第一回新学術領域ハイパーマテリアル
若手研究会@Web開催2020.5.28

準周期構造の理論的基礎
Theoretical introduction to quasiperiodic structures

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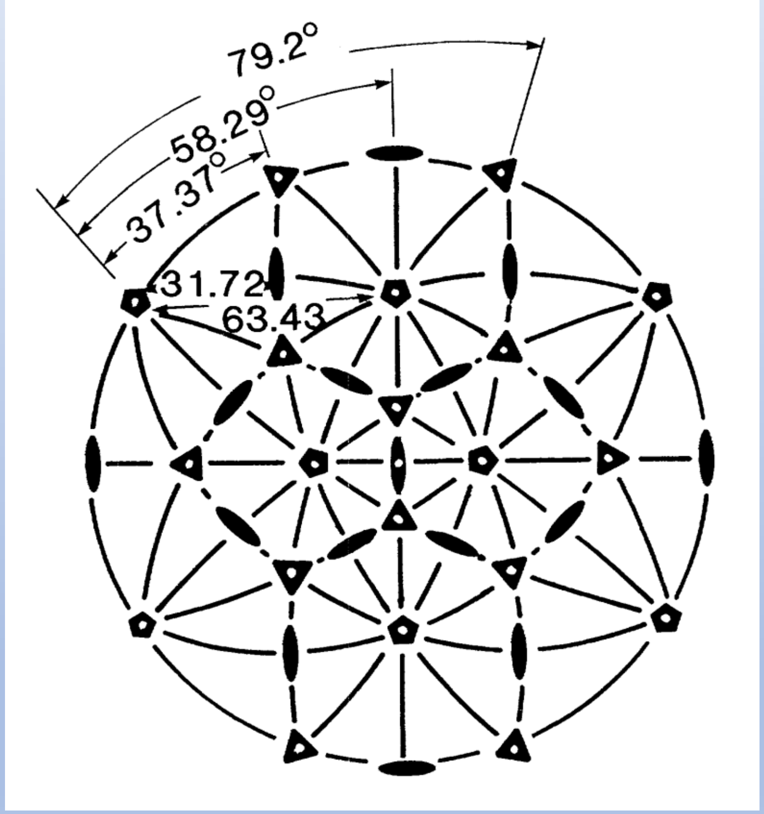
Outline

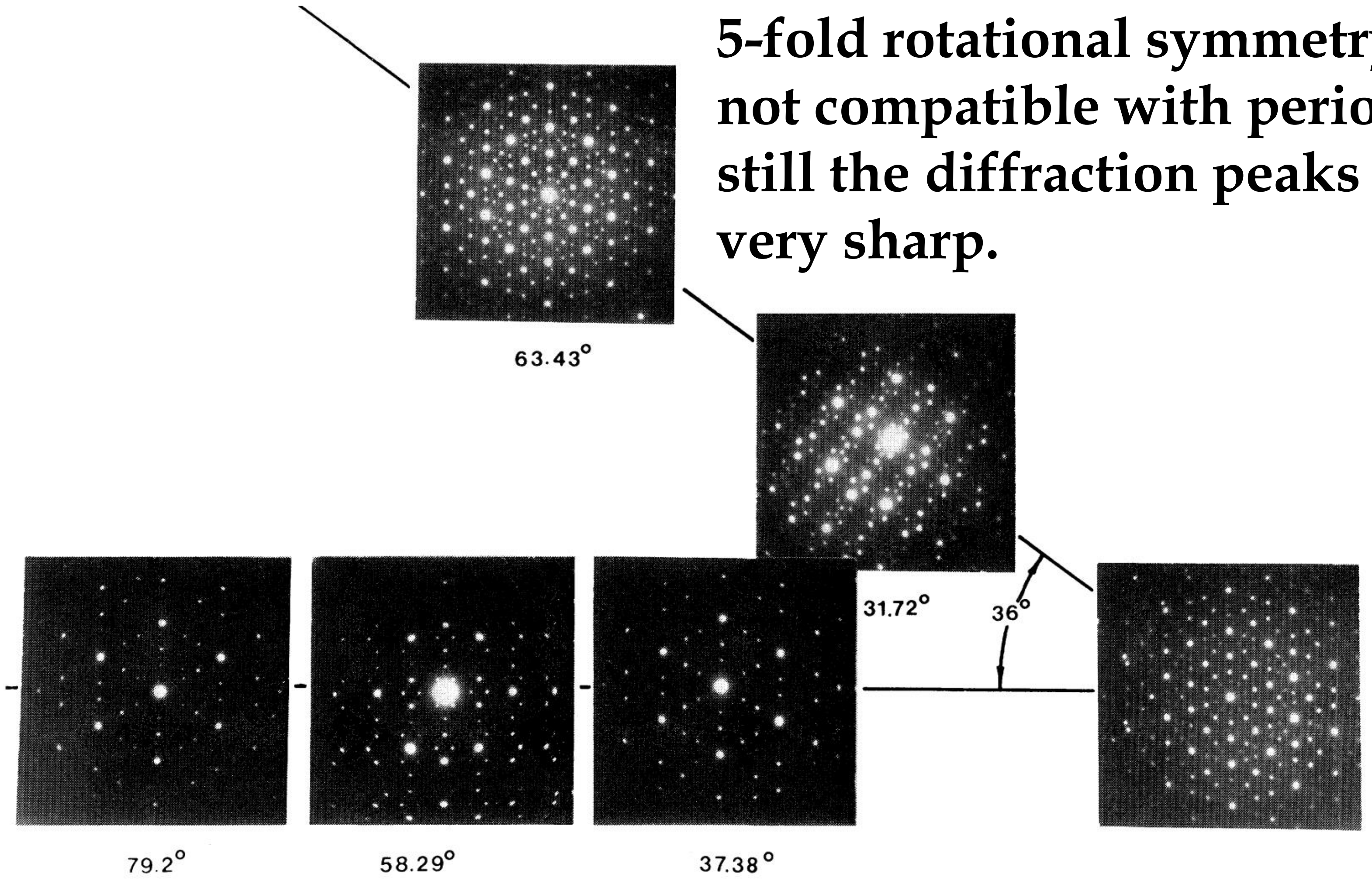
1. Introduction

ED pattern from a rapidly quenched Al-Mn alloy



D. Shechtman, *et al.*, *Phys. Rev. Lett.* 53 (1984) 1951–1953.

5-fold rotational symmetry is not compatible with periodicity, still the diffraction peaks are very sharp.



D. Shechtman, *et al.*, *Phys. Rev. Lett.* 53 (1984) 1951—1953.

Quasicrystals as a new class of ordered solids

1. Long-range quasiperiodic translational order

A QC exhibits a self-similar arrangement of Bragg peaks (δ functions), whose indexing needs k ($> d$) independent basis vectors for indexing (d: the number of space dimensions).

2. Non-crystallographic point group symmetry

A QC exhibits a point group symmetry forbidden in periodic crystals (*e.g.*, n-fold rotational axes with n being a natural number excluding 1, 2, 3, 4 and 6).

D. Levine and P.J. Steinhardt, *Phys. Rev. Lett.* 53 (1984) 2477—2480.

Paradigm shift in crystallography: the New definition of crystals (1992)

The definition proposed by the IUCr Commission on Aperiodic Structures (IUCr, 1991):

by *crystal* we mean <u>any solid having an essentially discrete diffraction diagram</u> and *aperiodic crystal* we mean <u>any crystal in which three-dimensional lattice periodicity can be considered to be absent</u>.

International Union of Crystallography, Report of the Executive Committee for 1991, *Acta Cryst.* A48 (1992) 922—946.

Aperiodic order: Three known categories

Quasiperiodic structure (QCs, incommensurate modulation, composite crystals)

A structure that show Bragg peaks (δ functions) in diffraction patterns which require k ($> d$) independent reciprocal basis vectors for indexing, where d is the # of space dimensions and $k < \infty$.

Limit-periodic structure

A structure with recursive (or hierarchical) superlattice structures superposed on a basic periodic lattice.

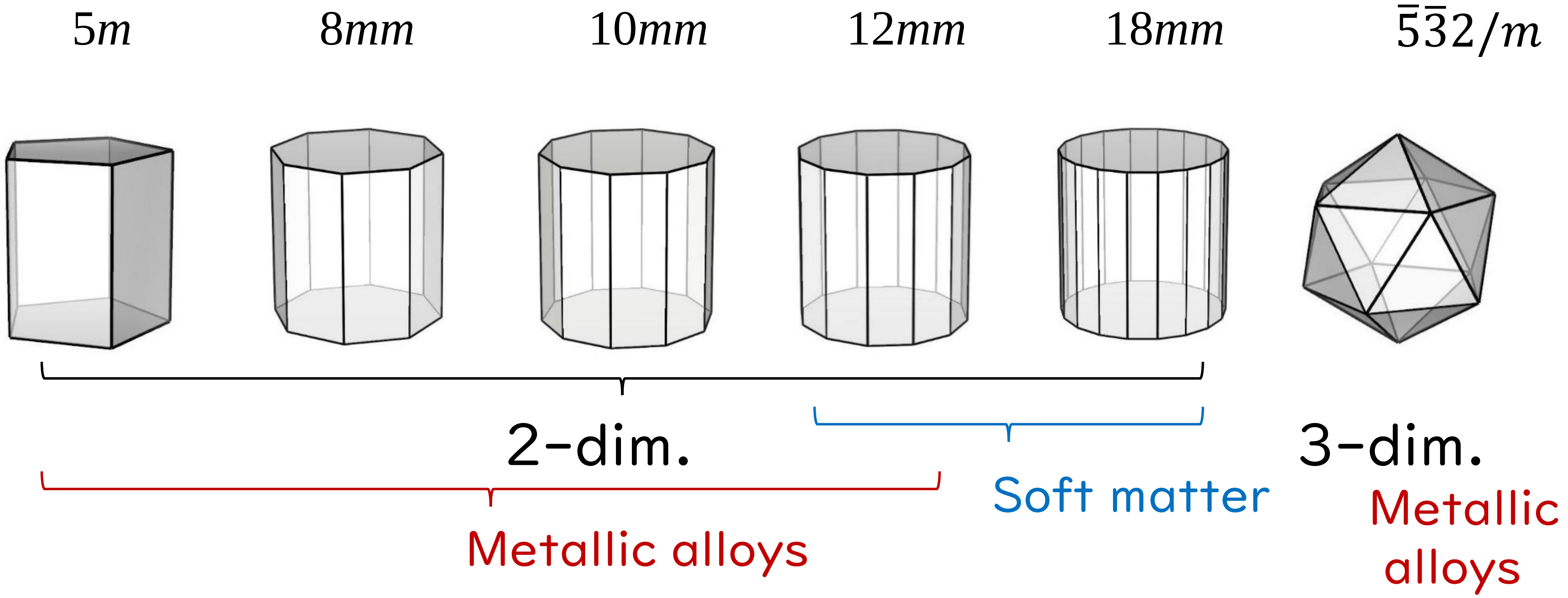
K. Niizeki and N. Fujita, *Philos. Mag.* 87 (2007) 3073—3078 and references cited therein.

Limit-quasiperiodic structure

A structure that can be obtained as an incommensurate section of a limit-periodic structure in higher dimensions.

K. Niizeki and N. Fujita, *J. Phys. A: Math. Gen.* 38 (2005) L199—L204 and references cited therein.

Non-crystallographic point groups for quasicrystals



2. Z-Modules for quasicrystals

(Z-加群) : Additive Abelian group over an integer ring (Z)

!! Alternatives to lattices for periodic crystals

Reciprocal (= Fourier) module, $\mathcal{M}^*$

≃ A *dense* (≠ *discrete*) point set in the *d*-dim. wave-number (or reciprocal) space generated as the integer linear combinations of *k* (> *d*) reciprocal basis vectors, used to index the Bragg peaks.

(*k*: rank, *d*: space dimensions)

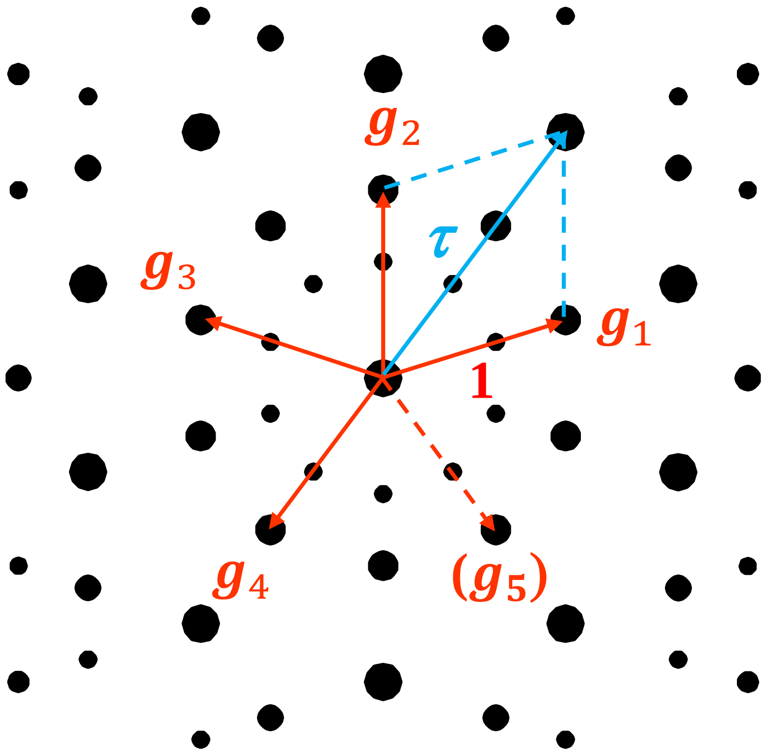
Direct (= Bravais) module, $\mathcal{M}$

≃ A *dense* (≠ *discrete*) point set in the *d*-dim. real (or direct) space generated as the integer linear combinations of *k* (> *d*) basis vectors, used to index the quasi-lattice points or tiling vertices.

Ex) Fourier module for decagonal QC

Point group

$10mm$



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

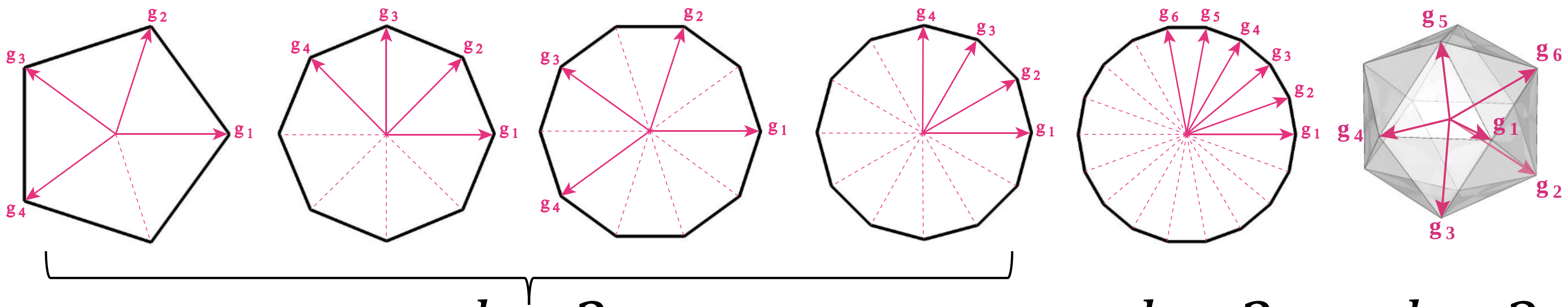
(golden mean)

$$\mathcal{M}_{10}^{*} = \{\sum_{j=1}^{4} n_j \boldsymbol{g}_j \,|\, n_j \in \mathbb{Z}\}$$

Minimal basis set for indexing the Bragg peaks

Point groups

$5m$ $8mm$ $10mm$ $12mm$ $18mm$ $\bar{5}\bar{3}2/m$



$d = 2$, $k = 4$ (pentagonal, octagonal, decagonal, dodecagonal)

$d = 2$, $k = 6$ (octakaidecagonal)

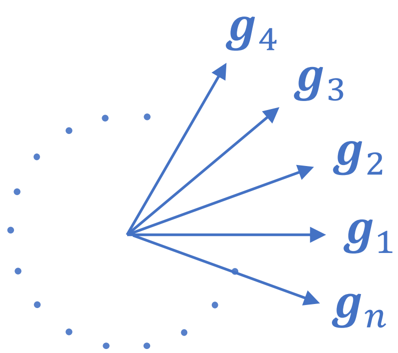
$d = 3$, $k = 6$ (icosahedral)

pentagonal octagonal decagonal dodecagonal octakaidecagonal icosahedral

For a planar n-gonal quasicrystal, the minimal number of basis vectors is $k = \phi(n)$, where $\phi(n)$ (Euler's ϕ-function) is the number of positive integers up to n that are co-prime with n.

$$\phi(n) = n \prod_j \left(1 - \frac{1}{p_j}\right) \qquad (p_j \in \{\text{all prime factors of } n\})$$

$$\sum_j \phi(d_j) = n \qquad (d_j \in \{\text{all divisors of } n\})$$

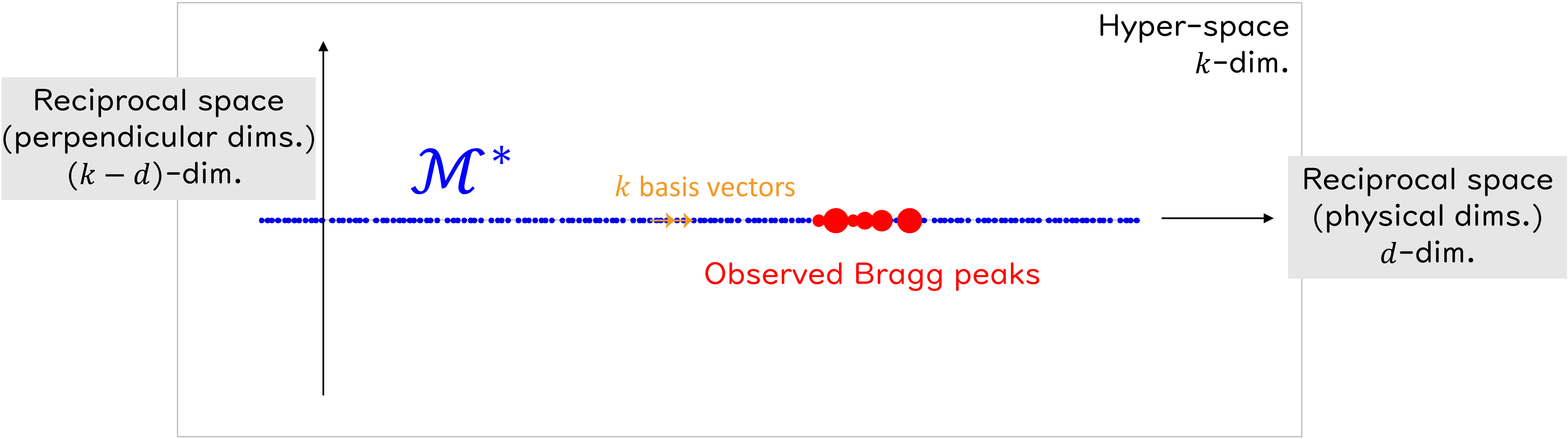


Check!! There are $n - \phi(n)$ independent constraints for the n unit vectors.

$$\left\{ g_\nu + g_{d_j+\nu} + g_{2d_j+\nu} + \cdots + g_{n-d_j+\nu} = 0 \mid 1 \le \nu \le \phi(d_j) \right\}_{1 \le d_j < n}$$

Lifting up the # of space dimensions

d-dim. Fourier module $\mathcal{M}^*$ of rank k can be lift up to k-dim. reciprocal hyper-lattice $\mathcal{L}^*$



Lifting up the # of space dimensions

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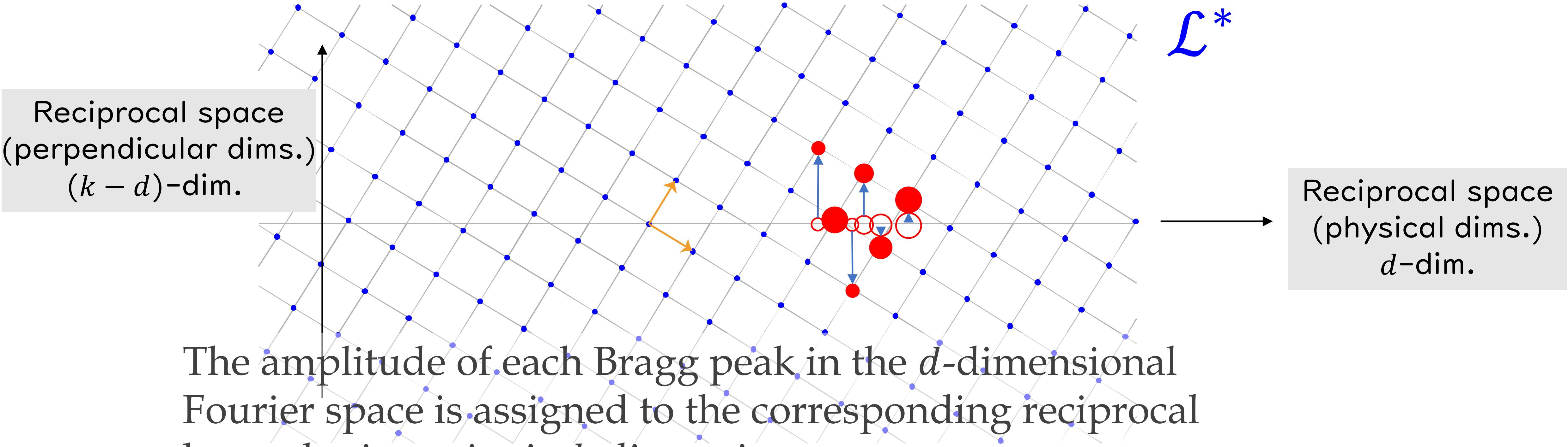


The amplitude of each Bragg peak in the d-dimensional Fourier space is assigned to the corresponding reciprocal hyper-lattice point in k dimensions

Complementary components, $g_j^\perp$

$G_{\mathcal{M}^*}$ **: point group of the Fourier module $\mathcal{M}^*$ of the QC**

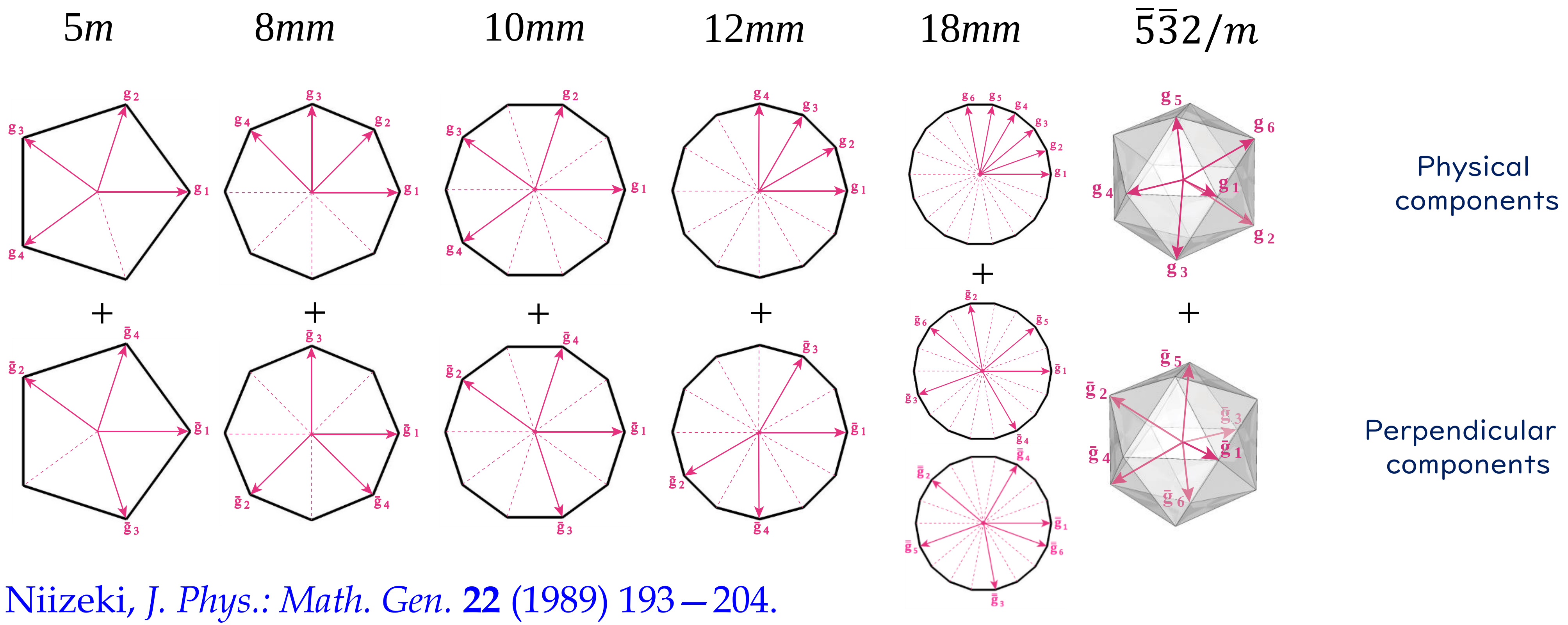
$G_{\mathcal{L}^*}$ **: point group of the k-dim. reciprocal hyper-lattice $\mathcal{L}^*$**

$G_{\mathcal{L}^*}$ should have a subgroup H which is isomorphic to $G_{\mathcal{M}^*}$ (i.e., $G_{\mathcal{L}^*} \supset H \cong G_{\mathcal{M}^*}$) and which does not mix the physical and orthogonal components, i.e.,

$$\bar{D} = \begin{pmatrix} D & 0 \\ 0 & D^\perp \end{pmatrix} \text{ where } \bar{D} \in H \text{ and } D \in G_{\mathcal{M}^*}$$

Lifting up the # of space dimensions

[k-dim. basis vectors, $\bar{g}_j = (g_j, g_j^{\perp})$ of $\mathcal{L}^*$]



[1] K. Niizeki, *J. Phys.: Math. Gen.* **22** (1989) 193 – 204.
[2] A. Yamamoto, *Acta Cryst.* A**52** (1996) 509 – 560.

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Structure factors

Fourier tr. ($\boldsymbol{d}$−dim.)

Physical dims. (d-dim.)

$$\{S(\boldsymbol{G})|\ \boldsymbol{G} \in \mathcal{M}^*\} \leftrightarrow \rho^d(\boldsymbol{r}) = \sum_{\boldsymbol{G}\in\mathcal{M}^*} S(\boldsymbol{G}) e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

∧

projection ↑ section ↑

Hyper-space (k-dim.)

