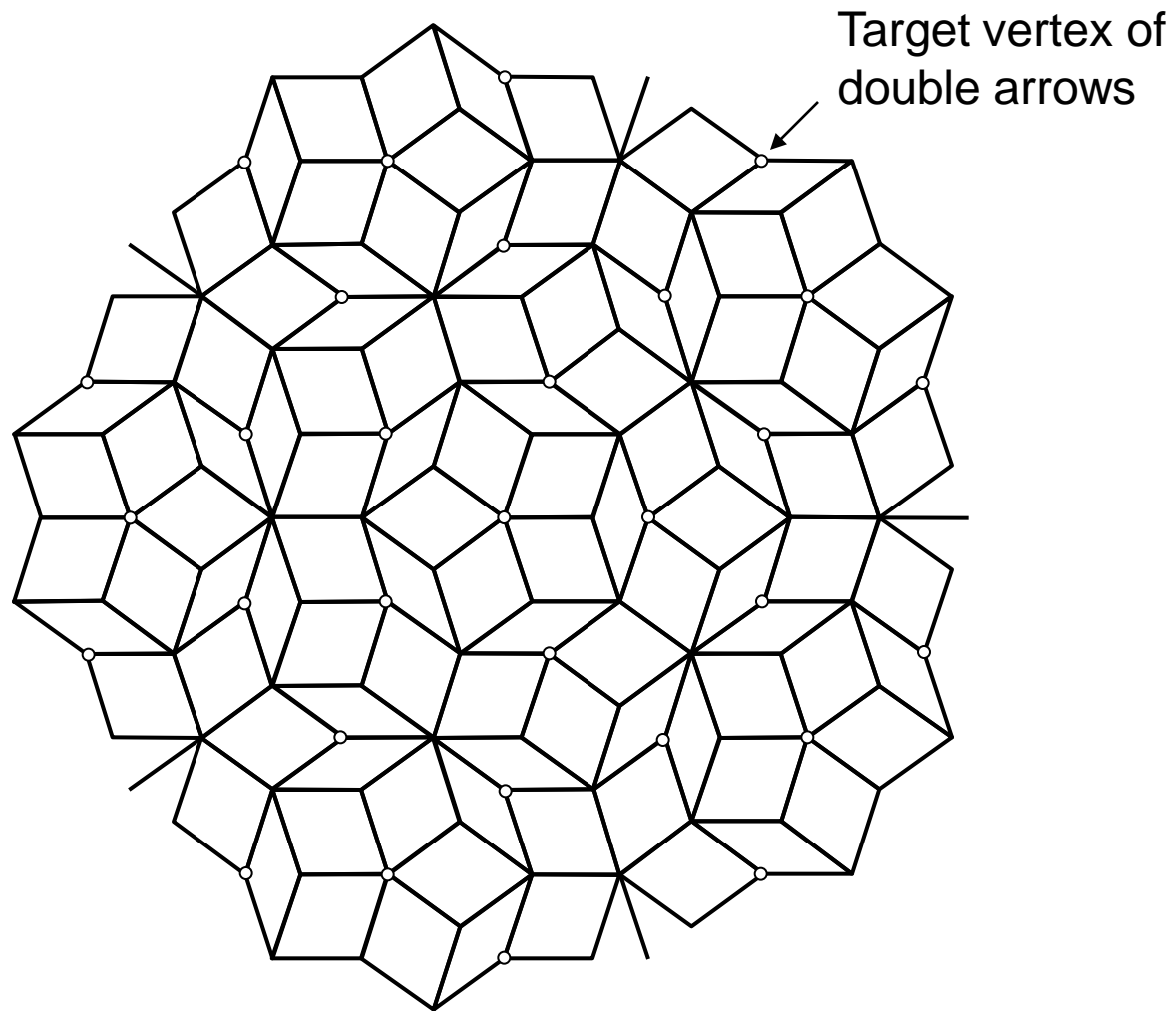
Mutual local derivability



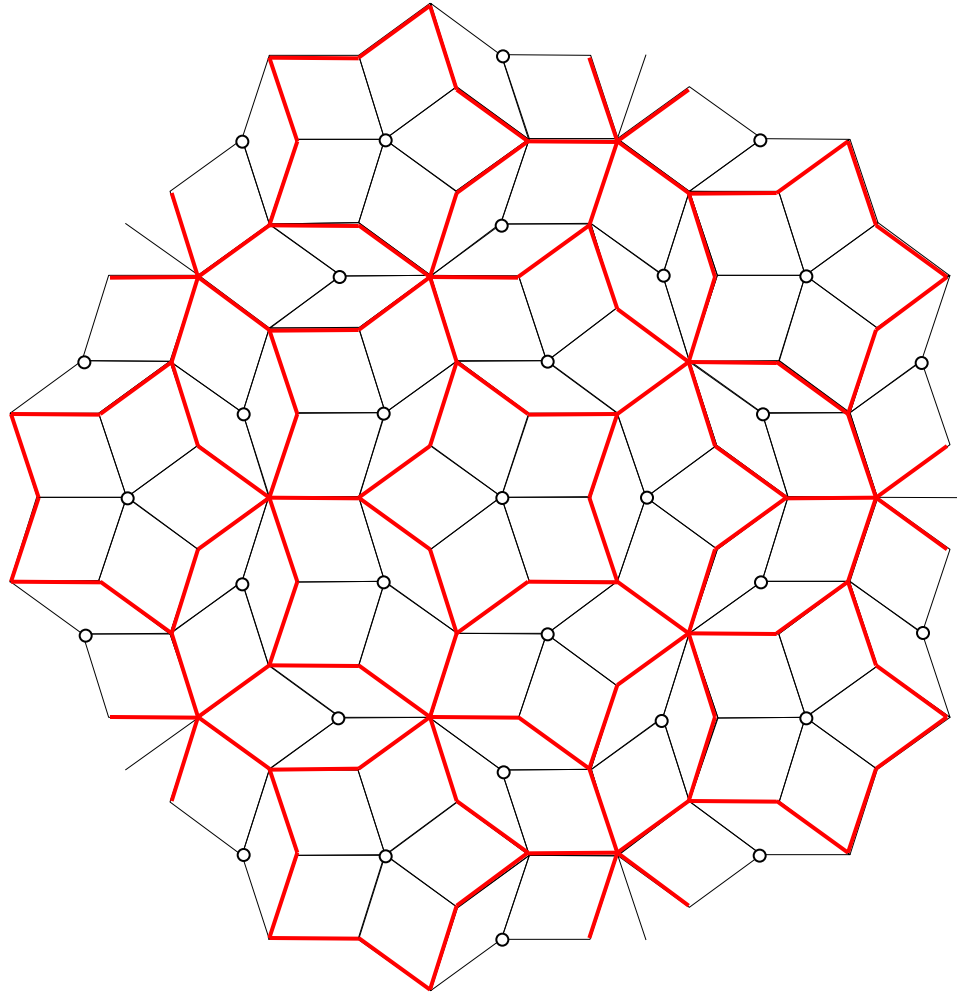
Local isomorphism

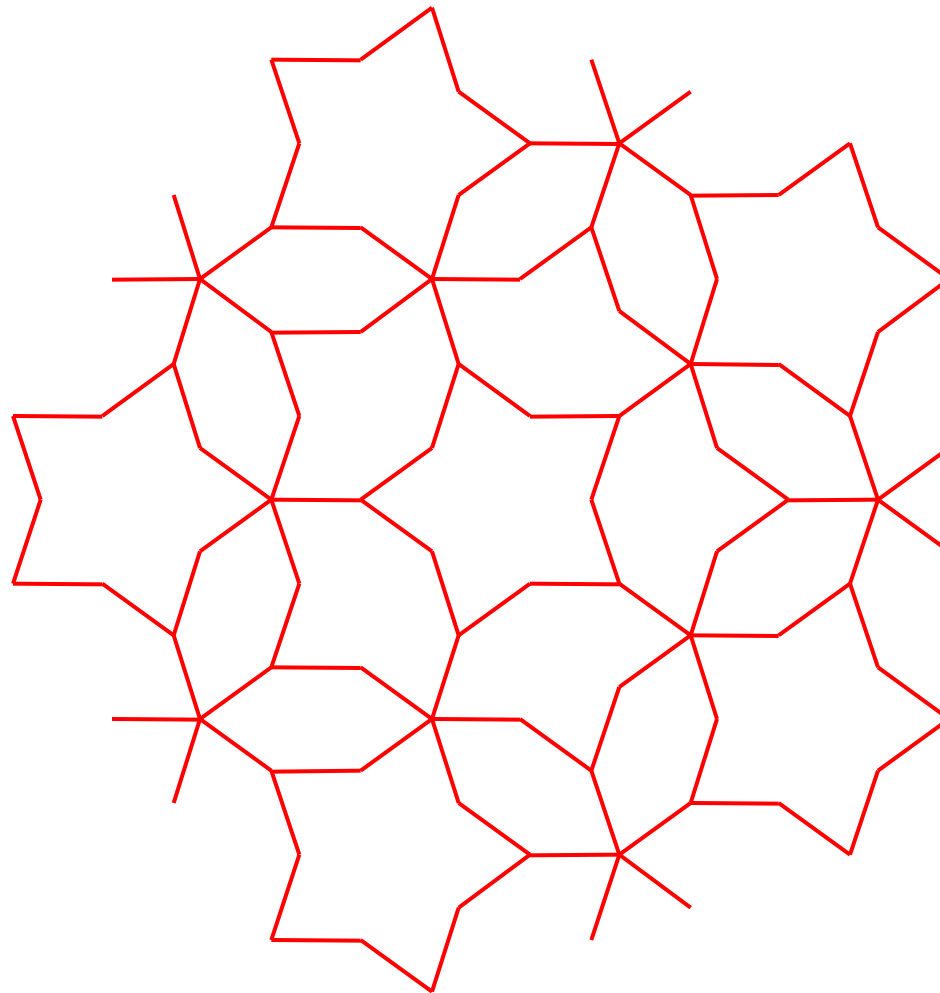
(Local indistinguishability)

A class in a higher layer is subdivided in a lower layer.



rhombic Penrose tiling (P3)

