

# Aperiodic tilings

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## Purpose:

A concise introduction to aperiodic tilings

A geometrical basis of the following lectures on modeling of quasicrystals

## Outline

- Part A:
  - 1. Introduction
  - 2. Hyper-space formalism
  - 3. Methods of construction
  - 4. Important examples
- Part B:
  - 5. Classification scheme
  - 6. Embedding lattices
  - 7. Approximants
  - 8. Phason flips

# **1. Introduction**

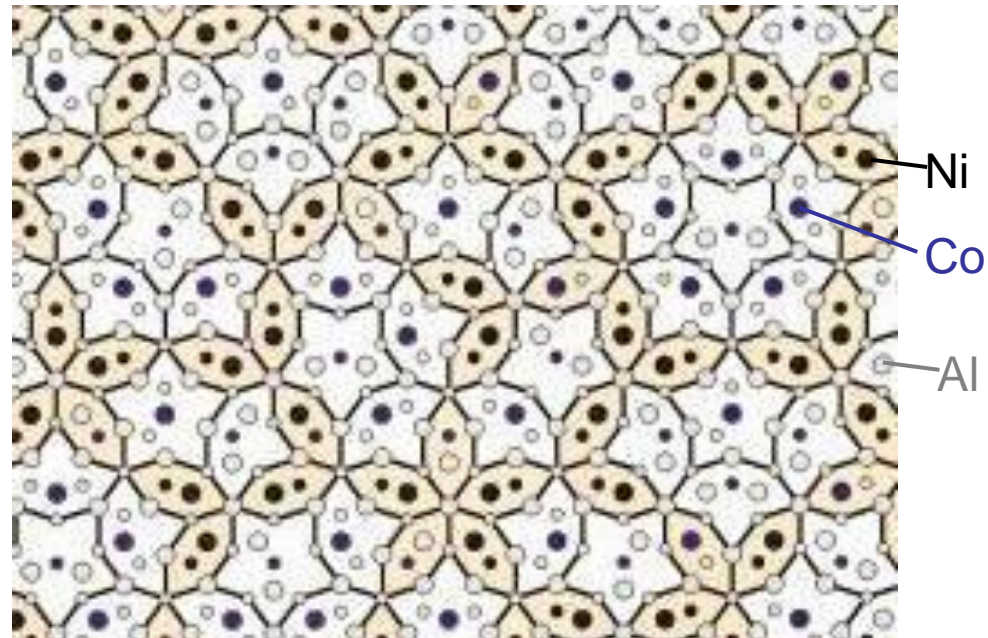
# Aperiodic crystals

No translation symmetry

Some kind of long-range orders (Bragg reflections)

## Quasicrystals

Decomposed into several types of building units (cells)



M. Mihalkovic et al., *Phys. Rev. B* 65, 104205 (2002)

# Tilings

**Tilings:** A mathematical representation of the space filling problem with a set of geometrical shapes (cells).

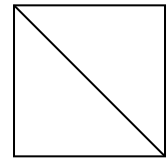
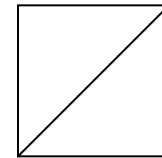
The theory of aperiodic tilings is a basis for understanding the structural properties of quasicrystals.

# An aperiodic tiling

$$v(m,n) = \text{Cos}(\pi p m + \phi) + \text{Cos}(\pi q n + \phi')$$

$$v \geq 0$$

$$v < 0$$



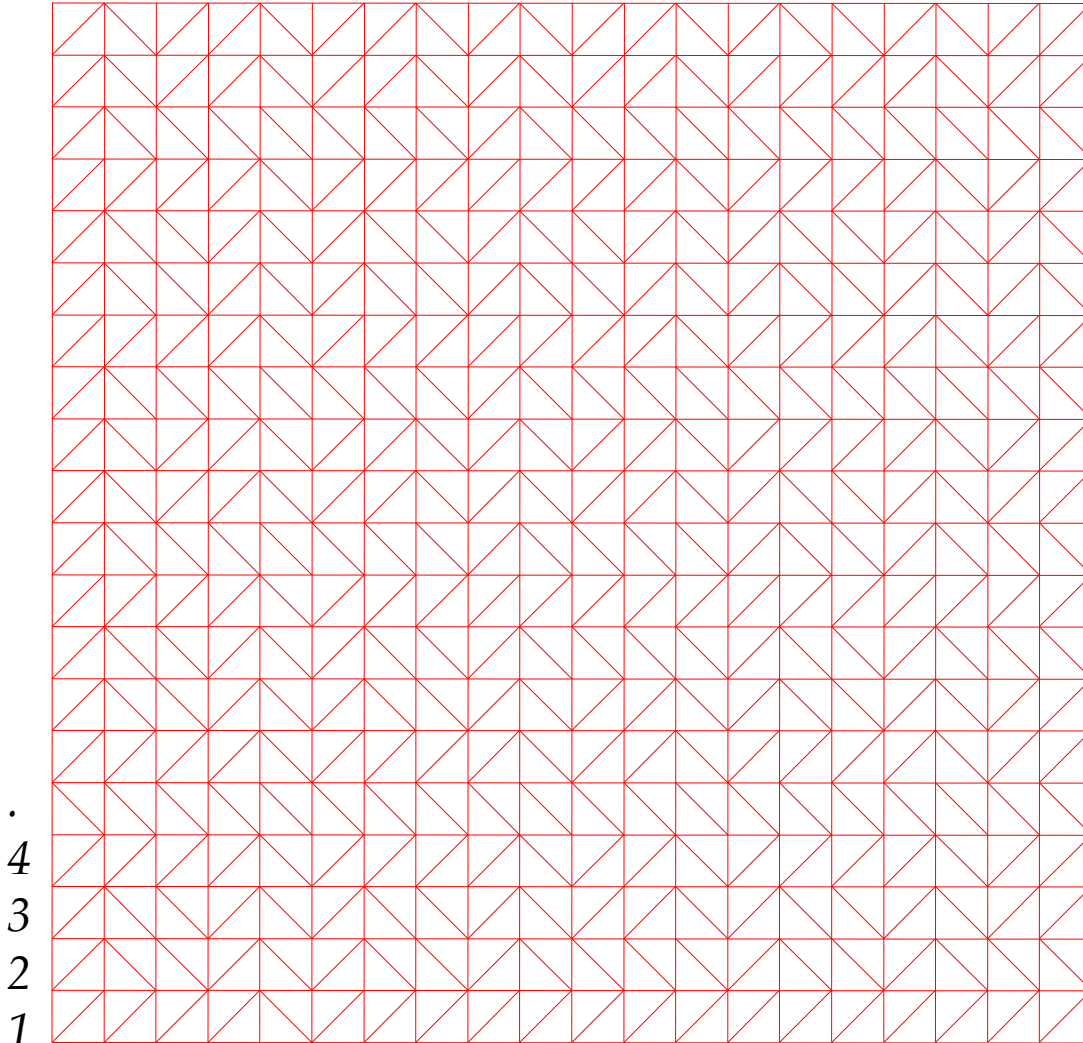
Mono-hedral tiling  
(there is only one type of tiles)

di-hedral

tri-hedral

.....

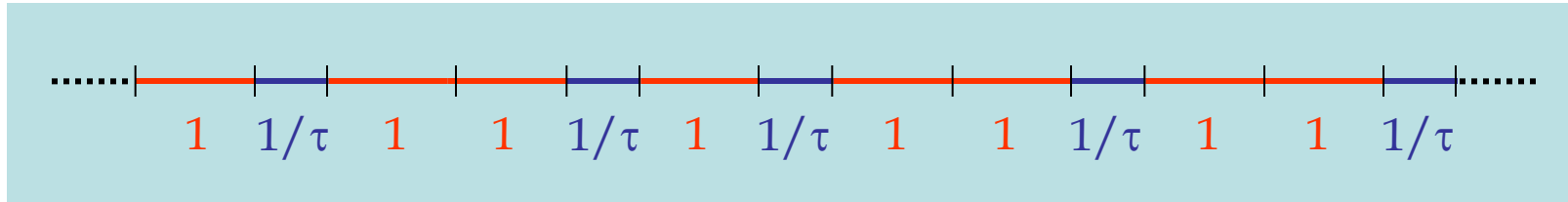
*k*-hedral



1 2 3 4...

$$(p,q) = (1/\tau, 1/\tau)$$

# Fibonacci chain



$$\tau = \frac{1 + \sqrt{5}}{2} \cong 1.618 \quad (\text{golden mean})$$

Aperiodic

Two types of tiles (di-hedral)

Bragg reflections (long-range ordered)

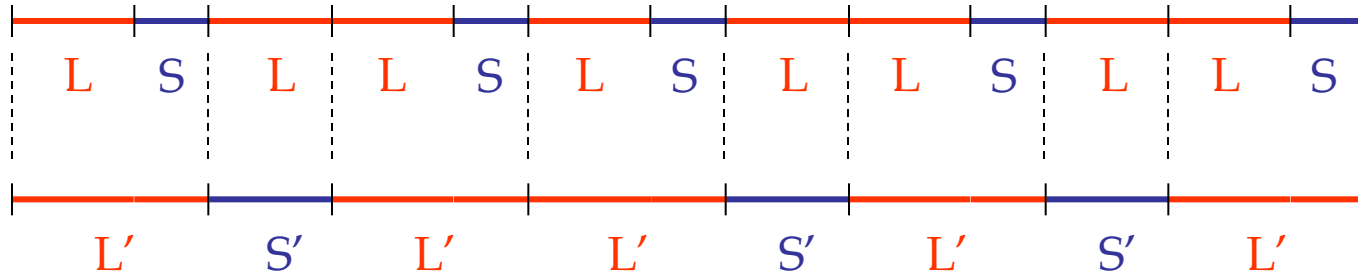
Self-similarity

Repetitivity  $\sim$  every patch in the tiling appear repeatedly with bounded distances between them.

The set of vertices  $\mathbb{V} \subset \mathbb{M} = \{n_1 + n_2 / \tau \mid n_1, n_2 \in \mathbb{Z}\}$   
(a module of rank 2)



# Self-similarity



$$LSLLSLSLLSLLS... \cong L'S'L'L'S'L'S'L'... \quad (L'=LS, S'=L)$$

## Substitution rule

$$\left\{ \begin{array}{l} L \rightarrow LS \\ S \rightarrow L \end{array} \right. \quad \begin{array}{l} L \rightarrow LS \rightarrow LSL \rightarrow LSLLS \rightarrow LSLLSLSL \\ (1) \quad (2) \quad (3) \quad (5) \quad (8) \\ \rightarrow LSLLSLSLLSLLS \rightarrow \dots \rightarrow \text{limit (fixed point)} \\ (13) \end{array}$$

$$F_{n+1} = F_n + F_{n-1} \quad (F_0=0, F_1=1, F_2=1, F_3=2, F_4=3, F_5=5, F_6=8, F_7=13, \dots)$$

(Fibonacci sequence)

# Rhombic Penrose tiling

Aperiodic

Di-hedral

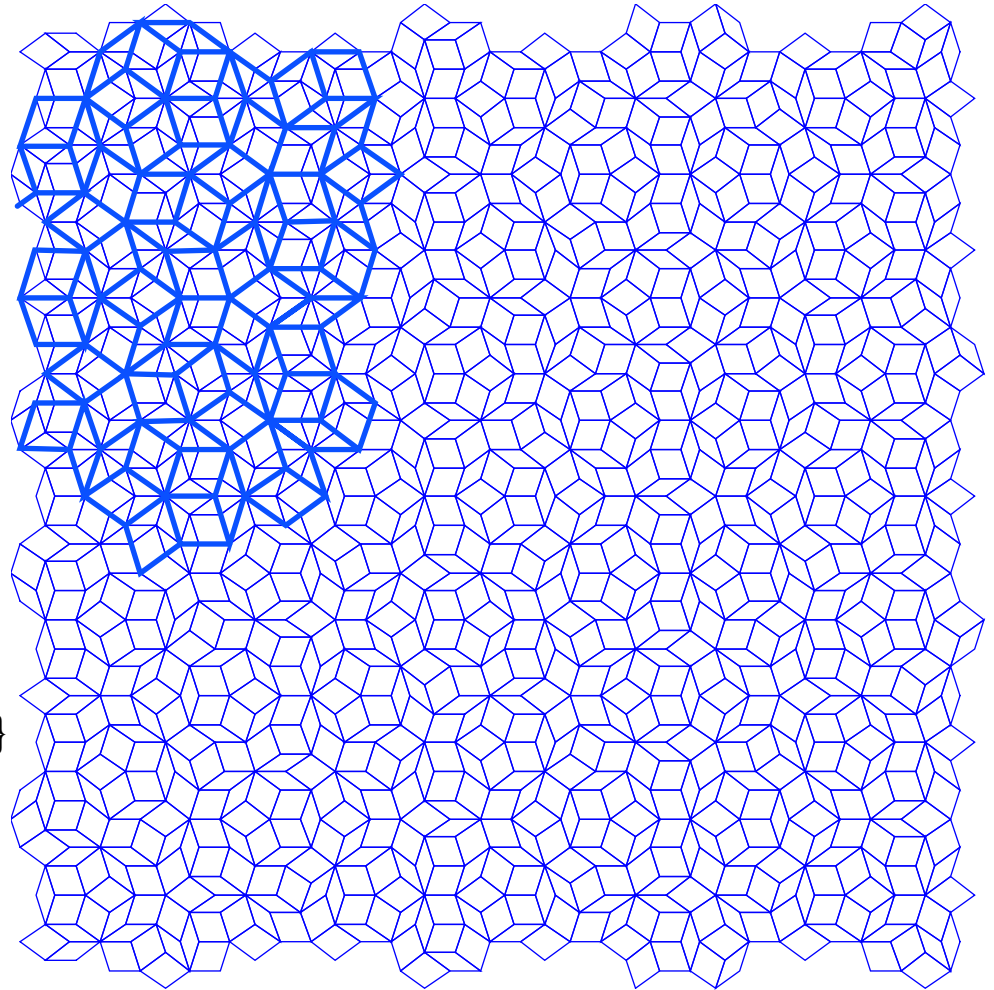
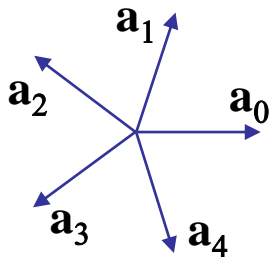
Bragg reflections