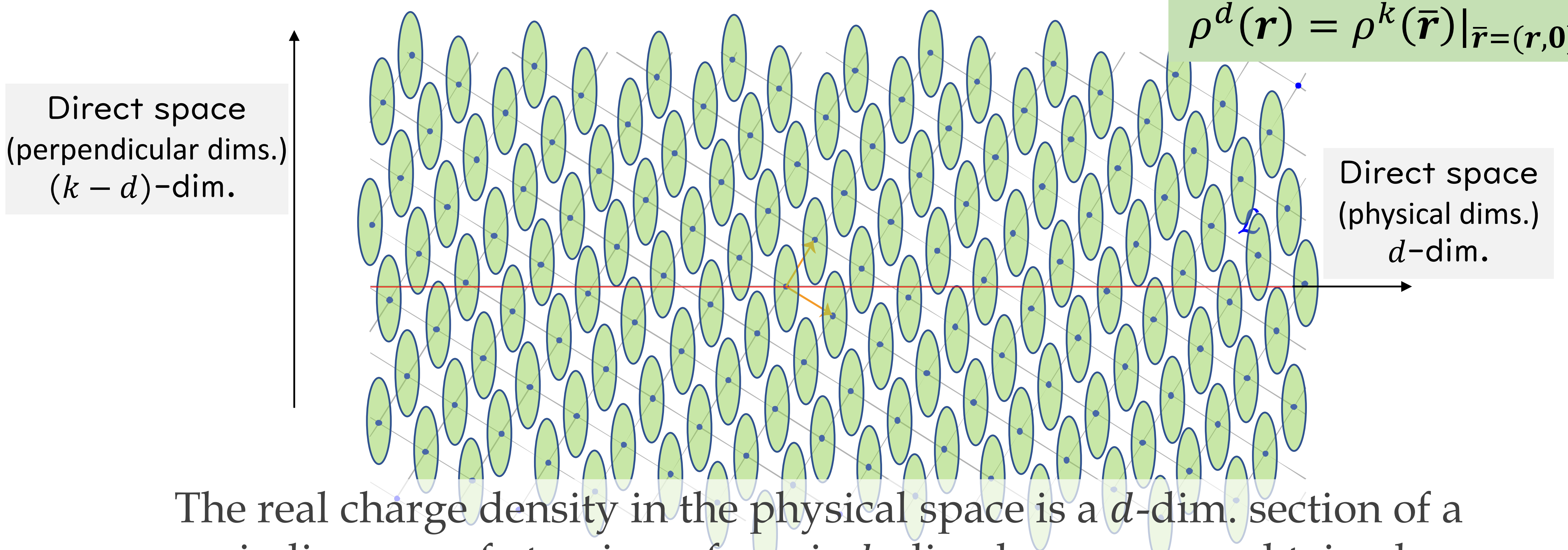
$$\{\bar{S}(\overline{\boldsymbol{G}})|\ \overline{\boldsymbol{G}} \in \mathcal{L}^*\} \leftrightarrow \rho^k(\bar{\boldsymbol{r}}) = \sum_{\overline{\boldsymbol{G}}\in\mathcal{L}^*} \bar{S}(\overline{\boldsymbol{G}}) e^{i\overline{\boldsymbol{G}}\cdot\bar{\boldsymbol{r}}}$$

Fourier tr. ($\boldsymbol{k}$−dim.)

(Reciprocal space) (Direct space)

Charge density (periodic in hyper-space)

$$\rho^d(\boldsymbol{r}) = \rho^k(\bar{\boldsymbol{r}})|_{\bar{\boldsymbol{r}}=(\boldsymbol{r},\boldsymbol{0})}$$



The real charge density in the physical space is a d-dim. section of a periodic array of atomic surfaces in k-dim. hyper-space obtained as the Fourier transform of the k-dim. structure factors.

k-dim. bases $\overline{\boldsymbol{a}}_j$ of the direct hyper-lattice $\mathcal{L}$ = Fourier tr. of the reciprocal hyper-lattice $\mathcal{L}^*$

$$\overline{\boldsymbol{a}}_i \cdot \overline{\boldsymbol{g}}_j = \boldsymbol{\delta}_{ij}$$

$$B = \begin{pmatrix} \overline{\boldsymbol{g}}_1 \\ \overline{\boldsymbol{g}}_2 \\ \vdots \\ \overline{\boldsymbol{g}}_n \end{pmatrix} \qquad A = \begin{pmatrix} \overline{\boldsymbol{a}}_1 \\ \overline{\boldsymbol{a}}_2 \\ \vdots \\ \overline{\boldsymbol{a}}_n \end{pmatrix} = (B^{-1})^T$$

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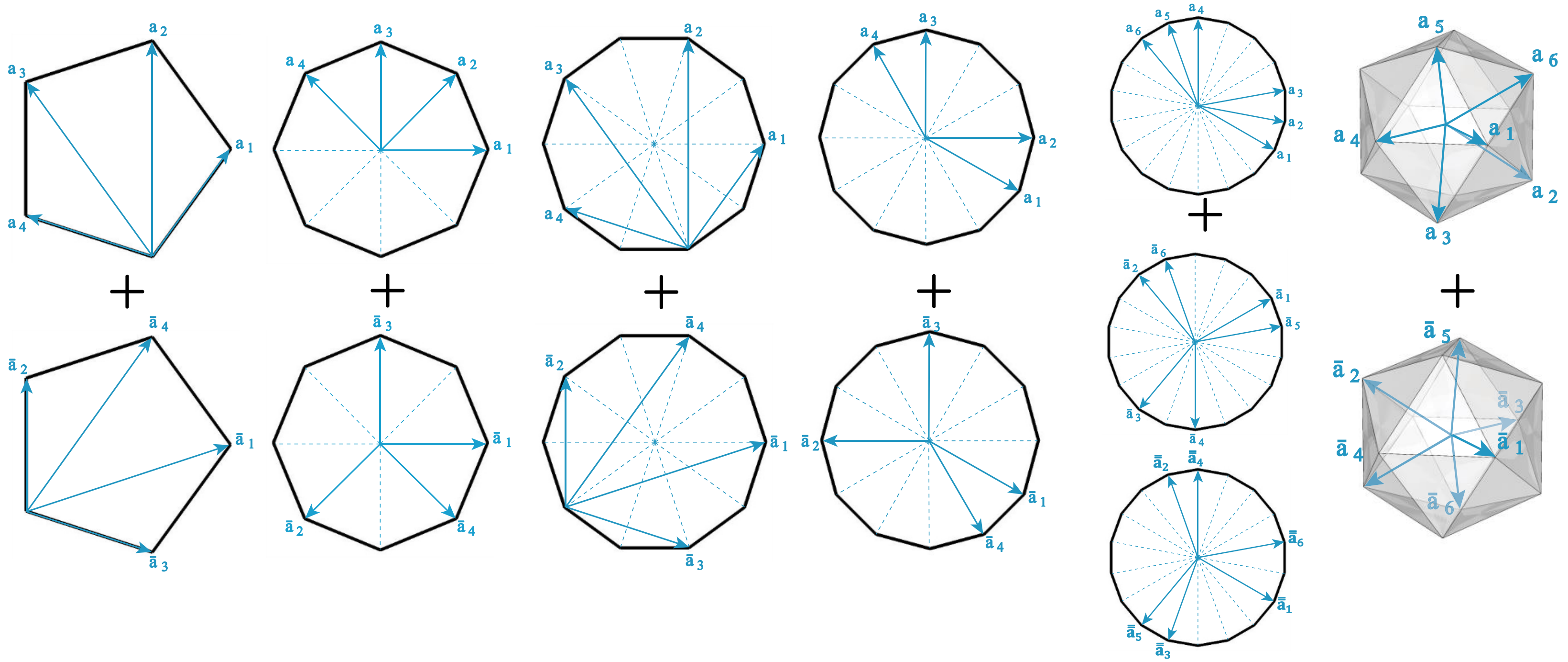
k-dimensional bases $\bar{\boldsymbol{a}}_j = (\boldsymbol{a}_j, \boldsymbol{a}_j^{\perp})$ of $\mathcal{L}$

$5m$ | $8mm$ | $10mm$ | $12mm$ | $18mm$ | $\bar{5}\bar{3}2/m$



Physical components

Perpendicular components

$\binom{\text{Direct}}{\text{Reciprocal}}$ hyper-lattices for quasicrystals

- 2-dim. QC : A unique hyper-lattice exists for n-gonal case $(n = 5, 8, 10, 12, 18, \ldots)$
- 3-dim. QC : Three hyper-lattices exist for icosahedral case P-type (SI) / F-type (FCI) / I-type (BCI)

$$\mathcal{L}_P := \{n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3 + n_4\bar{a}_4 + n_5\bar{a}_5 + n_6\bar{a}_6\}$$

$$\mathcal{L}_F := \left\{n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3 + n_4\bar{a}_4 + n_5\bar{a}_5 + n_6\bar{a}_6 \,\middle|\, \sum_{j=1}^{6} n_j = 0 \bmod 2\right\}$$

$$\mathcal{L}_I := \left\{n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3 + n_4\bar{a}_4 + n_5\bar{a}_5 + n_6\bar{a}_6 \,\middle|\, n_i = n_j \bmod 2\right\}$$

Direct (= Bravais) module $\mathcal{M}$
(projection of $\mathcal{L}$ onto the physical sub-space)

Df.) $\mathcal{M} = \left\{ \sum_{j=1}^{k} n_j \boldsymbol{a}_j \,\middle|\, n_j \in \mathbb{Z} \right\}$

	Physical dims. (*d*-dim.)		Hyper-space (*k*-dim.)		Perpendicular dims. ((*k*-*d*)-dim.)
Reciprocal space	$\mathcal{M}^*$	$\longleftrightarrow$	$\mathcal{L}^*$	$\longleftrightarrow$	$\mathcal{M}_\perp^*$
	$\Updownarrow$ (dashed)		$\updownarrow$		$\Updownarrow$ (dashed)
Direct space	$\mathcal{M}$	$\longleftrightarrow$	$\mathcal{L}$	$\longleftrightarrow$	$\mathcal{M}_\perp$

Self-similarity of $\mathcal{M}$ (and $\mathcal{M}^*$)

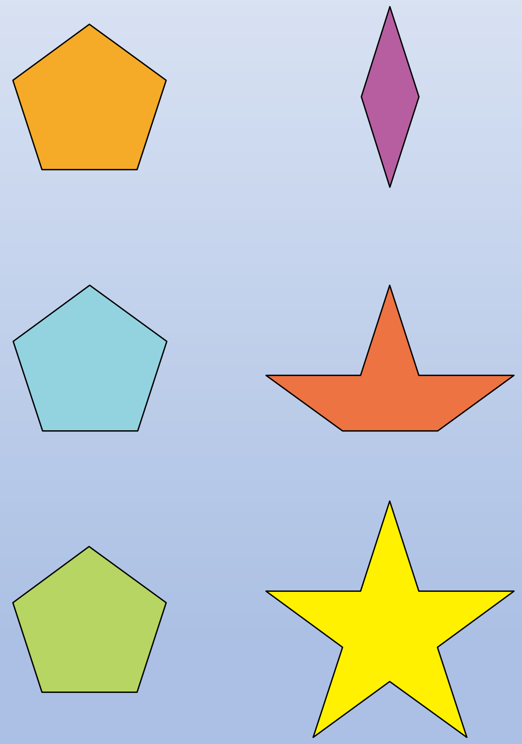
Z-modules for quasicrystals are scale invariant.
There exists an irrational number τ, called the *Pisot unit*, such that $\tau\mathcal{M}=\mathcal{M}$ **and** $\tau > 1$

Pisot unit for important classes of QCs:

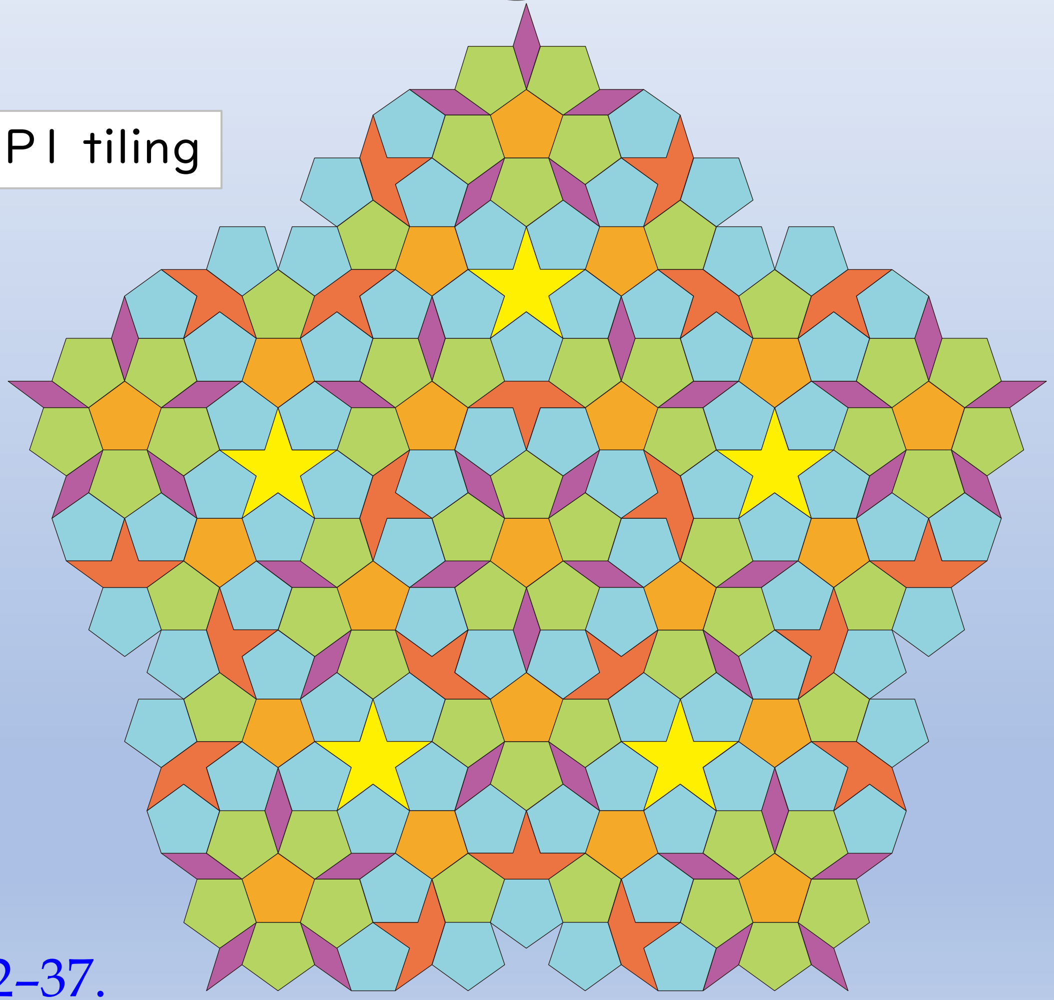
$1+\sqrt{2}$	$\dfrac{1+\sqrt{5}}{2}$	$2+\sqrt{3}$	$\tau_1 = 1+\varsigma+\varsigma^{-1}$, $\tau_2 = \tau_1(\tau_1-1)$ ($\varsigma = e^{\frac{\pi i}{9}}$)	$2+\sqrt{5}$	$\dfrac{1+\sqrt{5}}{2}$
$\mathcal{M}_8$ [3]	$\mathcal{M}_5$ [3], $\mathcal{M}_{10}$	$\mathcal{M}_{12}$ [3]	$\mathcal{M}_{18}$ [3]	$\mathcal{M}_{I_h}^{\mathrm{P}}$ [1,2]	$\mathcal{M}_{I_h}^{\mathrm{F}}$ [1,2], $\mathcal{M}_{I_h}^{\mathrm{I}}$

[1] D.S. Rokhsar, *et al.*, *Phys. Rev. B* **35** (1987)5487 – 5495.
[2] L.S. Levitov and J. Rhyner, *J. Phys. France* **49** (1988) 1835 – 1849.
[3] K. Niizeki, *J. Phys.: Math. Gen.* **22** (1989) 193 – 204.

3. Quasiperiodic tilings (QPTs)



P1 tiling



R. Penrose, *Math. Intel.* **2** (1979) 32–37.
B. Gruenbaum, G.C. Shephard, *Tilings and Patterns* (Freeman, New York, 1987) Chap. 10.

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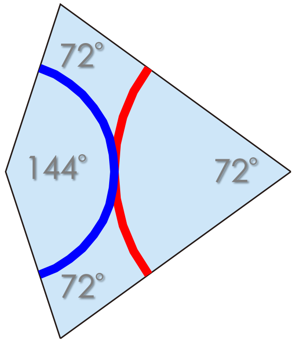
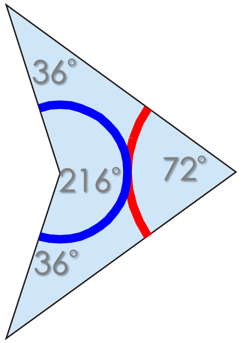
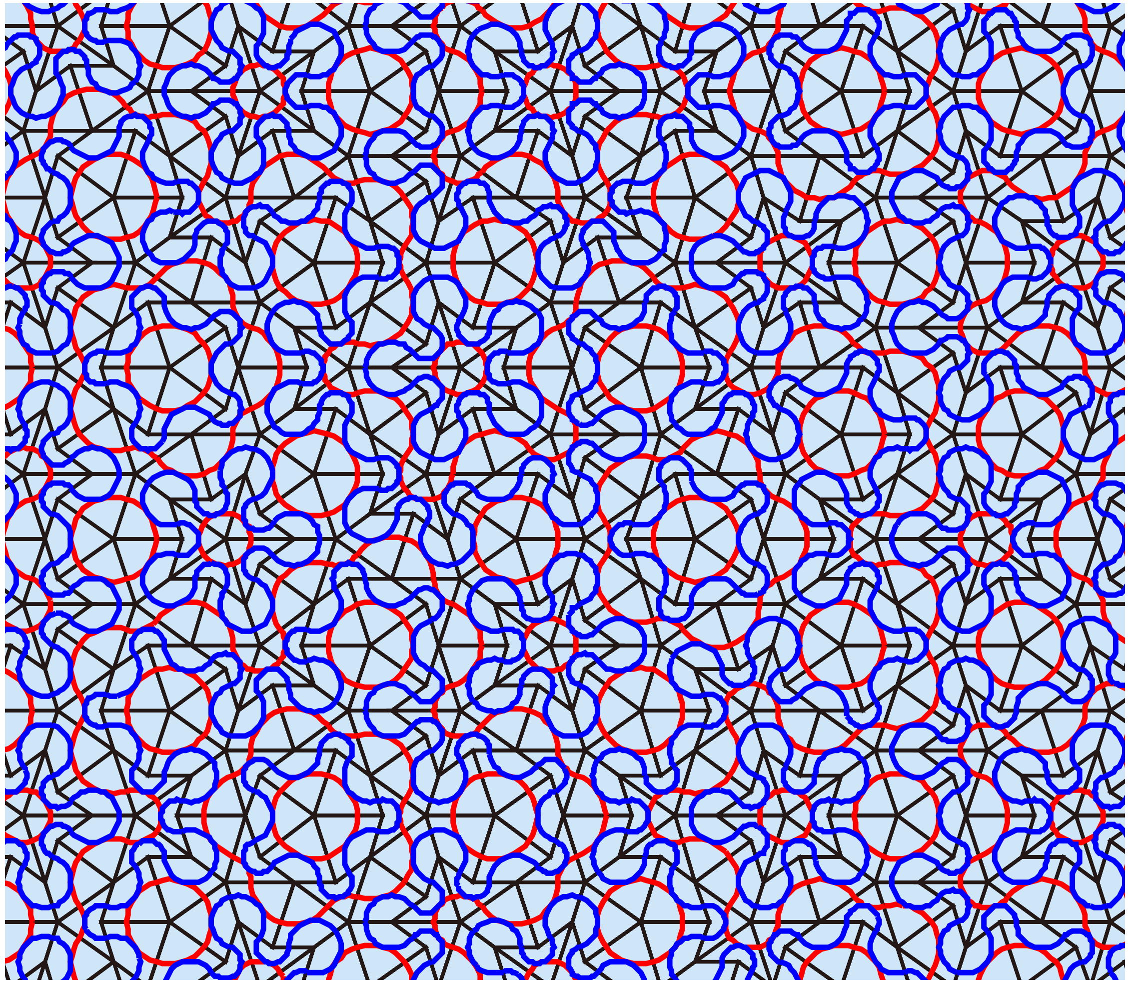
kite



dart



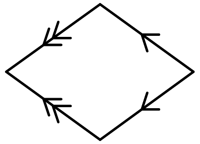
P2 tiling



R. Penrose, *Math. Intel.* **2** (1979) 32–37.
B. Gruenbaum, G.C. Shephard, *Tilings and Patterns* (Freeman, New York, 1987) Chap. 10.

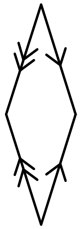
P3 tiling

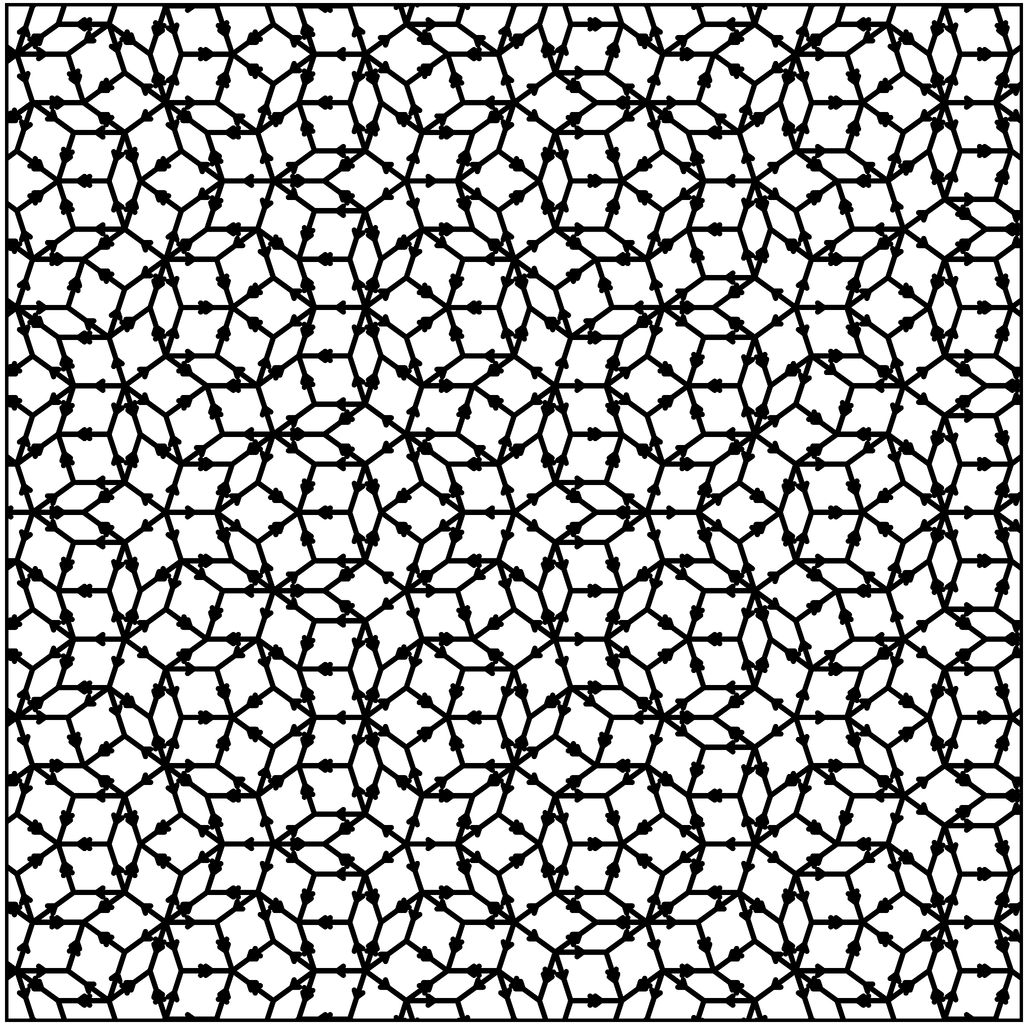
72°Rhombus



+

36°Rhombus



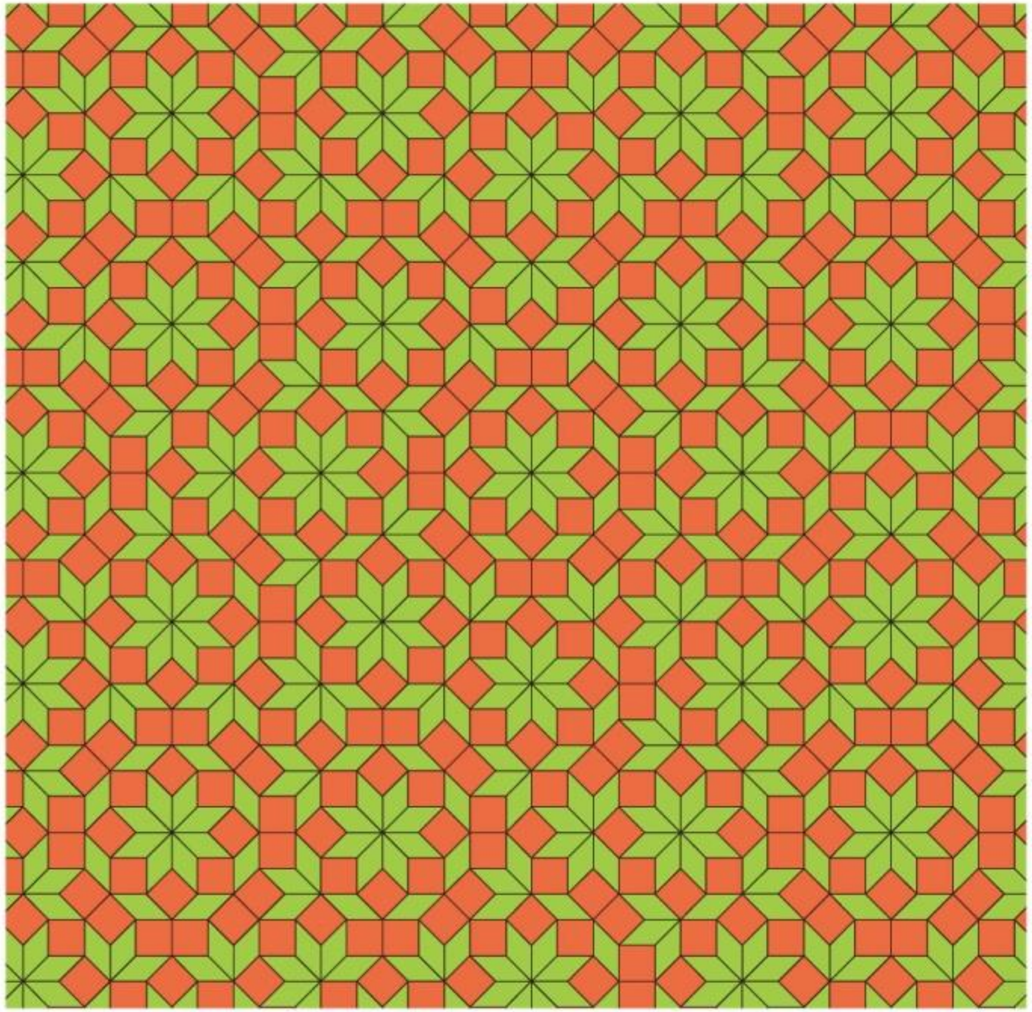


R. Penrose, *Math. Intel.* **2** (1979) 32–37.

B. Gruenbaum, G.C. Shephard, *Tilings and Patterns* (Freeman, New York, 1987) Chap. 10.

Ammann-Beenker tiling
(8*mm*)