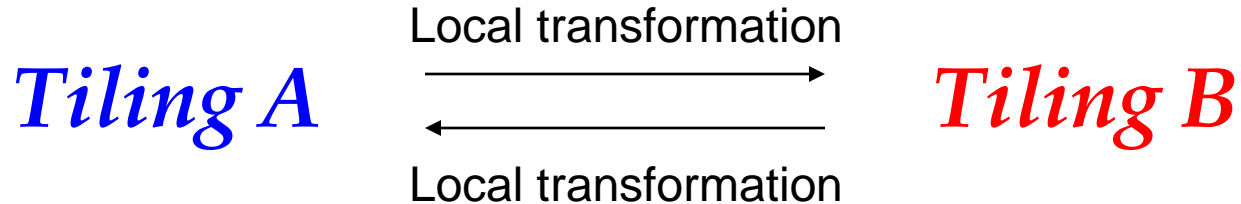




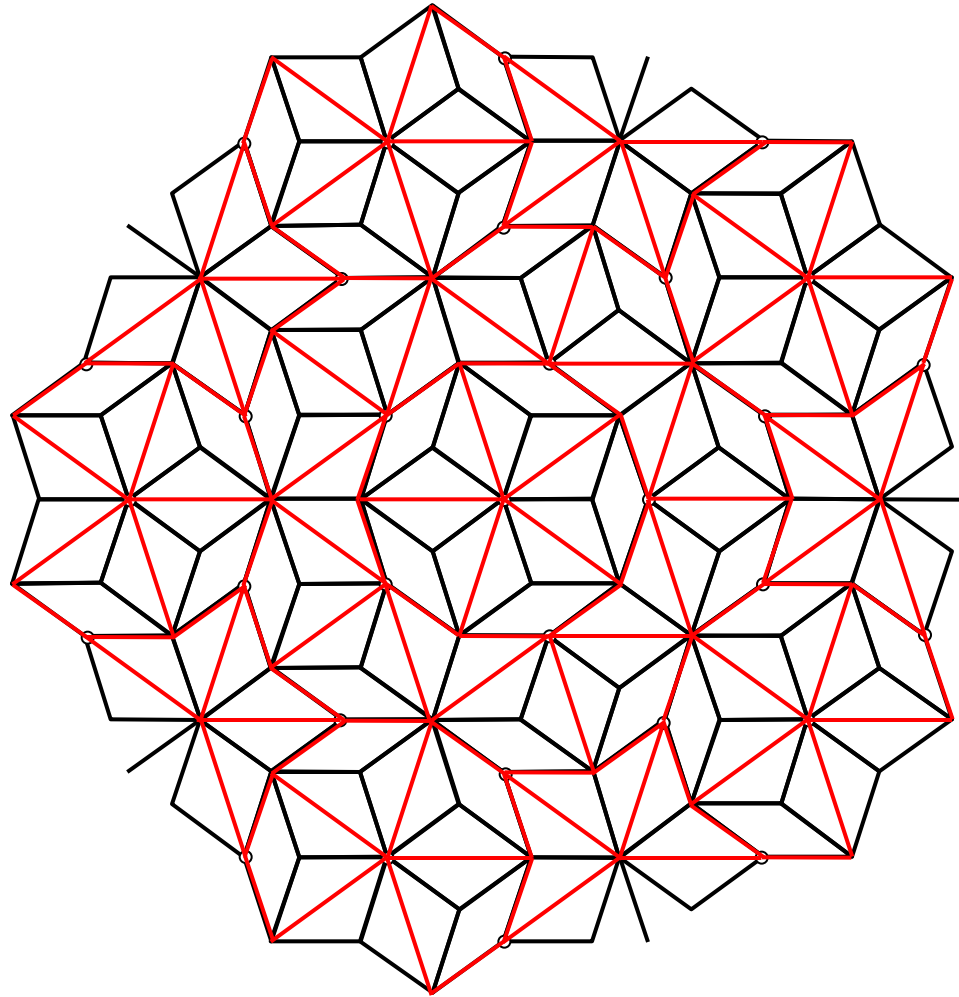
HBS (Hexagon-Boat-Star) tiling

Mutual local derivability

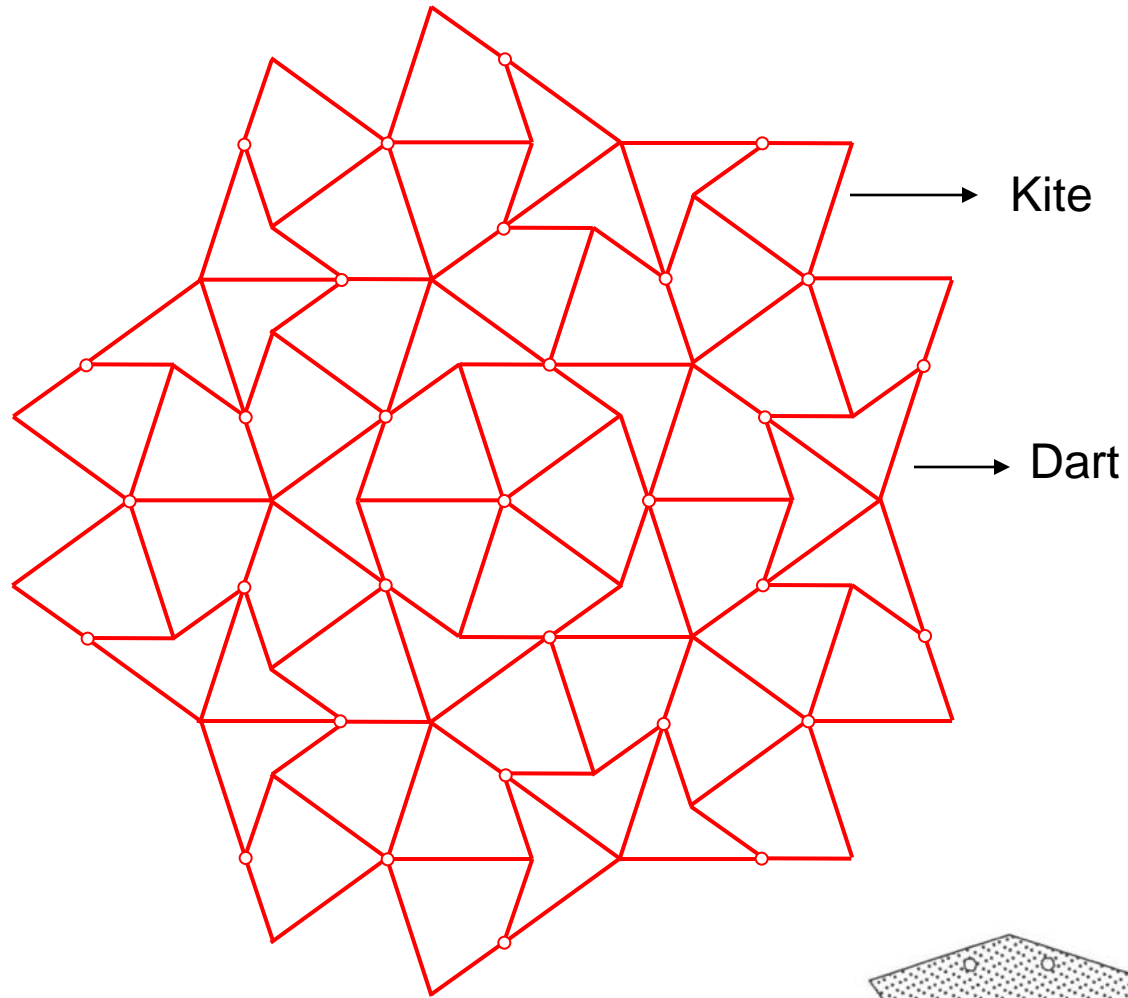
Two different tilings are said to be mutually-locally-derivable (MLD) iff one of them can be derived from the other through local transformation rules, and *vice versa*.



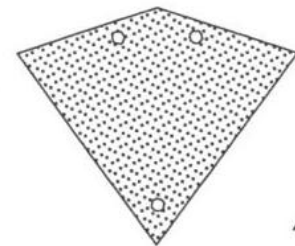
The tilings A and B are MLD: $A \sim B$



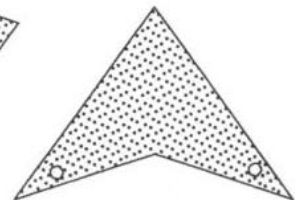
rhombic Penrose (P3) ~ **Kites & Darts (P2)**



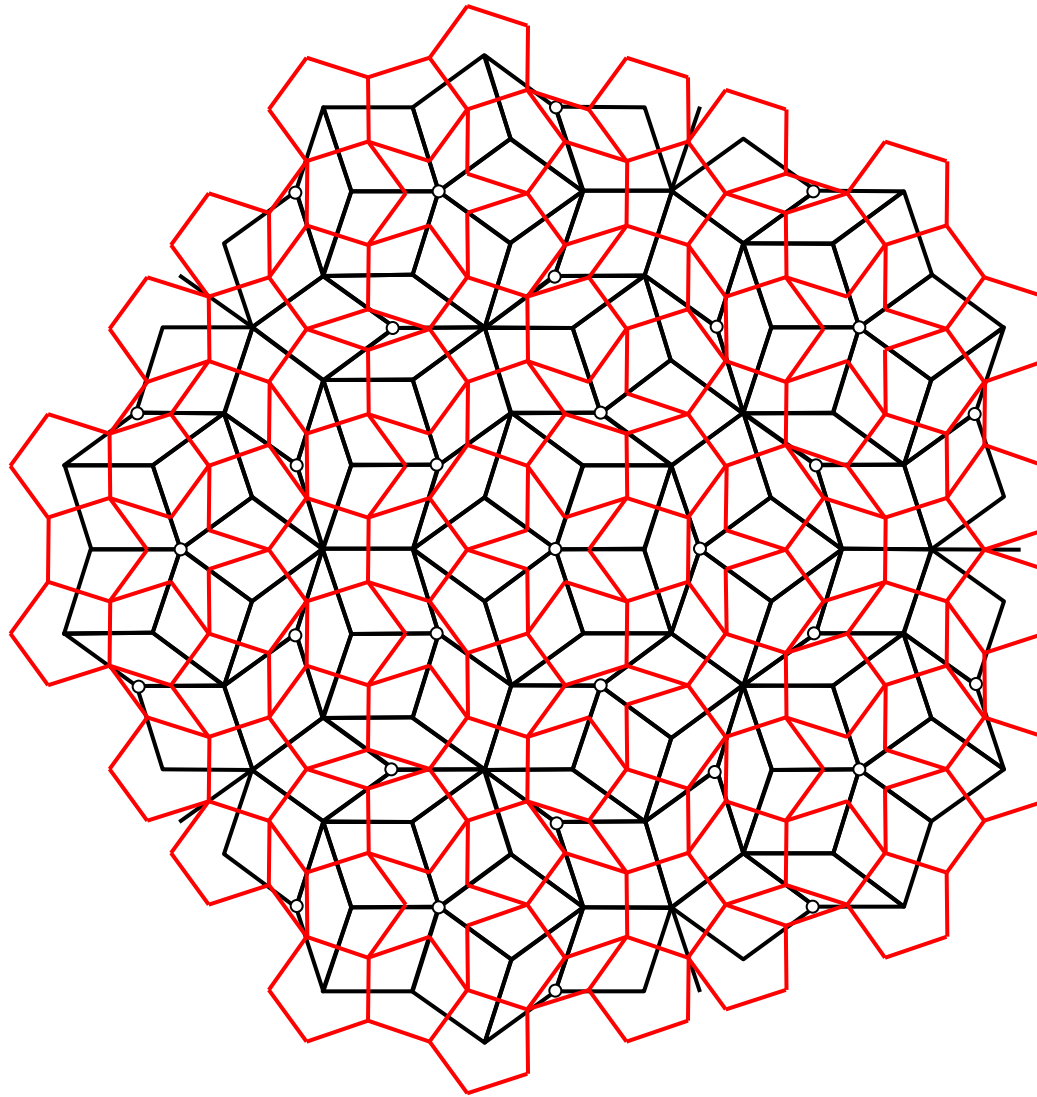
Kites and Darts (P2)