Self-similarity

Repetitivity

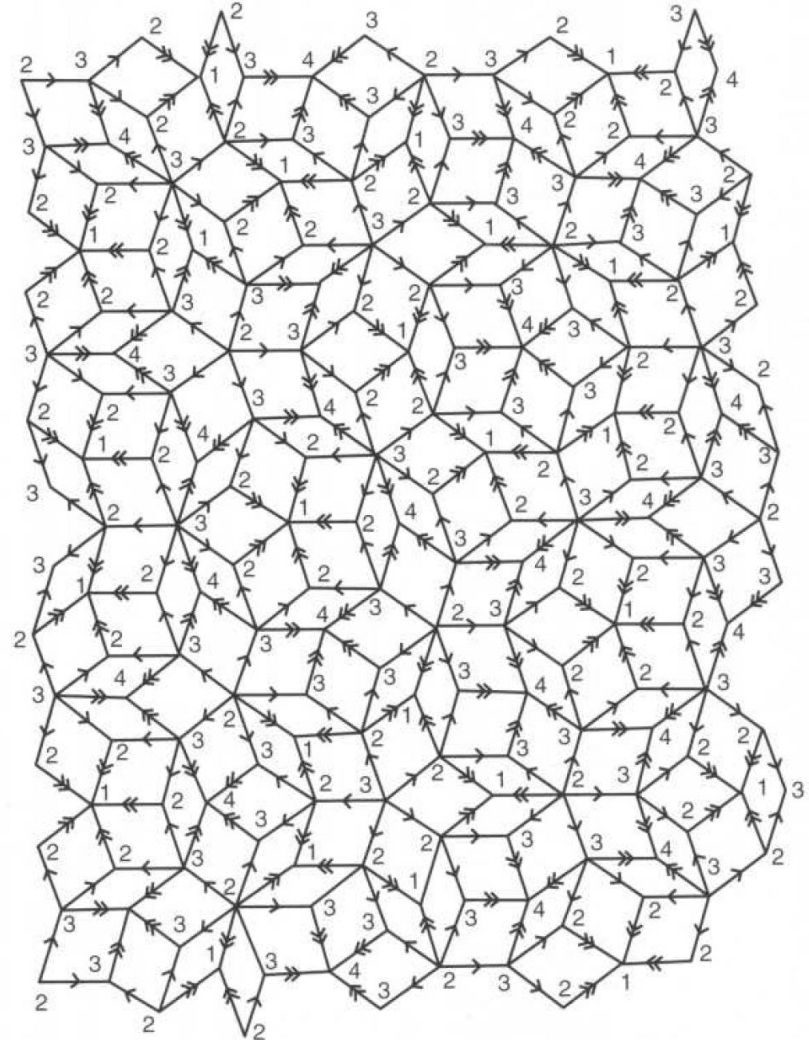
$\mathbb{V} \subset \mathbb{M}$  (rank 4)

$\mathbb{M} := \{n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 + n_4\mathbf{a}_4 \mid n_j \in \mathbb{Z}\}$



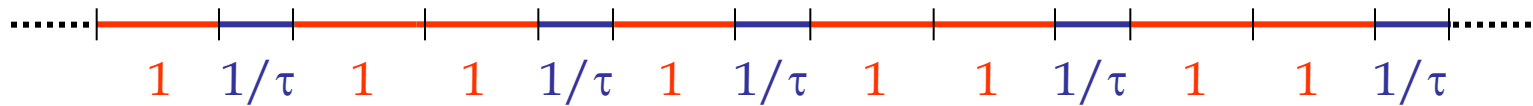
# Matching rules

The rhombic Penrose tiling is known to be a representative example of tilings whose aperiodicity is *enforced* by the tiles (decorated by arrows).



## **2. Hyper-space formalism**

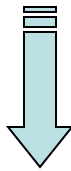
# The embedding of the Fibonacci chain



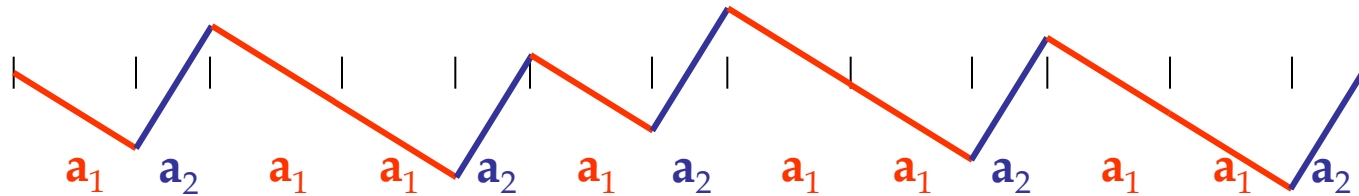
$$x_n = n_1 + n_2 / \tau \in \mathbb{M}$$

$$(x_0, y_0) = (0, \varphi)$$

$$(x_n, y_n) = (0, \varphi) + n_1 \vec{a}_1 + n_2 \vec{a}_2$$

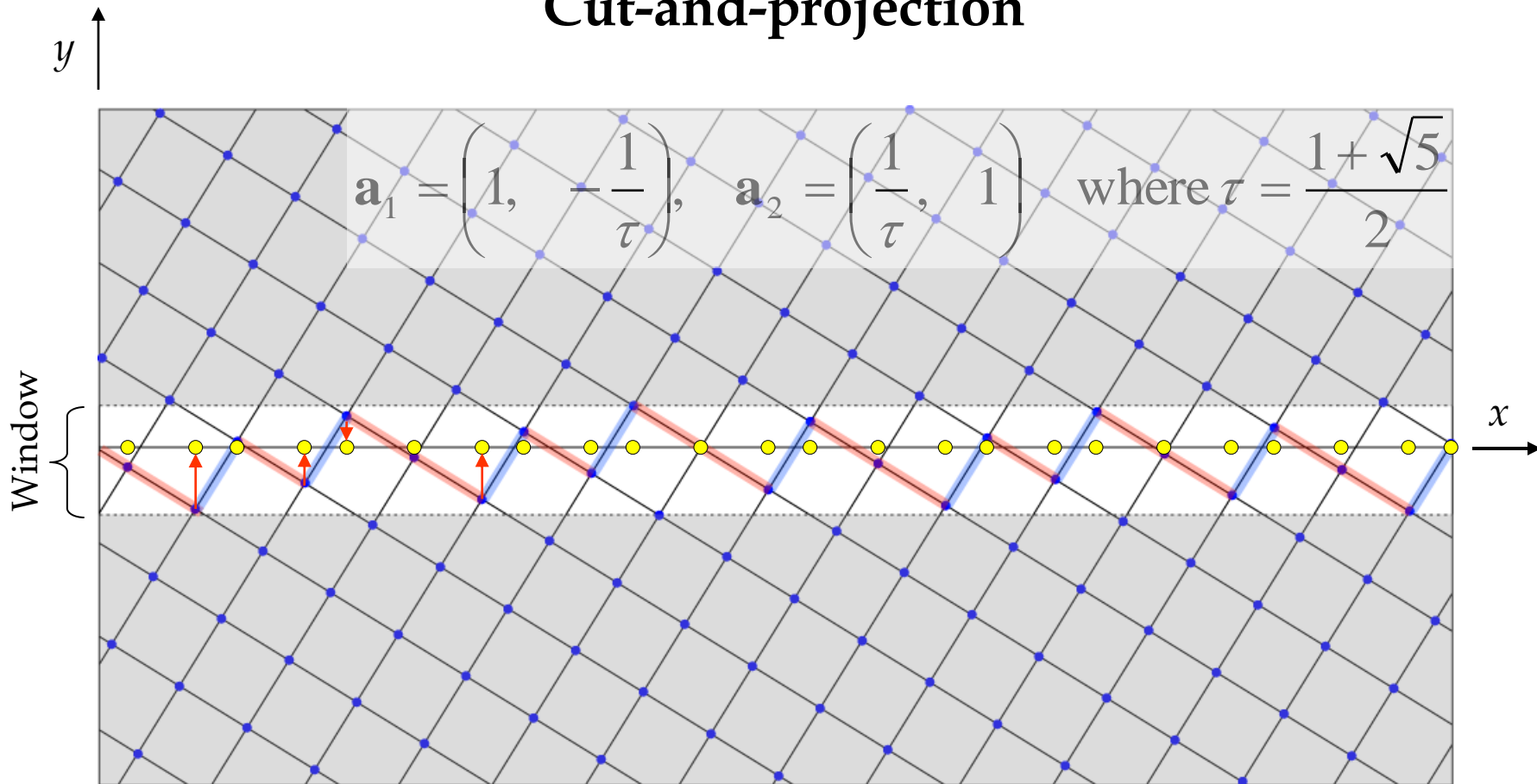


Zigzag chain



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

# Cut-and-projection



$$n = n_1 + n_2, \quad y_n = -n_1 \frac{1}{\tau} + n_2 + \varphi = \tau \operatorname{Frac}\left(\frac{n + \varphi}{\tau}\right)$$

$$\therefore x_n = n_1 + n_2 \frac{1}{\tau} = \left(\frac{3}{\tau} - 1\right)n + \left(\frac{1}{\tau} - 1\right)\operatorname{Frac}\left(\frac{n + \varphi}{\tau}\right) + \left(\frac{2}{\tau} - 1\right)\varphi$$

# Quasiperiodic tiling

hyper-lattice

... higher-dimensional lattice

hyper-space

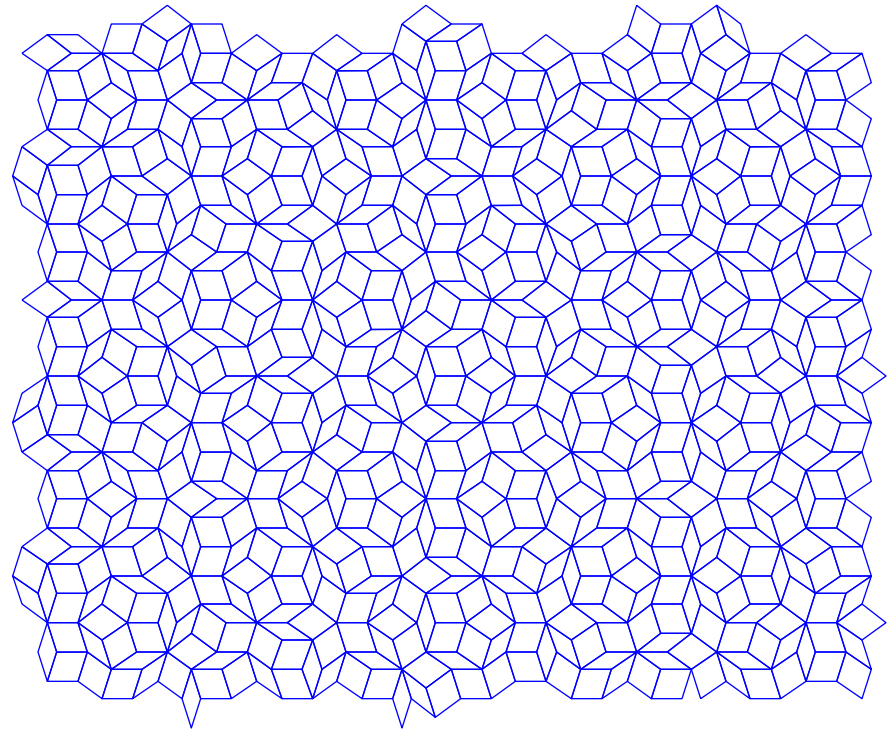
... higher-dimensional space

embedding dimensions ( $n$ )