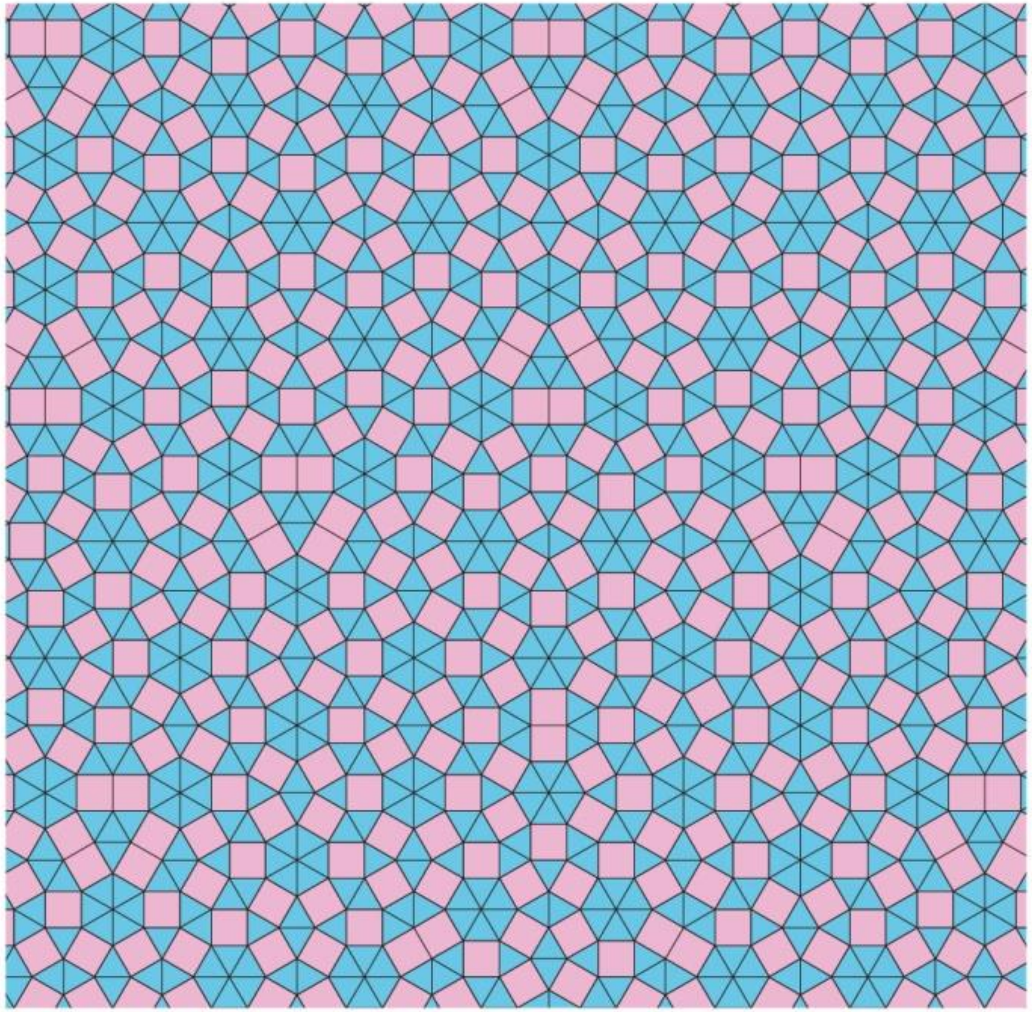
Square
+
45°Rhombus



F. P. M. Beenker, *Eindhoven University of Technology Report* No. 82-WSK-04. (Eindhoven , 1982).

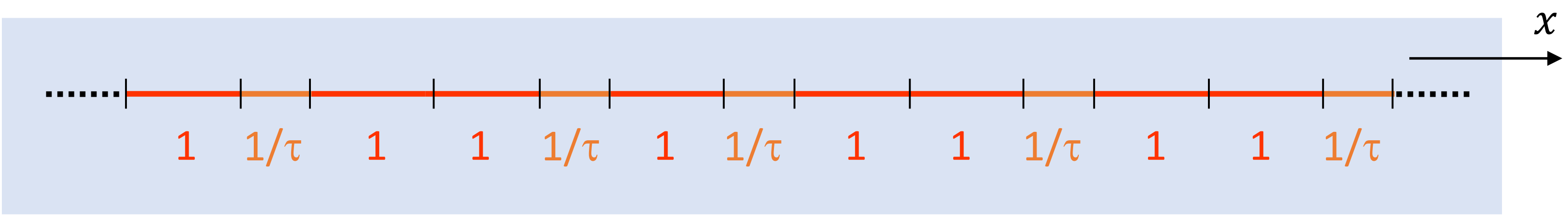
Stampfli tiling
(12*mm*)

Square
+
Equilateral
triangle



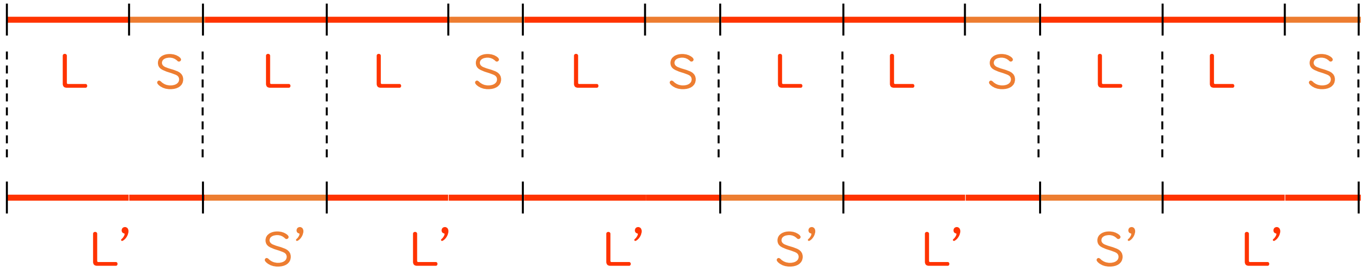
P. Stampfli, *Helv. Phys. Acta* **59** (1986) 1260–1263.
J. Hermisson, C. Richard, M. Baake, *J. Phys. I France* **7** (1997) 1003–1018.

Fibonacci chain (or tiling) (1-dim.)



$\tau = \frac{1+\sqrt{5}}{2}$ (golden mean)

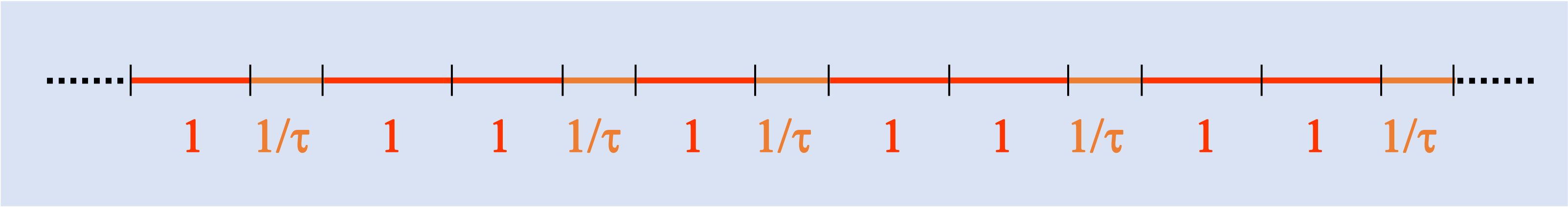
The x coordinate of every lattice point is represented as $x = i + \frac{j}{\tau}$, which belongs to the 1-dim. Z-module: $\mathcal{M} = \{m + n/\tau \mid m, n \in \mathbb{Z}\}$



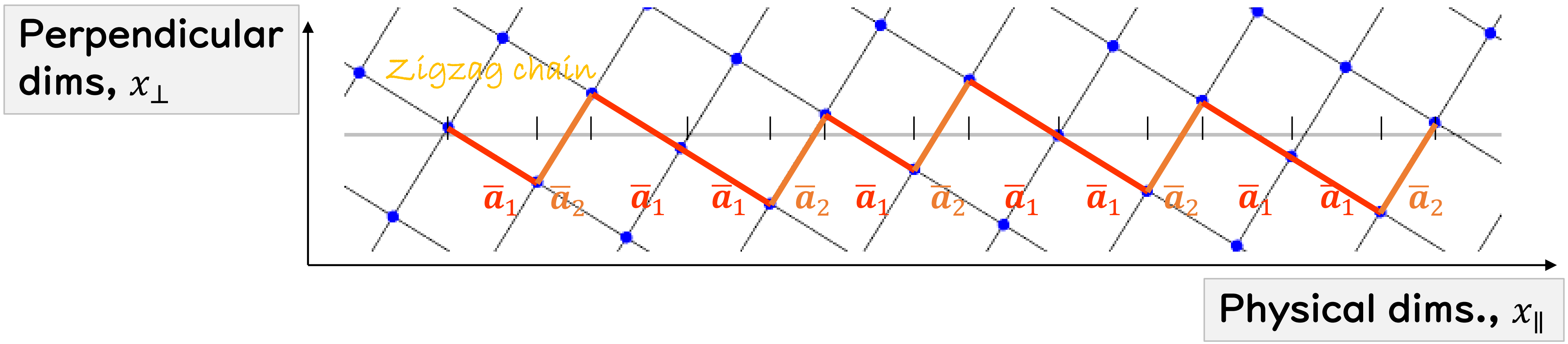
LSLLSLSLLSLLS⋯ ≅ L'S'L'L'S'L'S'L'⋯ (L'=LS, S'=L)

Cf. $\tau\mathcal{M}=\mathcal{M}$

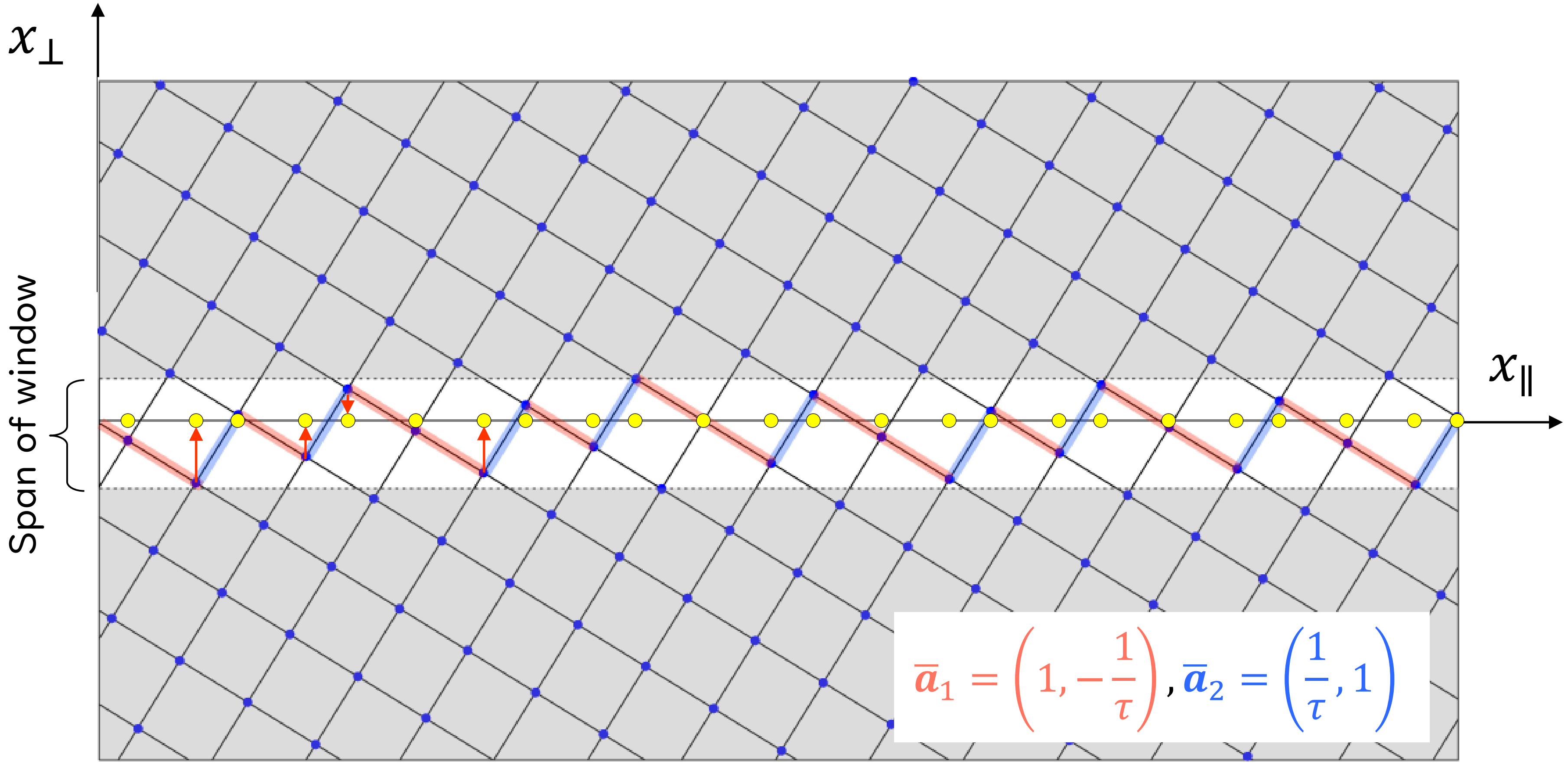
Lifting up the # of space dimensions



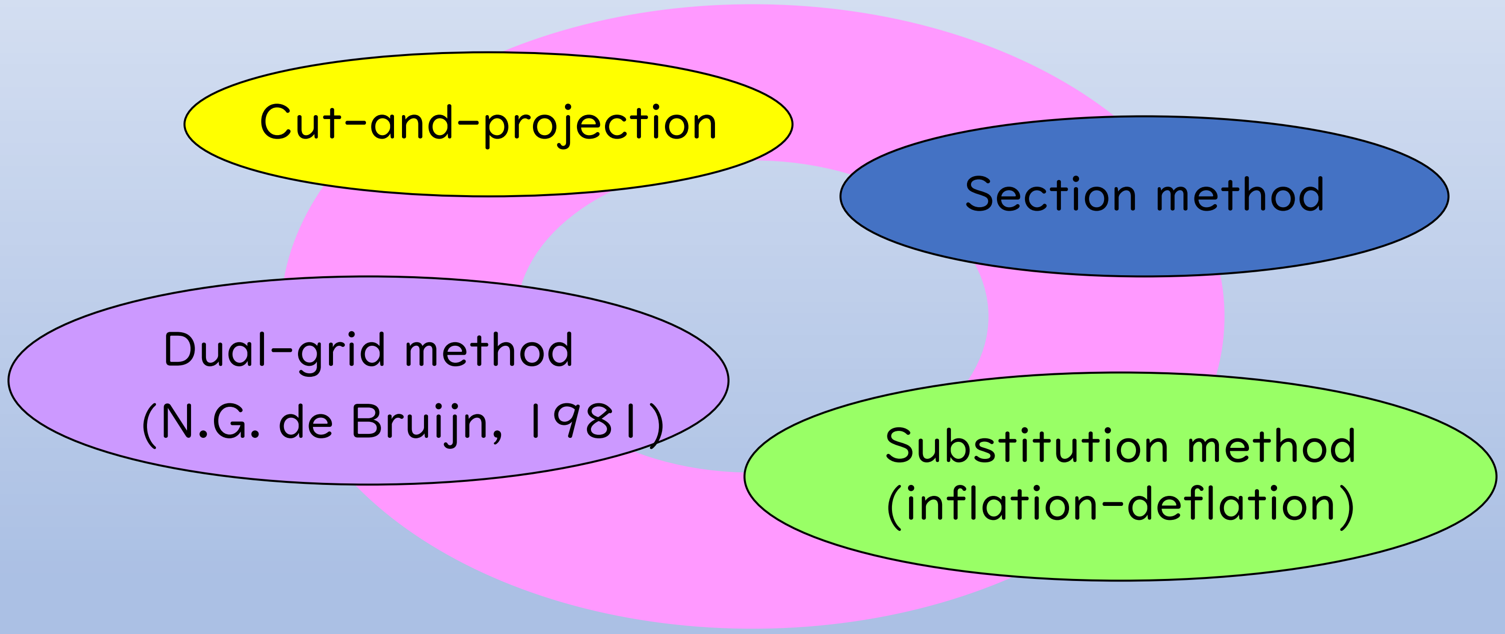
$$\bar{\boldsymbol{a}}_1 = \left(1, -\frac{1}{\tau}\right), \bar{\boldsymbol{a}}_2 = \left(\frac{1}{\tau}, 1\right)$$



Cut-and-project method

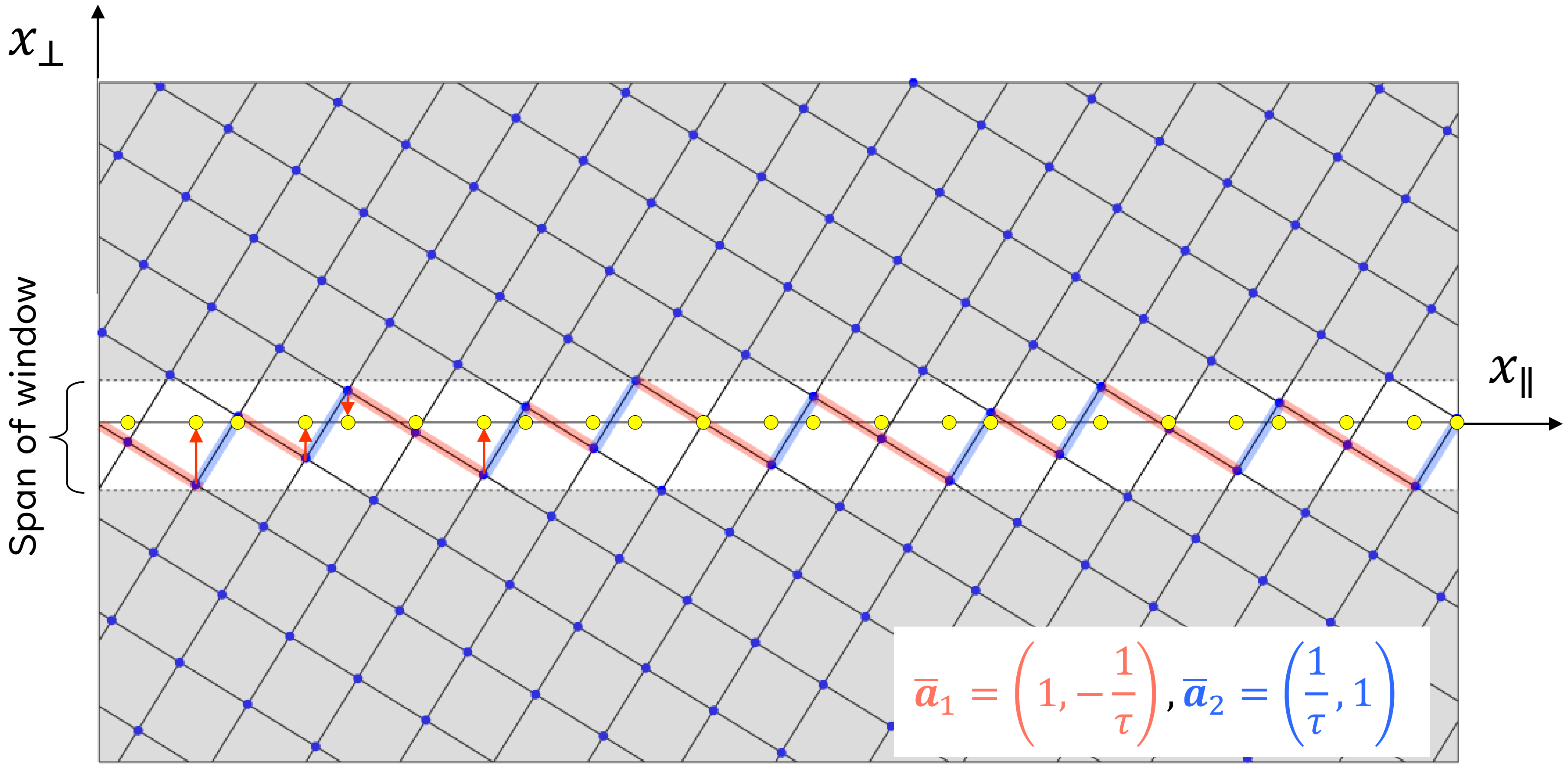


4. Methods for generating QPTs

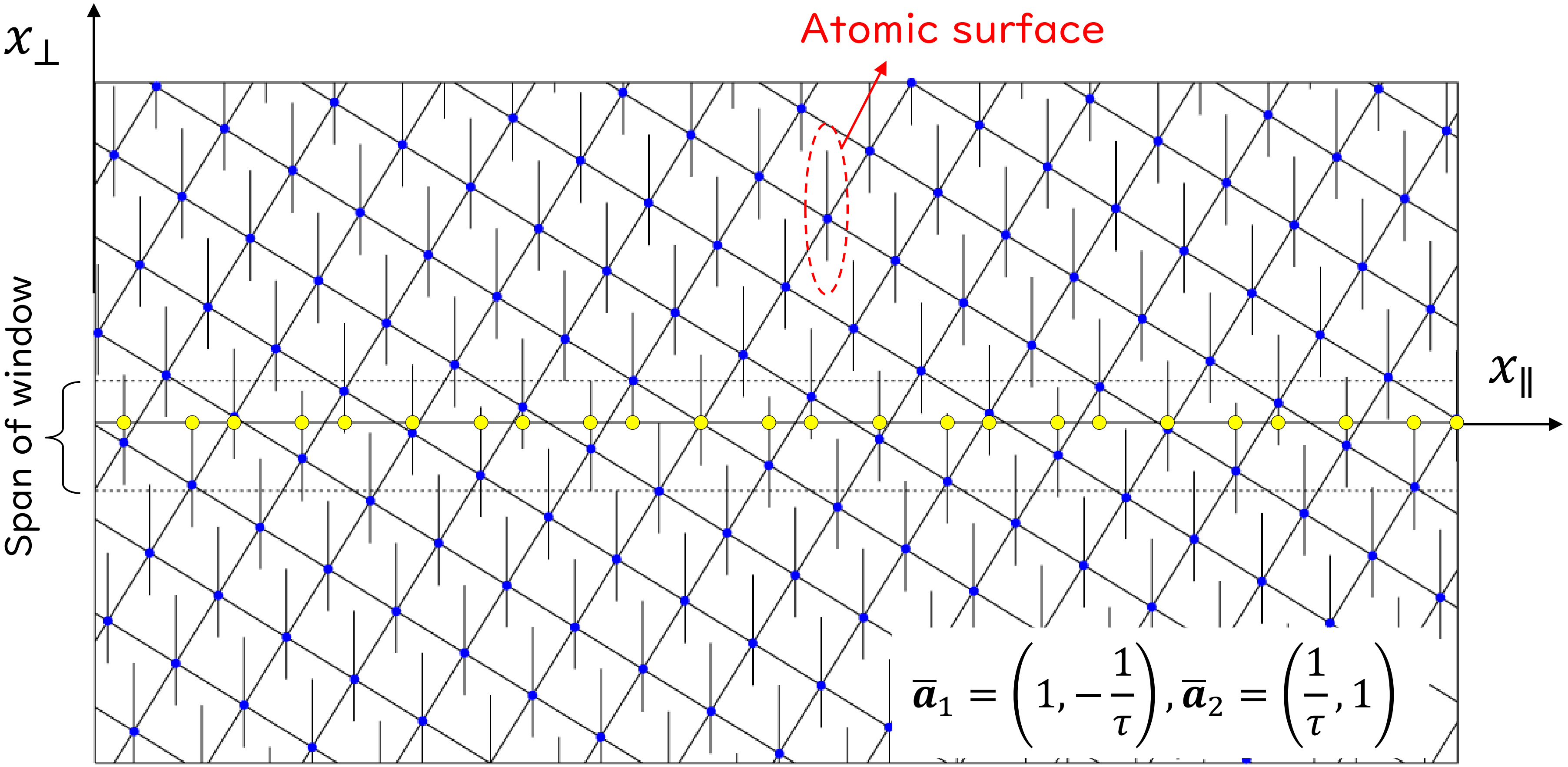


Methods for constructing QPTs

Cut-and-project method

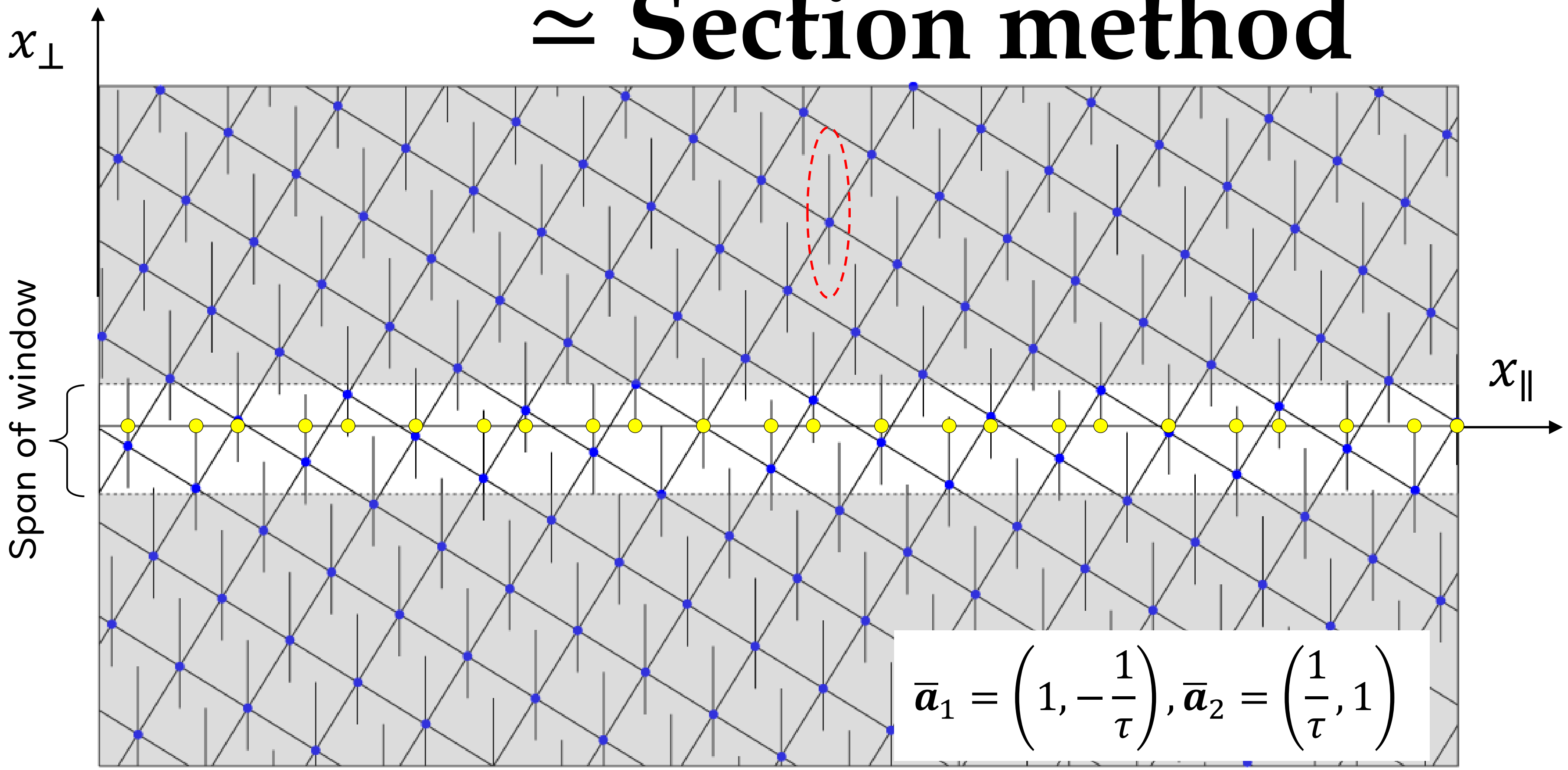


Section method



$$\bar{\boldsymbol{a}}_1 = \left(1, -\frac{1}{\tau}\right), \bar{\boldsymbol{a}}_2 = \left(\frac{1}{\tau}, 1\right)$$