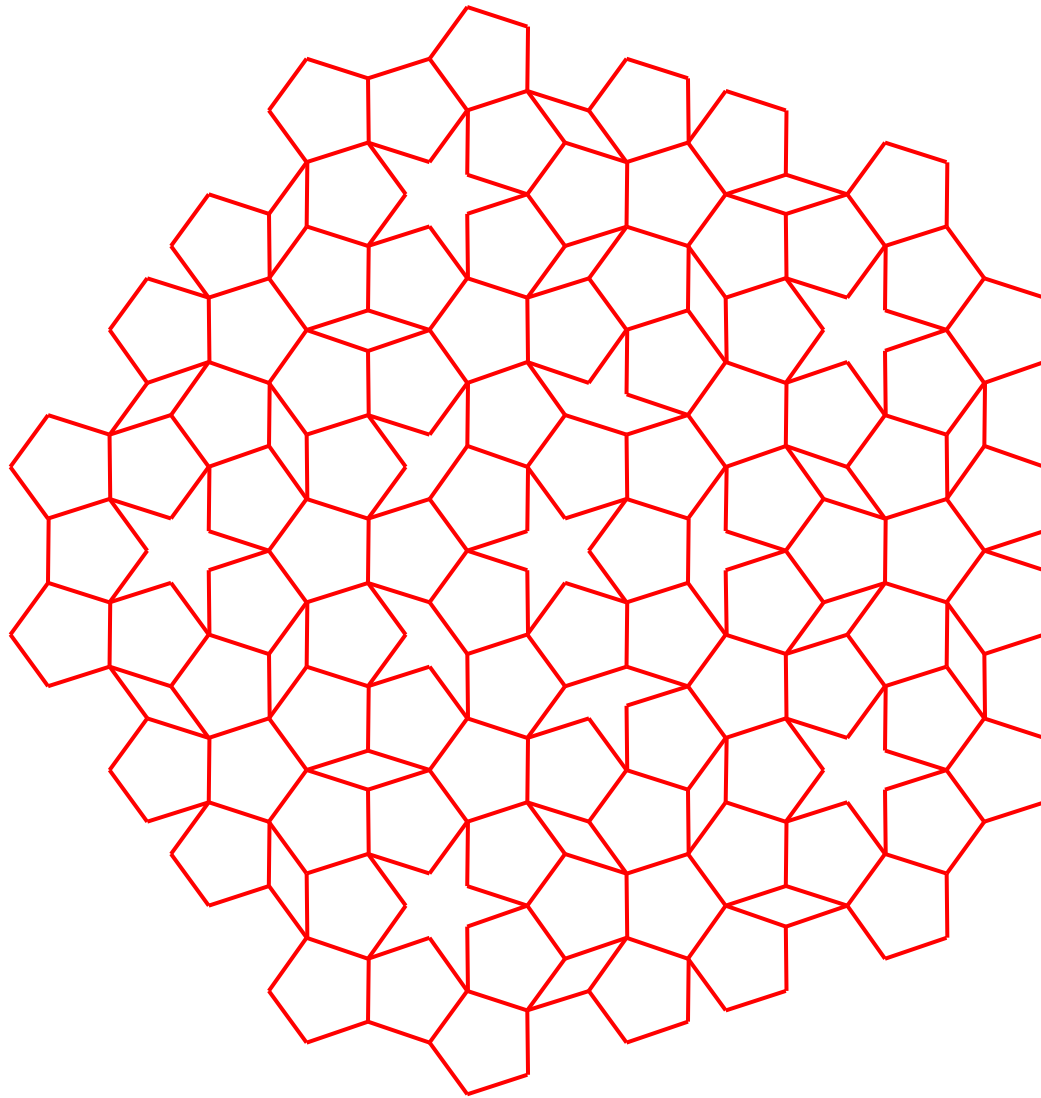
Kite



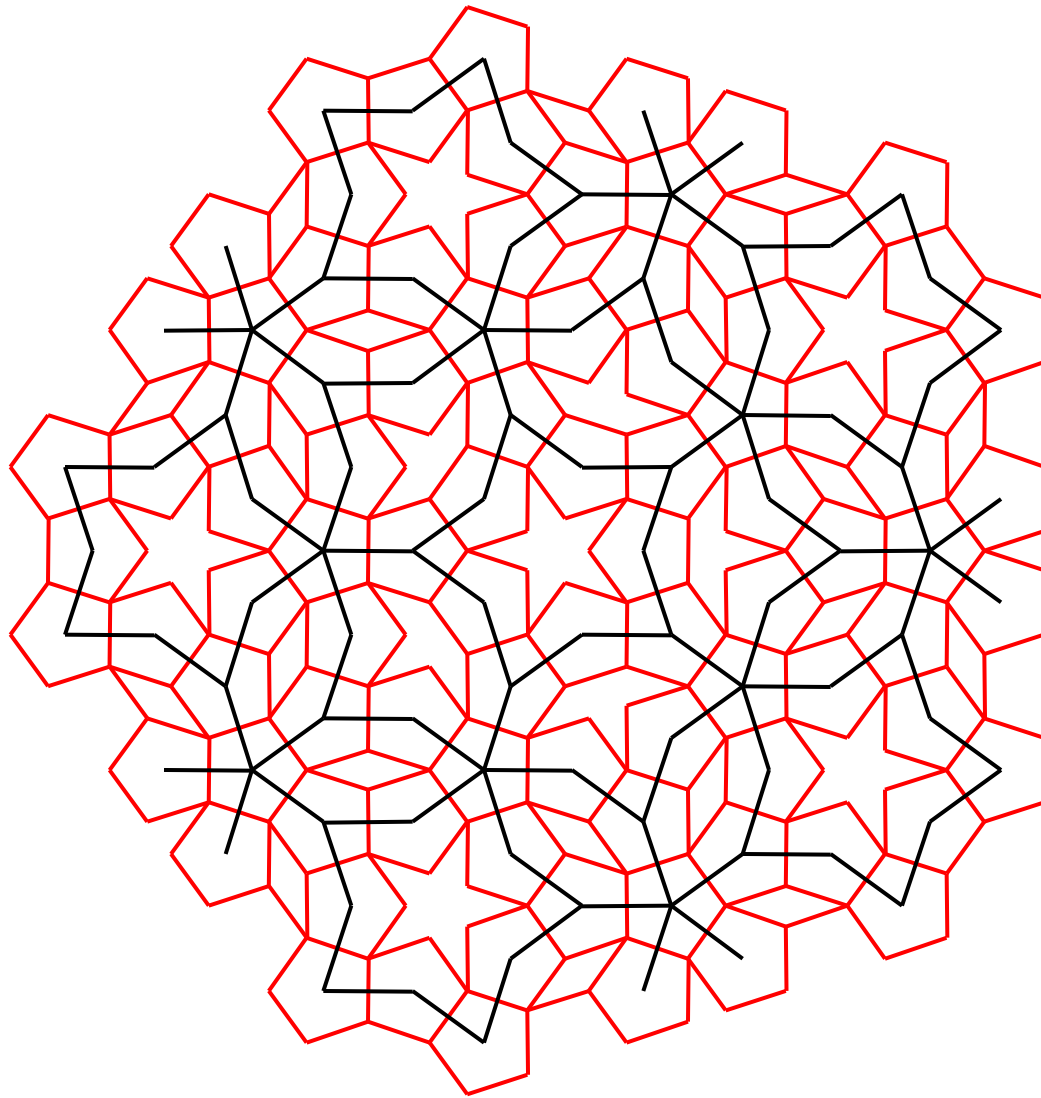
Dart



rhombic Penrose (P3) ~ pentagonal Penrose (P1)



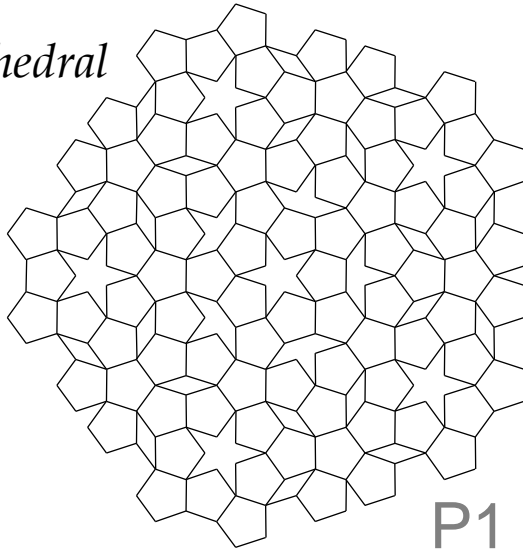
pentagonal Penrose (P1)



pentagonal Penrose (P1) ~ HBS

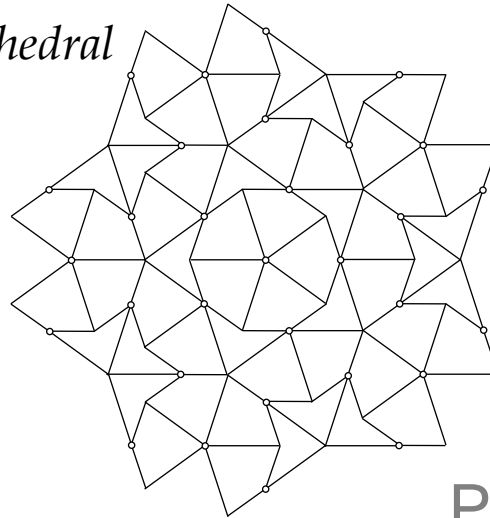
- the MLD class of the Penrose tilings -

4-hedral



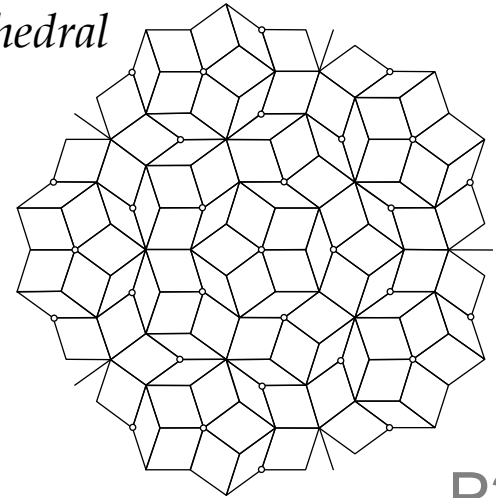
P1

di-hedral



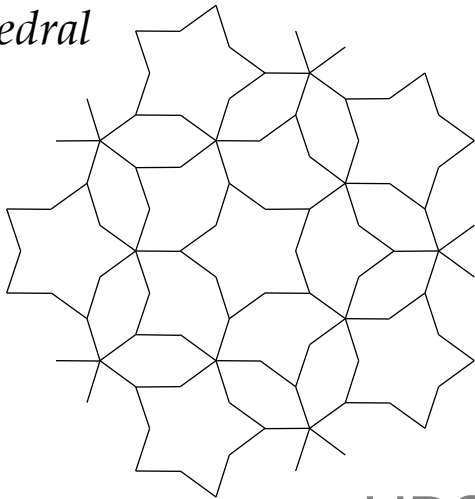
P2

di-hedral



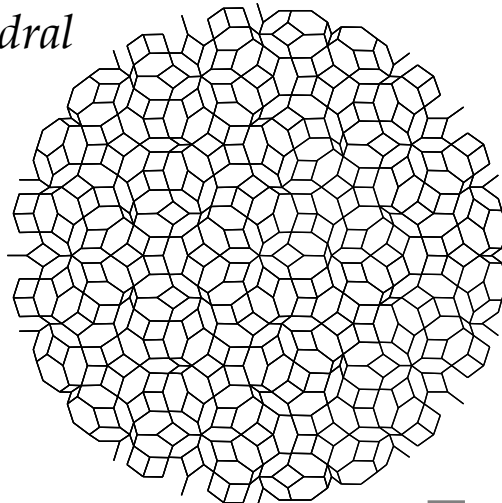
P3

tri-hedral



HBS

4-hedral



$T_{A_4^R}$

No simple rule
for the number
and the shapes
in general.

A hierarchy of the classification

Dimensions

Symmetry class

Mutual local derivability

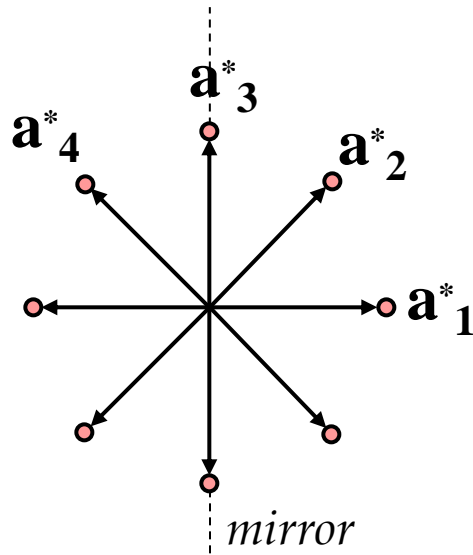
Local isomorphism

(Local indistinguishability)

A class in a higher layer is subdivided in a lower layer.