... dimensions of the hyper-space

$$n \geq r$$

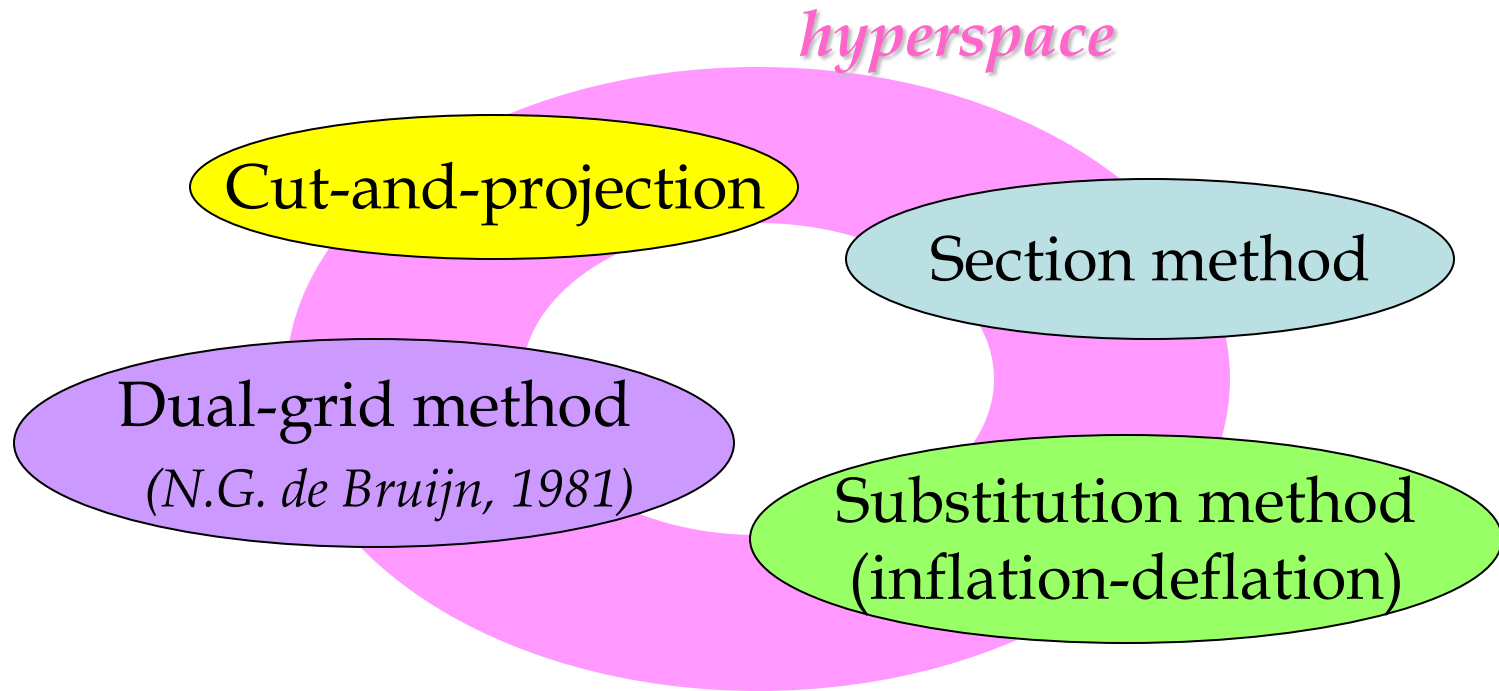
The rank ( $r$ ) of the module  $\mathbb{M}$  for the rhombic Penrose tiling is 4, while the most frequent choice for the hyper-lattice is a 5D hyper-cubic lattice.