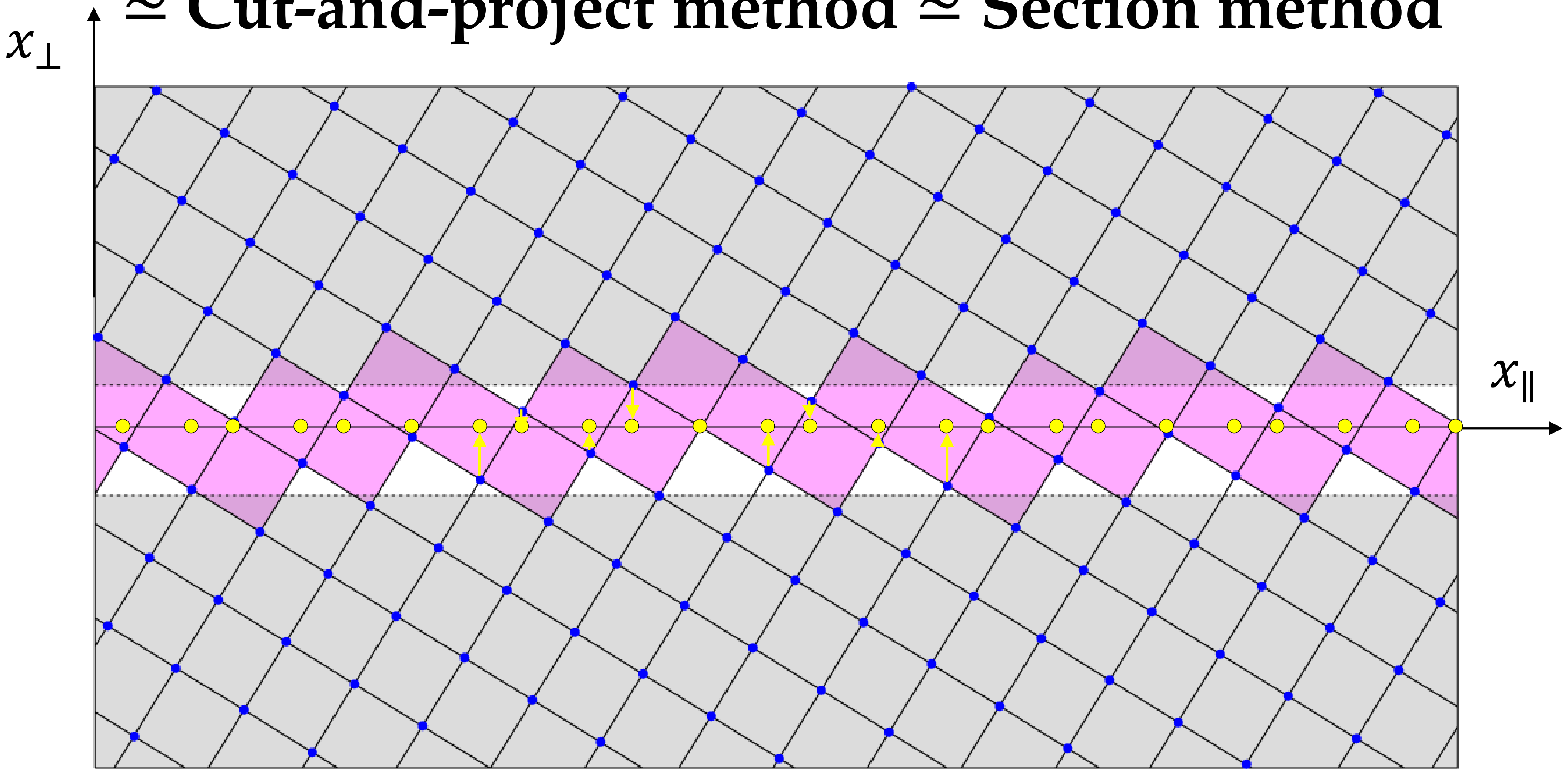
Cut-and-project method ≃ Section method



Check! An atomic surface intersect with the physical space if and only if the corresponding lattice point is within the strip.

Dual-grid method

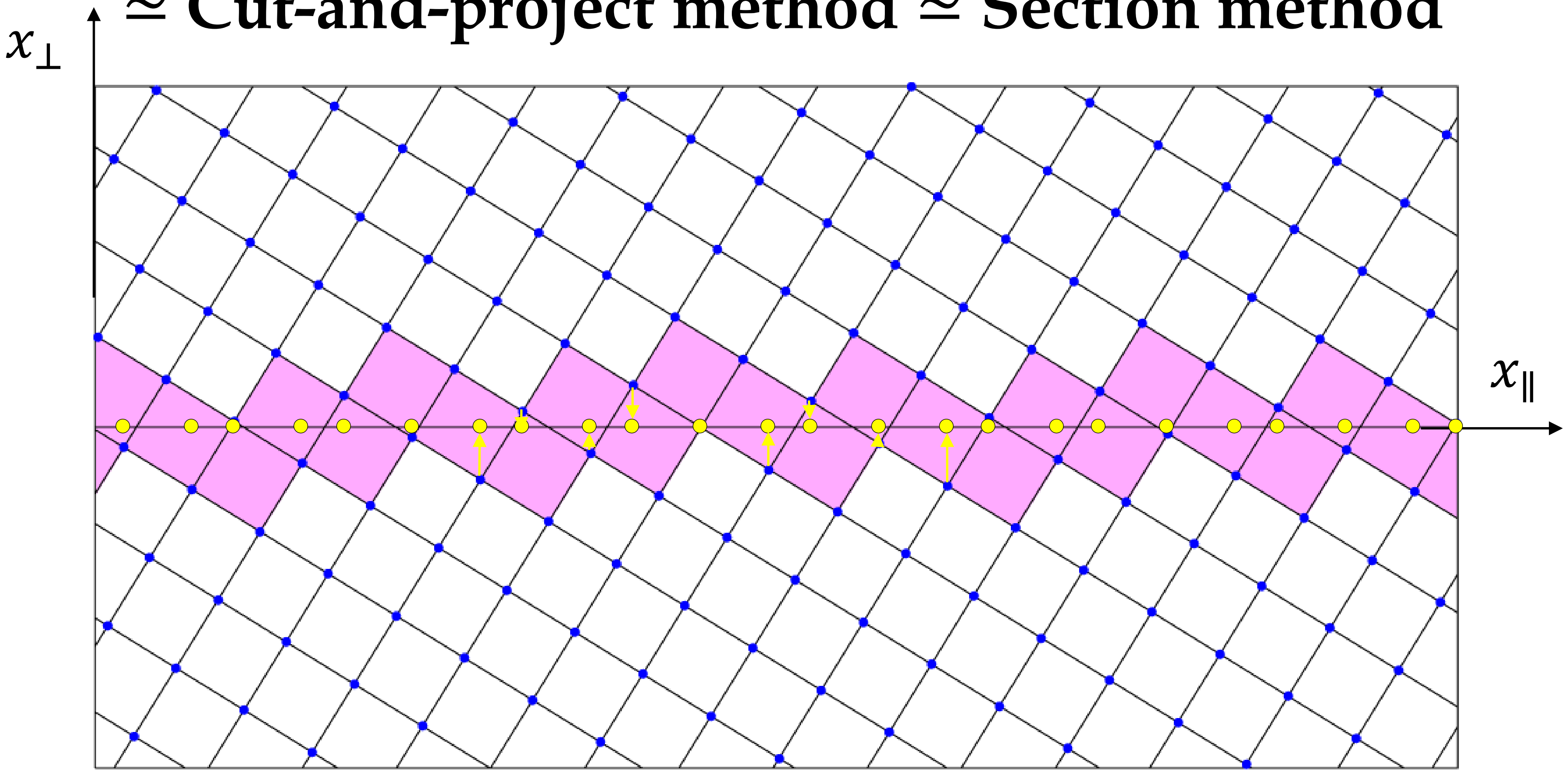
≃ Cut-and-project method ≃ Section method



Check! All the squares which intersect with the horizontal axis are colored in red. The left base points of the red square are inside the strip.

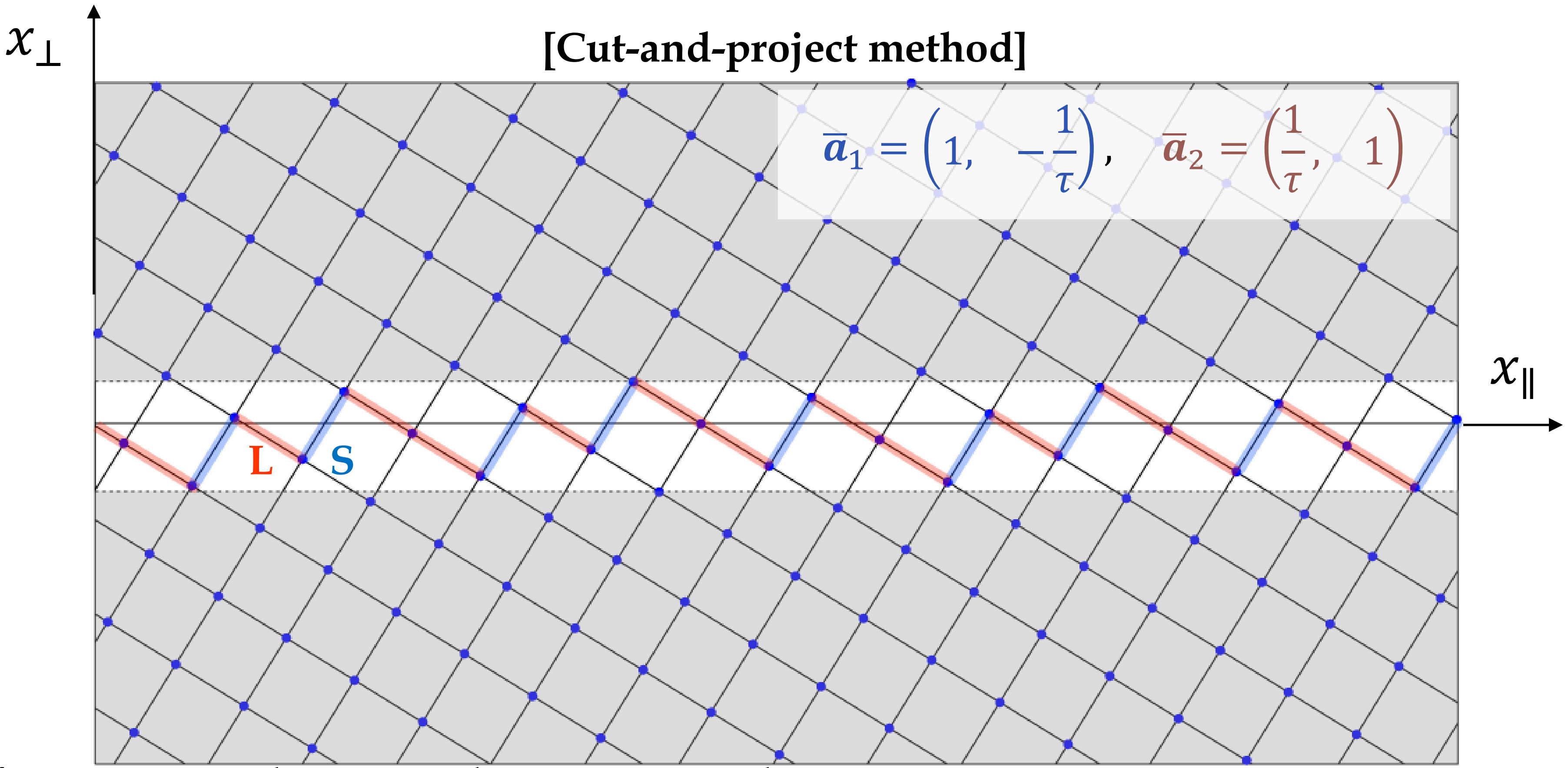
Dual-grid method

≃ Cut-and-project method ≃ Section method



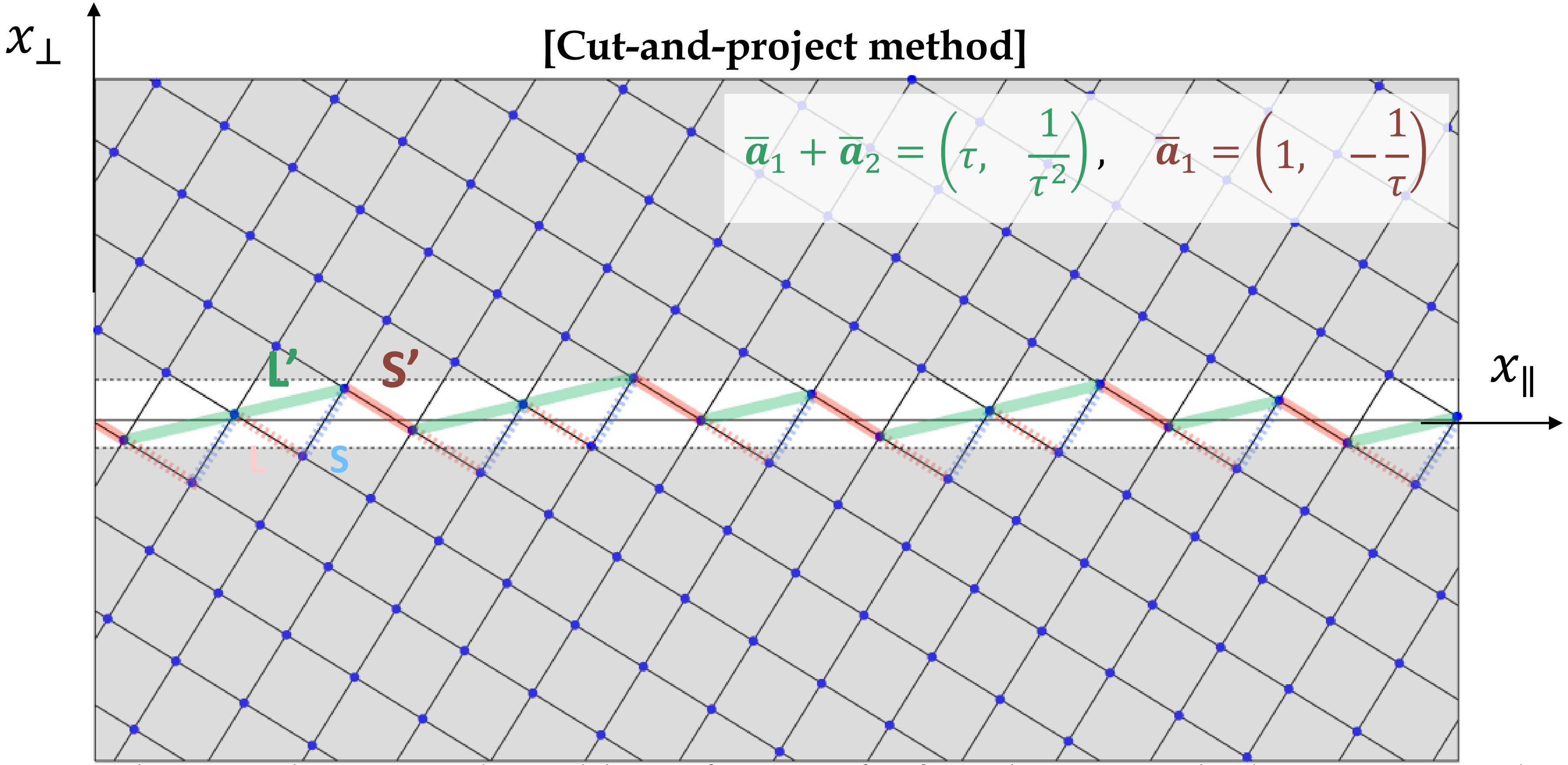
The base points of all the red squares are projected down to the physical space to form the vertices of the aperiodic tiling – the dual-grid method.

Self-similarity – an geometrical basis



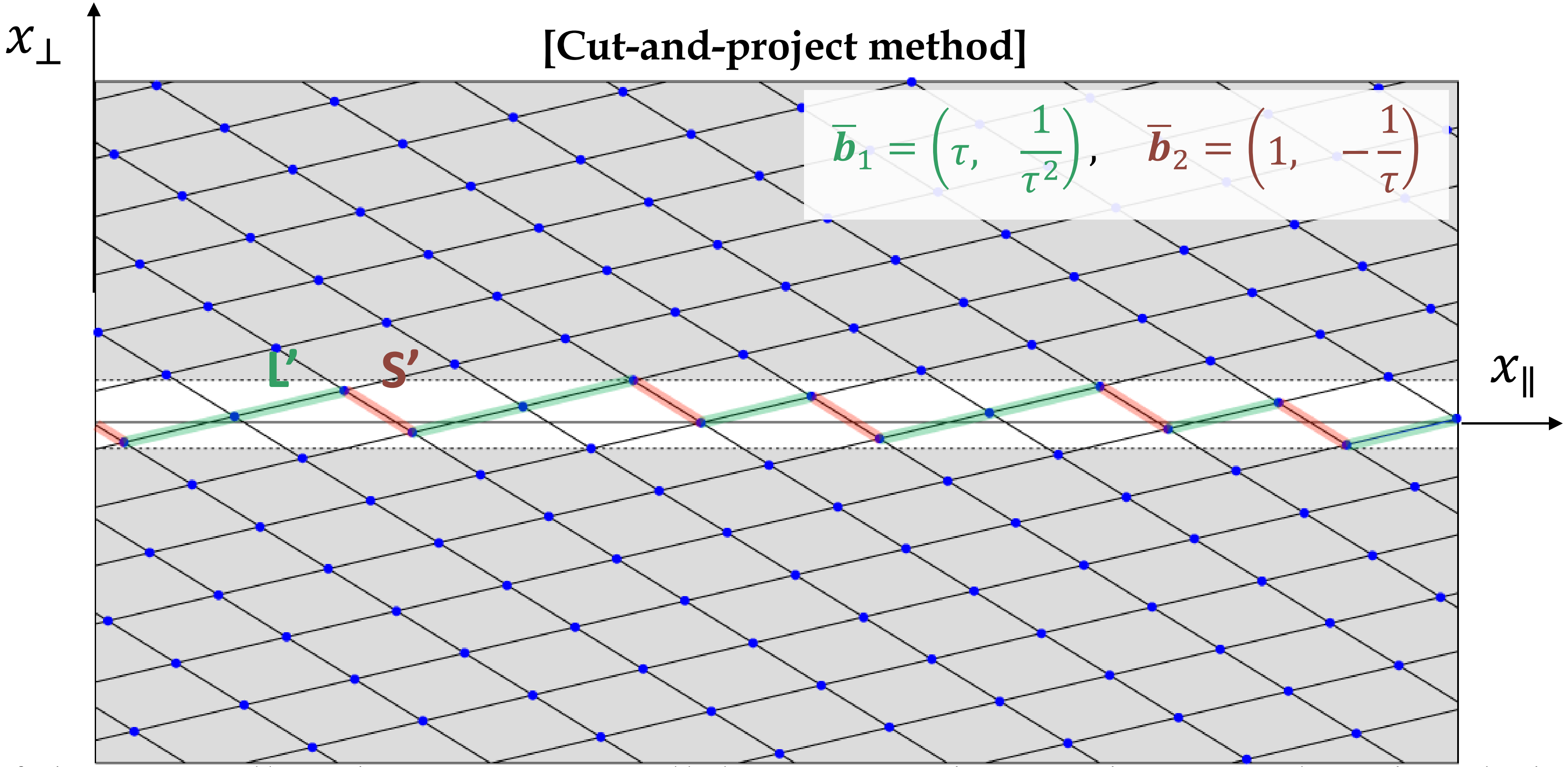
If we remove the vertex between L and S in every LS pair, we get a new segment, L′. This is done simply by narrowing the window.

Self-similarity – an geometrical basis



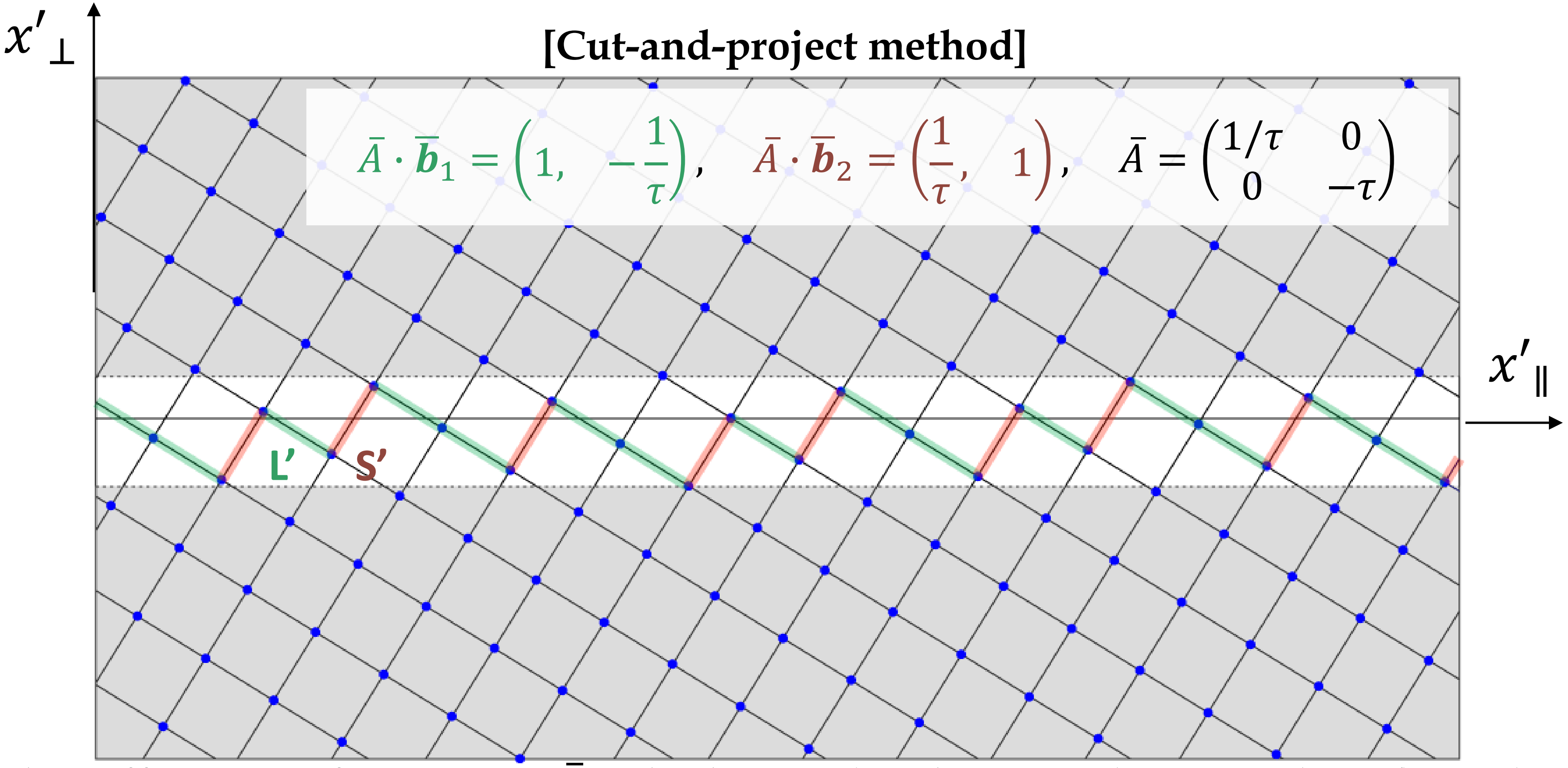
Here, the window is reduced by a factor of $1/\tau$. The new L′ tile corresponds to the projection of a diagonal of the square unit cell.