6. Embeddings of tilings

Case 1. Octagonal point symmetry (8mm, D_8)



$$\mathbf{a}_1^* = (1, 0)$$

$$\mathbf{a}_2^* = (\cos(\pi/4), \sin(\pi/4))$$

$$\mathbf{a}_3^* = (0, 1)$$

$$\mathbf{a}_4^* = (\cos(3\pi/4), \sin(3\pi/4))$$

$$D_8 = \{1, m\} \times \{1, C_8, C_8^2, C_8^3, C_8^4, C_8^5, C_8^6, C_8^7\}, \quad |D_8| = 16$$

Generators: m, C_8

$$\hat{m}\mathbf{a}_1^* = -\mathbf{a}_1^*, \quad \hat{m}\mathbf{a}_2^* = \mathbf{a}_4^*, \quad \hat{m}\mathbf{a}_3^* = \mathbf{a}_3^*, \quad \hat{m}\mathbf{a}_4^* = \mathbf{a}_2^*$$

$$\hat{C}_8\mathbf{a}_j^* = \mathbf{a}_{j+1}^* \quad (j = 1, 2, 3), \quad \hat{C}_8\mathbf{a}_4^* = -\mathbf{a}_1^*$$

The representation matrix of M :

$$\mathbf{q} = \sum_{j=1}^4 n_j \mathbf{a}_j^* = \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix}$$

$$\mathbf{q}' = \hat{m}\mathbf{x} = \hat{m} \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} = \begin{pmatrix} -\mathbf{a}_1^* & \mathbf{a}_4^* & \mathbf{a}_3^* & \mathbf{a}_2^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \Gamma^*(\hat{m}) \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix}$$

The representation matrix of C_8 :

$$\begin{aligned}
 \mathbf{q} &= \sum_{j=1}^4 n_j \mathbf{a}_j^* = \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} \\
 \mathbf{q}' &= \hat{C}_8 \mathbf{q} = \hat{C}_8 \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* & -\mathbf{a}_1^* \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} \\
 &= \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix} =: \begin{pmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* & \mathbf{a}_4^* \end{pmatrix} \Gamma^* (\hat{C}_8) \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix}
 \end{aligned}$$

$$\Gamma^*(\hat{m}) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \Gamma^*(\hat{C}_8) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Once we know the representation matrices for the generators, **the representation matrix for any symmetry operation in D_8 can be given as a suitable product of these two matrices.**

Since the representation matrices are orthogonal, the point group D_8 can be lifted to **a symmetry subgroup of a hyper-cubic lattice in four-dimensional space E_4 .**

The 4D space \mathbb{E}_4 can be decomposed into two 2D subspaces which are invariant against the point group:

$$\mathbb{E}_4 = \mathbb{E}_{\text{phys}} \text{ (physical space)} + \mathbb{E}_{\text{perp}} \text{ (perpendicular space)}$$

Basis vectors of \mathbb{E}_{phys} and \mathbb{E}_{perp} :

$$\mathbf{x}_{\text{phys}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \cos(\pi/4) \\ \cos(\pi/2) \\ \cos(3\pi/4) \end{pmatrix}, \quad \mathbf{y}_{\text{phys}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \sin(\pi/4) \\ \sin(\pi/2) \\ \sin(3\pi/4) \end{pmatrix}$$

$$\mathbf{x}_{\text{perp}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \cos(3\pi/4) \\ \cos(3\pi/2) \\ \cos(\pi/4) \end{pmatrix}, \quad \mathbf{y}_{\text{perp}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \sin(3\pi/4) \\ \sin(3\pi/2) \\ \sin(\pi/4) \end{pmatrix}$$

Orthogonal transformation:

$$\tilde{\Gamma}^*(\hat{R}) := O^T \Gamma^*(\hat{R}) O, \quad O = \begin{pmatrix} \mathbf{x}_{phys} & \mathbf{y}_{phys} & \mathbf{x}_{perp} & \mathbf{y}_{perp} \end{pmatrix}$$

$$\hat{R} = \hat{m}, \hat{C}_8$$

$$\tilde{\Gamma}^*(\hat{m}) := O^T \Gamma^*(\hat{m}) O = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Reflection w.r.t. the y-axis

Reflection w.r.t. the y-axis

$$\tilde{\Gamma}^*(\hat{C}_8) := O^T \Gamma^*(\hat{C}_8) O = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\pi/4) & -\sin(\pi/4) & 0 & 0 \\ \sin(\pi/4) & \cos(\pi/4) & 0 & 0 \\ 0 & 0 & \cos(3\pi/4) & -\sin(3\pi/4) \\ 0 & 0 & \sin(3\pi/4) & \cos(3\pi/4) \end{pmatrix}$$

Rotation by $\pi/4$

Rotation by $3\pi/4$ line

$$\mathbf{a}_1^* = \frac{1}{\sqrt{2}} \mathbf{O}^T \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} := \frac{1}{2} \begin{pmatrix} 1 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 1 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\mathbf{a}_2^* = \frac{1}{\sqrt{2}} \mathbf{O}^T \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} := \frac{1}{2} \begin{pmatrix} 1 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 1 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$\mathbf{a}_3^* = \frac{1}{\sqrt{2}} \mathbf{O}^T \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} := \frac{1}{2} \begin{pmatrix} 1 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 1 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\mathbf{a}_4^* = \frac{1}{\sqrt{2}} \mathbf{O}^T \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} := \frac{1}{2} \begin{pmatrix} 1 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 1 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

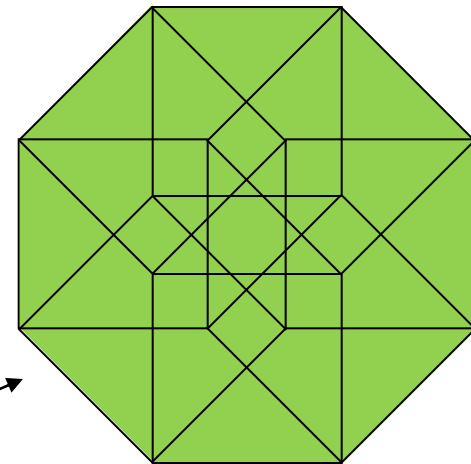
Basis vectors of
a four-dim.
Hypercubic
lattice Λ^* in
reciprocal space.

$$\mathbf{a}_j = 2 \mathbf{a}_j^* \quad (j = 1, 2, 3, 4)$$

Basis vectors of a four-dim.
Hypercubic lattice Λ in
direct space.

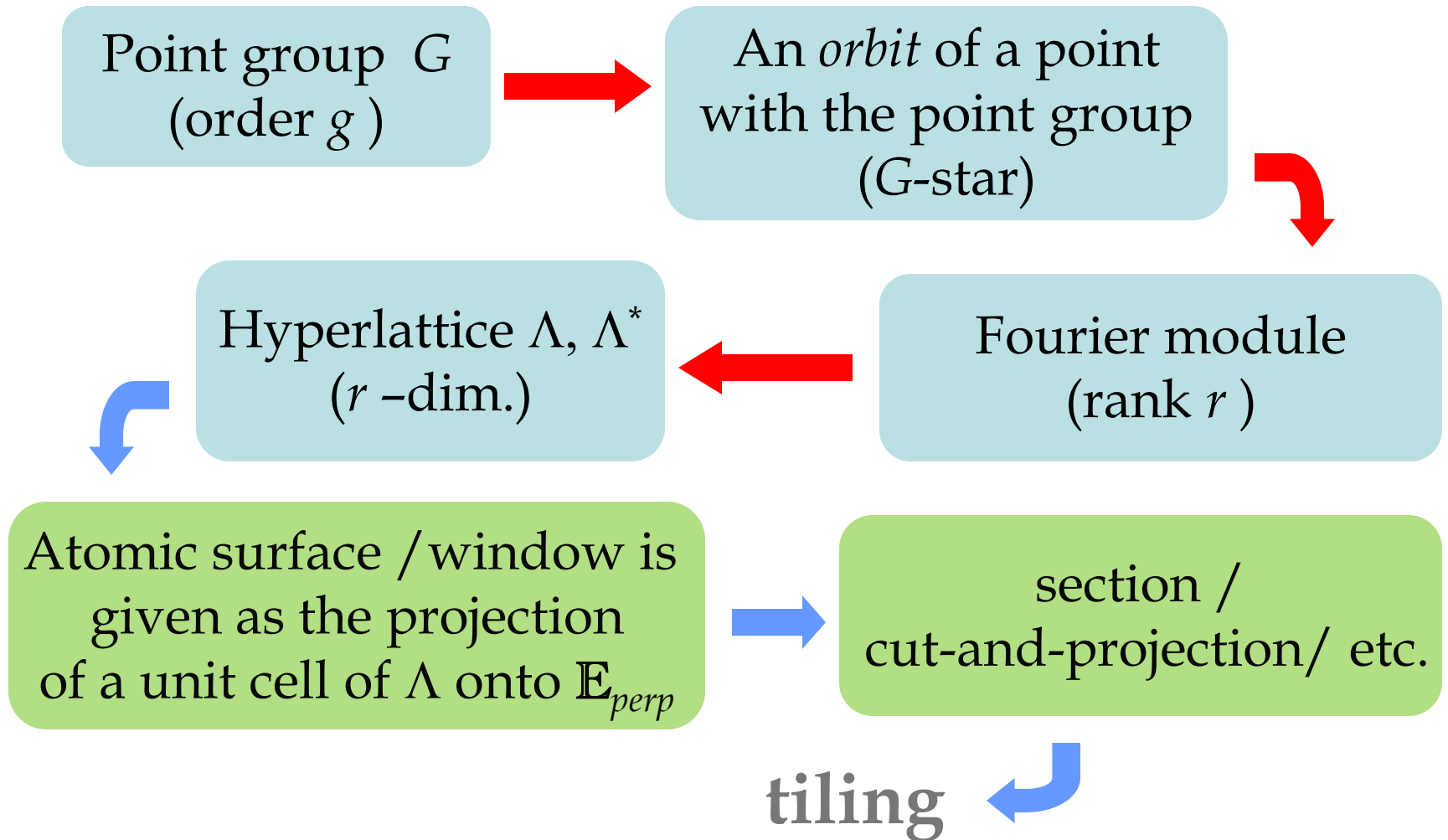
$$\text{Unitcell} = \left\{ \sum_{j=1}^4 t_j \mathbf{a}_j \mid 0 \leq t_j \leq 1 \right\}$$

$$\text{Atomicsurface} = \hat{\pi}_{\text{perp}}(\text{Unitcell})$$

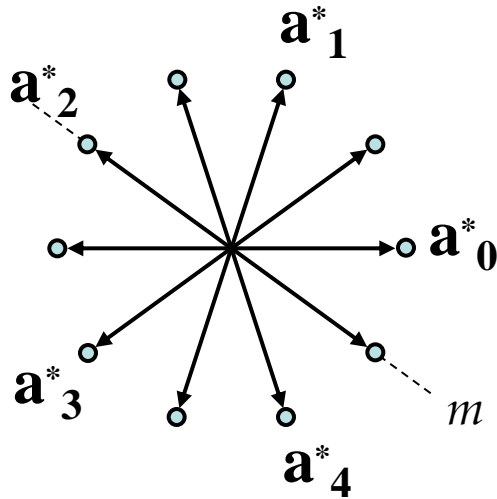


$$\hat{\pi}_{\text{phys}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \hat{\pi}_{\text{perp}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