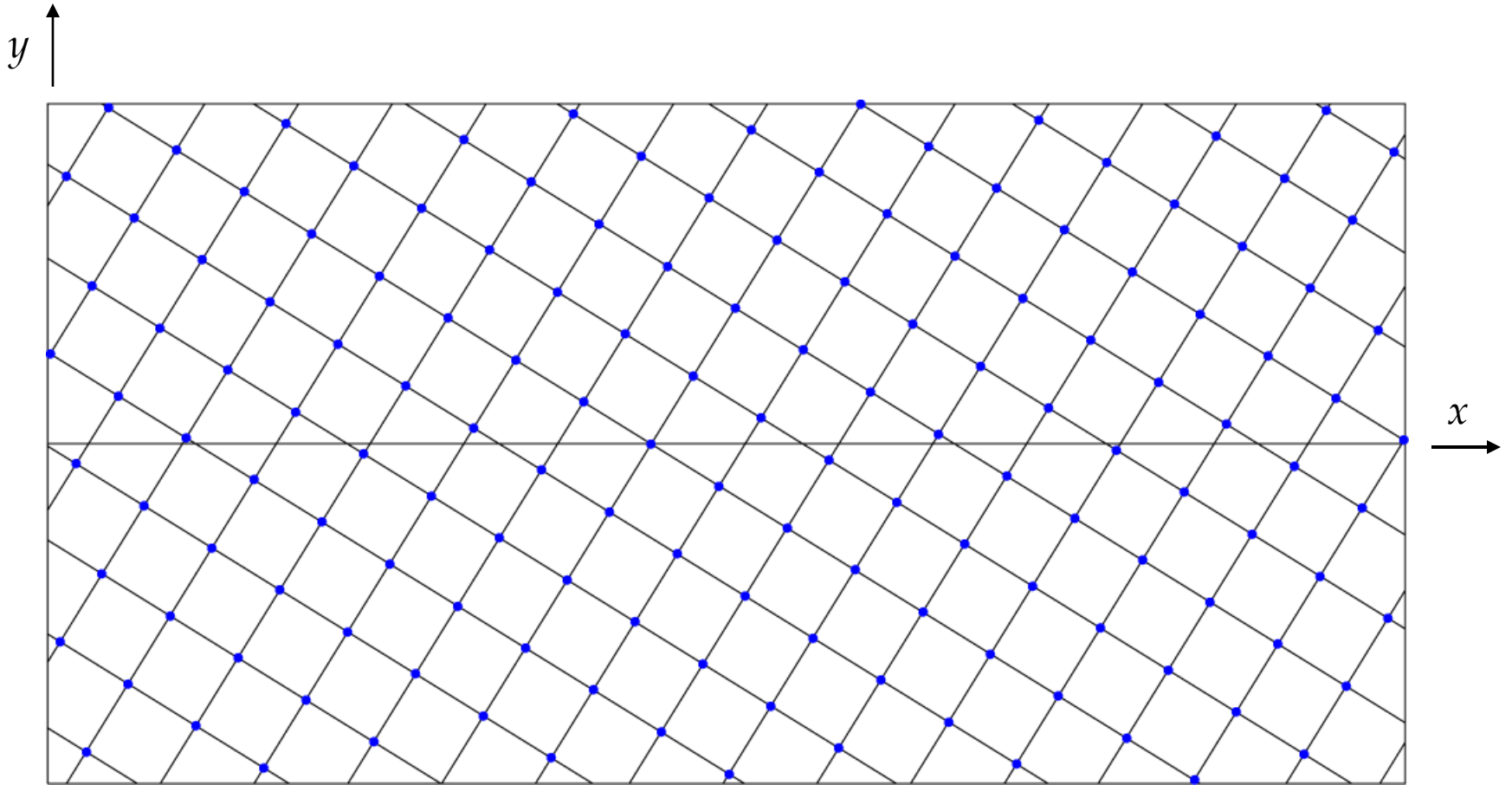


## **3. Methods of construction**

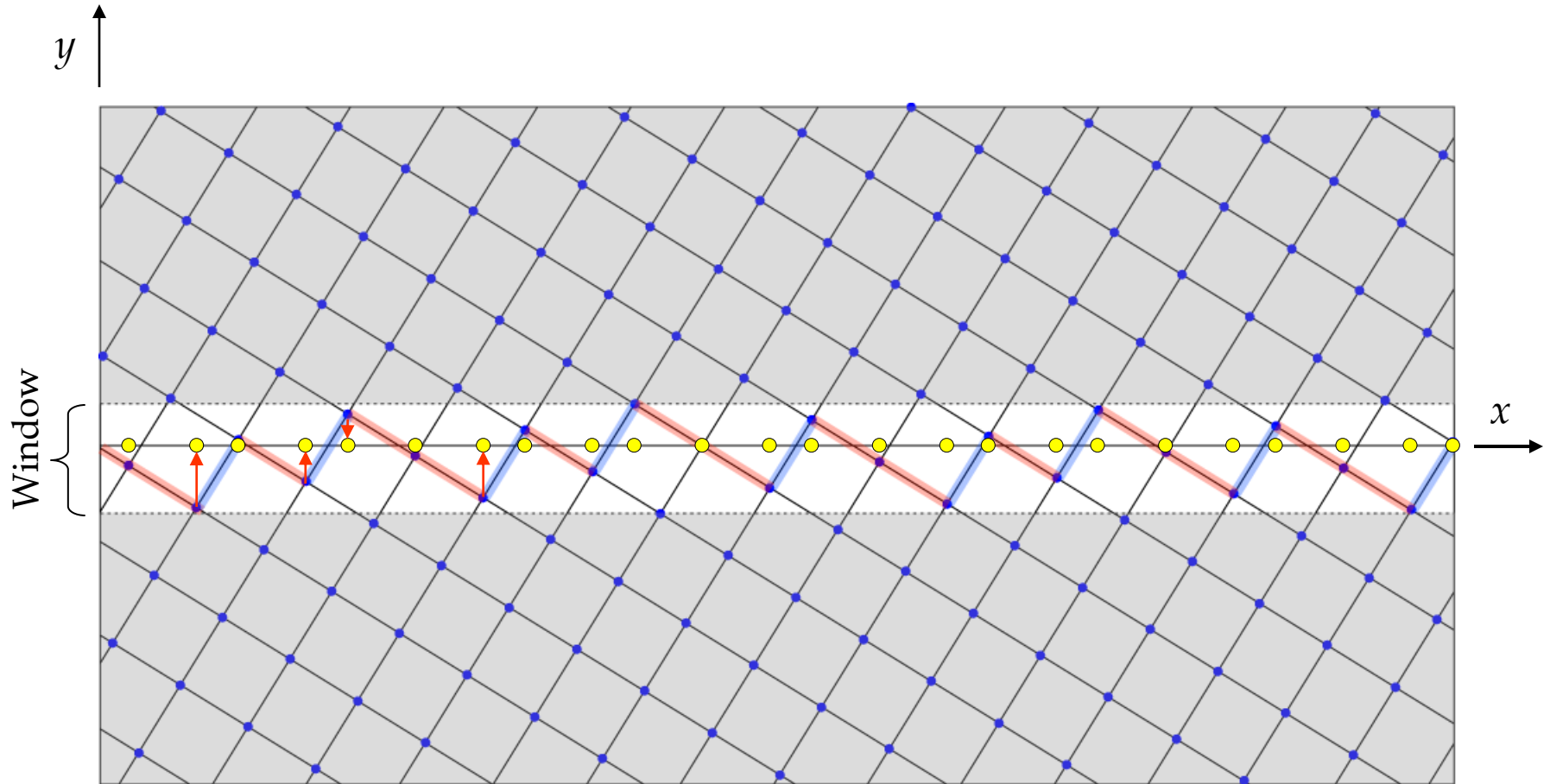


# Methods of construction

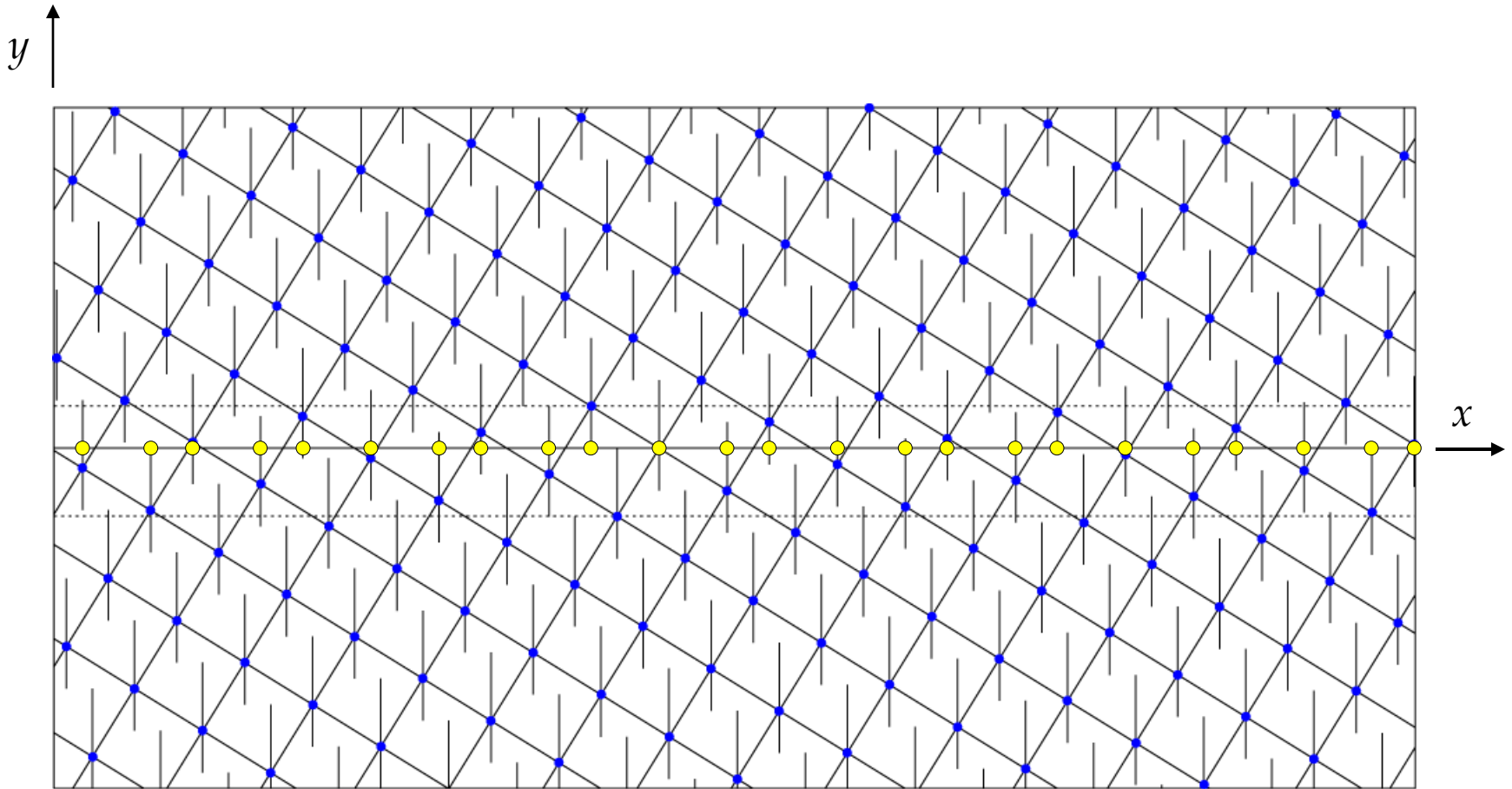




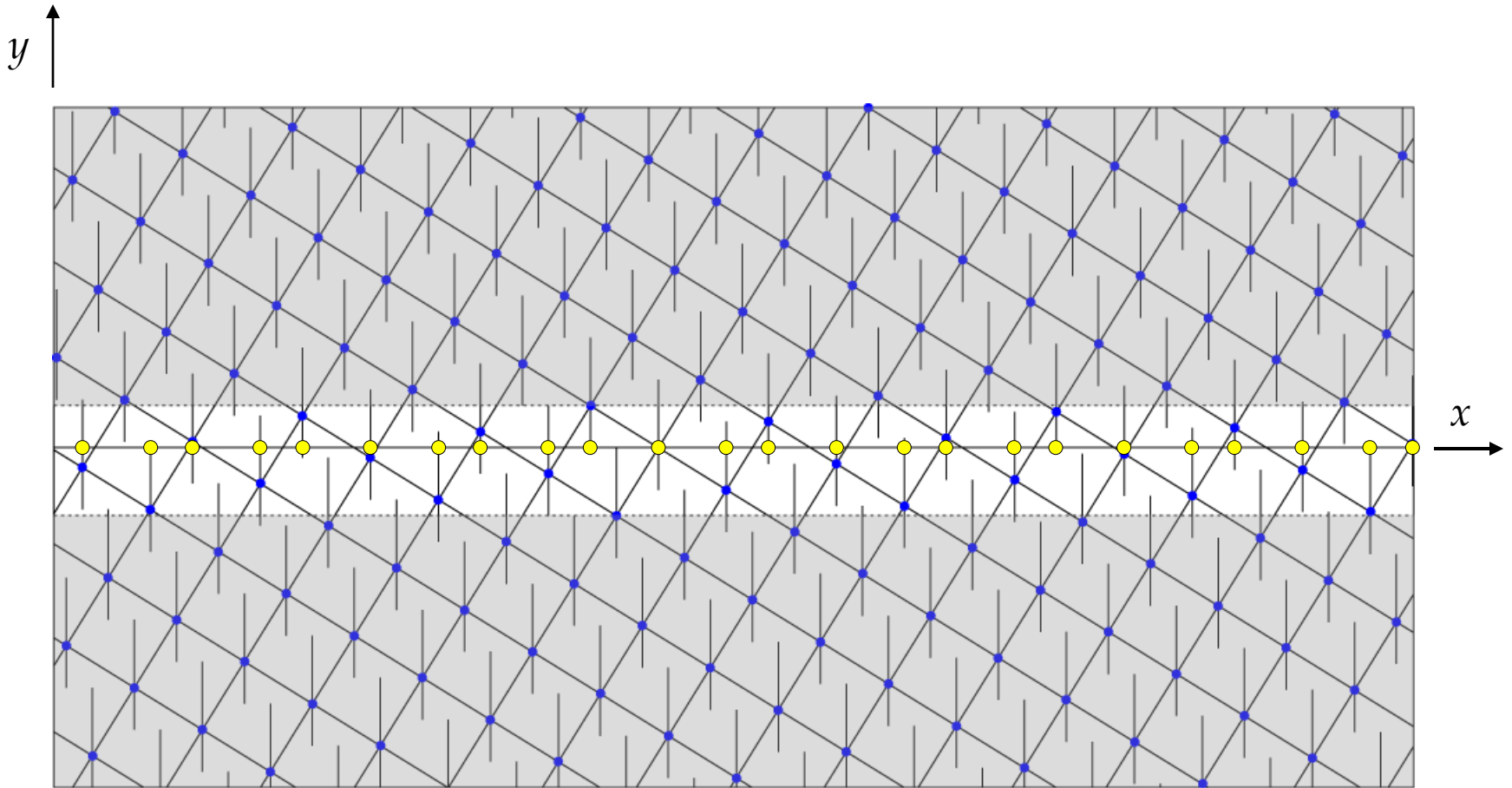
The  $D$ -dimensional physical space is embedded in an  $N$ -dimensional hyperspace, in which a periodic lattice is defined. Since the slope of the physical space relative to the lattice planes is incommensurate, the embedding lacks any periodicity.



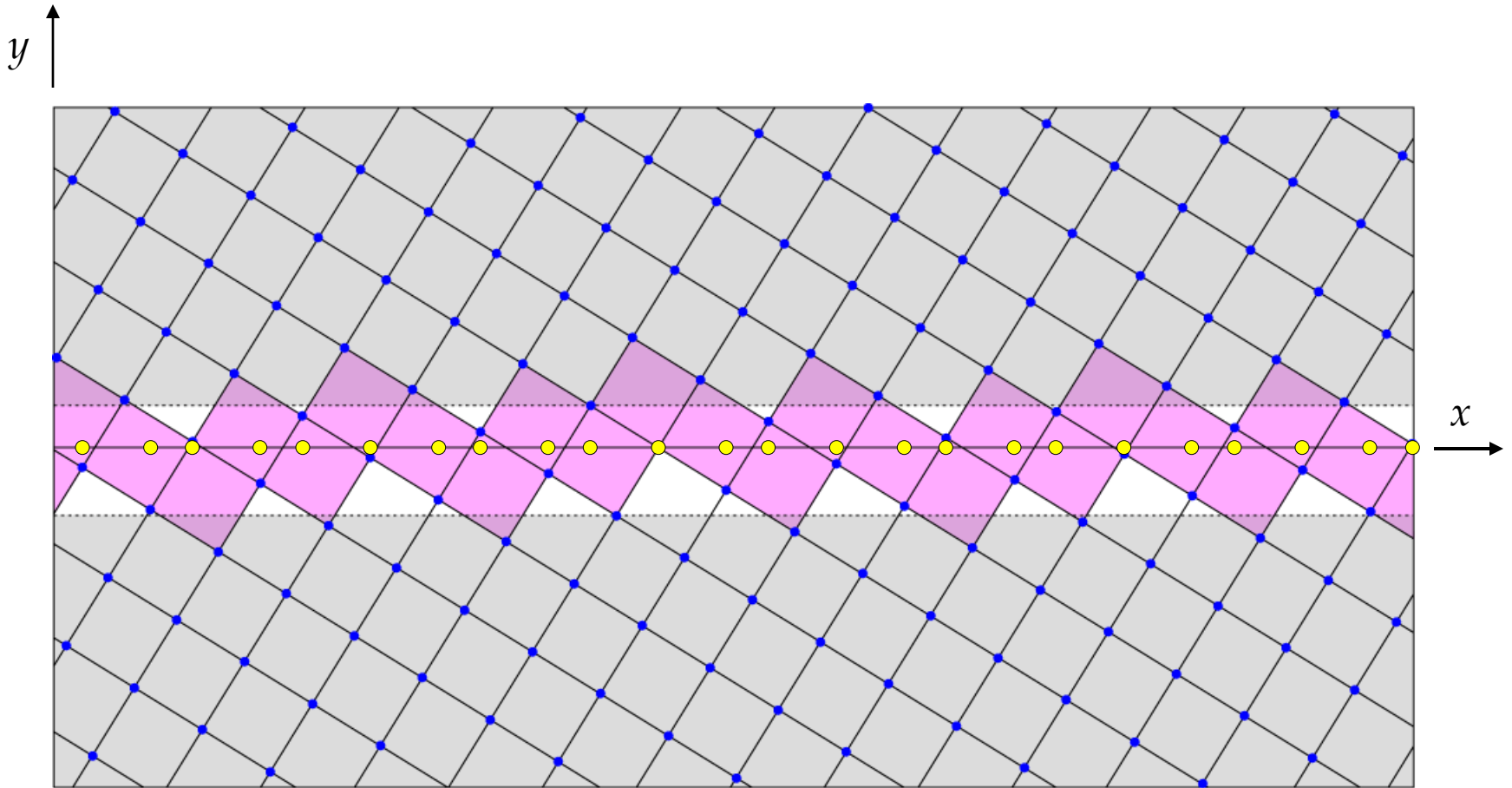
A strip along the physical space is drawn (white part). The cross section of the strip (window) is given by the projection of a unit cell (square) onto the internal space. The Fibonacci chain is obtained by projecting the points within the strip down to the physical space (x-axis). This is an easy-to-grasp way to construct aperiodic tilings, called the *cut-and-projection method*.



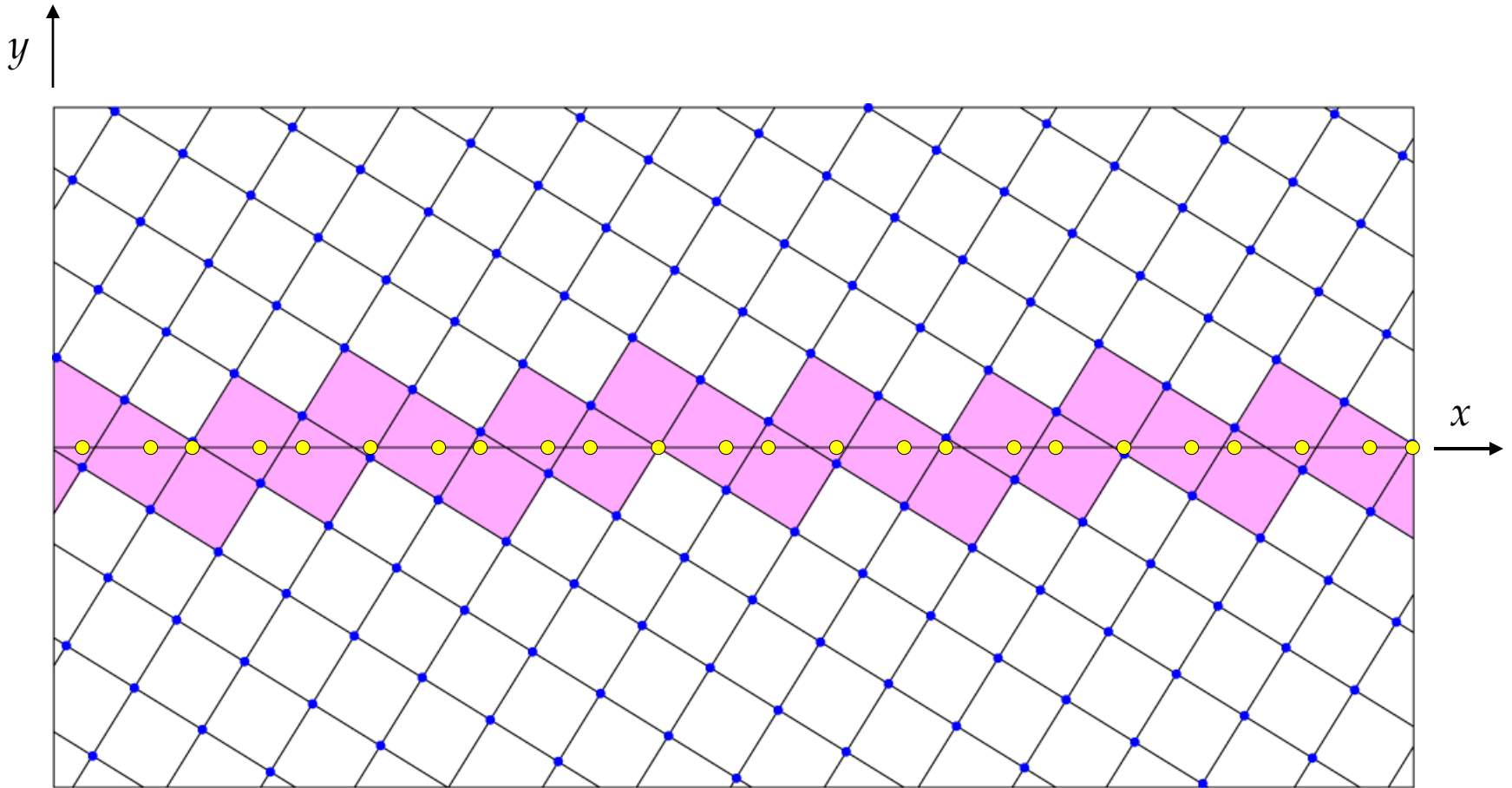
Here, we show the *section method*, in which the projected figure of each square down to the internal space (a line segment) is attached to the base point of the relevant square. The projected figure is called the *atomic surface*. Then the points in the physical space can be obtained as a section through the periodic arrangements of the atomic surfaces along the physical space.