Self-similarity – an geometrical basis



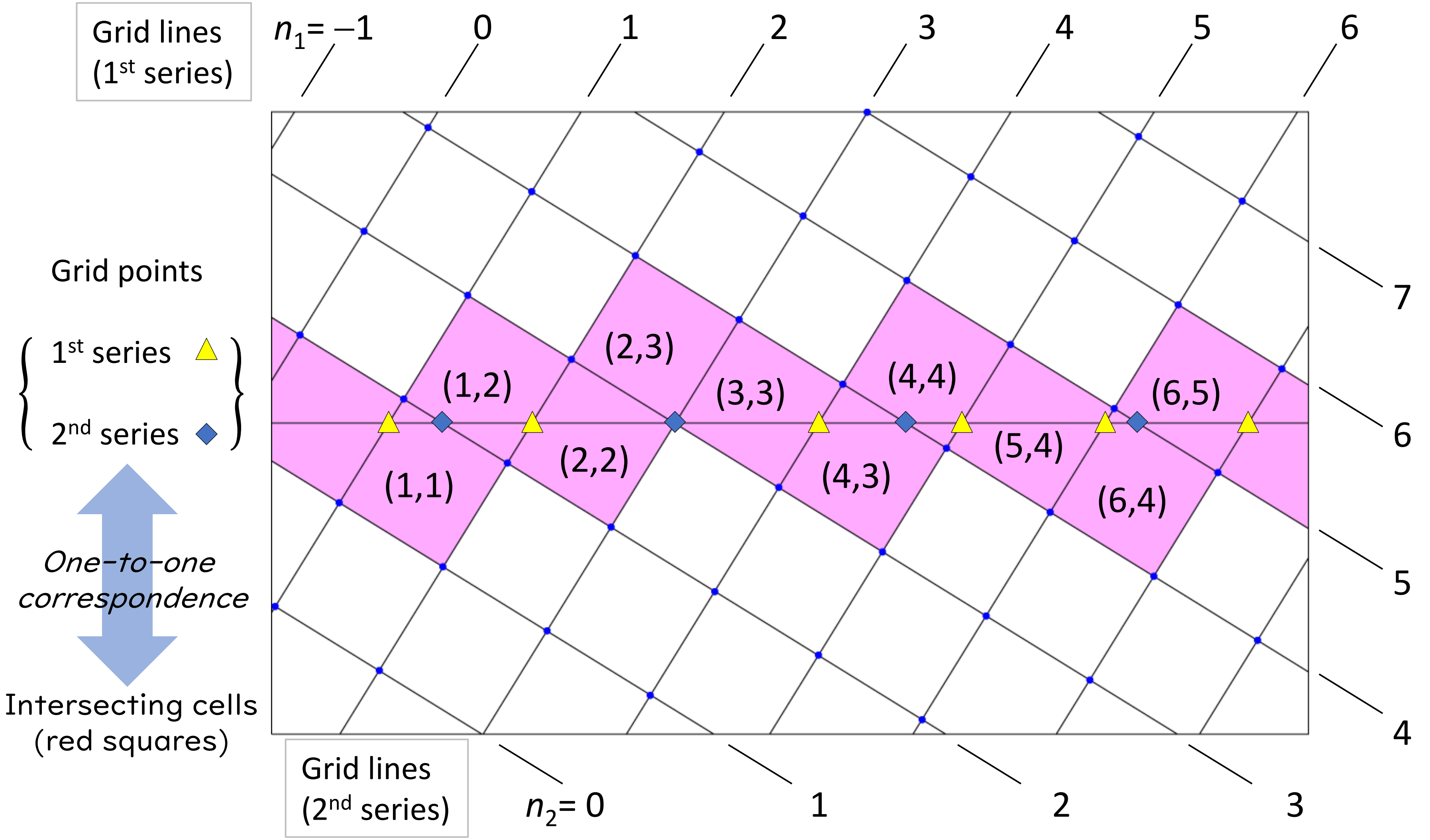
If the unit cell is chosen as a parallelogram as shown, the new tiles L′ and S′ correspond to the projection of the edges of the parallelogram.

Self-similarity – an geometrical basis



The Affine transformation, $\bar{A}$, which rescales the $x_\parallel$ and $x_\perp$ axes by $1/\tau$ and $-\tau$, respectively, will recover the original setting (cut-and-projection).

Dual-grid method – practice in 1 dim.



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Dual-grid method – practice in 1 dim.

Two-dimensional grid lines (in hyper-space)

$$\bar{\boldsymbol{a}}_1 = \left(1,\quad -\frac{1}{\tau}\right),\ \bar{\boldsymbol{a}}_2 = \left(\frac{1}{\tau},\quad 1\right)$$

$(n_1 + s_1)\bar{\boldsymbol{a}}_1 + \theta\bar{\boldsymbol{a}}_2$ $(-\infty < \theta < \infty)$ … 1st series

$\theta\bar{\boldsymbol{a}}_1 + (n_2 + s_2)\bar{\boldsymbol{a}}_2$ $(-\infty < \theta < \infty)$ … 2nd series

(s_1, s_2 … phason shift parameters)

One-dimensional grid points (in physical sub-space)

$(n_1 + s_1)\bar{\boldsymbol{a}}_1 + \theta\bar{\boldsymbol{a}}_2 = (x, 0) \rightarrow \theta = 1/\tau(n_1 + s_1)$

$\rightarrow x = (2 - 1/\tau)(n_1 + s_1)$ … 1st series △

$\theta\bar{\boldsymbol{a}}_1 + (n_2 + s_2)\bar{\boldsymbol{a}}_2 = (x, 0) \rightarrow \theta = \tau\,(n_2 + s_2)$

$\rightarrow x = (1 + 2/\tau)(n_2 + s_2)$ … 2nd series ◆

Dual-grid method – practice in 1 dim.

Base points of the two unit cells that contact each other at a grid point (in the physical space)

(1st series) $x = (2 - 1/\tau)(n_1+s_1)$, $\theta = 1/\tau(n_1+s_1)$

$n_2 = \theta - \mathrm{Frac}[\theta] = \mathrm{Floor}[\theta]$

(n_1, n_2), $(n_1\text{-}1, n_2)$ … indices for the squares

(2nd series) $x = (1 + 2/\tau)(n_2+s_2)$, $\theta = \tau(n_2+s_2)$

$n_1 = \theta - \mathrm{Frac}[\theta] = \mathrm{Floor}[\theta]$

(n_1, n_2), $(n_1, n_2\text{-}1)$ … indices for the squares

The vertices of the tiling are the projections of these base points.
base point, $(n_1, n_2) \leftrightarrow$ vertex coordinate $x = n_1 + n_2/\tau$

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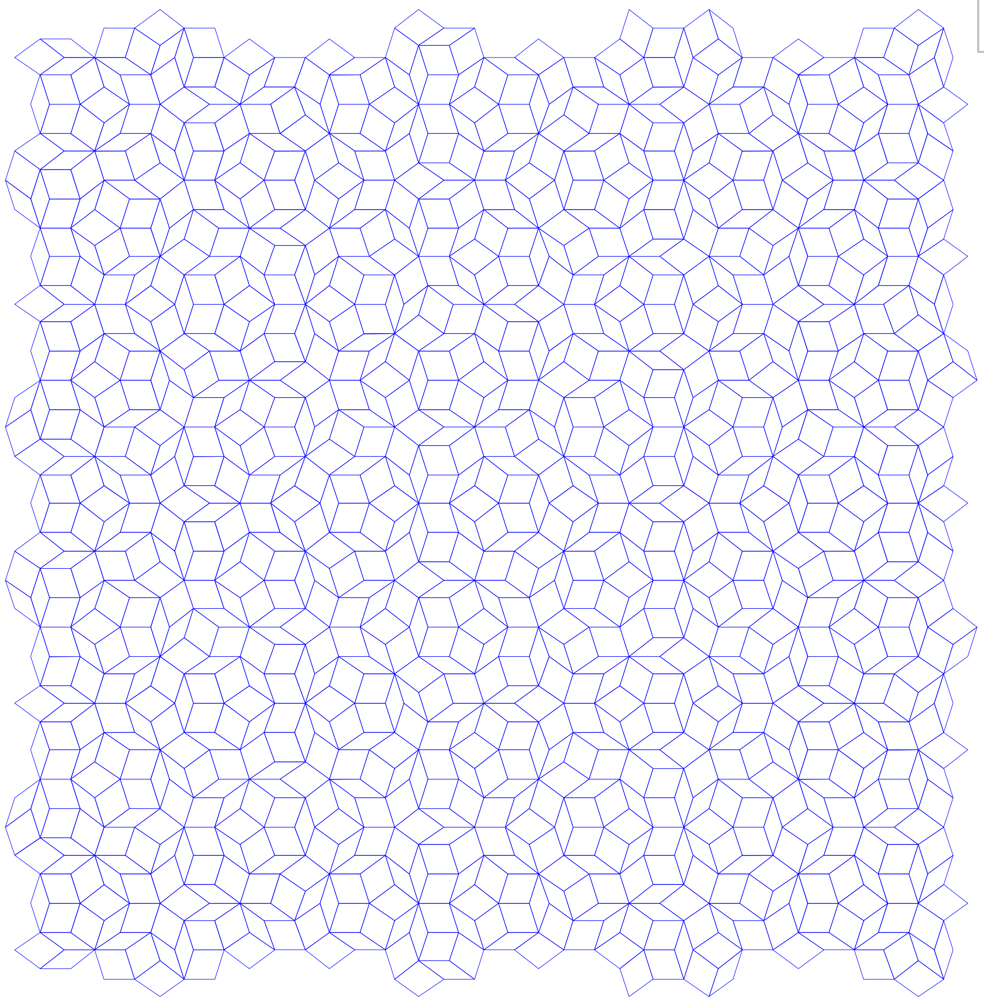
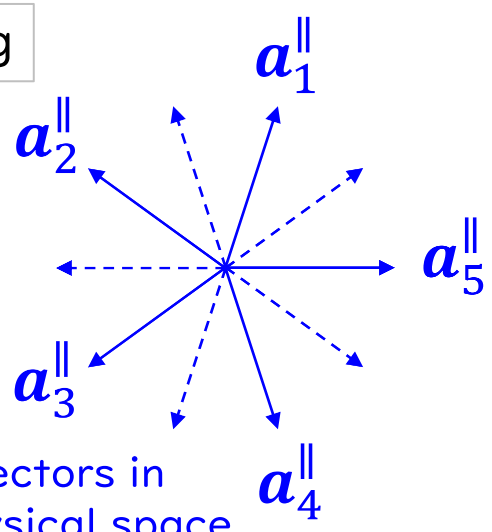
Dual-grid method – practice in 2 dims.



P3 tiling



edge vectors in the physical space

Embedding dimension = 5

$$(x, y, z, u, v)$$

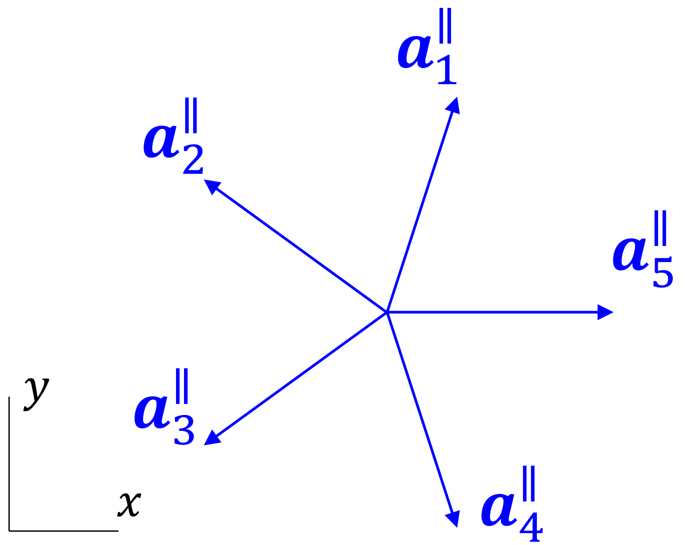
physical space (x, y) — *perpendicular space* (z, u, v)

Dual-grid method – practice in 2 dims.

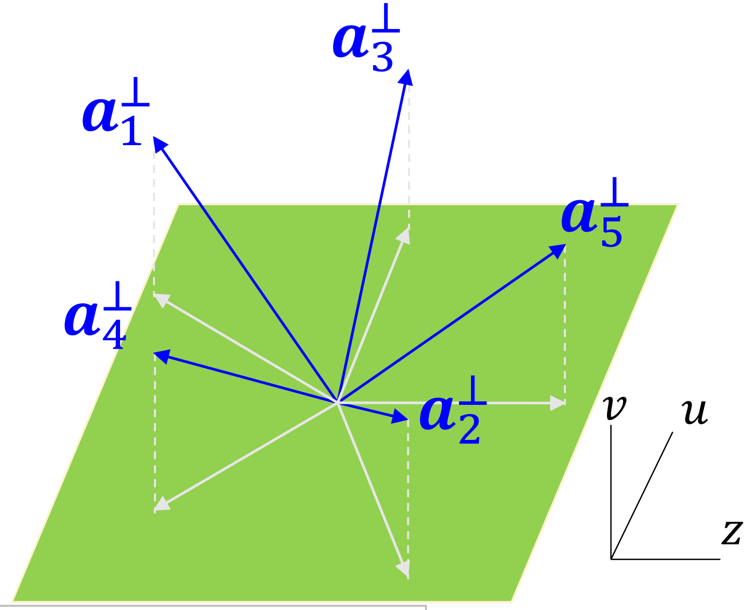
$$\bar{\boldsymbol{a}}_j = \sqrt{2/5}\left(\cos\varphi_j, \sin\varphi_j, \cos 2\varphi_j, \sin 2\varphi_j, \sqrt{1/2}\right)$$

where $\varphi_j = \frac{2\pi j}{5}$, $j = 1,2,3,4,5$

Check! $\bar{\boldsymbol{a}}_i \cdot \bar{\boldsymbol{a}}_j = \delta_{ij}$ … the Kronecker delta



physical space



perpendicular space

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Dual-grid method – practice in 2 dims.

5-dim. hyper-cubic lattice: $\mathcal{L} = \{n_1\bar{\boldsymbol{a}}_1 + n_2\bar{\boldsymbol{a}}_2 + n_3\bar{\boldsymbol{a}}_3 + n_4\bar{\boldsymbol{a}}_4 + n_5\bar{\boldsymbol{a}}_5\}$

Hyper-grids in 5-dim. hyper-space

Phason shifts

1st grids: $(n_1 + s_1)\bar{\boldsymbol{a}}_1 + \{\theta_2\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4 + \theta_5\bar{\boldsymbol{a}}_5\}$

2nd grids: $(n_2 + s_2)\bar{\boldsymbol{a}}_2 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4 + \theta_5\bar{\boldsymbol{a}}_5\}$

3rd grids: $(n_3 + s_3)\bar{\boldsymbol{a}}_3 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_2\bar{\boldsymbol{a}}_2 + \theta_4\bar{\boldsymbol{a}}_4 + \theta_5\bar{\boldsymbol{a}}_5\}$ (θ_j: free parameter)

4th grids: $(n_4 + s_4)\bar{\boldsymbol{a}}_4 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_2\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_5\bar{\boldsymbol{a}}_5\}$

5th grids: $(n_5 + s_5)\bar{\boldsymbol{a}}_5 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_2\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4\}$

2-dim. grid lines (the physical-space sections of the hyper-grids)

1st grids: $5/2(n_1 + s_1)\boldsymbol{a}_1^{\parallel} + \theta(\boldsymbol{a}_2^{\parallel} - \boldsymbol{a}_5^{\parallel}\}$

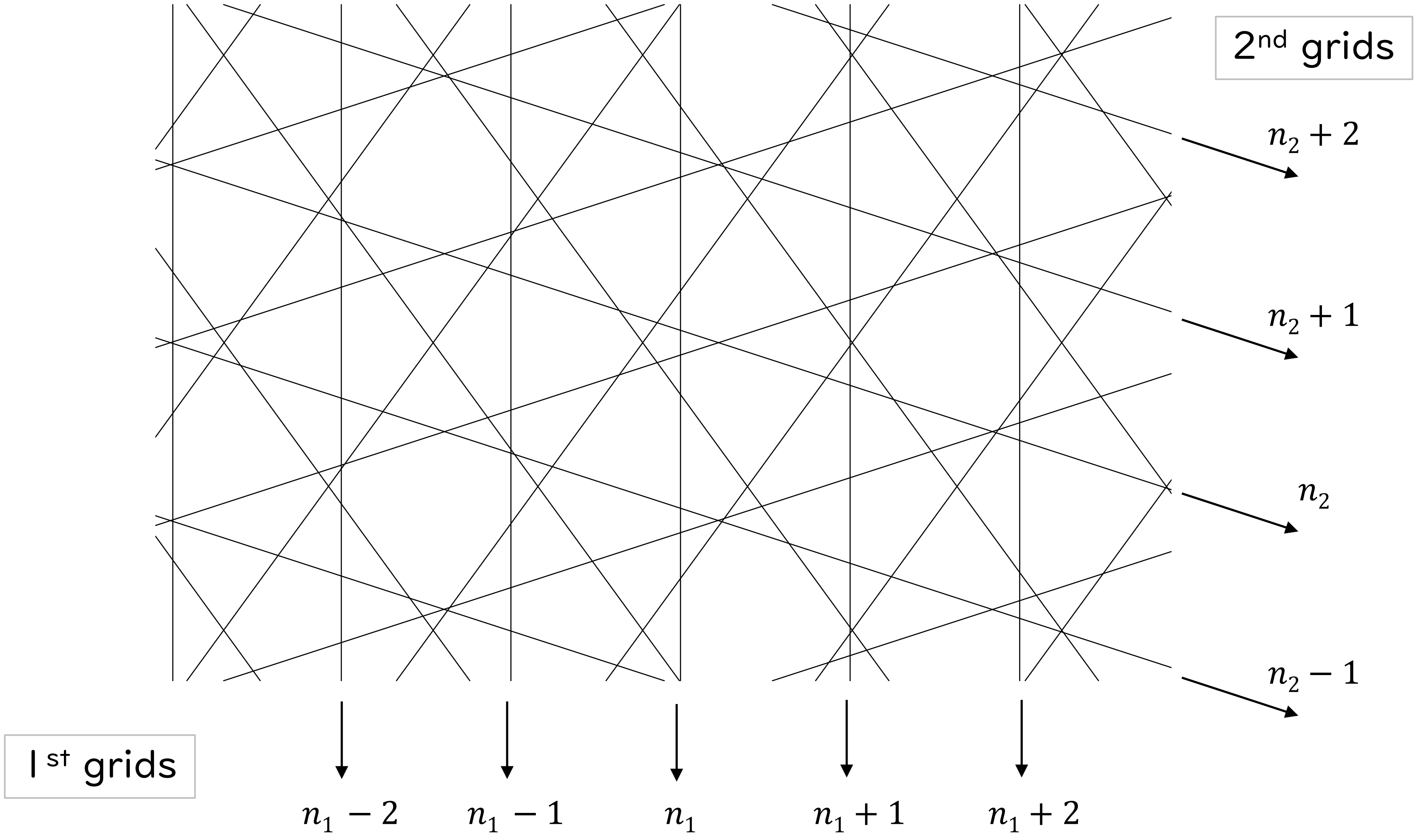
2nd grids: $5/2(n_2 + s_2)\boldsymbol{a}_2^{\parallel} + \theta(\boldsymbol{a}_3^{\parallel} - \boldsymbol{a}_1^{\parallel})$

3rd grids: $5/2(n_3 + s_3)\boldsymbol{a}_3^{\parallel} + \theta(\boldsymbol{a}_4^{\parallel} - \boldsymbol{a}_2^{\parallel})$ (θ: free parameter)

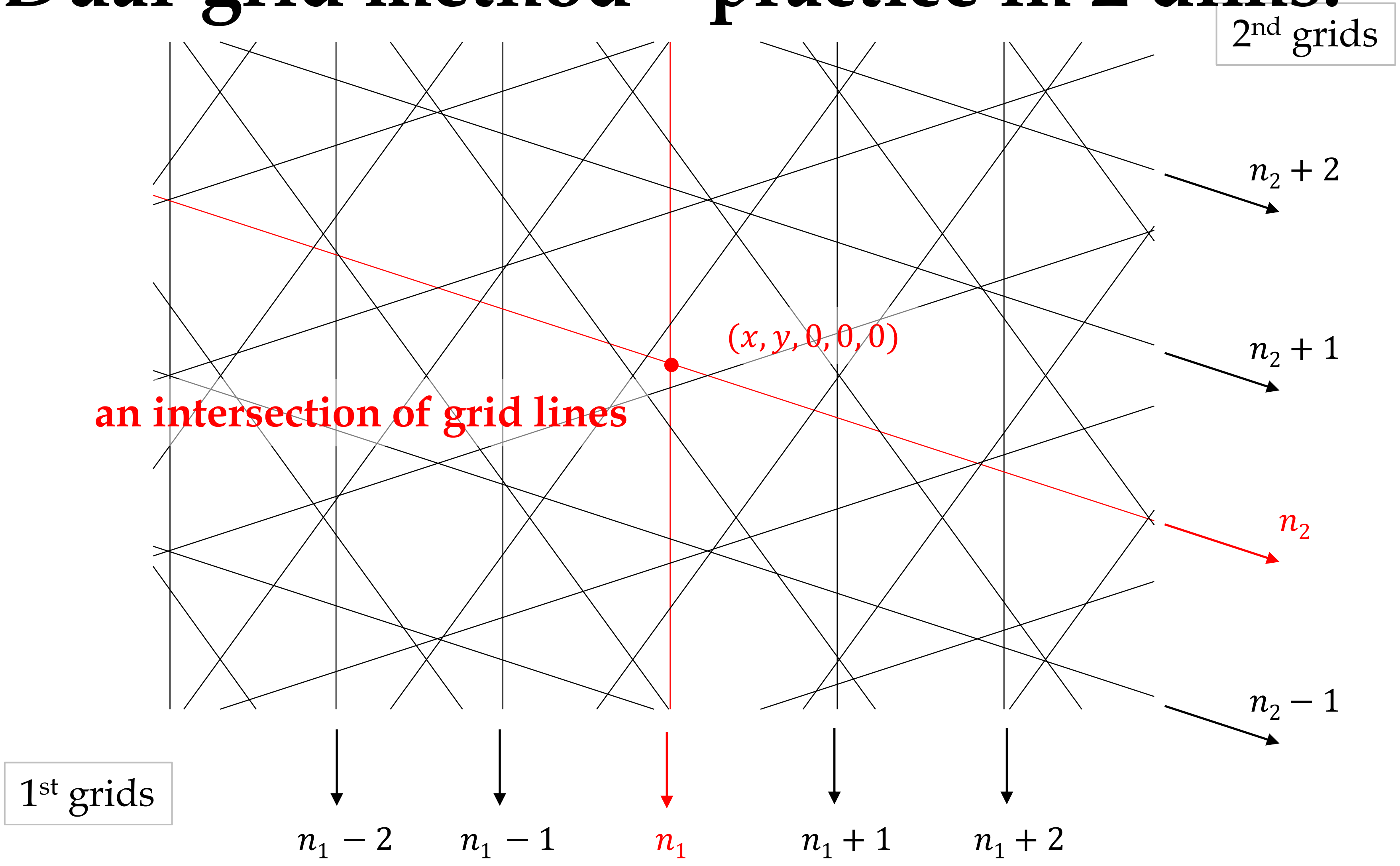
4th grids: $5/2(n_4 + s_4)\boldsymbol{a}_4^{\parallel} + \theta(\boldsymbol{a}_5^{\parallel} - \boldsymbol{a}_3^{\parallel})$

5th grids: $5/2(n_5 + s_5)\boldsymbol{a}_5^{\parallel} + \theta(\boldsymbol{a}_1^{\parallel} - \boldsymbol{a}_4^{\parallel})$

Dual-grid method – practice in 2 dims.



Dual-grid method – practice in 2 dims.



Dual-grid method – practice in 2 dims.

$$(x, y, 0, 0, 0) = (n_1 + s_1)\bar{\boldsymbol{a}}_1 + (n_2 + s_2)\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4 + \theta_5\bar{\boldsymbol{a}}_5$$

$$\theta_3 = \bar{\boldsymbol{g}}_3 \cdot (x, y, 0, 0, 0) = n_3 + s_3 + \delta,\ \ n_3 = [\theta_3 - s_3],\ \ \delta = Frac(\theta_3 - s_3)$$

$$\theta_4 = \bar{\boldsymbol{g}}_4 \cdot (x, y, 0, 0, 0) = n_4 + s_4 + \delta',\ \ n_4 = [\theta_4 - s_4],\ \ \delta' = Frac(\theta_4 - s_4)$$

$$\theta_5 = \bar{\boldsymbol{g}}_5 \cdot (x, y, 0, 0, 0) = n_5 + s_5 + \delta'',\ n_5 = [\theta_5 - s_5],\ \ \delta'' = Frac(\theta_5 - s_5)$$

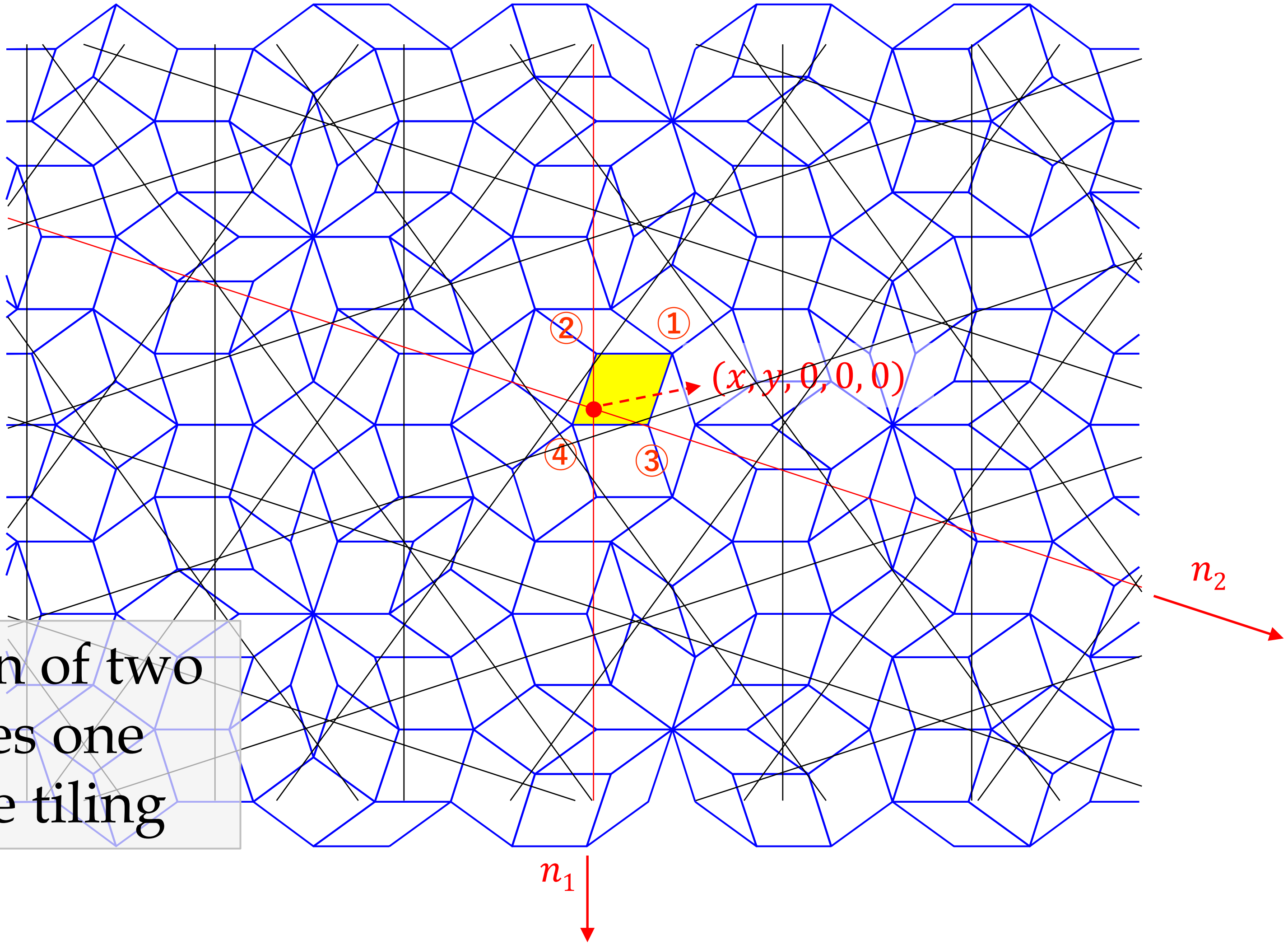
where $\bar{\boldsymbol{g}}_j = \bar{\boldsymbol{a}}_j$ $(j = 1, 2, 3, 4, 5)$ … 5-dim. reciprocal basis vecs.