A route to an aperiodic tiling



Case 2. Decagonal point symmetry (10mm, D_{10})



$$\mathbf{a}^*_0 = (1, 0)$$

$$\mathbf{a}^*_1 = (\cos(2\pi/5), \sin(2\pi/5))$$

$$\mathbf{a}^*_2 = (\cos(4\pi/5), \sin(4\pi/5))$$

$$\mathbf{a}^*_3 = (\cos(6\pi/5), \sin(6\pi/5))$$

$$\mathbf{a}^*_4 = (\cos(8\pi/5), \sin(8\pi/5))$$

$$D_{10} = \{1, m\} \{1, C_{10}, C_{10}^2, C_{10}^3, C_{10}^4, C_{10}^5, C_{10}^6, C_{10}^7, C_{10}^8, C_{10}^9\},$$

$$|D_{10}| = 20$$

$$\text{Generators: } m, C_{10}^2$$

$$\hat{m}\mathbf{a}^*_0 = \mathbf{a}^*_4, \hat{m}\mathbf{a}^*_1 = \mathbf{a}^*_3, \hat{m}\mathbf{a}^*_2 = \mathbf{a}^*_2, \hat{m}\mathbf{a}^*_3 = \mathbf{a}^*_1, \hat{m}\mathbf{a}^*_4 = \mathbf{a}^*_0$$

$$(\hat{C}_{10}^2)\mathbf{a}^*_j = \mathbf{a}^*_{j+1} \quad (j=0,1,2,3), \quad (\hat{C}_{10}^2)\mathbf{a}^*_4 = \mathbf{a}^*_0$$

$$\Gamma^*(\hat{m}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Gamma^*(\hat{C}_{10}^2) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Once we know the representation matrices for the generators, **the representation matrix for any symmetry operation in D_{10} can be given as a suitable product of these two matrices.**

Since the representation matrices are orthogonal, the point group D_{10} can be lifted to **a symmetry subgroup of a hyper-cubic lattice in five-dimensional space E_5 .**

The 5D space \mathbb{E}_5 can be decomposed into two subspaces (2D+3D) which are invariant against the point group:

$$\mathbb{E}_4 = \mathbb{E}_{\text{phys}} \text{ (2D, physical space)} + \mathbb{E}_{\text{perp}} \text{ (3D, perpendicular space)}$$

Basis vectors of \mathbb{E}_{phys} and \mathbb{E}_{perp} :

$$\mathbf{x}_{\text{phys}} = \sqrt{\frac{2}{5}} \begin{pmatrix} 1 \\ \cos(2\pi/5) \\ \cos(4\pi/5) \\ \cos(6\pi/5) \\ \cos(8\pi/5) \end{pmatrix}, \quad \mathbf{y}_{\text{phys}} = \sqrt{\frac{2}{5}} \begin{pmatrix} 0 \\ \sin(2\pi/5) \\ \sin(4\pi/5) \\ \sin(6\pi/5) \\ \sin(8\pi/5) \end{pmatrix}$$

$$\mathbf{x}_{\text{perp}} = \sqrt{\frac{2}{5}} \begin{pmatrix} 1 \\ \cos(4\pi/5) \\ \cos(8\pi/5) \\ \cos(2\pi/5) \\ \cos(6\pi/5) \end{pmatrix}, \quad \mathbf{y}_{\text{perp}} = \sqrt{\frac{2}{5}} \begin{pmatrix} 0 \\ \sin(4\pi/5) \\ \sin(8\pi/5) \\ \sin(2\pi/5) \\ \sin(6\pi/5) \end{pmatrix}, \quad \mathbf{z}_{\text{perp}} = \sqrt{\frac{1}{5}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Orthogonal transformation:

$$\tilde{\Gamma}^*(\hat{R}) := O^T \Gamma^*(\hat{R}) O, \quad O = \begin{pmatrix} \mathbf{x}_{phys} & \mathbf{y}_{phys} & \mathbf{x}_{perp} & \mathbf{y}_{perp} & \mathbf{z}_{perp} \end{pmatrix}$$

$$\hat{R} = \hat{m}, \hat{C}_{10}^2$$

Reflection w.r.t. $\theta = -\pi/5$ line

$$\tilde{\Gamma}^*(\hat{m}) := \begin{pmatrix} \cos(2\pi/5) & -\sin(2\pi/5) & 0 & 0 & 0 \\ -\sin(2\pi/5) & -\cos(2\pi/5) & 0 & 0 & 0 \\ 0 & 0 & \cos(4\pi/5) & -\sin(4\pi/5) & 0 \\ 0 & 0 & -\sin(4\pi/5) & -\cos(4\pi/5) & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

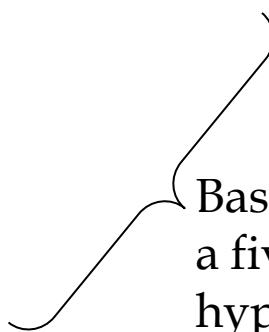
Reflection w.r.t. $\theta = -2\pi/5$ line

Rotation by $2\pi/5$

$$\tilde{\Gamma}^*(\hat{C}_{10}^2) := \begin{pmatrix} \cos(2\pi/5) & -\sin(2\pi/5) & 0 & 0 & 0 \\ \sin(2\pi/5) & \cos(2\pi/5) & 0 & 0 & 0 \\ 0 & 0 & \cos(4\pi/5) & -\sin(4\pi/5) & 0 \\ 0 & 0 & \sin(4\pi/5) & \cos(4\pi/5) & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Rotation by $4\pi/5$

$$\begin{aligned}
\mathbf{a}_0^* &= \mathcal{O}^T \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \sqrt{\frac{2}{5}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1/\sqrt{2} \end{pmatrix}, &
\mathbf{a}_1^* &= \mathcal{O}^T \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \sqrt{\frac{2}{5}} \begin{pmatrix} \cos(2\pi/5) \\ \sin(2\pi/5) \\ \cos(4\pi/5) \\ \sin(4\pi/5) \\ 1/\sqrt{2} \end{pmatrix}, &
\mathbf{a}_2^* &= \mathcal{O}^T \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \sqrt{\frac{2}{5}} \begin{pmatrix} \cos(4\pi/5) \\ \sin(4\pi/5) \\ \cos(8\pi/5) \\ \sin(8\pi/5) \\ 1/\sqrt{2} \end{pmatrix} \\
\mathbf{a}_3^* &= \mathcal{O}^T \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} := \sqrt{\frac{2}{5}} \begin{pmatrix} \cos(6\pi/5) \\ \sin(6\pi/5) \\ \cos(2\pi/5) \\ \sin(2\pi/5) \\ 1/\sqrt{2} \end{pmatrix}, &
\mathbf{a}_4^* &= \mathcal{O}^T \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} := \sqrt{\frac{2}{5}} \begin{pmatrix} \cos(8\pi/5) \\ \sin(8\pi/5) \\ \cos(6\pi/5) \\ \sin(6\pi/5) \\ 1/\sqrt{2} \end{pmatrix}
\end{aligned}$$


 Basis vectors of
 a five-dim.
 hyper-cubic
 lattice Λ^* in
 reciprocal space.

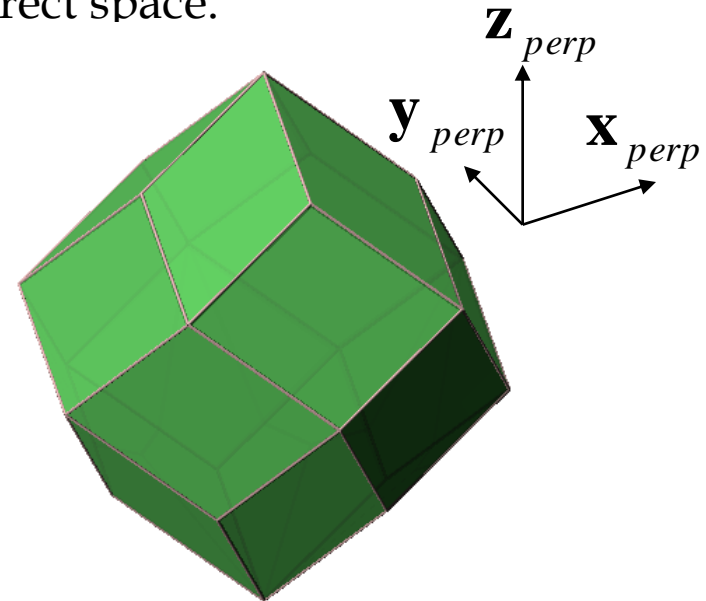
$$\mathbf{a}_j = \mathbf{a}_j^* \quad (j = 0, 1, 2, 3, 4)$$

$$\text{Unitcell} = \left\{ \sum_{j=0}^4 t_j \mathbf{a}_j \mid 0 \leq t_j \leq 1 \right\}$$

$$\text{Atomicsurface} = \hat{\pi}_{perp}(\text{Unitcell})$$

$$\hat{\pi}_{phys} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{\pi}_{perp} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Basis vectors of a five-dim.
hyper-cubic lattice Λ in
direct space.



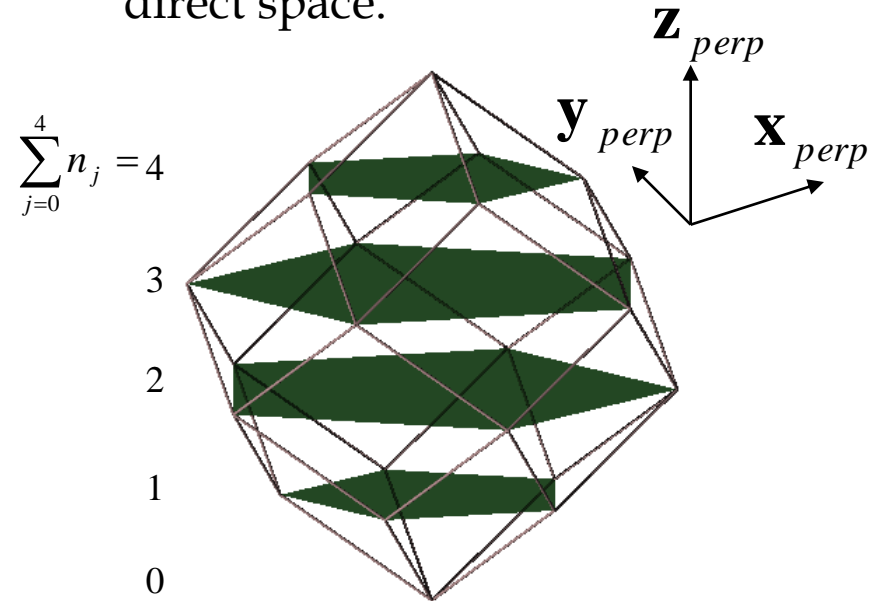
$$\mathbf{a}_j = \mathbf{a}_j^* \quad (j = 0, 1, 2, 3, 4)$$

$$\text{Unitcell} = \left\{ \sum_{j=0}^4 t_j \mathbf{a}_j \mid 0 \leq t_j \leq 1 \right\}$$