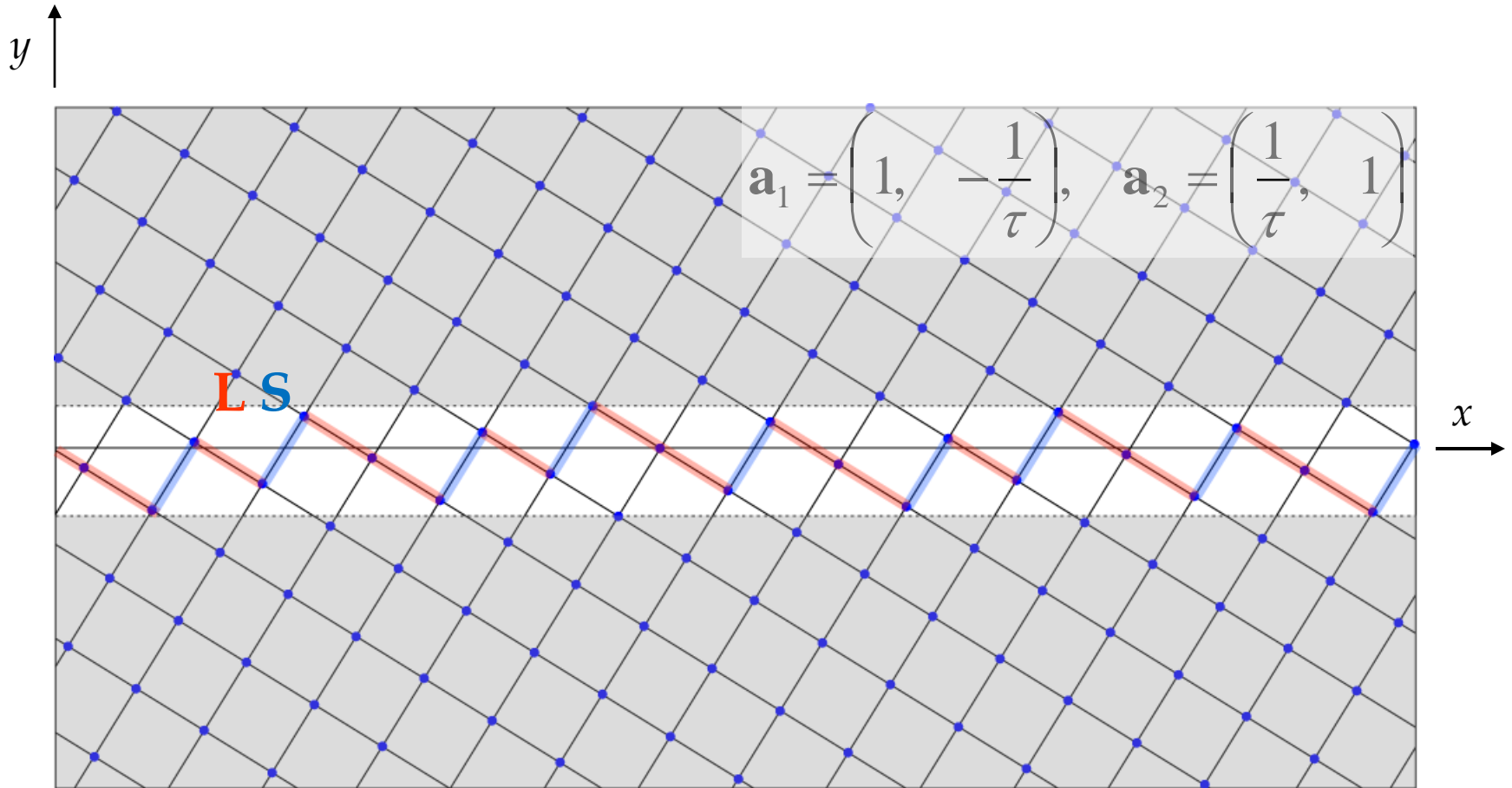
It is very easy to check that the point set obtained by the section method is equivalent to the one obtained by projecting the points within the strip, whose cross section is congruent with the atomic surface. It is easy to see that an atomic surface has an intersection with the physical space if and only if the corresponding lattice point is within the strip.



Here is yet another way to look at the hyperspace scheme. In the above figure, one can recognize that a lattice point lies within the strip if and only if the relevant square has an intersection with the physical space. All the squares which are intersected with the  $x$ -axis are colored in red.



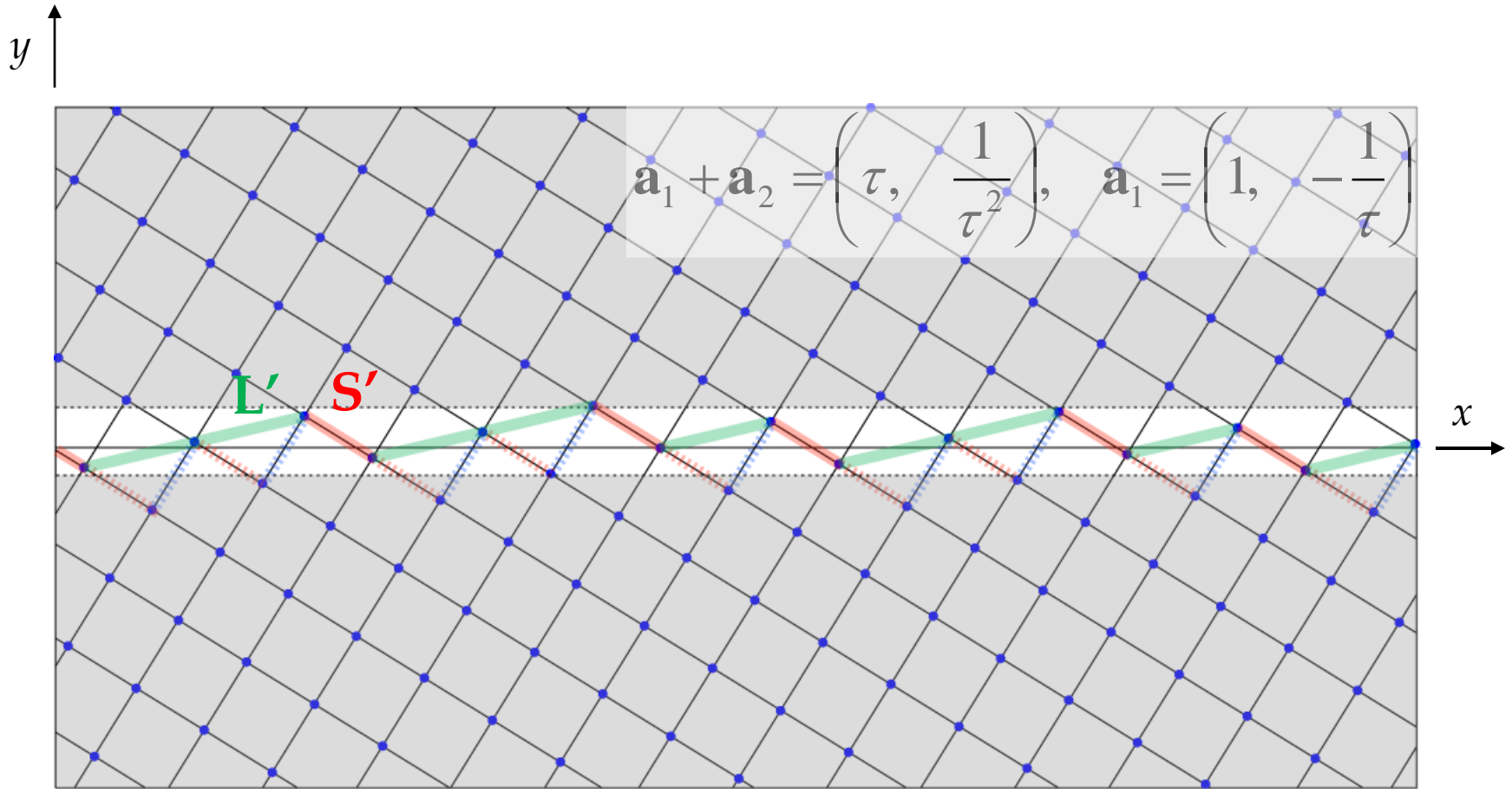
If we forget about the window or atomic surface, it looks like a barbecue skewer (yakitori stick) penetrating pieces of meat. If the base points of the pieces of meat are projected down to the physical space, we get the aperiodic tiling. This is the basic idea underlying the *dual-grid method*.



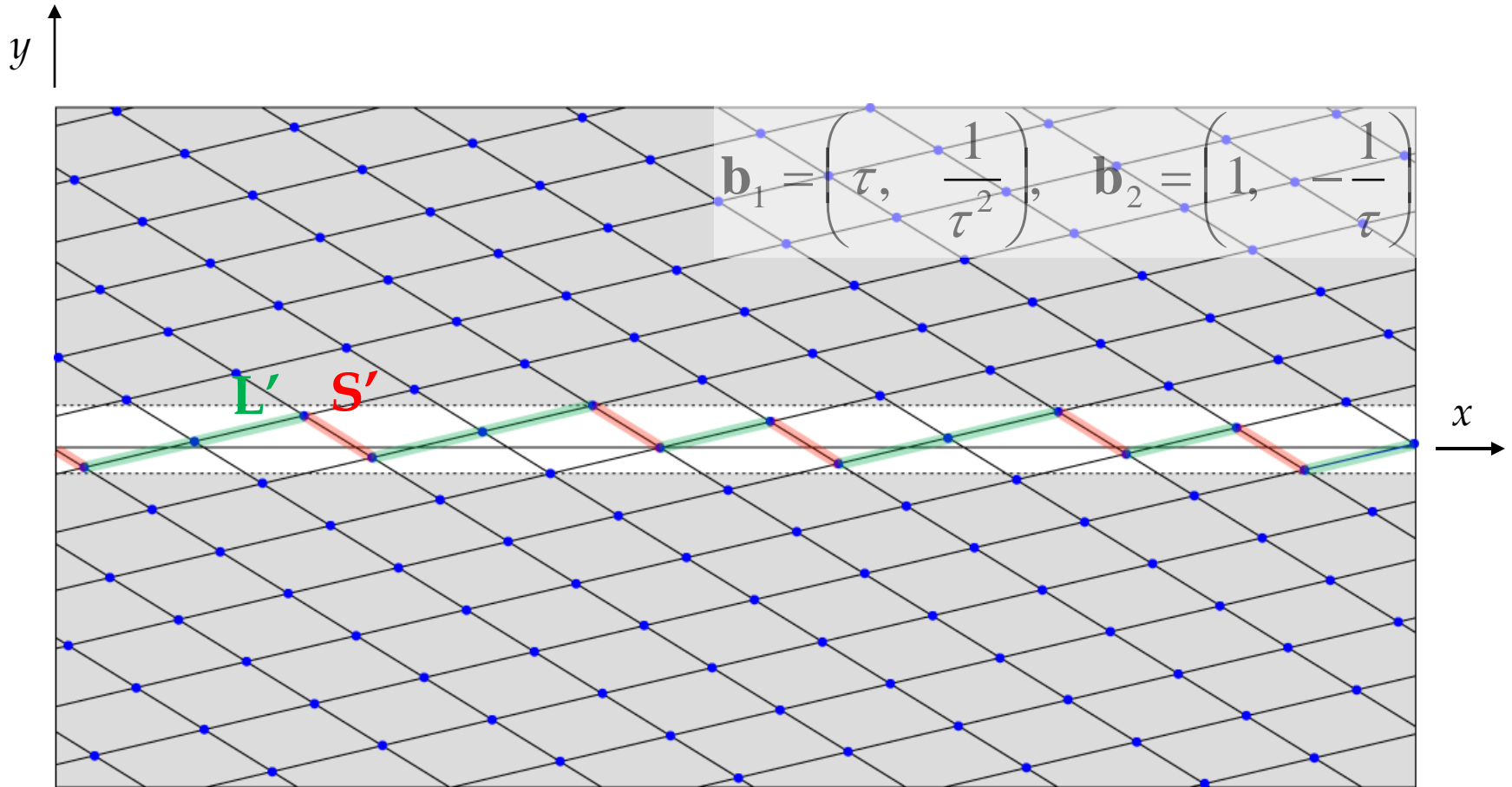
Let's see how the cut-and-projection method is connected with the substitution rule. To identify an  $L'S$  pair with an  $L'$ , we need to remove the vertex between  $L$  and  $S$ . This is achieved by narrowing the window by a certain amount.