These equations determine five integers n_1, n_2, n_3, n_4, n_5, which provide the indices of the base points of the four 5-dim. unit cells that contact each other at the above intersection point (x,y) of the 1st and 2nd grid lines →

① $(n_1, n_2, n_3, n_4, n_5)$
② $(n_1 - 1, n_2, n_3, n_4, n_5)$
③ $(n_1, n_2 - 1, n_3, n_4, n_5)$
④ $(n_1 - 1, n_2 - 1, n_3, n_4, n_5)$

(similar formulas can be obtained for an intersection of ith and jth grid lines)

Dual-grid method – practice in 2 dims.

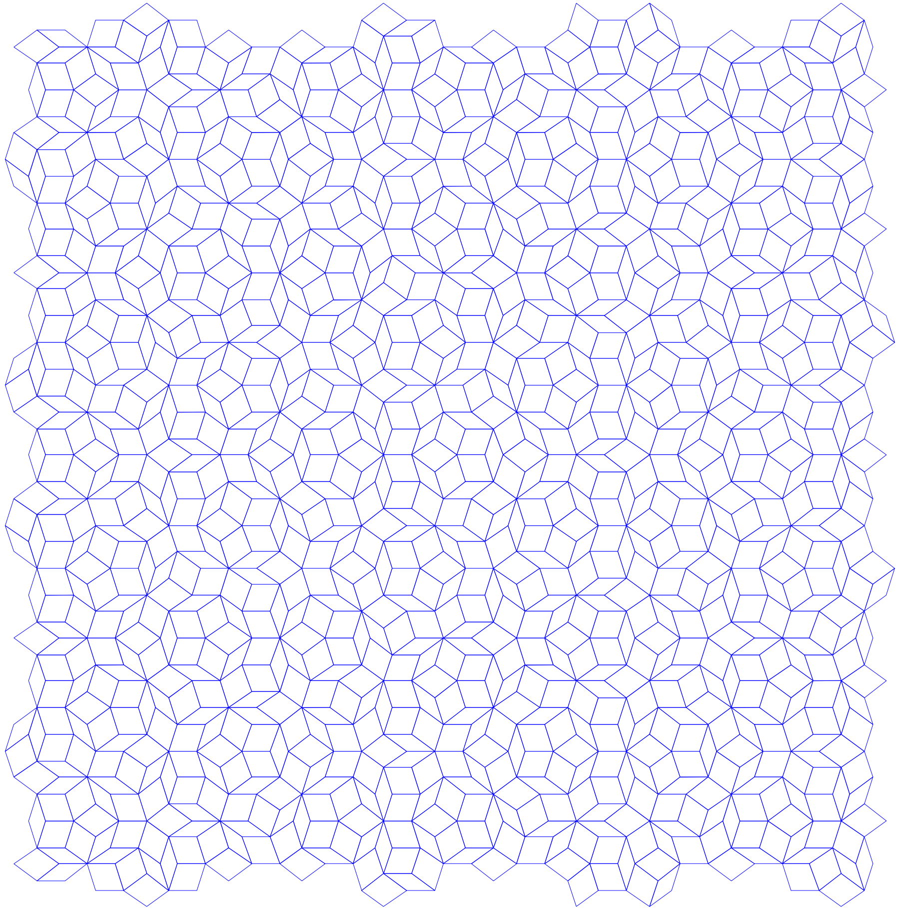


Each intersection of two grid lines gives one rhombus in the tiling

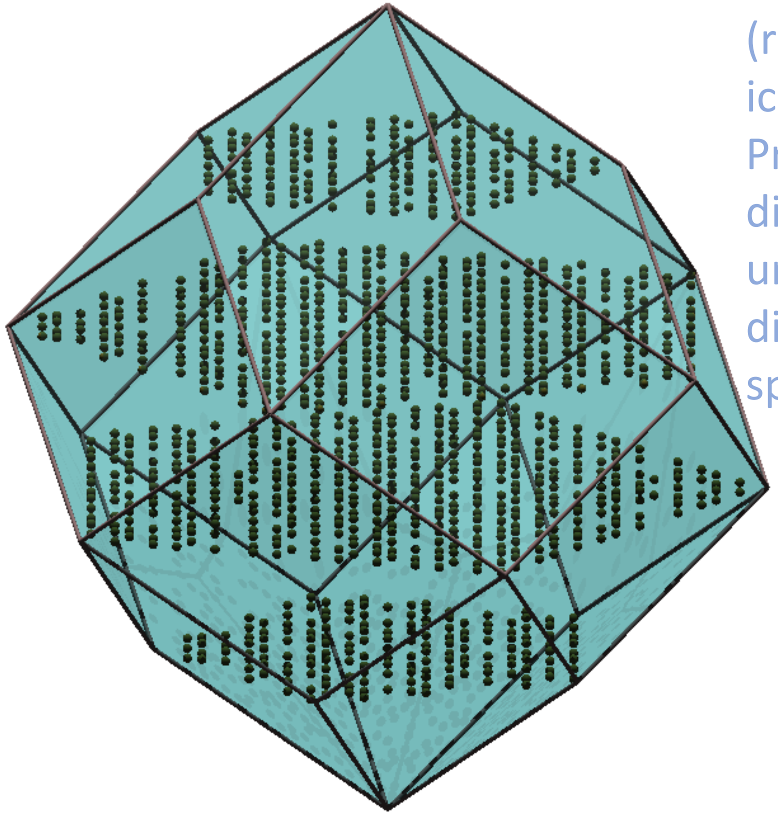
Dual-grid method – practice in 2 dims.

Rhombic Penrose tiling (in 2-dim. physical space)

P3 tiling



Mapping the vertices of the tiling into the orthogonal complement (3-dim.)



Outer boundary (rhombic icosahedron)
Projection of a 5-dim hyper-cubic unit cell into the 3-dim. perpendicular space.

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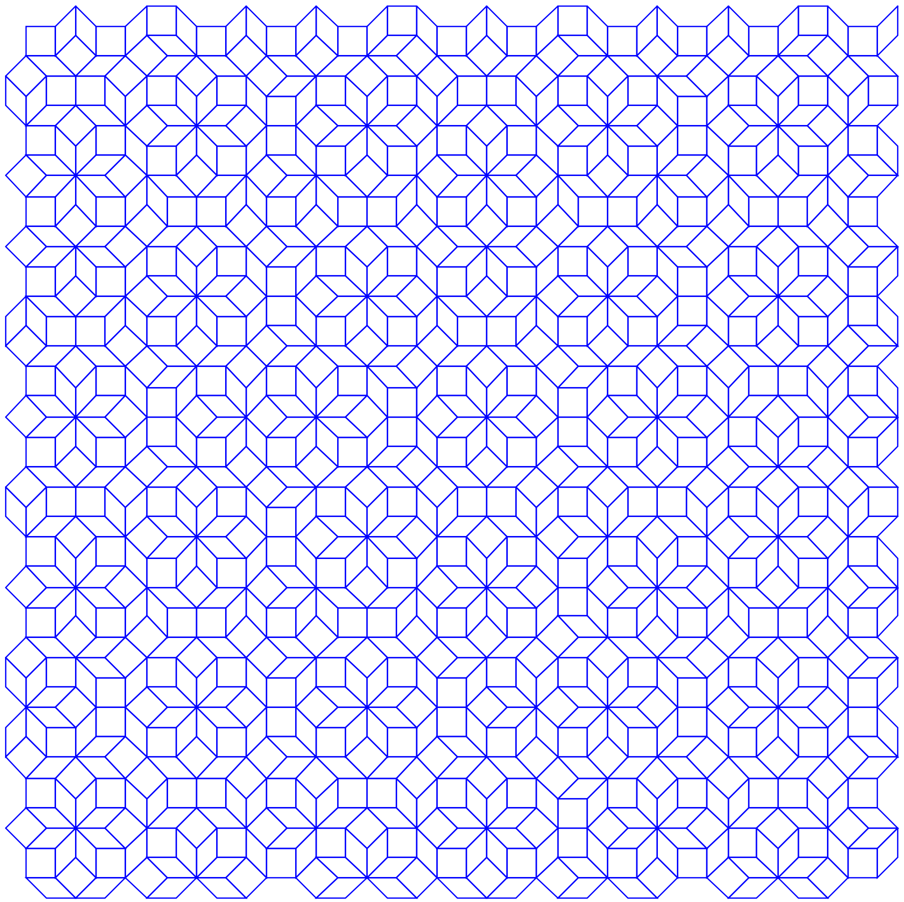
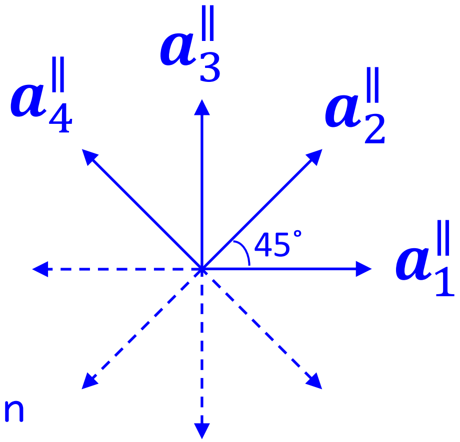
Dual-grid method – practice in 2 dims.



Ammann-Beenker tiling



edge vectors in the physical space

Embedding dimension = 4

$$(x, y, z, u)$$

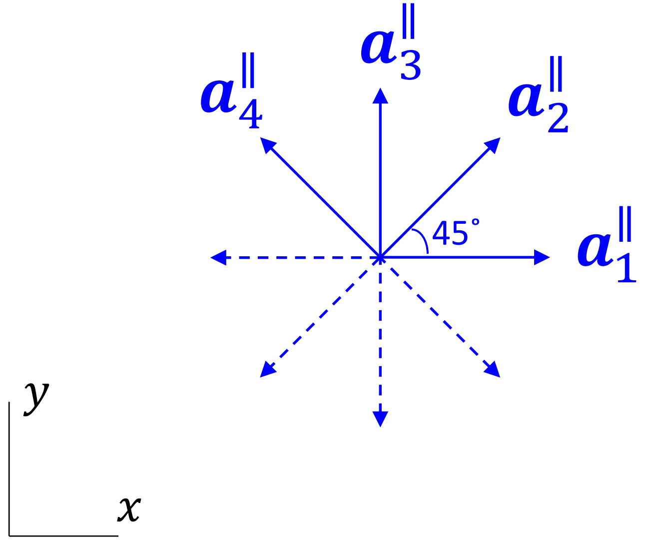
physical space (x, y) *perpendicular space* (z, u)

Dual-grid method – practice in 2 dims.

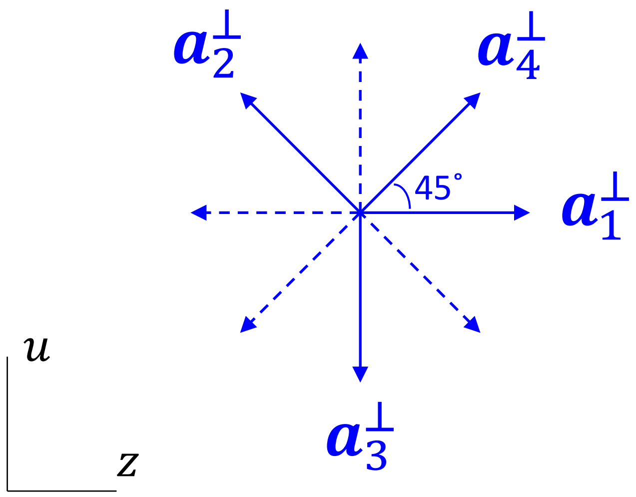
$$\bar{\boldsymbol{a}}_j = 1/\sqrt{2}\left(\cos(\varphi_j)\,,\sin(\varphi_j)\,,\cos(3\,\varphi_j),\sin(3\,\varphi_j)\right)$$

where $\varphi_j = \frac{\pi(j-1)}{4}, j = 1,2,3,4$

Check! $\bar{\boldsymbol{a}}_i \cdot \bar{\boldsymbol{a}}_j = \delta_{ij}$ … the Kronecker delta



physical space



perpendicular space

Dual-grid method – practice in 2 dims.

4-dim. hyper-cubic lattice: $\mathcal{L} = \{n_1\bar{\boldsymbol{a}}_1 + n_2\bar{\boldsymbol{a}}_2 + n_3\bar{\boldsymbol{a}}_3 + n_4\bar{\boldsymbol{a}}_4\}$

Hyper-grids in 4-dim. hyper-space

Phason shifts

1st grids: $(n_1 + s_1)\bar{\boldsymbol{a}}_1 + \{\theta_2\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4\}$
2nd grids: $(n_2 + s_2)\bar{\boldsymbol{a}}_2 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_3\bar{\boldsymbol{a}}_3 + \theta_4\bar{\boldsymbol{a}}_4\}$
3rd grids: $(n_3 + s_3)\bar{\boldsymbol{a}}_3 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_2\bar{\boldsymbol{a}}_2 + \theta_4\bar{\boldsymbol{a}}_4\}$
4th grids: $(n_4 + s_4)\bar{\boldsymbol{a}}_4 + \{\theta_1\bar{\boldsymbol{a}}_1 + \theta_2\bar{\boldsymbol{a}}_2 + \theta_3\bar{\boldsymbol{a}}_3\}$

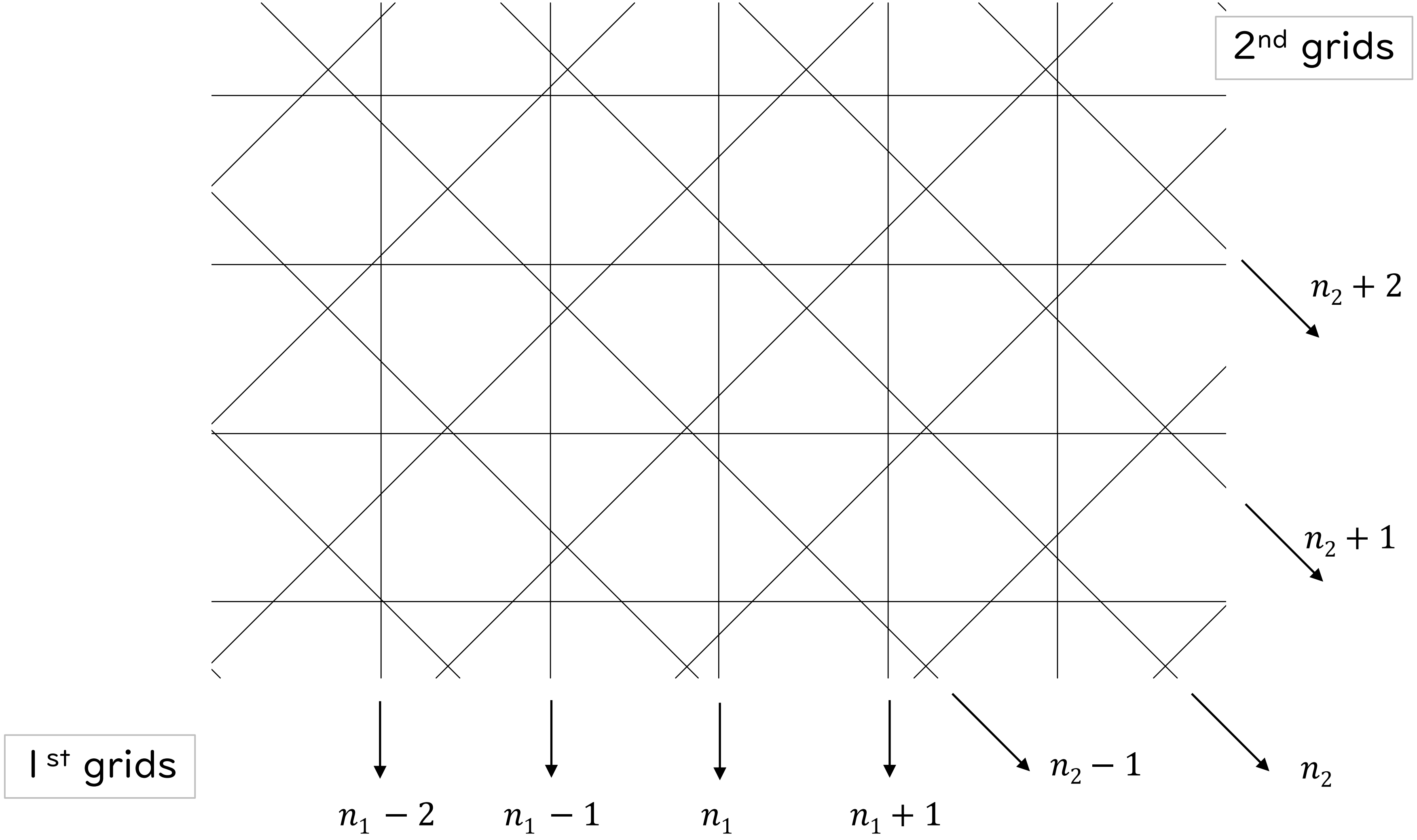
(θ_j: free parameter)

2-dim. grid lines (the physical-space sections of the hyper-grids)

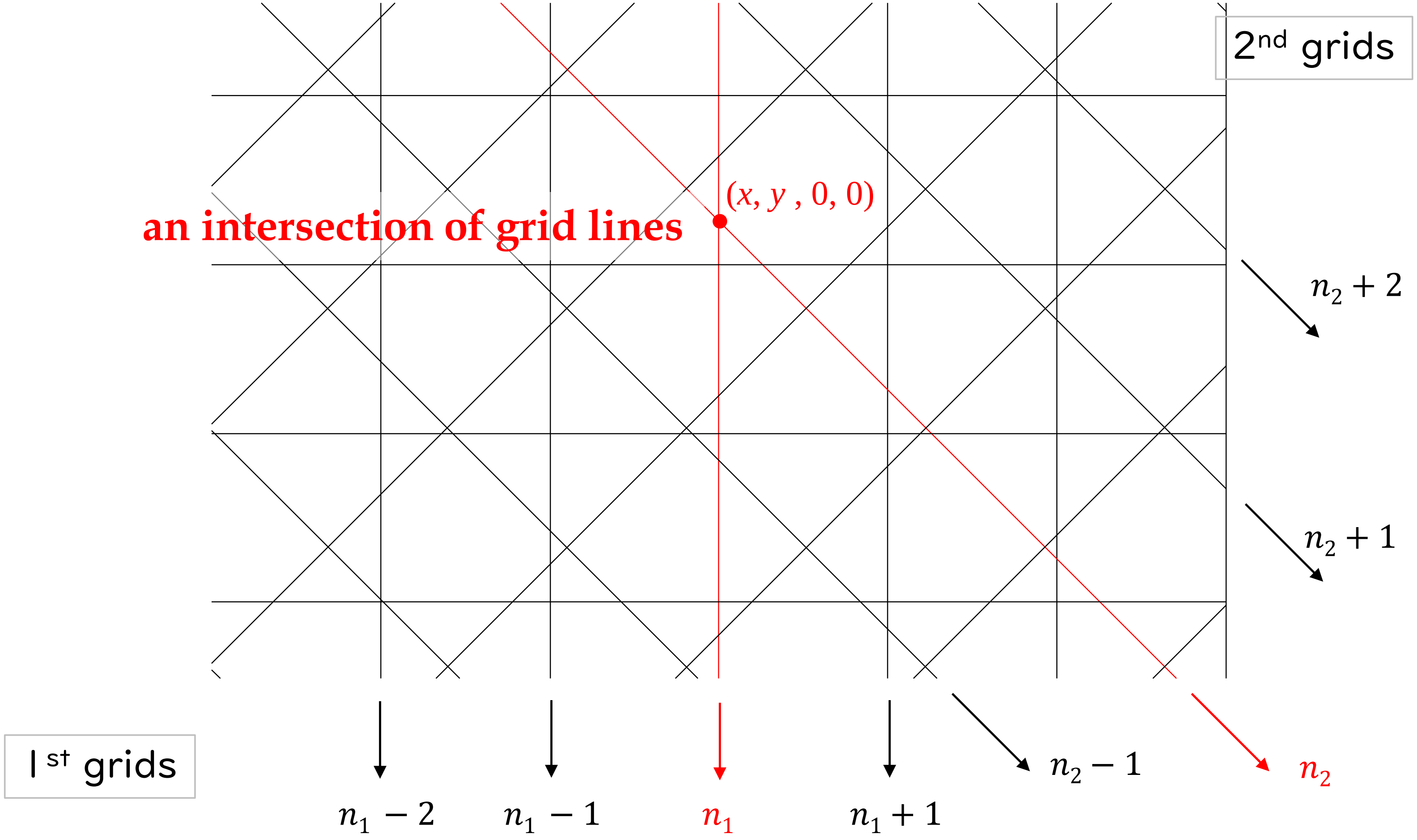
1st grids: $2(n_1 + s_1)\boldsymbol{a}_1^{\parallel} + \theta\boldsymbol{a}_3^{\parallel}$
2nd grids: $2(n_2 + s_2)\boldsymbol{a}_2^{\parallel} + \theta\boldsymbol{a}_4^{\parallel}$
3rd grids: $2(n_3 + s_3)\boldsymbol{a}_3^{\parallel} + \theta\boldsymbol{a}_1^{\parallel}$
4th grids: $2(n_4 + s_4)\boldsymbol{a}_4^{\parallel} + \theta\boldsymbol{a}_2^{\parallel}$

(θ: free parameter)

Dual-grid method – practice in 2 dims.



Dual-grid method – practice in 2 dims.



Dual-grid method – practice in 2 dims.

$$(x, y, 0, 0, 0) = (n_1 + s_1)\bar{a}_1 + (n_2 + s_2)\bar{a}_2 + \theta_3\bar{a}_3 + \theta_4\bar{a}_4$$

$$\theta_3 = \bar{\boldsymbol{g}}_3 \cdot (x, y, 0, 0) = n_3 + s_3 + \delta, \;\; n_3 = [\theta_3 - s_3], \;\; \delta = Frac(\theta_3 - s_3)$$

$$\theta_4 = \bar{\boldsymbol{g}}_4 \cdot (x, y, 0, 0) = n_4 + s_4 + \delta', \;\; n_4 = [\theta_4 - s_4], \;\; \delta' = Frac(\theta_4 - s_4)$$

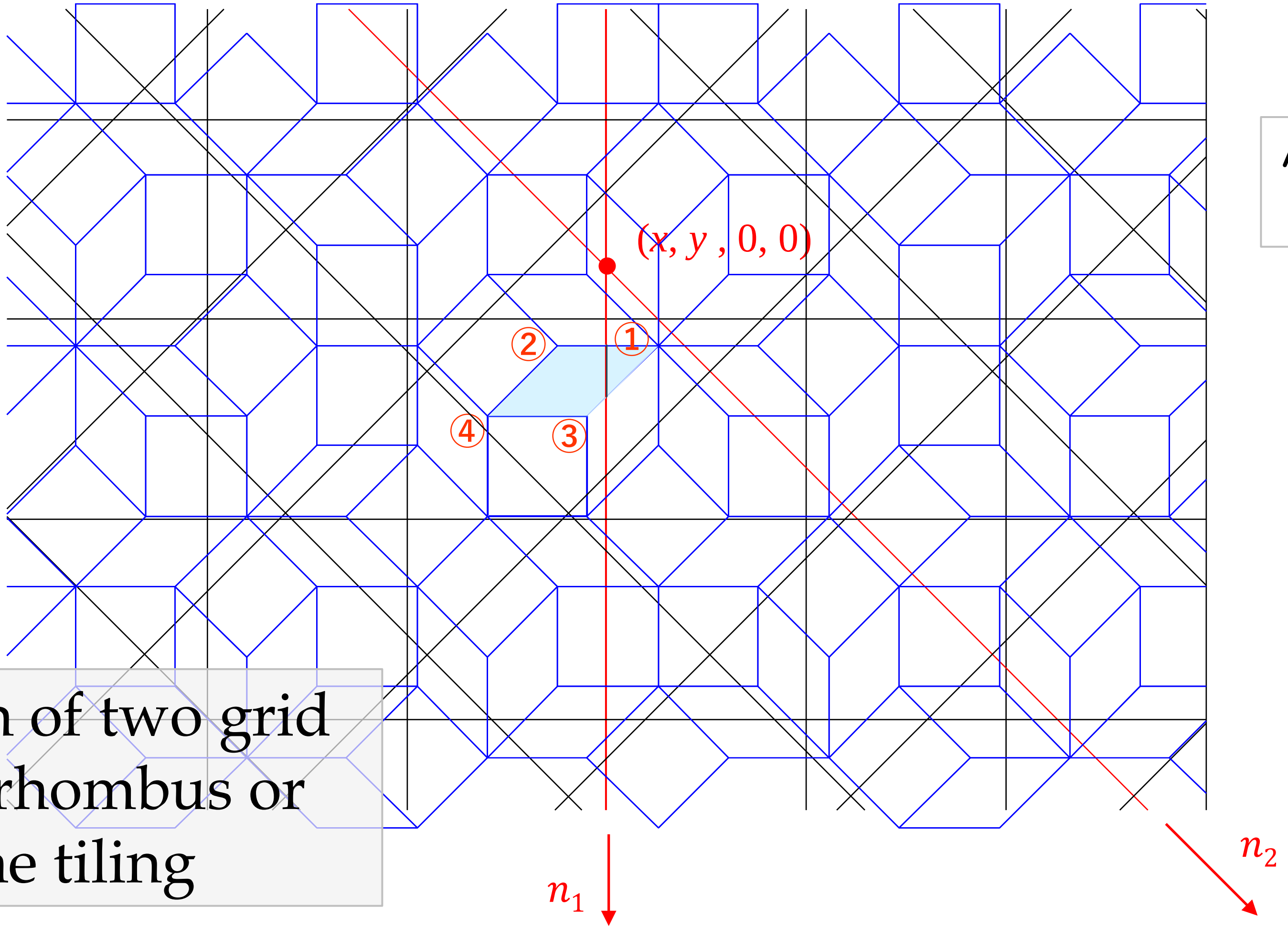
where $\bar{\boldsymbol{g}}_j = \bar{\boldsymbol{a}}_j \; (j = 1, 2, 3, 4)$ … 4-dim. reciprocal basis vecs.

These equations determine four integers n_1, n_2, n_3, n_4, which provide the indices of the base points of the four 4-dim. unit cells that contact each other at the intersection *(x,y)* of the 1st and 2nd grid lines →

(similar formulas can be obtained for an intersection of ith and jth grid lines)

① (n_1, n_2, n_3, n_4)
② $(n_1 - 1, n_2, n_3, n_4)$
③ $(n_1, n_2 - 1, n_3, n_4)$
④ $(n_1 - 1, n_2 - 1, n_3, n_4)$

Dual-grid method – practice in 2 dims.