$$\text{Atomicsurface} = \hat{\pi}_{perp}(\text{Unitcell})$$

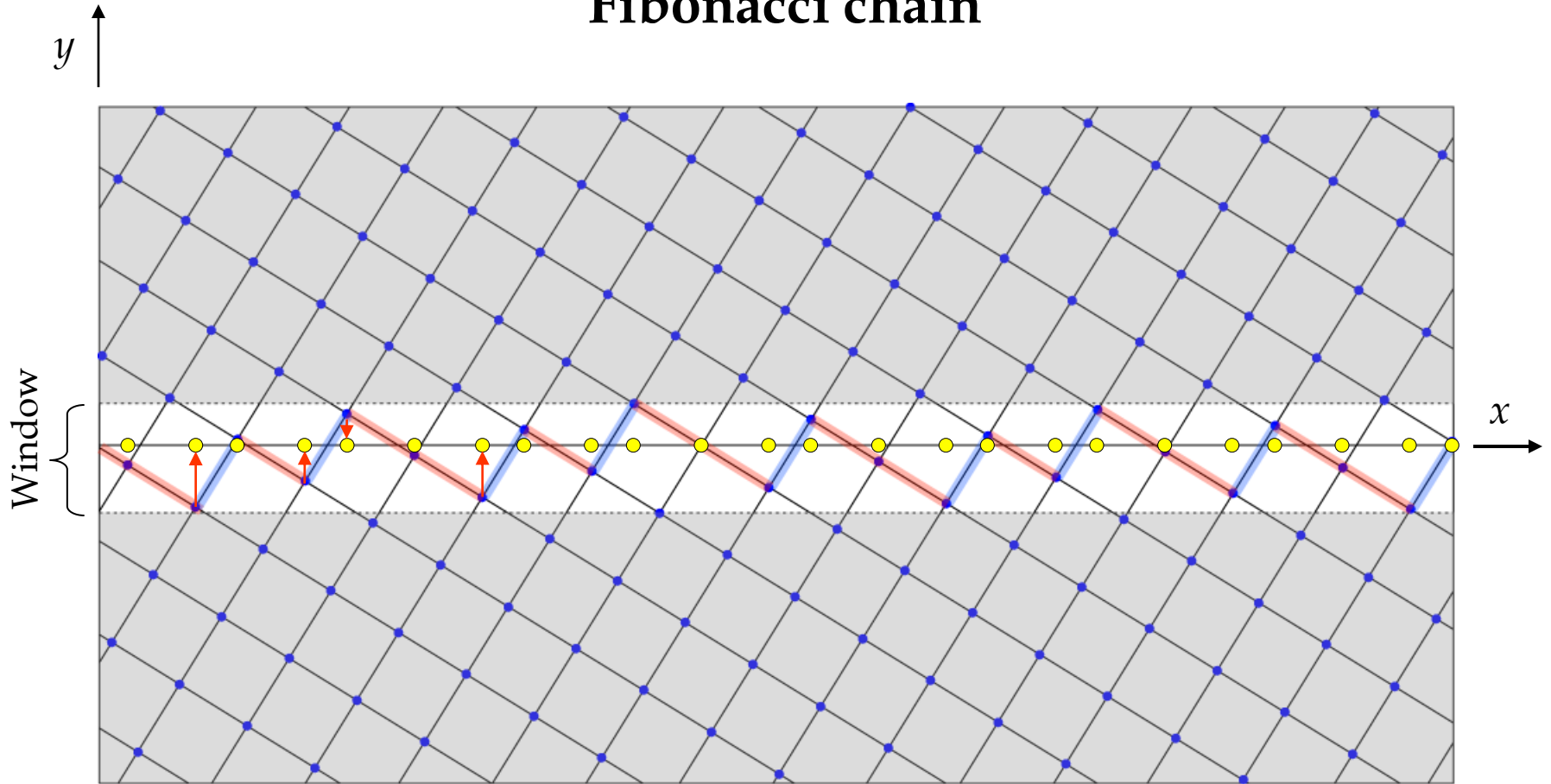
$$\hat{\pi}_{phys} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{\pi}_{perp} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Basis vectors of a five-dim.
hyper-cubic lattice Λ in
direct space.



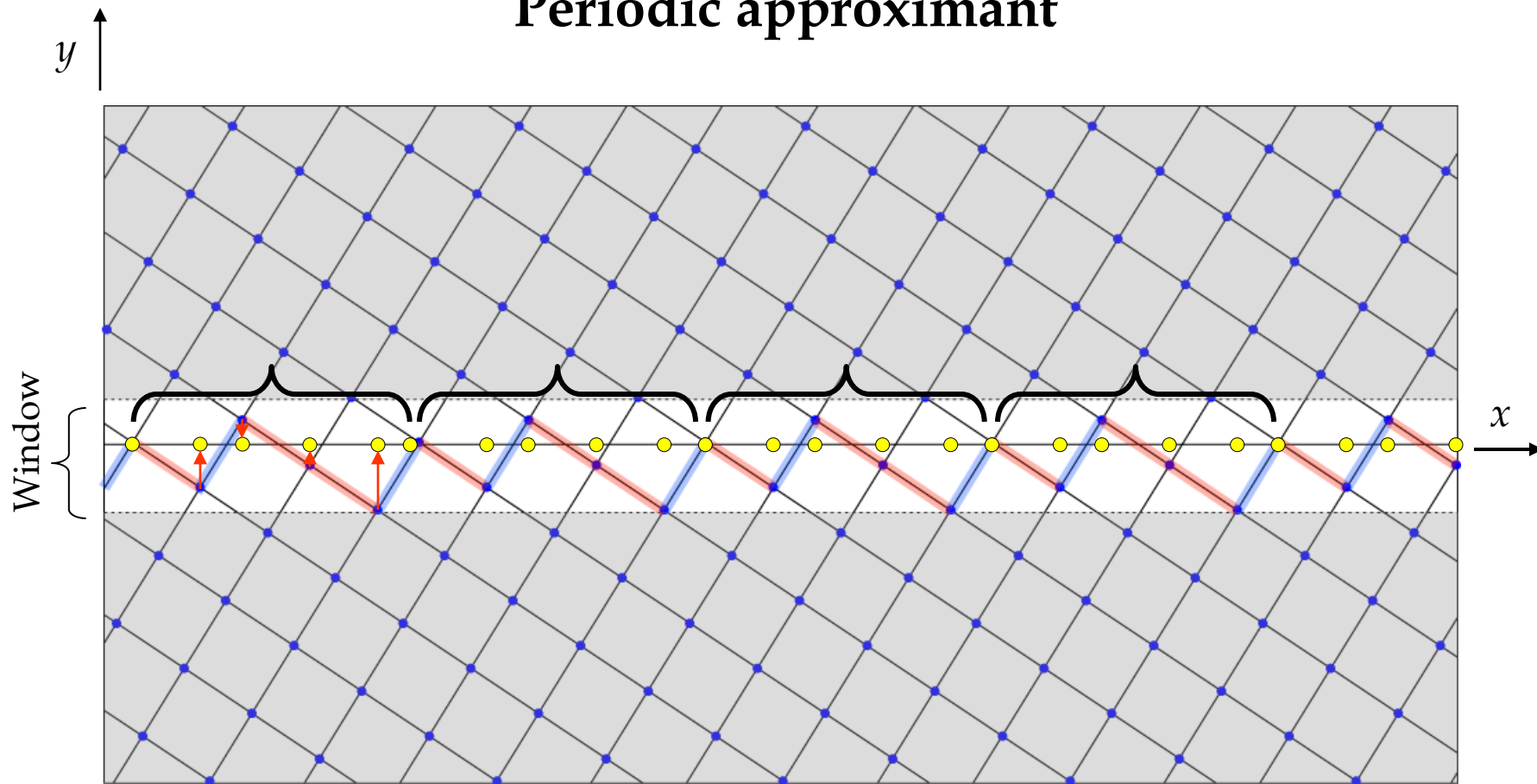
7. Approximants

Fibonacci chain



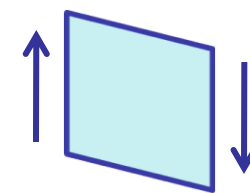
$$\mathbf{a}_1 = \left(1, -\frac{1}{\tau} \right), \quad \mathbf{a}_2 = \left(\frac{1}{\tau}, 1 \right) \quad \text{where } \tau = \frac{1 + \sqrt{5}}{2}$$

Periodic approximant



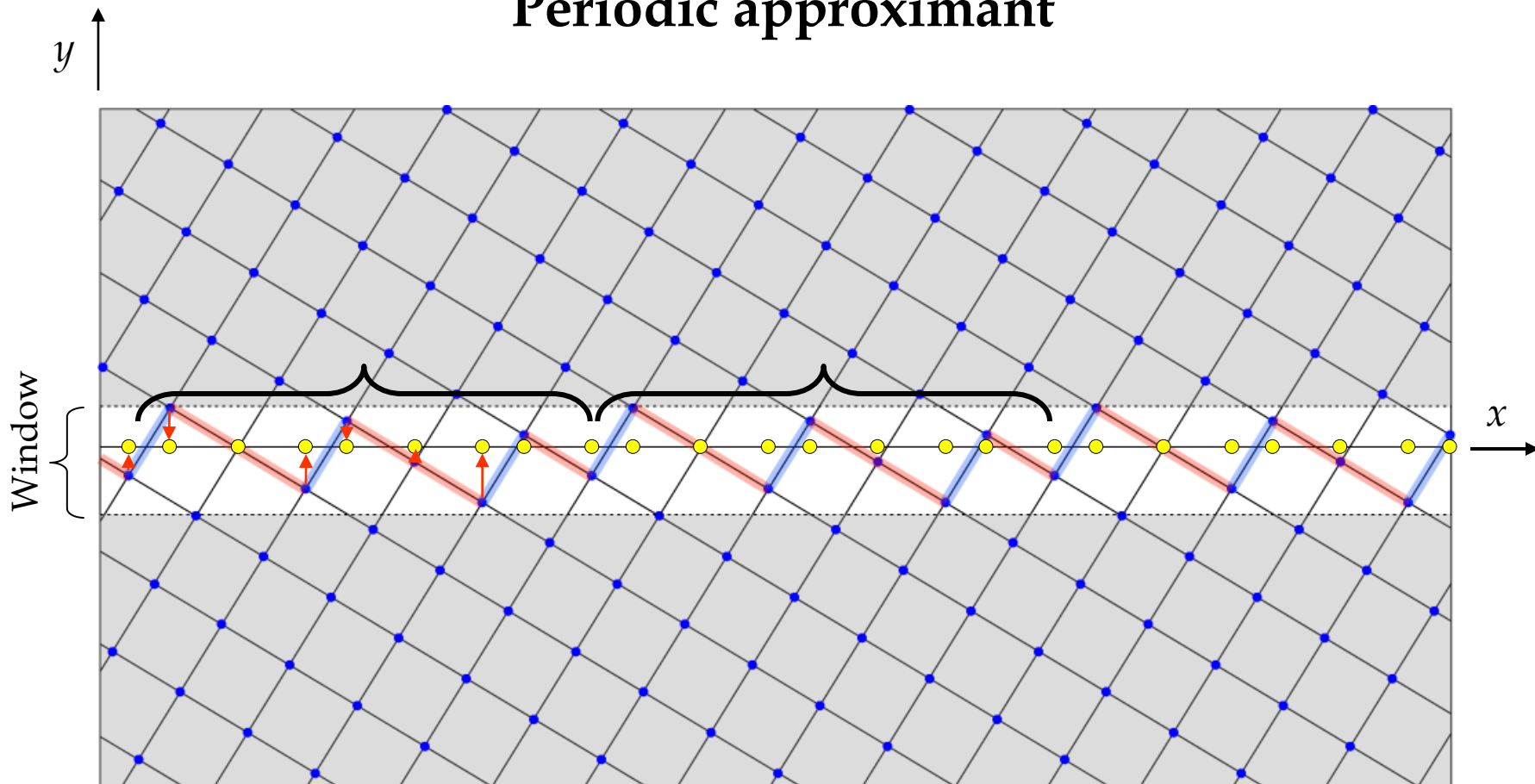
$$\mathbf{a}_1 = \left(1, -\frac{1}{\tau'} \right), \quad \mathbf{a}_2 = \left(\frac{1}{\tau}, 1 \right) \quad \text{where } \tau' = \frac{3}{2}$$