$$\left\{ \begin{array}{l} L' = LS \\ S' = L \end{array} \right.$$

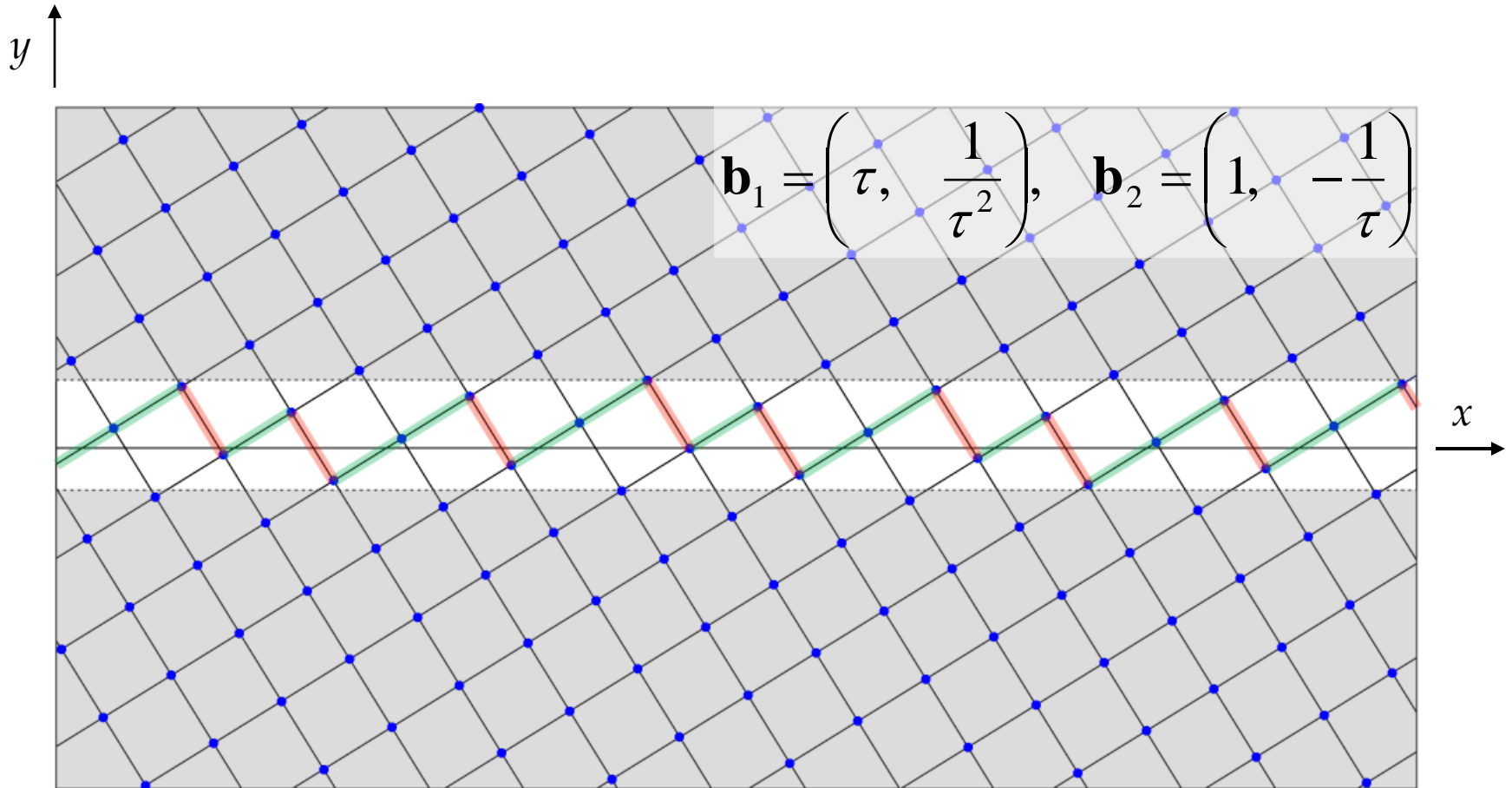




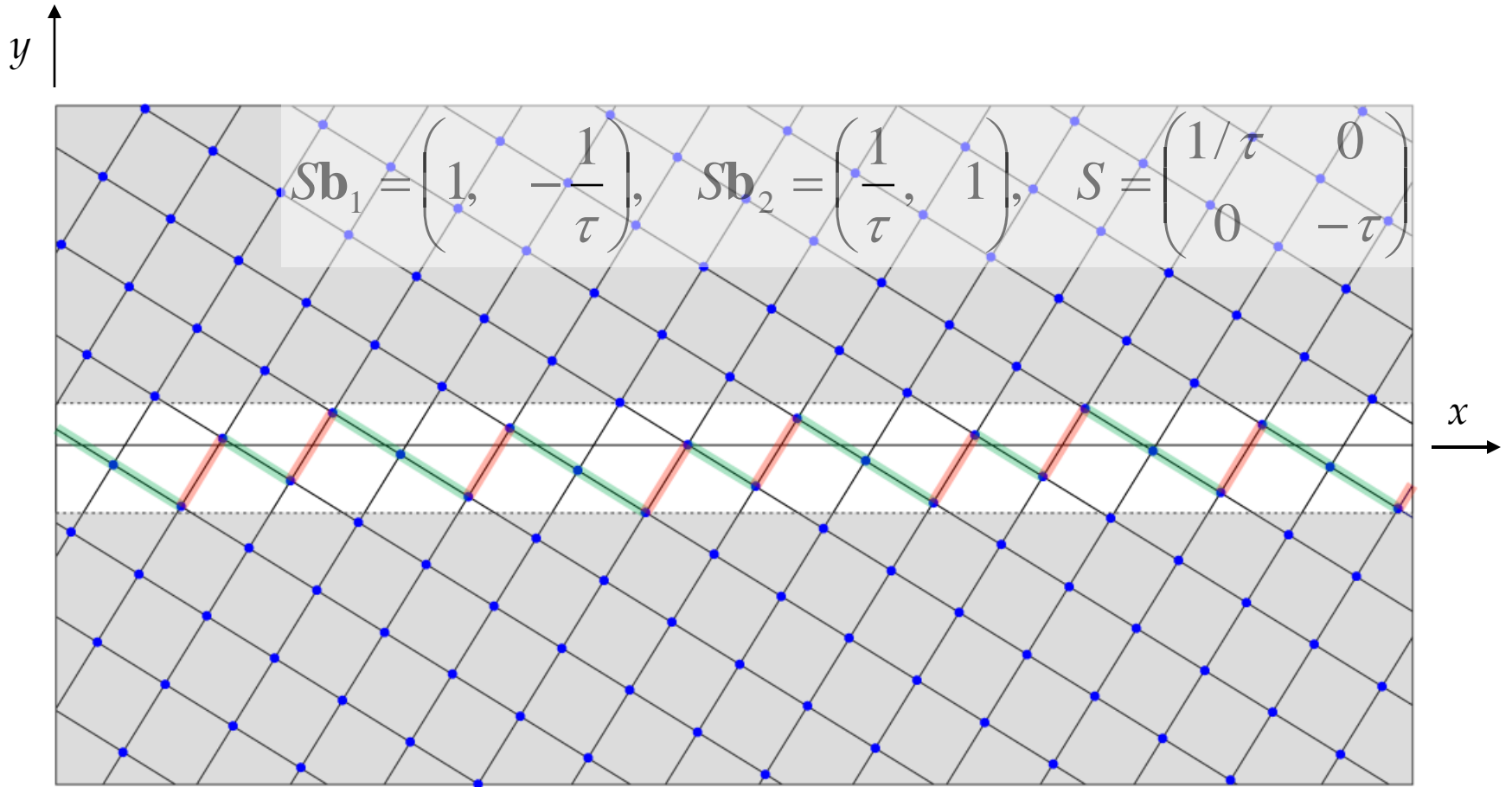
Here, the window is reduced by a factor of  $1/\tau$ , where  $\tau$  is the golden mean. The  $L'$  tiles are shown by green color. Note that the tile does not correspond to the projection of an edge of the square unit cell.



However, if we remember that unit cell can also be taken as a parallelogram, the new tile will be the projection of an edge of a parallelogram. Now we will change the scale of  $x$  and  $y$  by  $1/\tau$  and  $\tau$ , respectively.

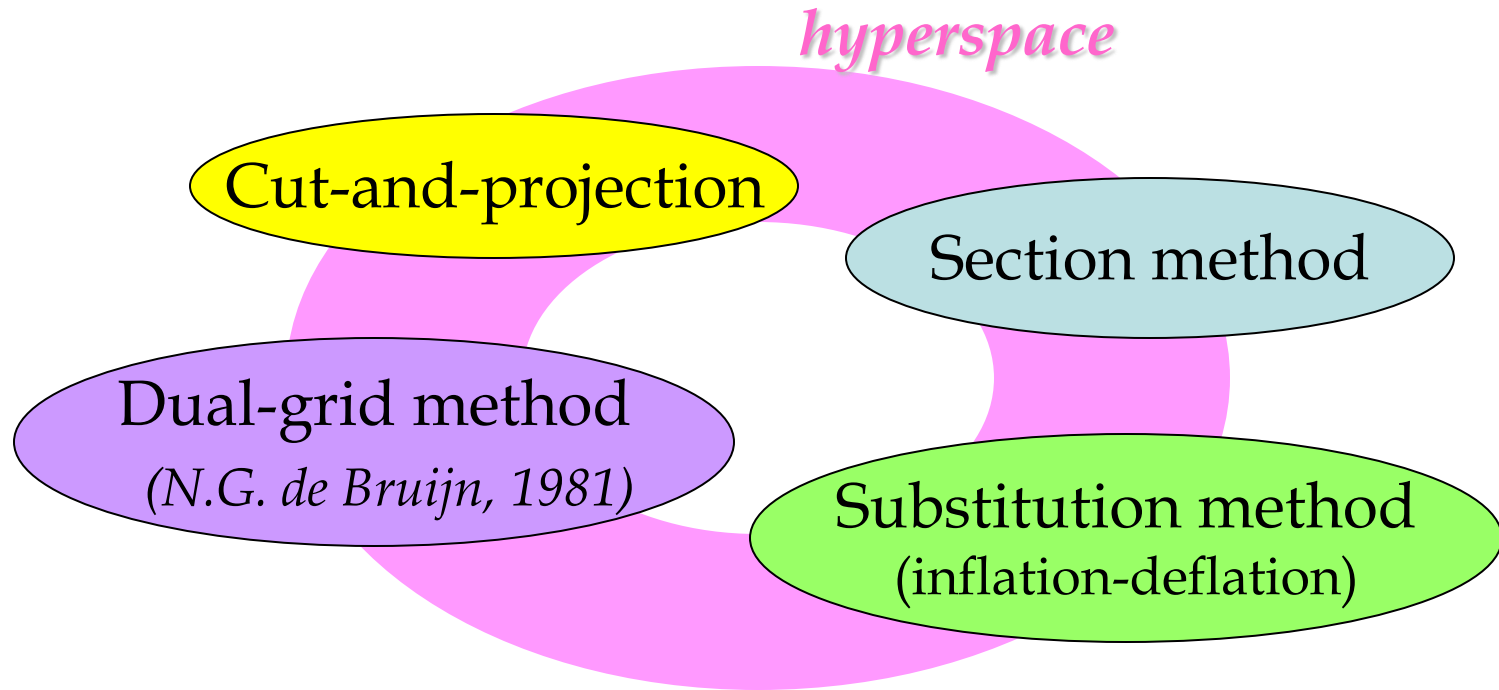


Then what happens is that the parallelogram will turn to a square again. In fact we need to reverse the sign of  $y$  in order to fully recover the square lattice in the same orientation.

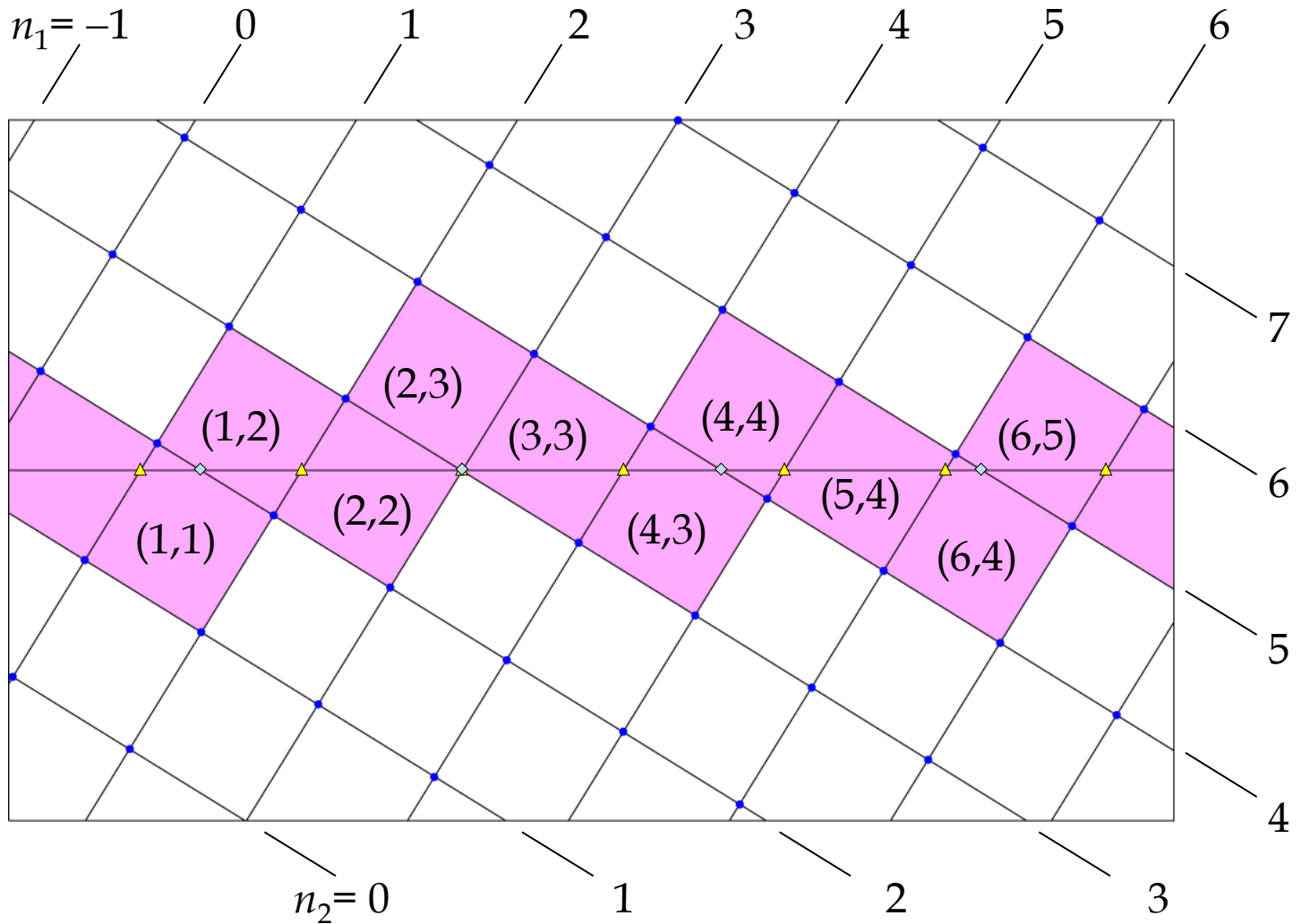


Now, we have seen that even the self-similarity and the substitution rule of the Fibonacci lattice can be explained within the framework of hyper-space geometry.