Ammann-Beenker tiling (8mm)

Each intersection of two grid lines gives one rhombus or square in the tiling

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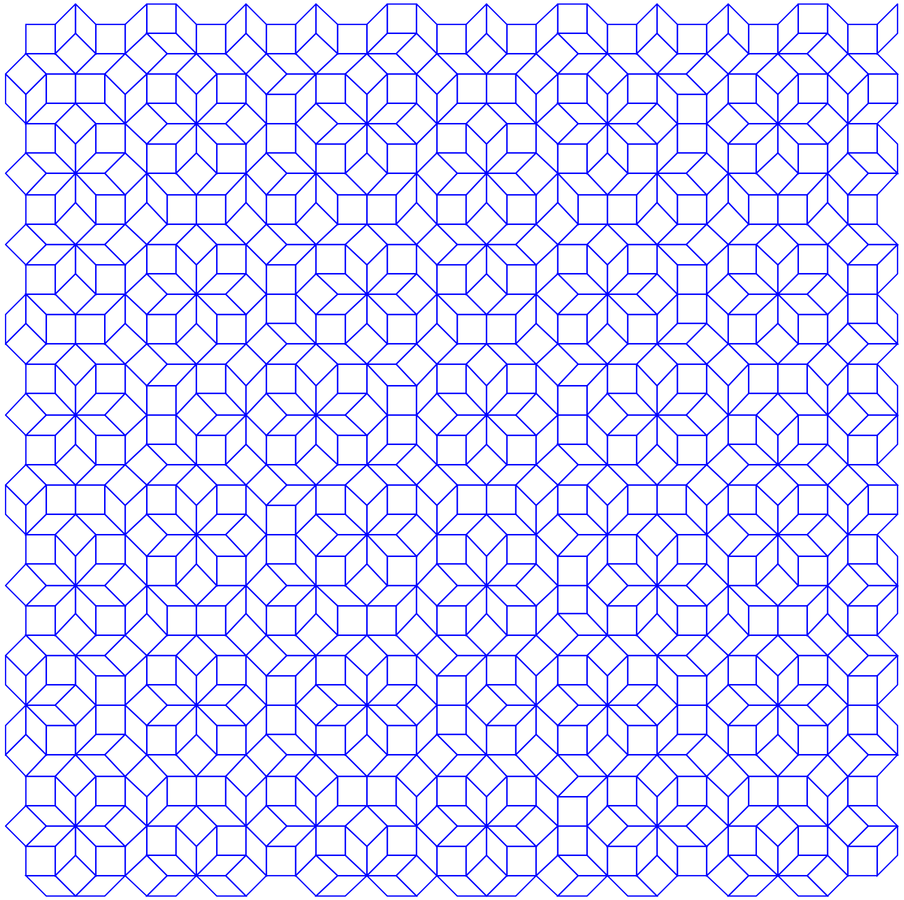
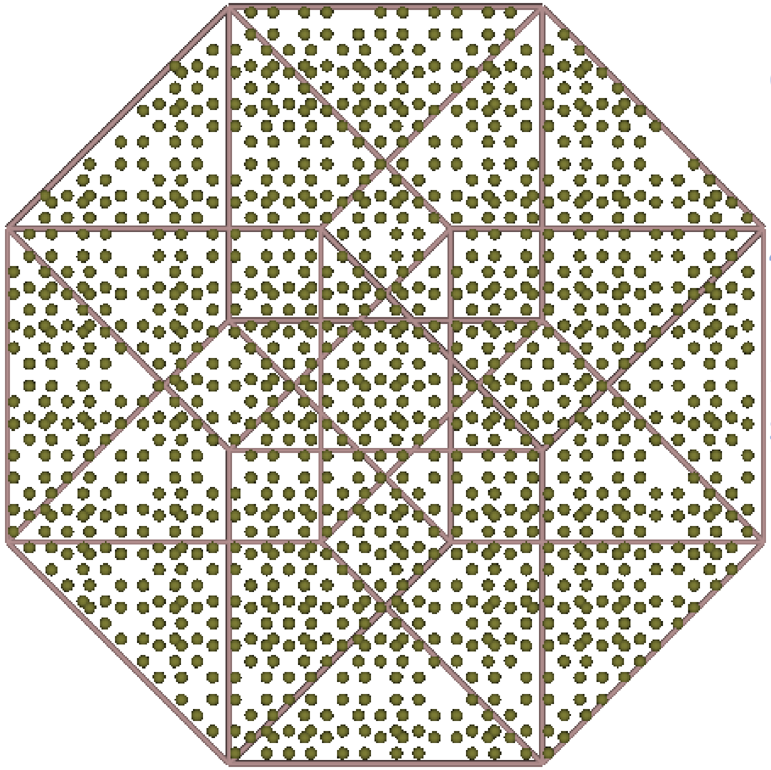
Dual-grid method – practice in 2 dims.

Ammann-Beenker tiling (in 2-dim. physical space)



Mapping the vertices of the tiling into the orthogonal complement (2-dim.)



Outer boundary (regular octagon) Projection of the 4-dim. hyper-cubic unit cell into the 2-dim. perpendicular space.

Some resources on aperiodic tilings:

Perl scripts for constructing the rhombic Penrose tiling (P3) and the Ammann-Beenker tiling:

http://www.tagen.tohoku.ac.jp/labo/tsai/nobuhisa/Penrose2pov.pl

$s_1 + s_2 + s_3 + s_4 + s_5$ = integer → rhombic Penrose tiling (P3)

$s_1 + s_2 + s_3 + s_4 + s_5$ = half integer → anti-Penrose tiling

http://www.tagen.tohoku.ac.jp/labo/tsai/nobuhisa/AmmannBeenker2pov.pl

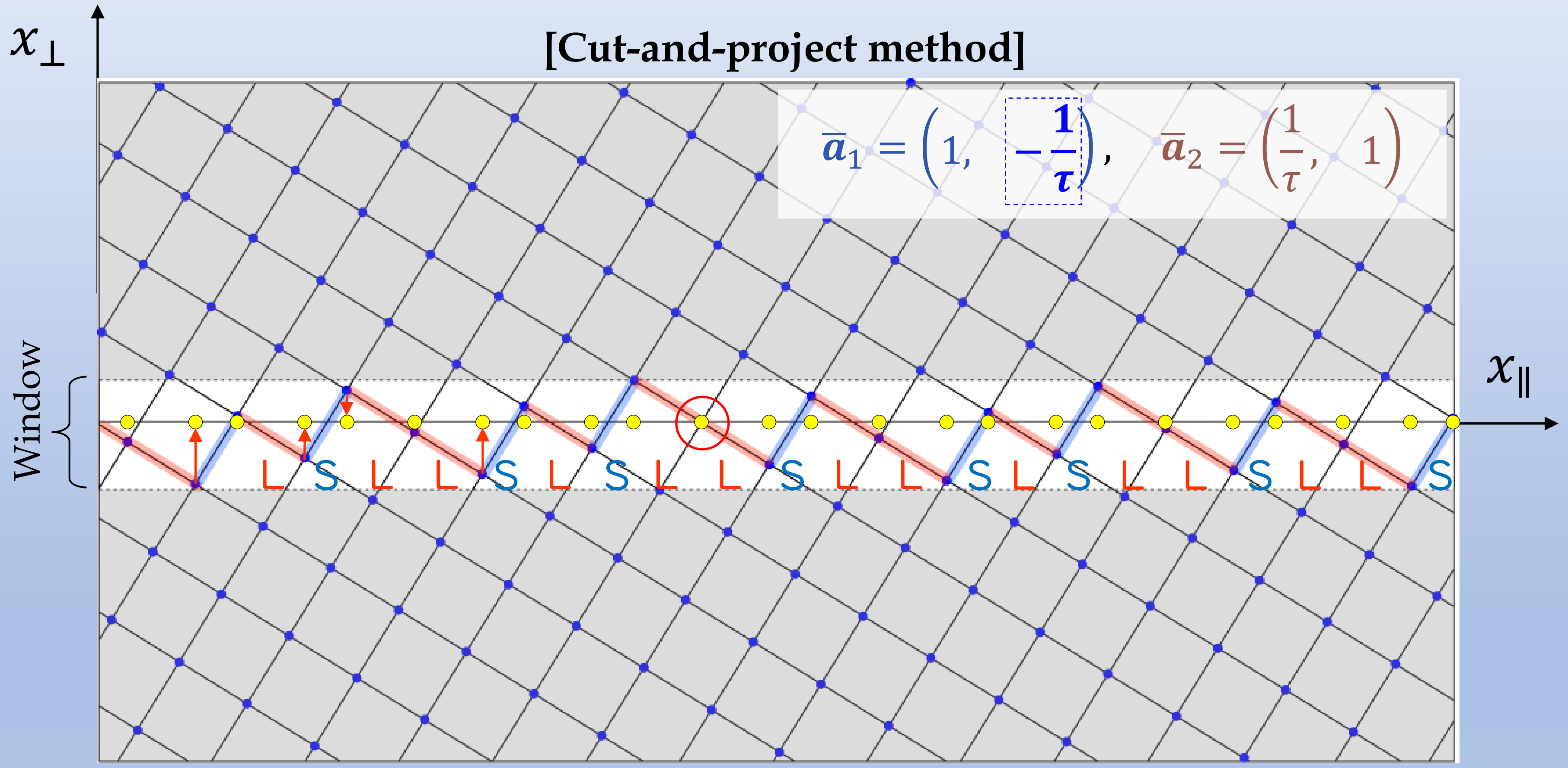
Tilings encyclopedia:

http://tilings.math.uni-bielefeld.de/

Book:

B. Gruenbaum, G.C. Shephard, Tilings and Patterns,
W. H. Freeman and Company, New York, 1987 (Chapter 10).

5. Approximants

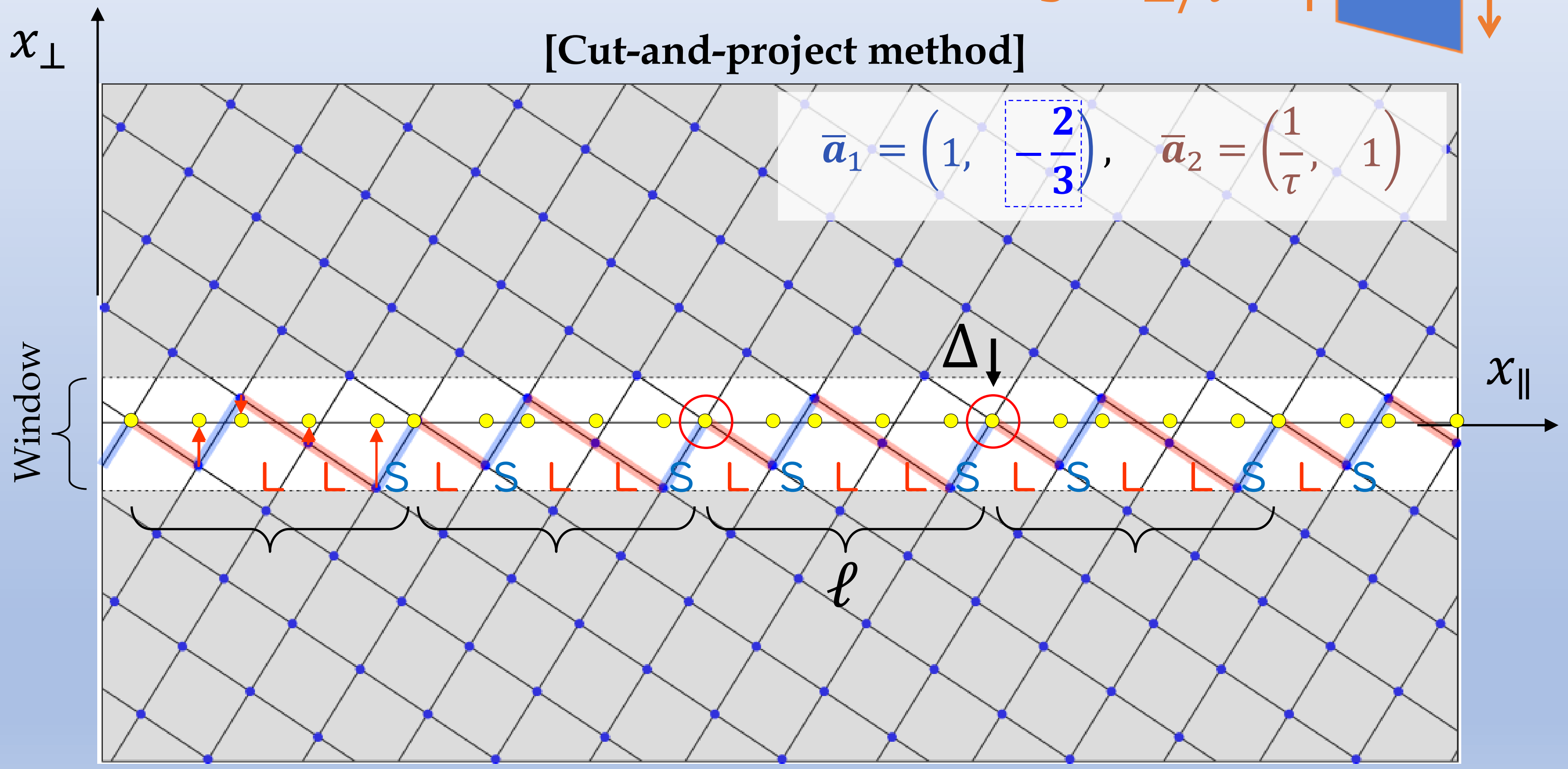


Fibonacci chain (without linear phason strain)

5. Approximants

Phason strain

$S = \Delta/\ell$



3/2 approximant to Fibonacci chain

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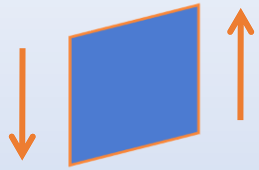
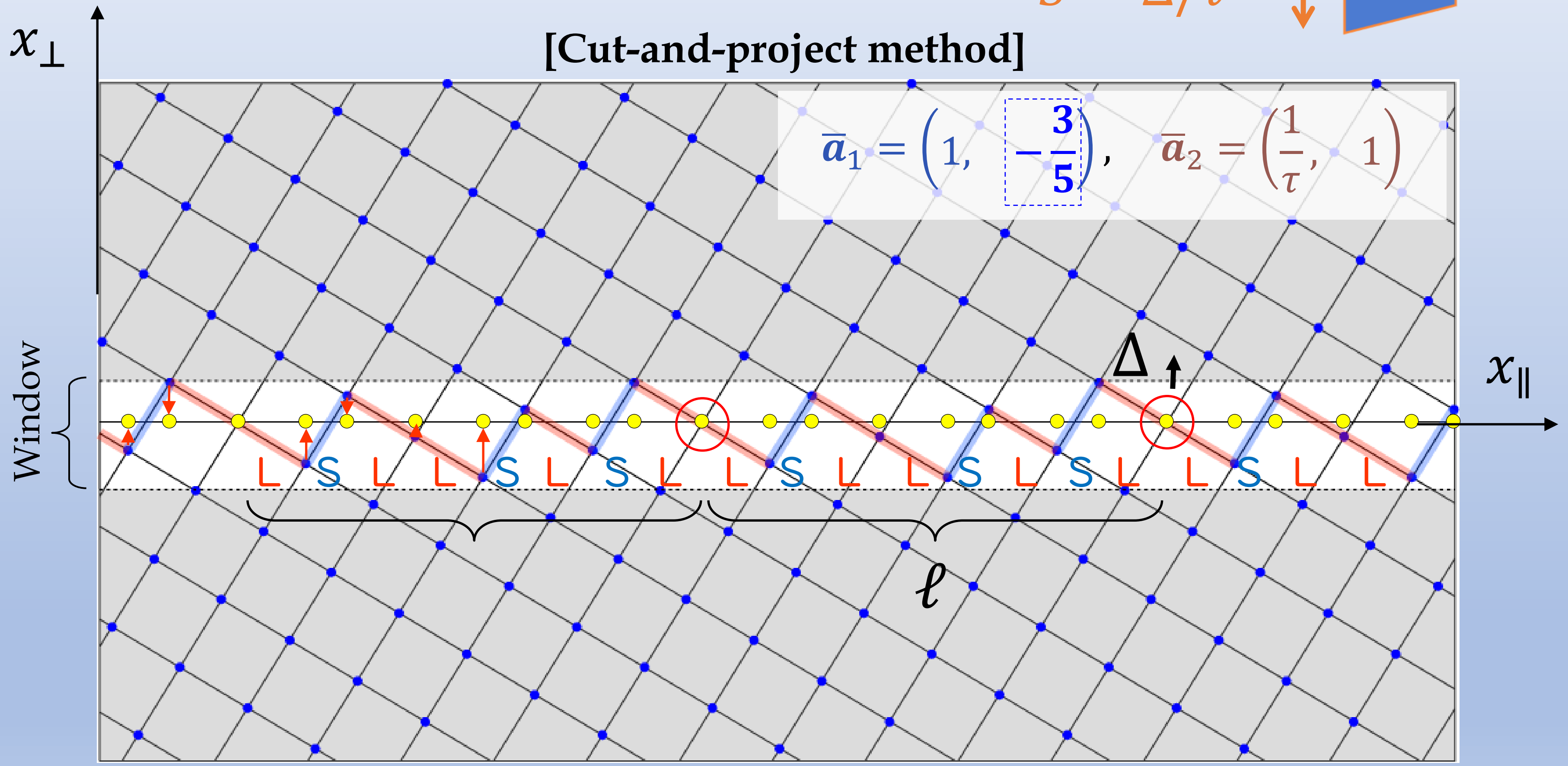
5. Approximants

Phason strain
$S = \Delta/\ell$





5/3 approximant to Fibonacci chain

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Rational approximations of τ

Continued fraction expansion of $\tau = \frac{1+\sqrt{5}}{2}$ (golden mean)

$$\tau = \frac{1+\sqrt{5}}{2} = 1 + \frac{1}{\tau} = 1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1+\dots}}}}$$

Rational approximation of τ; $\tau \cong \frac{F_{n+1}}{F_n}$

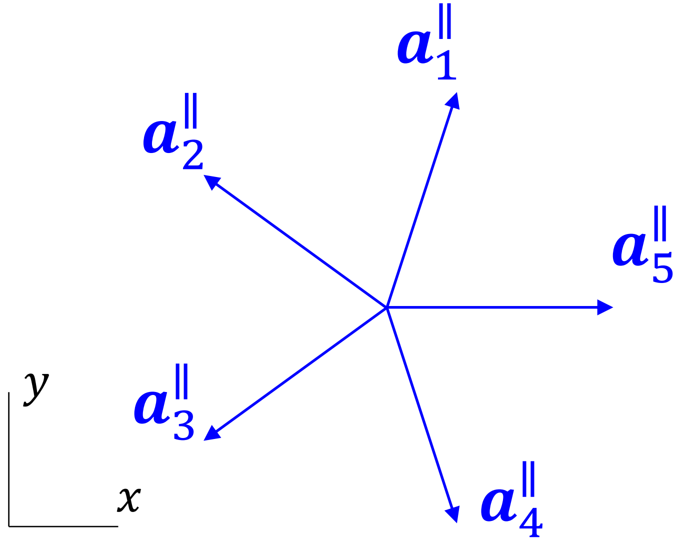
$$\tau \cong 1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1+1}}} = 1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{F_2}{F_3}}} = 1 + \cfrac{1}{1 + \cfrac{F_3}{F_4}} = 1 + \frac{F_4}{F_5} = \frac{F_6}{F_5}$$

Fibonacci numbers

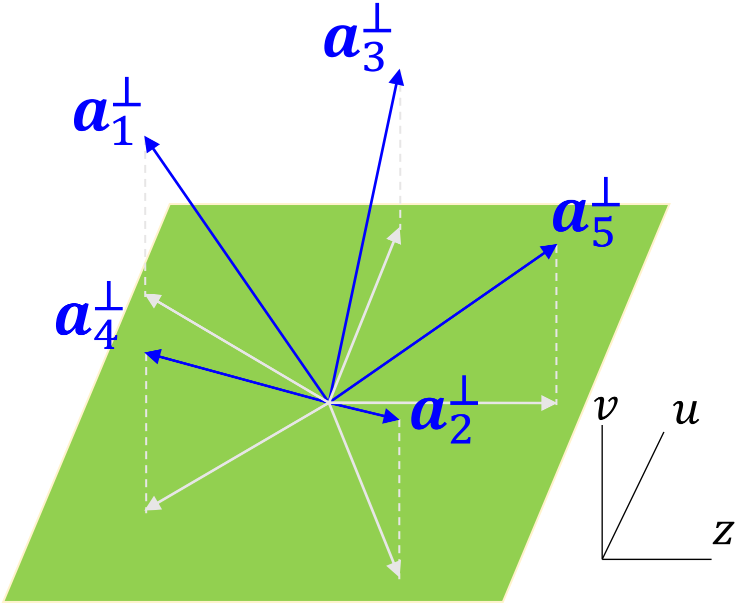
$$F_{n+1} = F_n + F_{n-1} \ \ (F_0 = 0, F_1 = 1, F_2 = 1, F_3 = 2, F_4 = 3, F_5 = 5, F_6 = 8, \dots)$$

5-dim. basis vectors of the P3 tiling

(with no linear phason strain)



physical space



perpendicular space

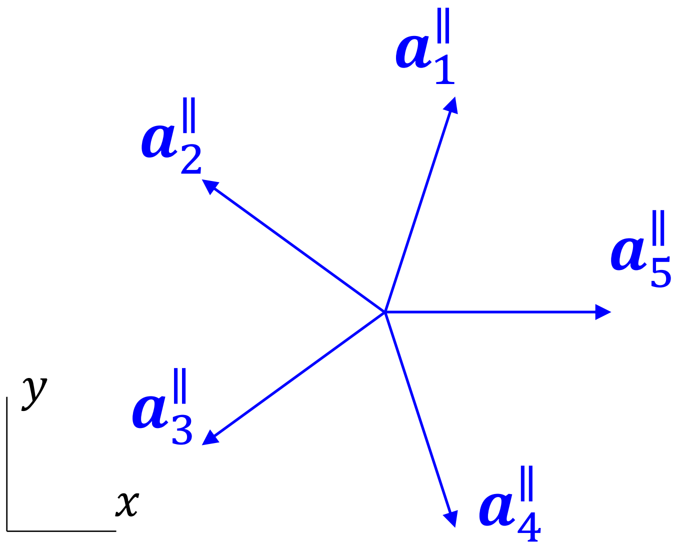
$\boldsymbol{a}_5^{\parallel} - \tau(\boldsymbol{a}_1^{\parallel} + \boldsymbol{a}_4^{\parallel}) = \boldsymbol{0}$ *x−direction*

$\boldsymbol{a}_1^{\parallel} - \boldsymbol{a}_4^{\parallel} - \tau(\boldsymbol{a}_2^{\parallel} - \boldsymbol{a}_3^{\parallel}) = \boldsymbol{0}$ *y−dir.*

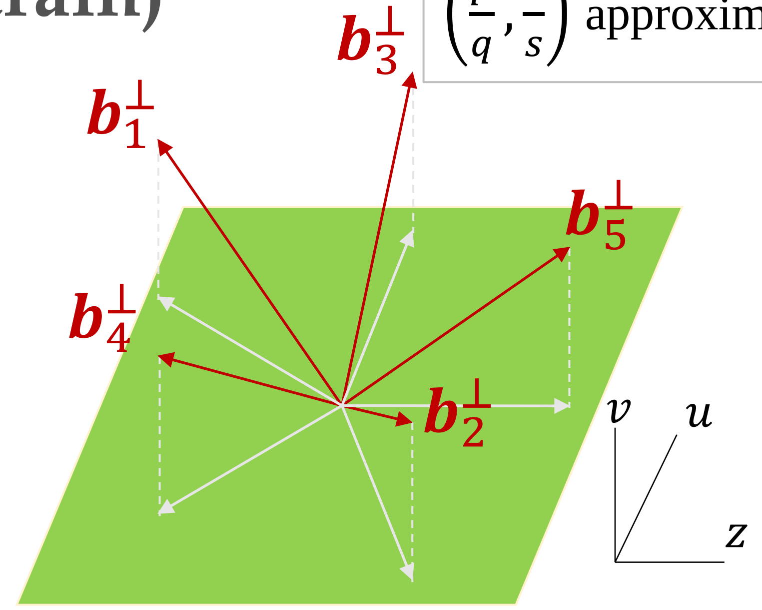
$\boldsymbol{a}_5^{\perp} + \frac{1}{\tau}(\boldsymbol{a}_1^{\perp} + \boldsymbol{a}_4^{\perp}) = \boldsymbol{0}$ *z−dir.*

$\boldsymbol{a}_1^{\perp} - \boldsymbol{a}_4^{\perp} + \frac{1}{\tau}(\boldsymbol{a}_2^{\perp} - \boldsymbol{a}_3^{\perp}) = \boldsymbol{0}$ *u−dir.*

5-dim. basis vectors of an approximant
(modified with a linear phason strain)



physical space



$\left(\frac{p}{q}, \frac{r}{s}\right)$ approximation

perpendicular space

$$\boldsymbol{a}_5^{\parallel} - \tau(\boldsymbol{a}_1^{\parallel} + \boldsymbol{a}_4^{\parallel}) = \mathbf{0} \qquad x\text{−}direction$$

$$\boldsymbol{a}_1^{\parallel} - \boldsymbol{a}_4^{\parallel} - \tau(\boldsymbol{a}_2^{\parallel} - \boldsymbol{a}_3^{\parallel}) = \mathbf{0} \qquad y\text{−}dir.$$

$$\boldsymbol{b}_5^{\perp} + \frac{q}{p}(\boldsymbol{b}_1^{\perp} + \boldsymbol{b}_4^{\perp}) = \mathbf{0} \qquad z\text{−}dir.$$

$$\boldsymbol{b}_1^{\perp} - \boldsymbol{b}_4^{\perp} + \frac{s}{r}(\boldsymbol{b}_2^{\perp} - \boldsymbol{b}_3^{\perp}) = \mathbf{0} \qquad u\text{−}dir.$$

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5-dim. basis vectors of an approximant
(modified with a linear phason strain)

$\left(\frac{p}{q}, \frac{r}{s}\right)$ approximation

$$\tilde{\boldsymbol{a}}_1 = \begin{pmatrix} 1/(2\tau) \\ \sqrt{4\tau+3}/(2\tau) \\ -p \\ s \\ 1/\sqrt{2} \end{pmatrix},\quad \tilde{\boldsymbol{a}}_2 = \begin{pmatrix} -\tau/2 \\ \sqrt{3-\tau}/2 \\ p-q \\ -r \\ 1/\sqrt{2} \end{pmatrix},\quad \tilde{\boldsymbol{a}}_3 = \begin{pmatrix} -\tau/2 \\ -\sqrt{3-\tau}/2 \\ p-q \\ r \\ 1/\sqrt{2} \end{pmatrix},$$

$$\tilde{\boldsymbol{a}}_4 = \begin{pmatrix} 1/(2\tau) \\ -\sqrt{4\tau+3}/(2\tau) \\ -p \\ -s \\ 1/\sqrt{2} \end{pmatrix},\quad \tilde{\boldsymbol{a}}_5 = \begin{pmatrix} 1 \\ 0 \\ 2q \\ 0 \\ 1/\sqrt{2} \end{pmatrix}$$

$$\tilde{\boldsymbol{a}}_j = \begin{pmatrix} \boldsymbol{a}_j^{||} \\ \boldsymbol{b}_j^{\perp} \\ 1/\sqrt{2} \end{pmatrix}$$

N.B. z and u axes are arbitrarily scaled

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Periodicity of $\left(\frac{p}{q}, \frac{r}{s}\right)$ approximant

A general 5-dim. lattice vector with indices $(h_1, h_2, h_3, h_4, h_5)$

→ Perpendicular space components:

$$h_1 b_1^{\perp} + h_2 b_2^{\perp} + h_3 b_3^{\perp} + h_4 b_4^{\perp} + h_5 b_5^{\perp}$$
$$= \begin{pmatrix} 2qh_5 - ph_1 + (p-q)h_2 + (p-q)h_3 - ph_4 \\ sh_1 - rh_2 + rh_3 - sh_4 \\ (h_1 + h_2 + h_3 + h_4 + h_5)/\sqrt{2} \end{pmatrix}$$

Note that the 2-dim. lattice basis vectors, $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, of $\left(\frac{p}{q}, \frac{r}{s}\right)$ approximant along the x and y directions should in general be indexed as (j, k, k, j, i) and $(l, m, -m, -l, 0)$, respectively.