rational approximation



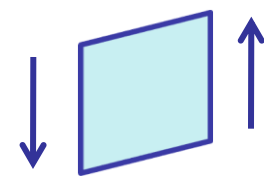
Phason strain

Periodic approximant



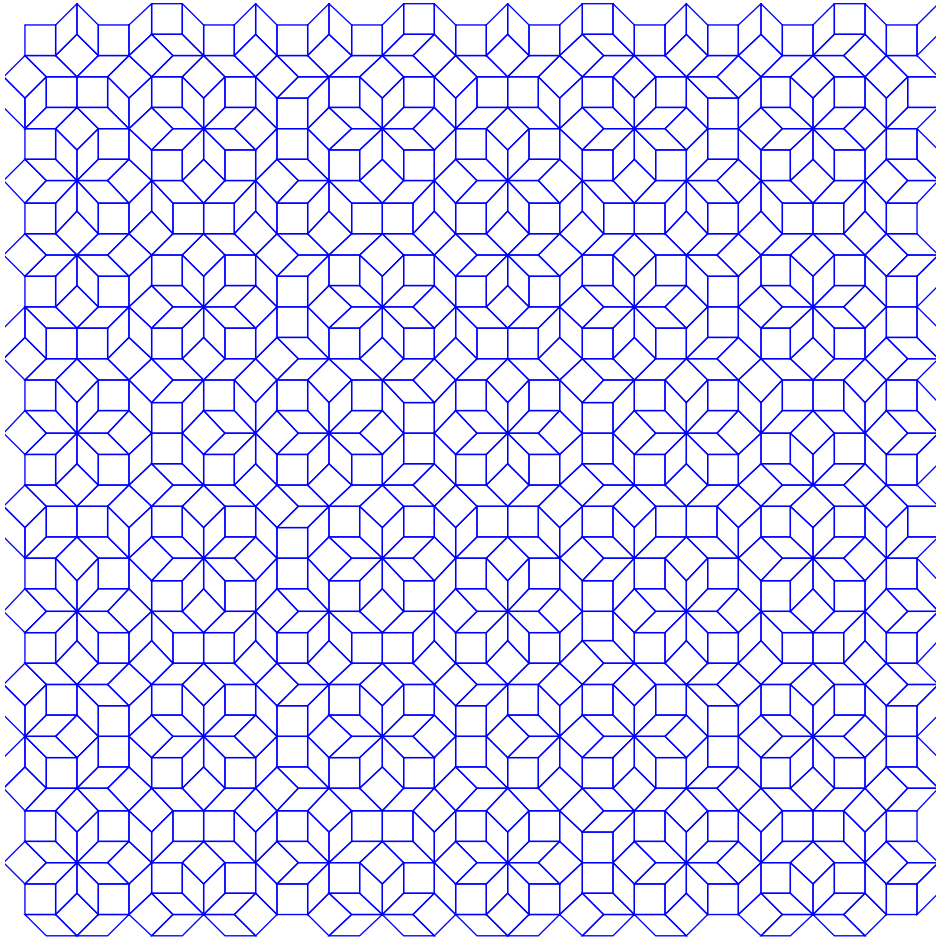
$$\mathbf{a}_1 = \left(1, -\frac{1}{\tau''} \right), \quad \mathbf{a}_2 = \left(\frac{1}{\tau}, 1 \right) \quad \text{where } \tau'' = \frac{5}{3}$$

rational approximation



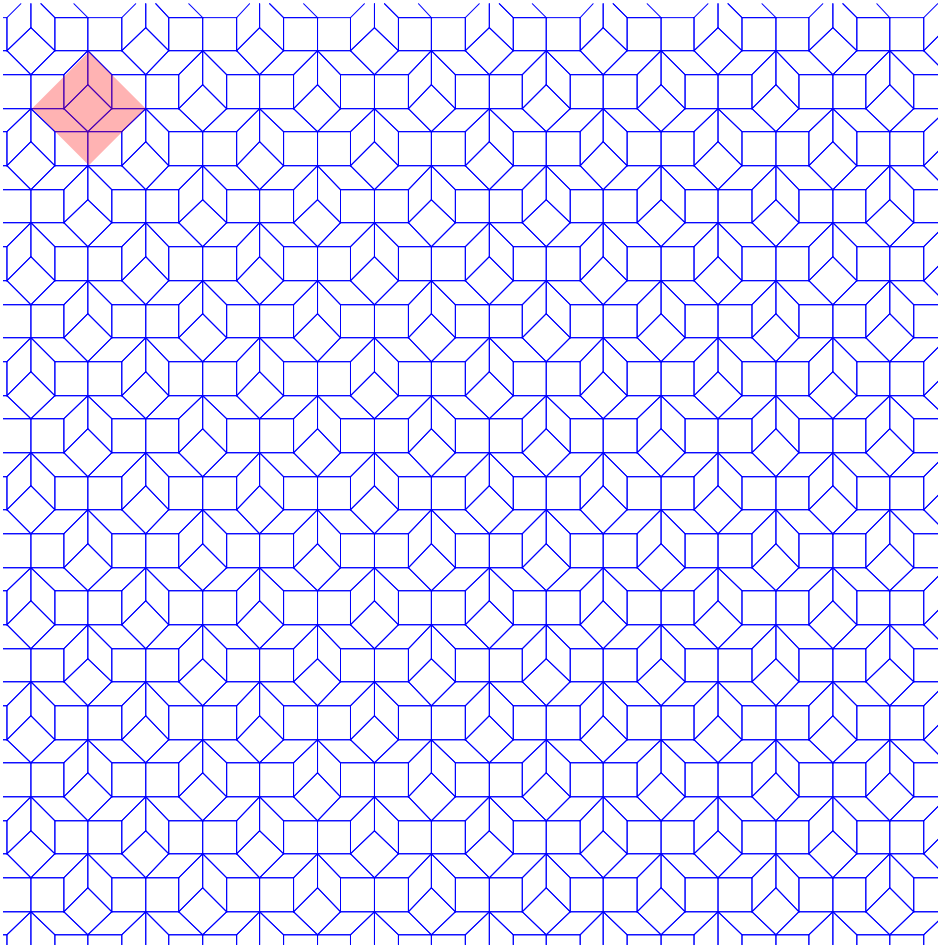
Phason strain

Ammann-Beenker tiling



$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix},$$
$$\mathbf{a}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{a}_4 = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

Periodic approximant

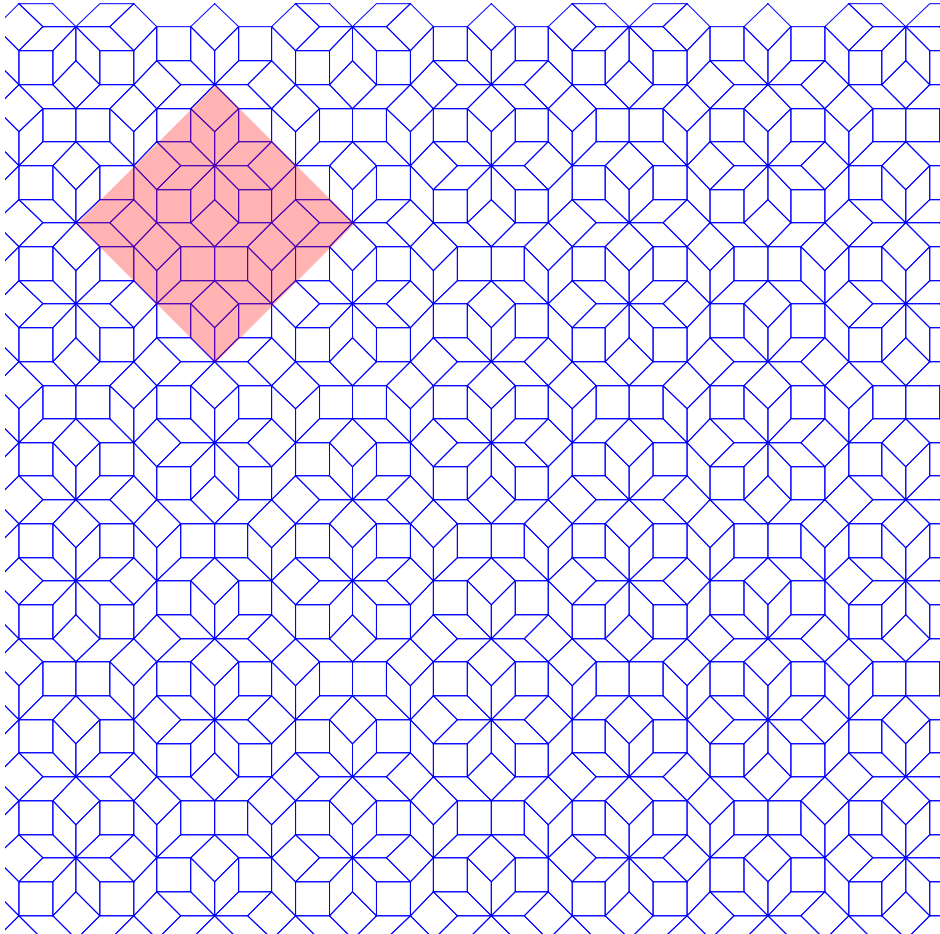


$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1 \\ 1 \end{pmatrix},$$

$$\mathbf{a}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{a}_4 = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 1 \\ 1 \end{pmatrix}$$

rational approximation

Periodic approximant



$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -2/3 \\ 2/3 \end{pmatrix},$$
$$\mathbf{a}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{a}_4 = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 2/3 \\ 2/3 \end{pmatrix}$$

rational approximation

The resulting tiling will have a crystallographic point group which is a subgroup of the 8-fold point group.

8. Phason flips

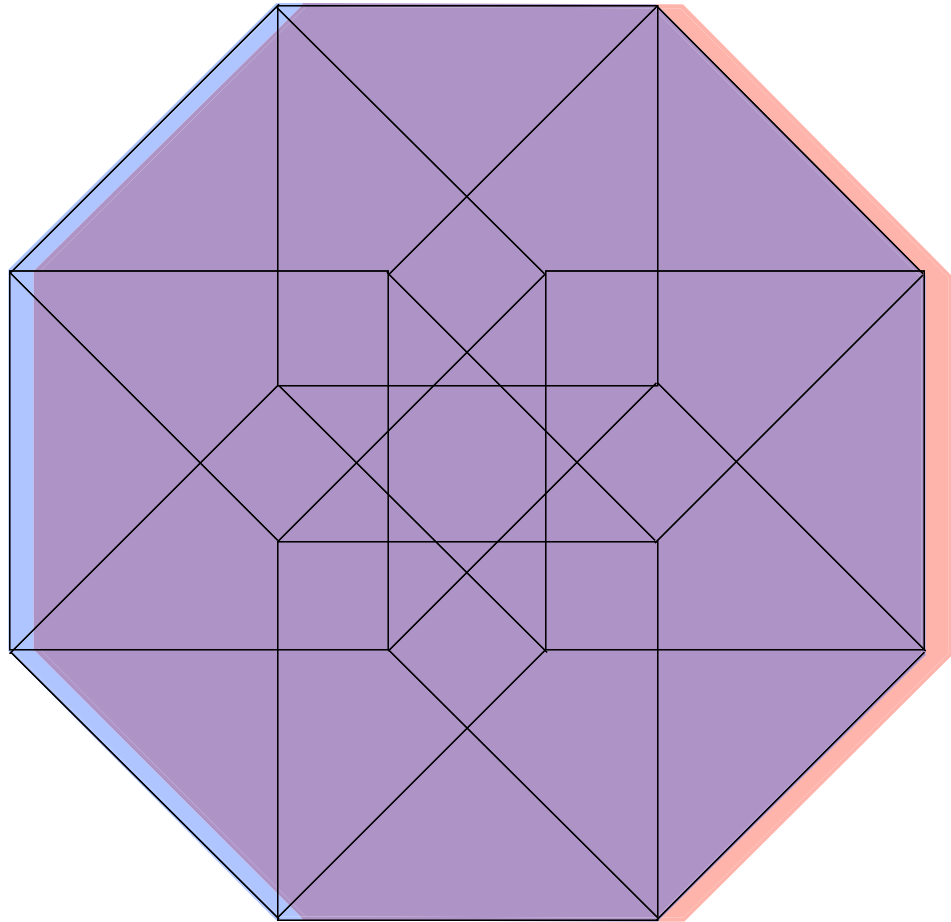
Phason shift

Phason shift:

Let's see what happens if the atomic surface is shifted in the perpendicular space.