# Methods of construction



# Dual-grid method for the Fibonacci chain



# Dual-grid method for the Fibonacci chain

Two sets of grids in the hyper space:

$$n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$$

... lattice point

$$(n_1 + s_1) \mathbf{a}_1 + \theta \mathbf{a}_2 \quad (-\infty < \theta < \infty)$$

... grid lines 1

$$\theta \mathbf{a}_1 + (n_2 + s_2) \mathbf{a}_2 \quad (-\infty < \theta < \infty)$$

... grid lines 2

$$s_1, s_2$$

... shift parameters

$$\mathbf{a}_1 = \begin{pmatrix} 1 & -\frac{1}{\tau} \end{pmatrix}$$

$$\mathbf{a}_2 = \begin{pmatrix} \frac{1}{\tau} & 1 \end{pmatrix}$$

Two sets of grids in the physical space:

$$(n_1 + s_1) \mathbf{a}_1 + \theta \mathbf{a}_2 = (x, 0)$$

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

... grid points 1 

$$\theta \mathbf{a}_1 + (n_2 + s_2) \mathbf{a}_2 = (x, 0)$$

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

... grid points 2 

# Dual-grid method for the Fibonacci chain

Indices for the two unit cells on both sides of a grid point

$$\text{(for grid points 1) } x = (2 - 1/\tau) (n_1 + s_1), \theta = 1/\tau (n_1 + s_1)$$

$$n_2 = \theta - \text{Frac}[\theta]$$

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

$$\text{(for grid points 2) } x = (1 + 2/\tau) (n_2 + s_2), \theta = \tau (n_2 + s_2)$$

$$n_1 = \theta - \text{Frac}[\theta]$$

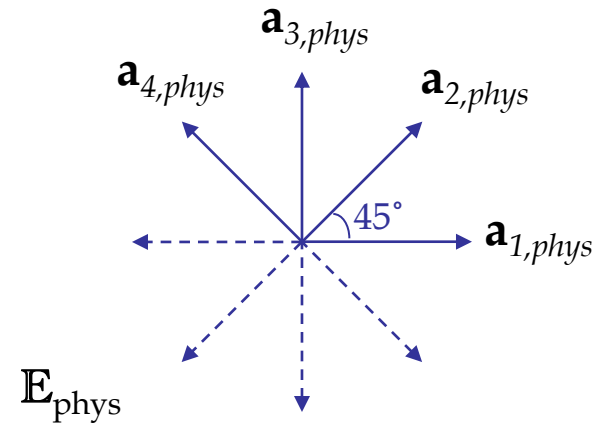
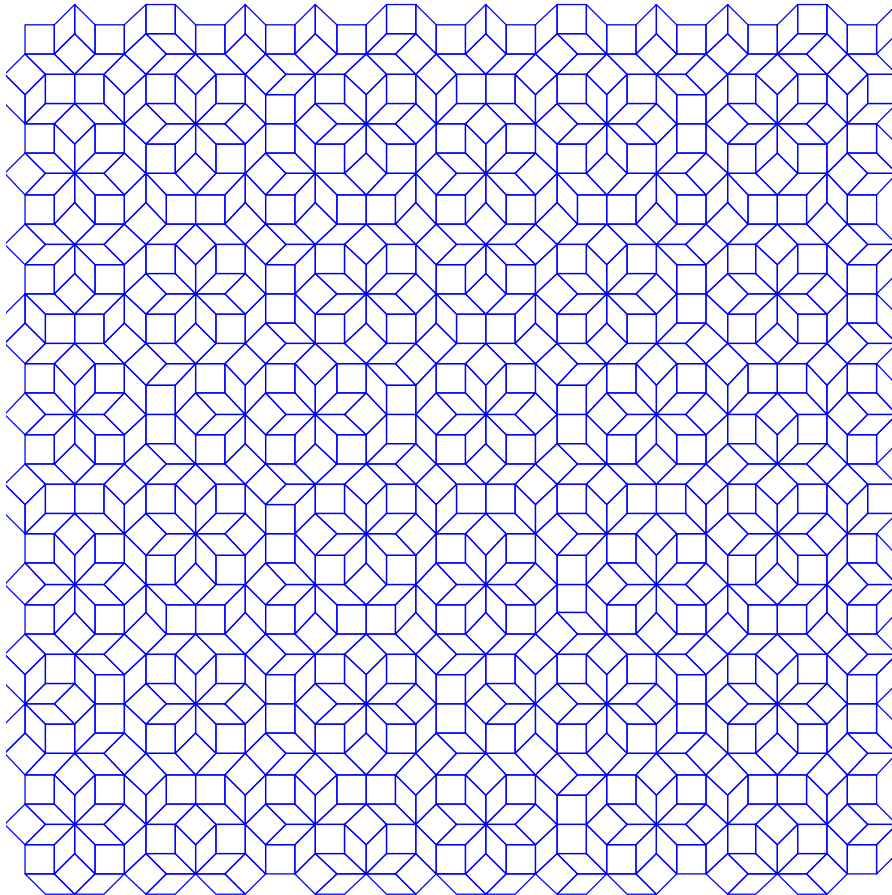
$$(n_1, n_2), (n_1, n_2 - 1) \quad \dots \text{ indices for the squares}$$

Once the indices are obtained, the vertices of the tiling are just the projection of them onto the physical space. Use  $x = n_1 + n_2/\tau$



## **4. Important examples**

# Example 1: Ammann-Beenker tiling (8mm)



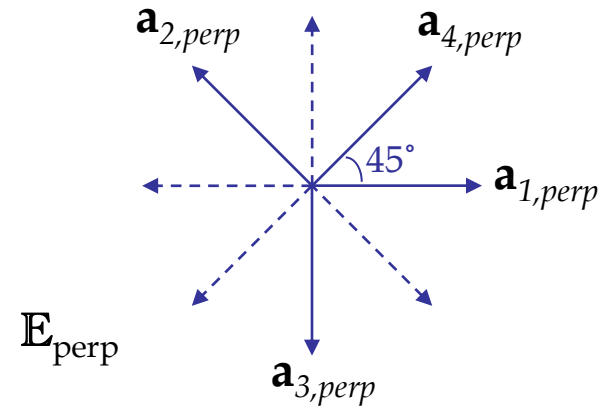
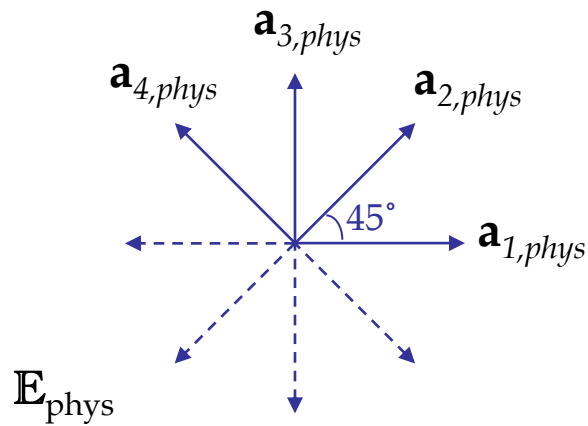
Embedding dimension = 4

$$\{(x, y, z, u)\} = \{(x, y)\} \oplus \{(z, u)\}$$

*hyperspace*      *physical*      *perpendicular*  
*space*       $\mathbb{E}_{\text{phys}}$       *space*       $\mathbb{E}_{\text{perp}}$

$$\mathbf{a}_j = (\cos(\phi_j), \sin(\phi_j), \cos(3\phi_j), \sin(3\phi_j)), \quad j = 1, 2, 3, 4; \quad \phi_j = \pi(j-1)/4$$

$$\mathbf{a}_i \cdot \mathbf{a}_j = 2\delta_{ij} \quad (4\text{D hypercubic lattice})$$



$\mathbf{L} = \{(n_1+s_1) \mathbf{a}_1 + (n_2+s_2)\mathbf{a}_2 + (n_3+s_3)\mathbf{a}_3 + (n_4+s_4)\mathbf{a}_4\}$  ... hyper-cubic lattice

$$\mathbf{g}_1(n_1) = (n_1 + s_1) \mathbf{a}_1 + \{t_2\mathbf{a}_2 + t_3\mathbf{a}_3 + t_4\mathbf{a}_4\}$$

$$\mathbf{g}_2(n_2) = (n_2 + s_2) \mathbf{a}_2 + \{t_1\mathbf{a}_1 + t_3\mathbf{a}_3 + t_4\mathbf{a}_4\}$$

... hyper grids

$$\mathbf{g}_3(n_3) = (n_3 + s_3) \mathbf{a}_3 + \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + t_4\mathbf{a}_4\}$$

$$\mathbf{g}_4(n_4) = (n_4 + s_4) \mathbf{a}_4 + \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + t_3\mathbf{a}_3\}$$

$$\mathbf{g}_1(n_1) \cap \mathbf{E}_{\text{phys}} = 2(n_1 + s_1) \mathbf{a}_{1,\text{phys}} + \{2 t_3 \mathbf{a}_{3,\text{phys}}\} =: \mathbf{h}_1(n_1)$$

$$\mathbf{g}_2(n_2) \cap \mathbf{E}_{\text{phys}} = 2(n_2 + s_2) \mathbf{a}_{2,\text{phys}} + \{2 t_4 \mathbf{a}_{4,\text{phys}}\} =: \mathbf{h}_2(n_2)$$

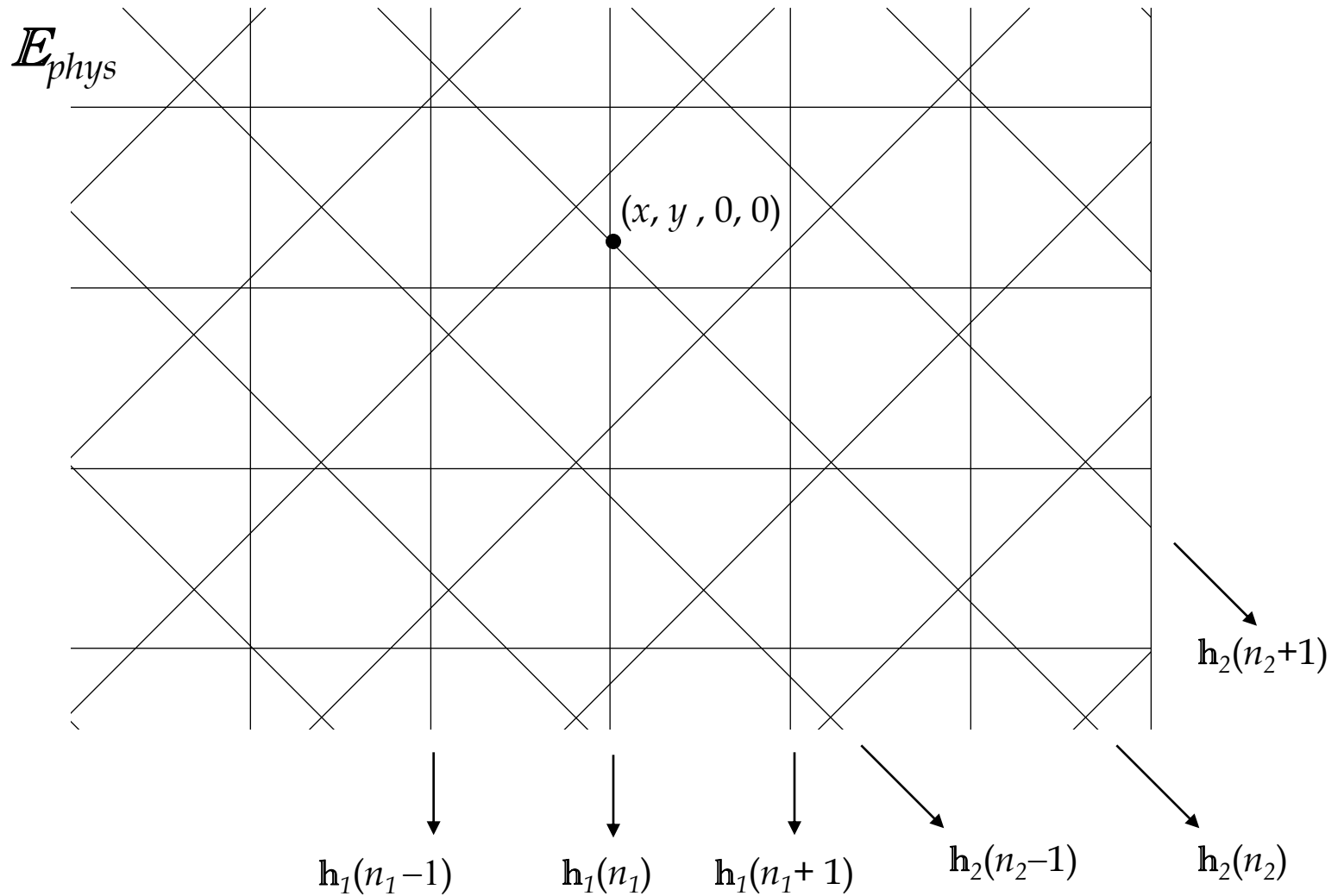
$$\mathbf{g}_3(n_3) \cap \mathbf{E}_{\text{phys}} = 2(n_3 + s_3) \mathbf{a}_{3,\text{phys}} + \{2 t_1 \mathbf{a}_{1,\text{phys}}\} =: \mathbf{h}_3(n_3)$$

$$\mathbf{g}_4(n_4) \cap \mathbf{E}_{\text{phys}} = 2(n_4 + s_4) \mathbf{a}_{4,\text{phys}} + \{2 t_2 \mathbf{a}_{2,\text{phys}}\} =: \mathbf{h}_4(n_4)$$