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Periodicity of $\left(\frac{p}{q},\frac{r}{s}\right)$ approximant

Their modified perpendicular space components would then be

$$\boldsymbol{R}_1{}' = jb_1^\perp + kb_2^\perp + kb_3^\perp + jb_4^\perp + ib_5^\perp = \begin{pmatrix} 2\{p(k-j)-q(k-i)\} \\ 0 \\ (i+2j+2k)/\sqrt{2} \end{pmatrix}$$

$$\boldsymbol{R}_2{}' = lb_1^\perp + mb_2^\perp - mb_3^\perp - lb_4^\perp = \begin{pmatrix} 0 \\ 2(sl-rm) \\ 0 \end{pmatrix}$$

These perpendicular space components would vanish if $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are the lattice bases of the approximant, so that

$$\frac{p}{q}=\frac{k-i}{k-j}, \qquad \frac{r}{s}=\frac{l}{m}, \qquad i+2j+2k=0$$

$$(i-k)+2(j-k)+5k=0$$

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Periodicity of $\left(\frac{p}{q}, \frac{r}{s}\right)$ approximant

There exists non-zero integer, n, such that

$$i - k = pn,\ j - k = qn \text{ and}$$
$$5k = -(p + 2q)n$$

p+2qと5の最小公倍数を
与えるようにnを決める。

Thus the values of i, j and k are determined uniquely (up to a sign) according to the values of p and q, and so are the values l and m according to the values of r and s through

$$l = \pm r,\ m = \pm s$$

Periodicity of $\left(\frac{p}{q}, \frac{r}{s}\right)$ approximant

Lattice basis vectors in the physical space

$$\boldsymbol{R}_1 = j\boldsymbol{a}_1^{||} + k\boldsymbol{a}_2^{||} + k\boldsymbol{a}_3^{||} + j\boldsymbol{a}_4^{||} + i\boldsymbol{a}_5^{||} = qn\boldsymbol{a}_1^{||} + qn\boldsymbol{a}_4^{||} + pn\boldsymbol{a}_5^{||}$$

$$\boldsymbol{R}_2 = r\boldsymbol{a}_1^{||} + s\boldsymbol{a}_2^{||} - s\boldsymbol{a}_3^{||} - r\boldsymbol{a}_4^{||}$$

The corresponding increments in the perpendicular space

$$\boldsymbol{R}_1{}^{\perp} = j\boldsymbol{a}_1^{\perp} + k\boldsymbol{a}_2^{\perp} + k\boldsymbol{a}_3^{\perp} + j\boldsymbol{a}_4^{\perp} + i\boldsymbol{a}_5^{\perp} = qn\boldsymbol{a}_1^{\perp} + qn\boldsymbol{a}_4^{\perp} + pn\boldsymbol{a}_5^{\perp}$$

$$\boldsymbol{R}_2{}^{\perp} = r\boldsymbol{a}_1^{\perp} + s\boldsymbol{a}_2^{\perp} - s\boldsymbol{a}_3^{\perp} - r\boldsymbol{a}_4^{\perp}$$

The linear phason strain tensor, S (Definition: $\boldsymbol{x}^{\perp} \sim S\boldsymbol{x}^{\|}$)

$$\begin{pmatrix}\boldsymbol{R}_1{}^{\perp} & \boldsymbol{R}_2{}^{\perp}\end{pmatrix} = \boldsymbol{S}\begin{pmatrix}\boldsymbol{R}_1 & \boldsymbol{R}_2\end{pmatrix}$$

$$\boldsymbol{S} = \begin{pmatrix}\boldsymbol{R}_1{}^{\perp} & \boldsymbol{R}_2{}^{\perp}\end{pmatrix}\begin{pmatrix}\boldsymbol{R}_1 & \boldsymbol{R}_2\end{pmatrix}^{-1}$$

N.B.) $\boldsymbol{S}$ is a 3x2 matrix in the present case

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How to generate an approximant with dual-grids

Replace the hyper-cubic lattice basis vectors ($\bar{\boldsymbol{a}}_j$ and $\bar{\boldsymbol{g}}_j$) into modified basis vectors ($\tilde{\boldsymbol{a}}_j$ and $\tilde{\boldsymbol{g}}_j$) while performing the dual-grid method (see, p.50)

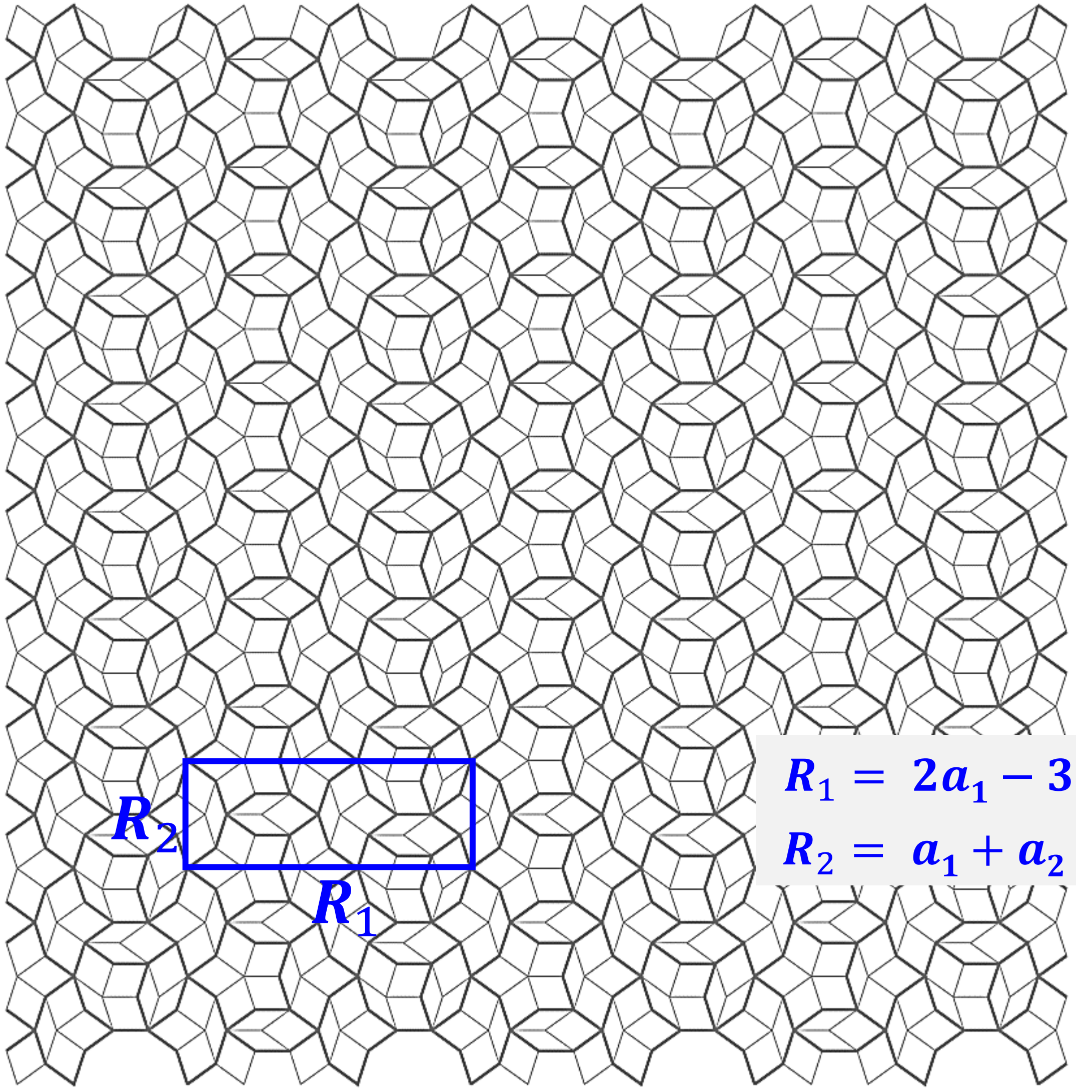
$$\bar{\boldsymbol{a}}_j = \left(\boldsymbol{a}_j^{||}, \boldsymbol{a}_j^{\perp}\right) \quad \rightarrow \quad \tilde{\boldsymbol{a}}_j = \left(\boldsymbol{a}_j^{||}, \boldsymbol{b}_j^{\perp}\right)$$

$$\bar{\boldsymbol{g}}_j \quad (\text{def: } \bar{\boldsymbol{a}}_j \cdot \bar{\boldsymbol{g}}_j = \boldsymbol{\delta}_{ij}) \quad \rightarrow \quad \tilde{\boldsymbol{g}}_j \quad (\text{def: } \tilde{\boldsymbol{a}}_j \cdot \tilde{\boldsymbol{g}}_j = \boldsymbol{\delta}_{ij})$$

Examples

Approximant No.1

$$\left(\frac{1}{1},\frac{1}{1}\right)$$



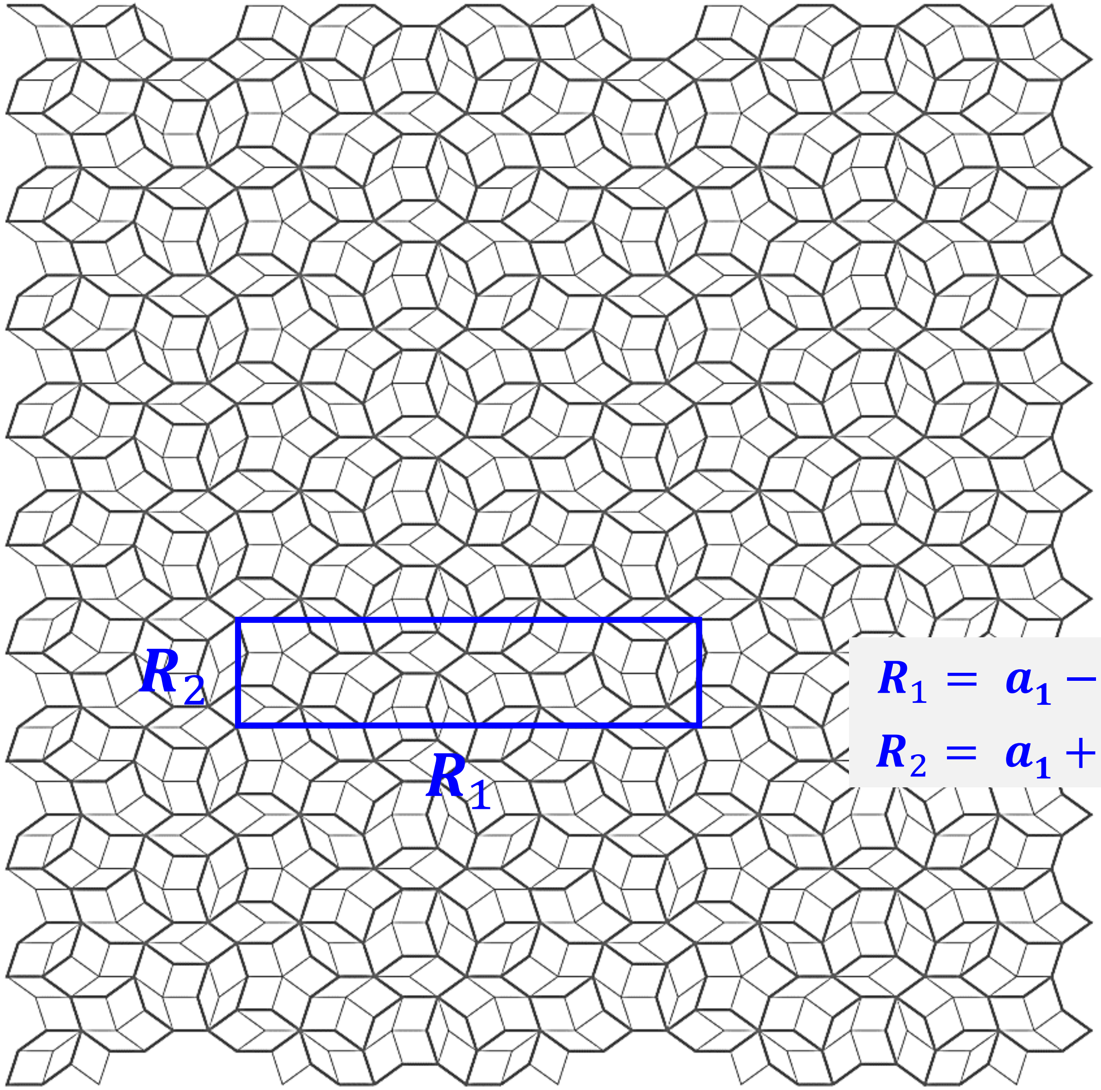
$$\boldsymbol{R}_1 = 2\boldsymbol{a}_1 - 3\boldsymbol{a}_2 - 3\boldsymbol{a}_3 + 2\boldsymbol{a}_4 + 2\boldsymbol{a}_5$$

$$\boldsymbol{R}_2 = \boldsymbol{a}_1 + \boldsymbol{a}_2 - \boldsymbol{a}_3 - \boldsymbol{a}_4$$

Examples

Approximant No.2

$$\left(\frac{2}{1},\frac{1}{1}\right)$$



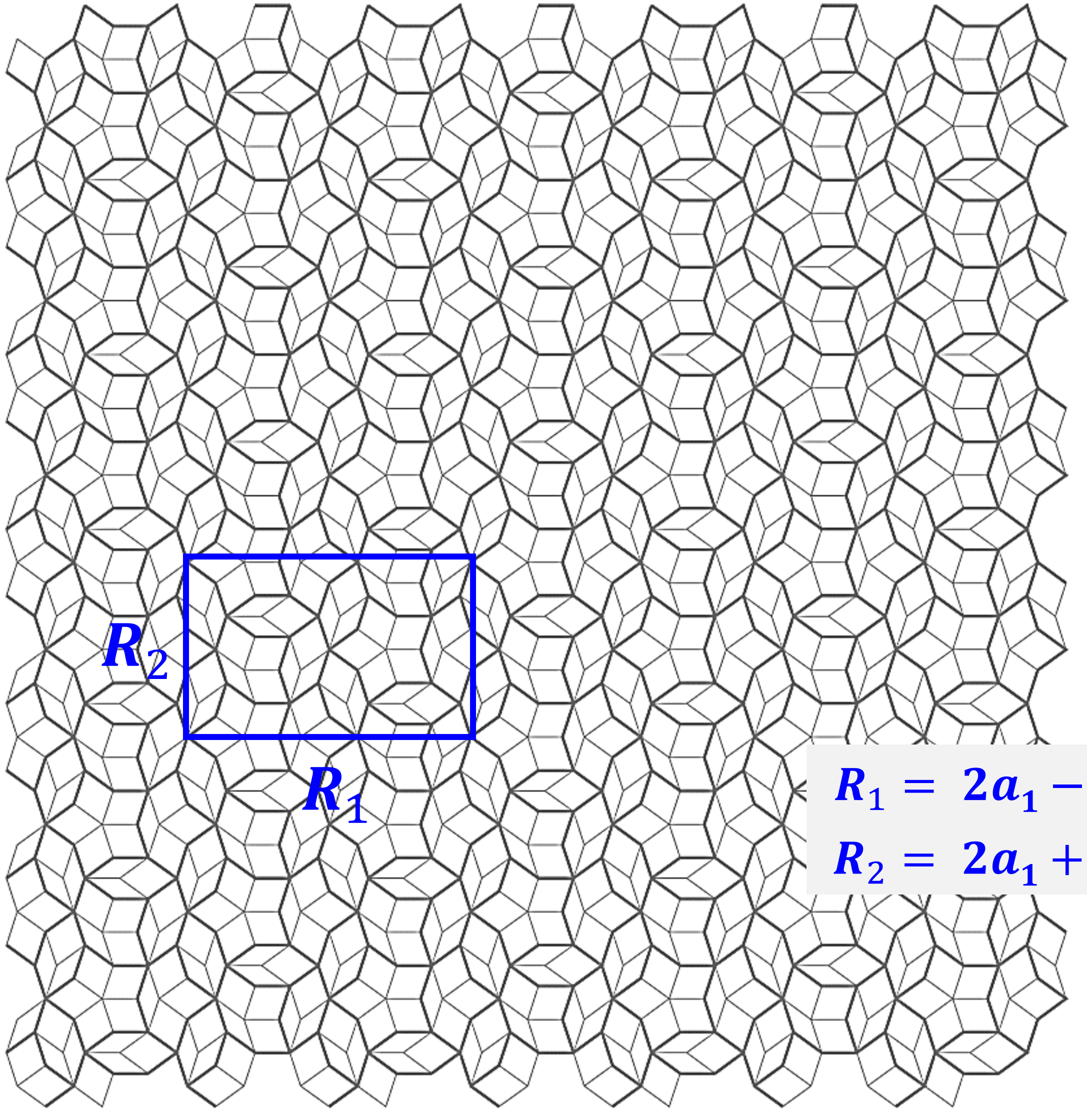
$$R_1 = a_1 - 4a_2 - 4a_3 + a_4 + 6a_5$$

$$R_2 = a_1 + a_2 - a_3 - a_4$$

Examples

Approximant No.3

$$\left(\frac{1}{1},\frac{2}{1}\right)$$



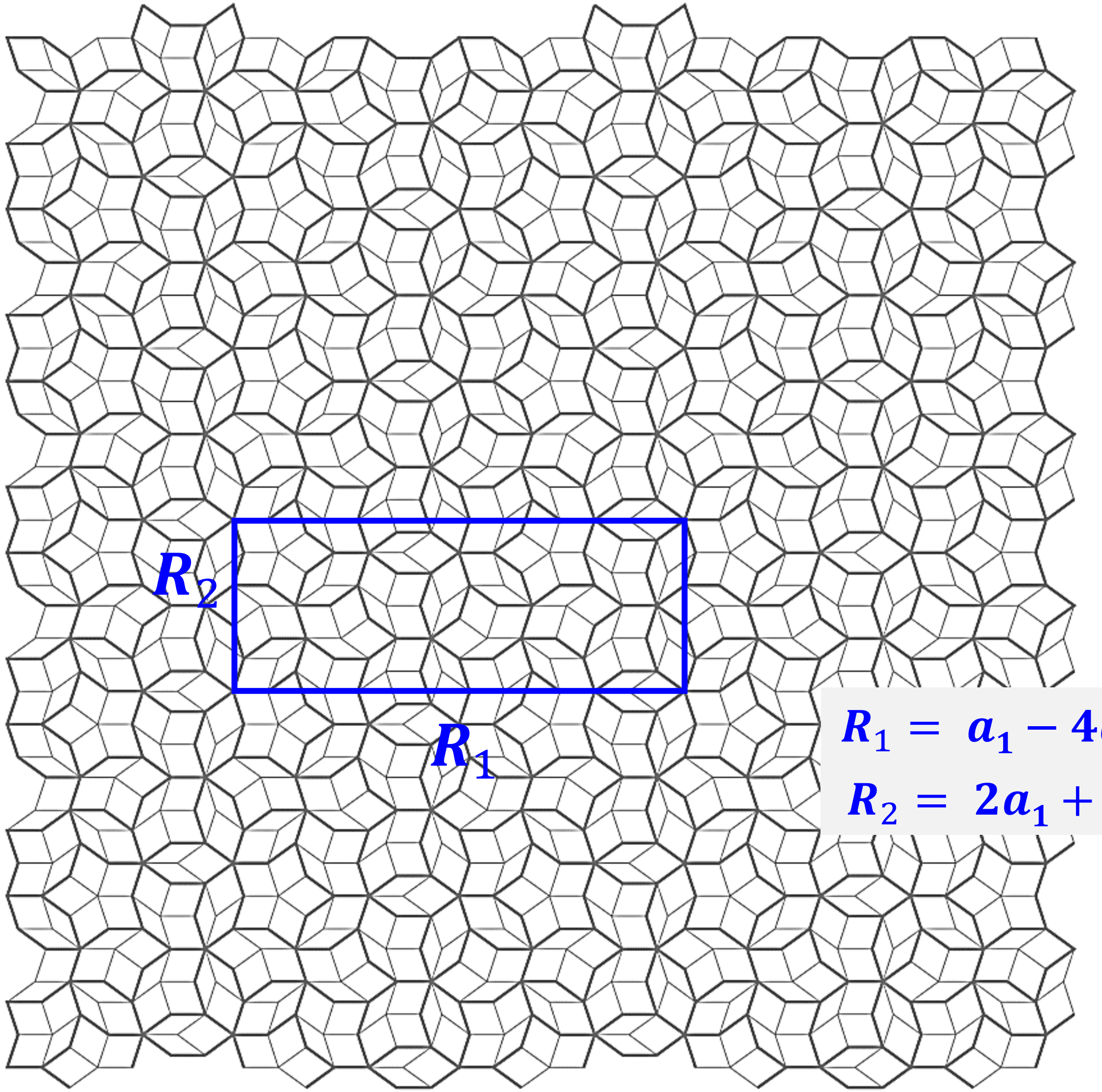
$$R_1 = 2a_1 - 3a_2 - 3a_3 + 2a_4 + 2a_5$$

$$R_2 = 2a_1 + a_2 - a_3 - 2a_4$$

Examples

Approximant No.4

$$\left(\frac{2}{1},\frac{2}{1}\right)$$



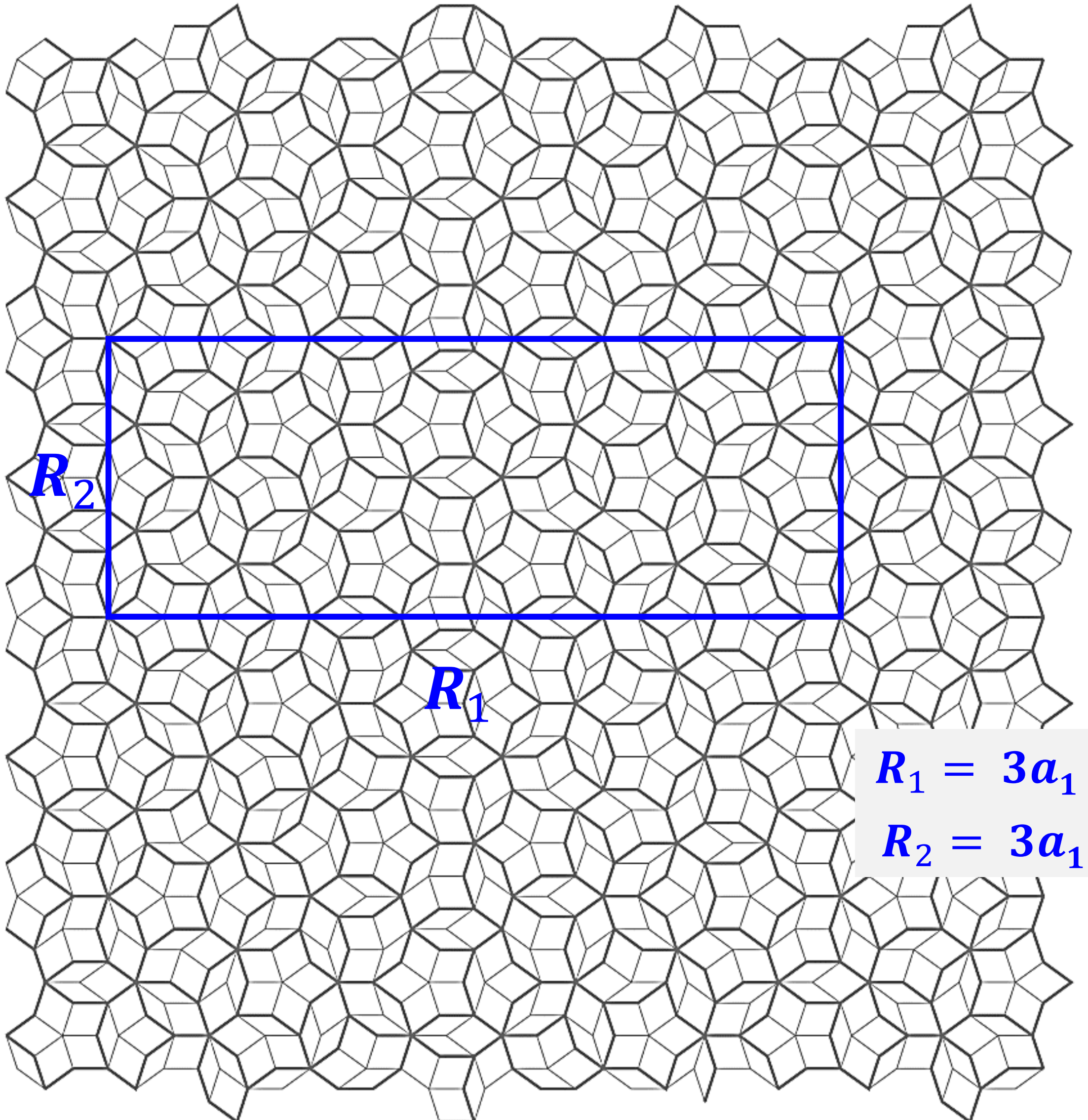
$$\boldsymbol{R}_1 = \boldsymbol{a}_1 - 4\boldsymbol{a}_2 - 4\boldsymbol{a}_3 + \boldsymbol{a}_4 + 6\boldsymbol{a}_5$$

$$\boldsymbol{R}_2 = 2\boldsymbol{a}_1 + \boldsymbol{a}_2 - \boldsymbol{a}_3 - 2\boldsymbol{a}_4$$

Examples

Approximant No.5

$$\left(\frac{3}{2},\frac{3}{2}\right)$$



$$R_1 = 3a_1 - 7a_2 - 7a_3 + 3a_4 + 8a_5$$
$$R_2 = 3a_1 + 2a_2 - 2a_3 - 3a_4$$

Exercises

a. **Compare approximant tilings generated with different values of phason shifts.**

b. **Apply the dual-grid method for generating Ammann-Beenker tiling (octagonal, or 8-gonal, QC).**

c. **Generate a few simplest approximants to the Ammann-Beenker tiling.**