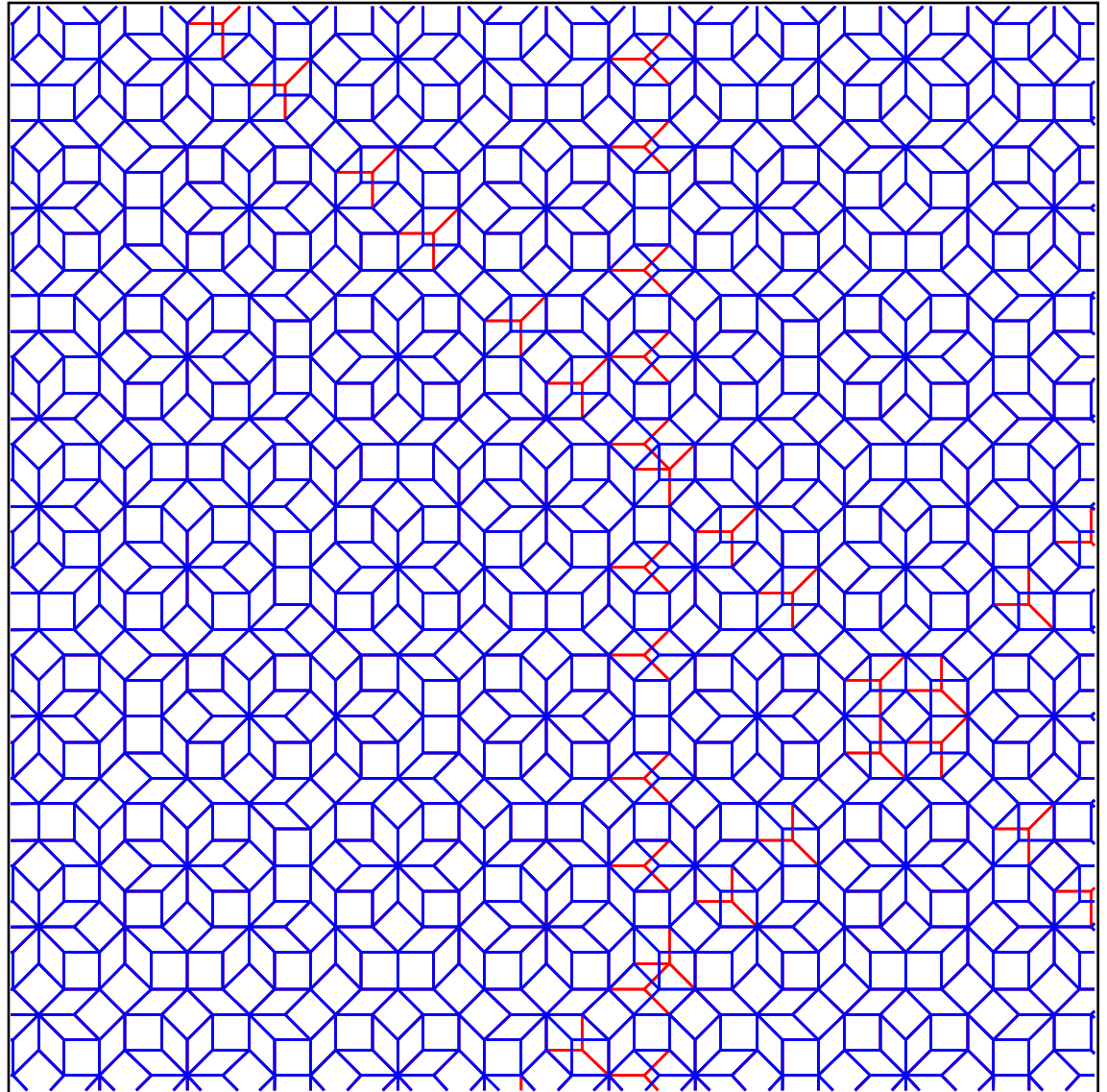
(blue) original

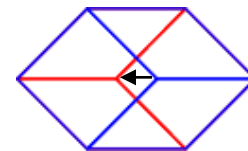
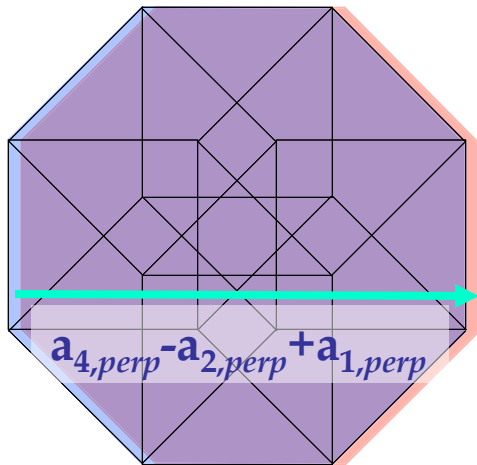
(red) shifted



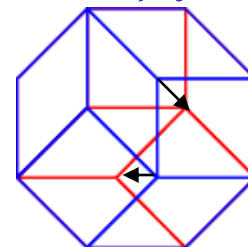
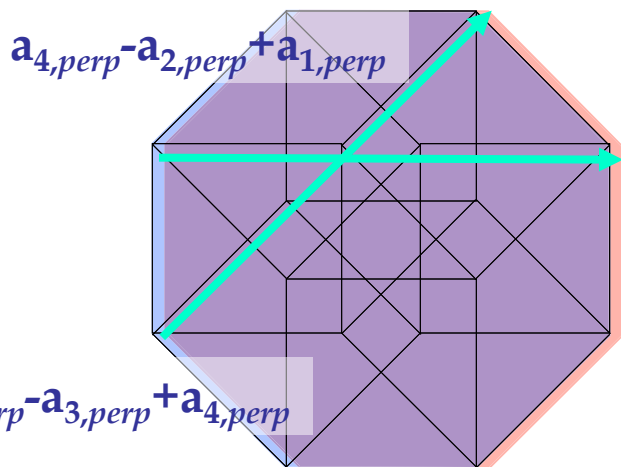
Rearrangement of tiles
due to local flips called

phason flips
or singleton flips
or phason jumps.





$a_{4,phys} - a_{2,phys} + a_{1,phys}$

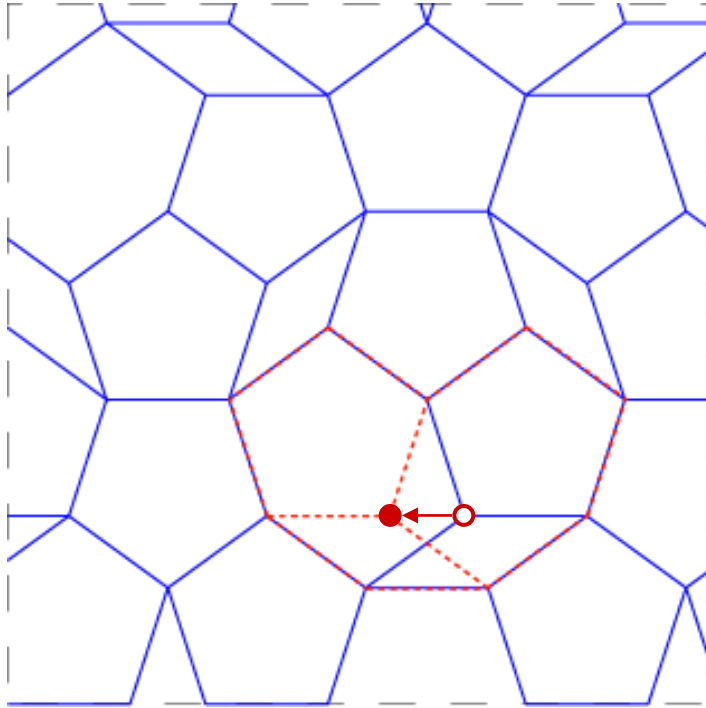


$a_{4,phys} - a_{2,phys} + a_{1,phys}$

$a_{1,phys} - a_{3,phys} + a_{4,phys}$

The cost of energy is very small for phason flips.
They are closely connected to defects and dynamics in quasicrystals.

**K. Edagawa, K. Suzuki & S. Takeuchi,
Phys. Rev. Lett. 85 (2000) 1674.**



Decagonal QC $\text{Al}_{65}\text{Cu}_{20}\text{Co}_{15}$
Real time observation (1123K)

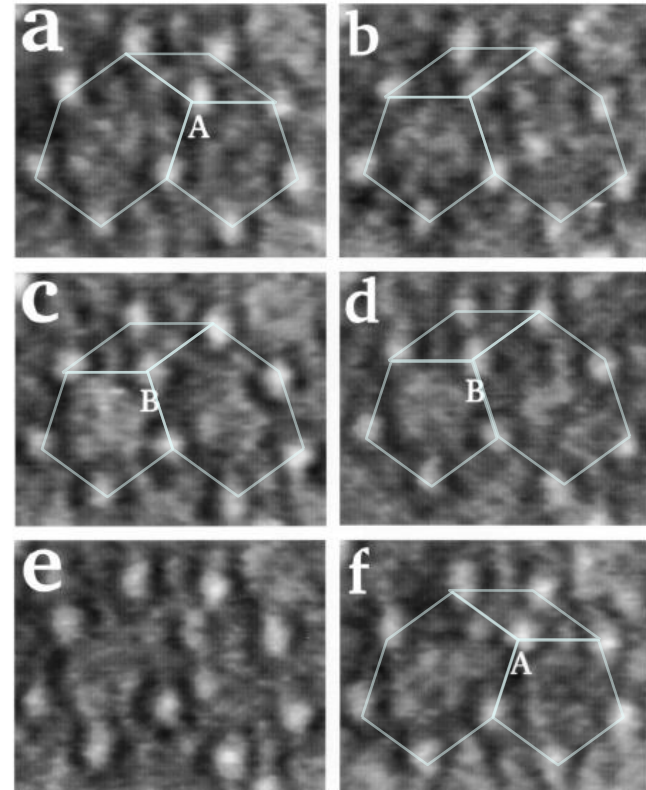


FIG. 2. An example of the change in the HRTEM image observed at 1123 K. Elapsed times for (a)–(f) are 0, 5, 8, 110, 113, and 115 s, respectively. The scale bar indicates 2.0 nm.

Summary of Part B

- 1. The classification of aperiodic tilings can be done on the basis of dimensionality, symmetry and the MLD concept.**
- 2. A proper hyperlattice for a given Bravais class can be chosen.**
- 3. Approximants are obtained by introducing a phason strain into the hyperlattice.**
- 4. Phason flips are associated with a shift of the atomic surfaces along the perpendicular space.**

Remarks

- 1. There are a lot more different tilings than those shown in this lecture. For some of them, not all the four techniques can be applied for construction.**
- 2. In my view, the substitution method can handle the broadest class of deterministic tilings, which even include those with fractal atomic surfaces.**
- 3. Some aperiodic tilings do not exhibit Bragg reflections but are constructed deterministically. What kind of order do they have?**

c.f.

Tiling encyclopedia (germany): <http://tilings.math.uni-bielefeld.de/>