... grids in the physical space (intersection of the hyper grids with the physical space)

$\mathbf{h}_i(n_i) \cap \mathbf{h}_j(n_j)$

... intersection of grid lines (point)



$$(x, y, 0, 0) = (n_1 + s_1) \mathbf{a}_1 + (n_2 + s_2) \mathbf{a}_2 + t_3 \mathbf{a}_3 + t_4 \mathbf{a}_4$$

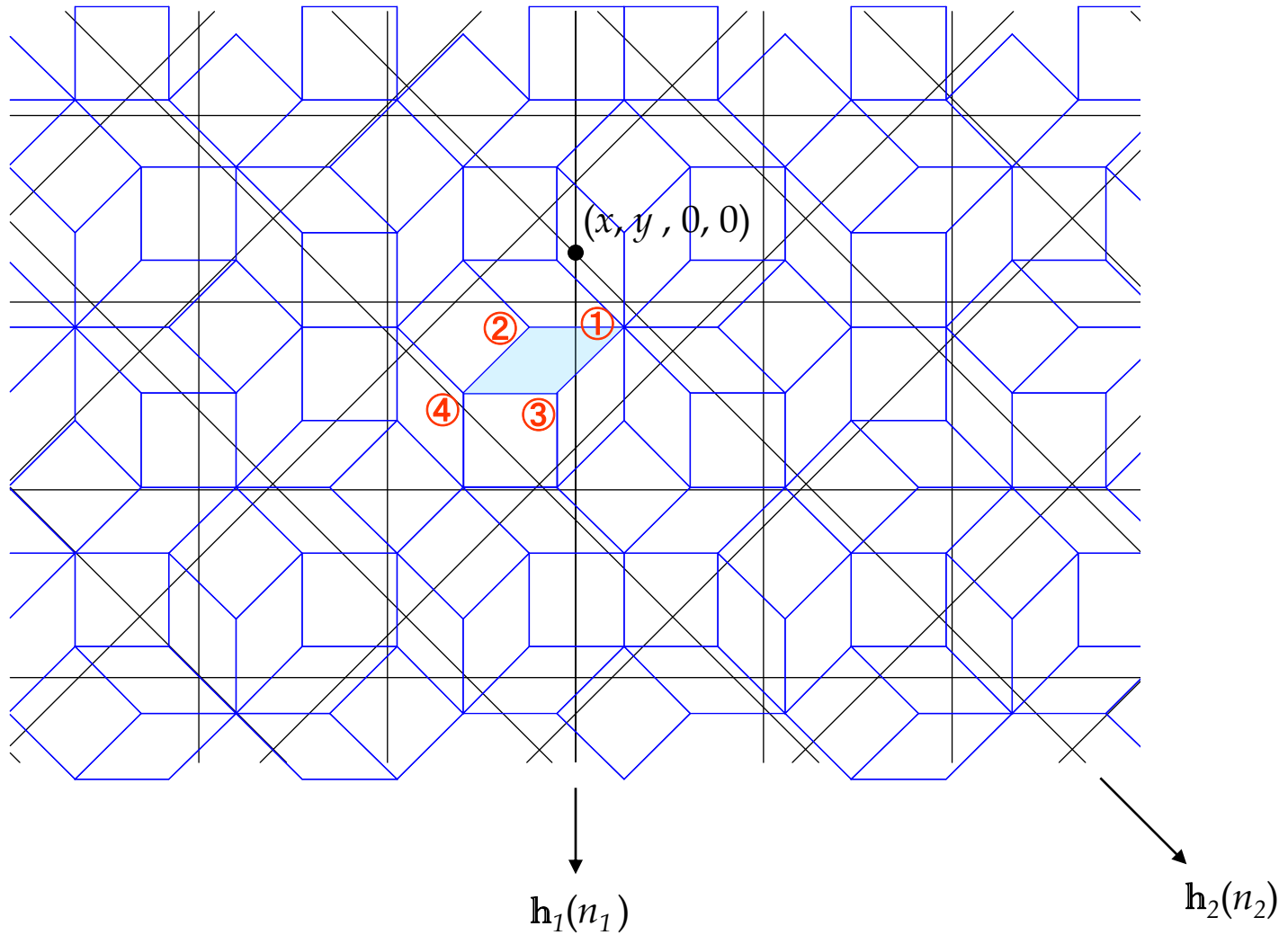
$$\left. \begin{aligned} t_3 &= \mathbf{a}_3^* \cdot (x, y, 0, 0) = n_3 + s_3 + \delta \left( \begin{array}{l} n_3 = [t_3 - s_3], \quad \delta = \text{Frac}(t_3 - s_3) \\ n_4 = [t_4 - s_4], \quad \delta' = \text{Frac}(t_4 - s_4) \\ \mathbf{a}_j^* = 1/2 \mathbf{a}_j \quad (j = 1, 2, 3, 4) \\ \dots \text{ the reciprocal basis vectors} \end{array} \right) \\ t_4 &= \mathbf{a}_4^* \cdot (x, y, 0, 0) = n_4 + s_4 + \delta' \end{aligned} \right\}$$

At the intersection point, the physical space cut through four hypercubic unit cells. The base points of these unit cells are:

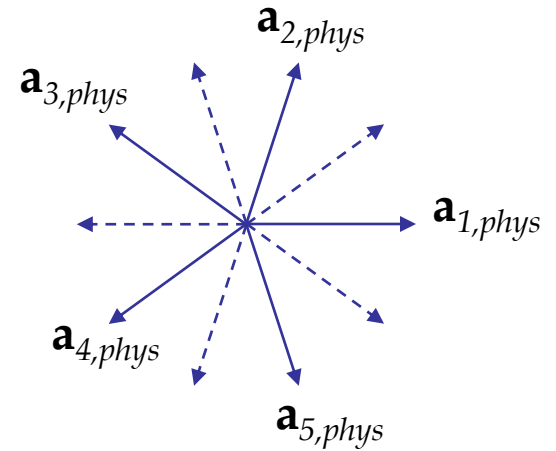
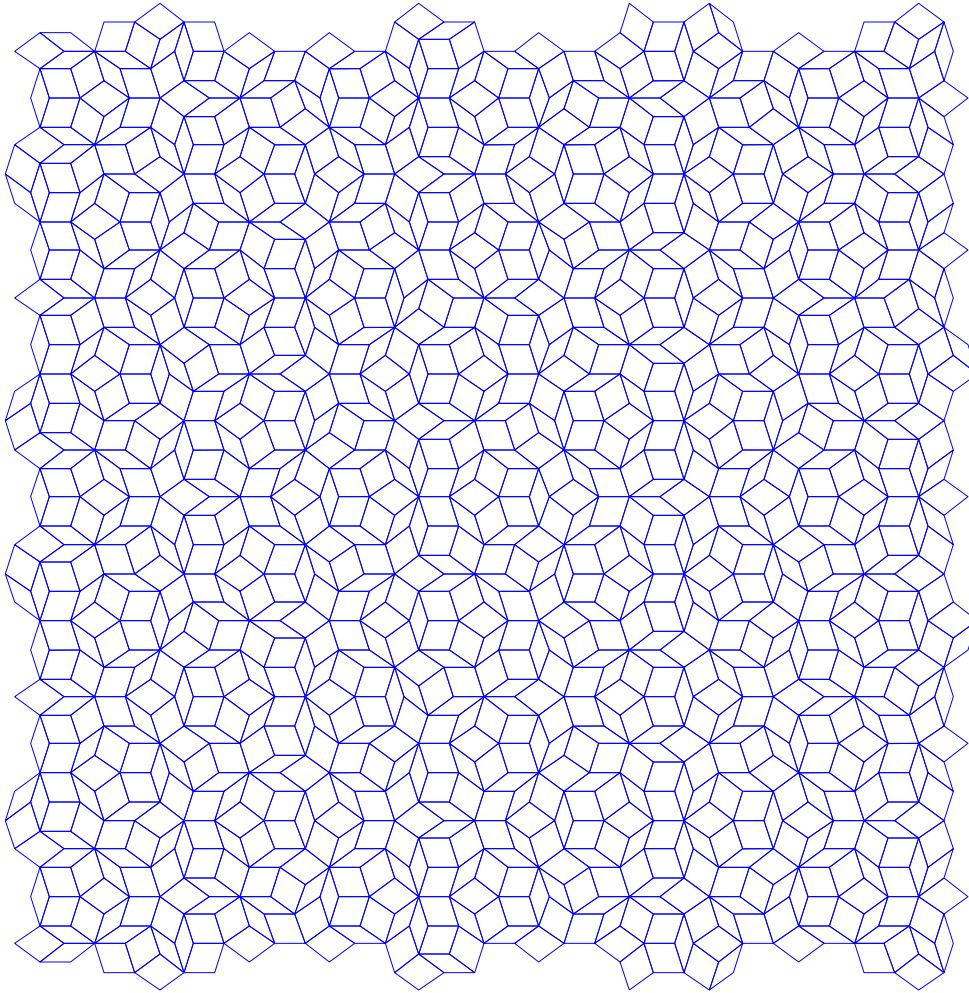
- ①  $(n_1, n_2, n_3, n_4)$
- ②  $(n_1 - 1, n_2, n_3, n_4)$
- ③  $(n_1, n_2 - 1, n_3, n_4)$
- ④  $(n_1 - 1, n_2 - 1, n_3, n_4)$

For general interaction points,  $\mathbf{h}_i(n_i) \cap \mathbf{h}_j(n_j)$ , the relevant four hypercubes are identified in a similar manner; for  $k \neq i, j$ .

# Ammann-Beenker tiling (8mm)



## Example 2: Rhombic Penrose tiling (10mm)



$\mathbf{E}_{\text{phys}}$

Embedding dimension = 5

$$\{(x, y, z, u, v)\} = \{(x, y)\} \oplus \{(z, u, v)\}$$

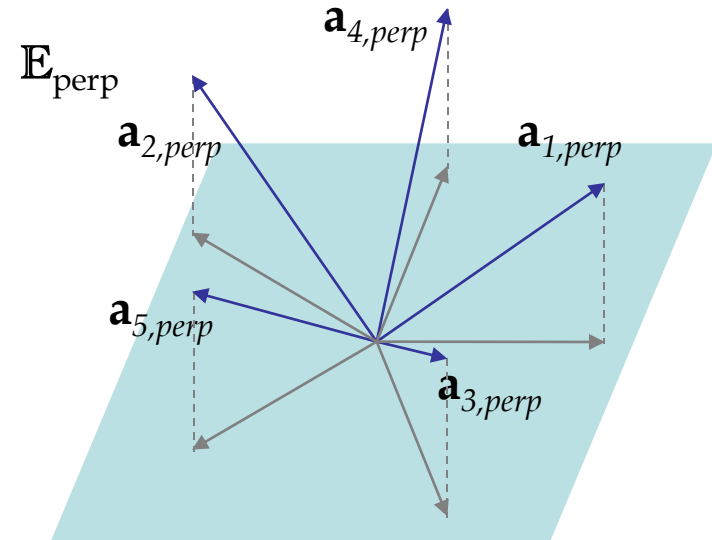
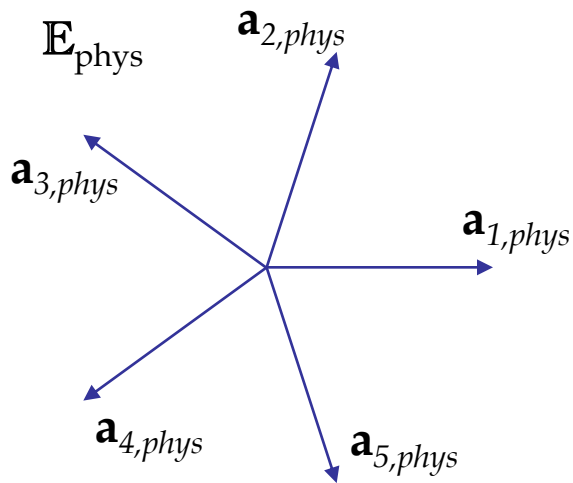
*hyperspace*      *physical*      *perpendicular*  
*space*       $\mathbf{E}_{\text{phys}}$       *space*       $\mathbf{E}_{\text{perp}}$



$$\mathbf{a}_j = \sqrt{2/5} \left( \cos \phi_j, \sin \phi_j, \cos 2\phi_j, \sin 2\phi_j, \sqrt{1/2} \right),$$

$$j = 1, 2, 3, 4, 5 ; \phi_j = 2\pi(j-1)/5$$

$$\mathbf{a}_i \cdot \mathbf{a}_j = \delta_{ij} \quad (5\text{D hyper-cubic lattice})$$



$$\mathbf{L} = \{(n_1+s_1)\mathbf{a}_1 + (n_2+s_2)\mathbf{a}_2 + (n_3+s_3)\mathbf{a}_3 + (n_4+s_4)\mathbf{a}_4 + (n_5+s_5)\mathbf{a}_5\}$$

... hyper-cubic lattice

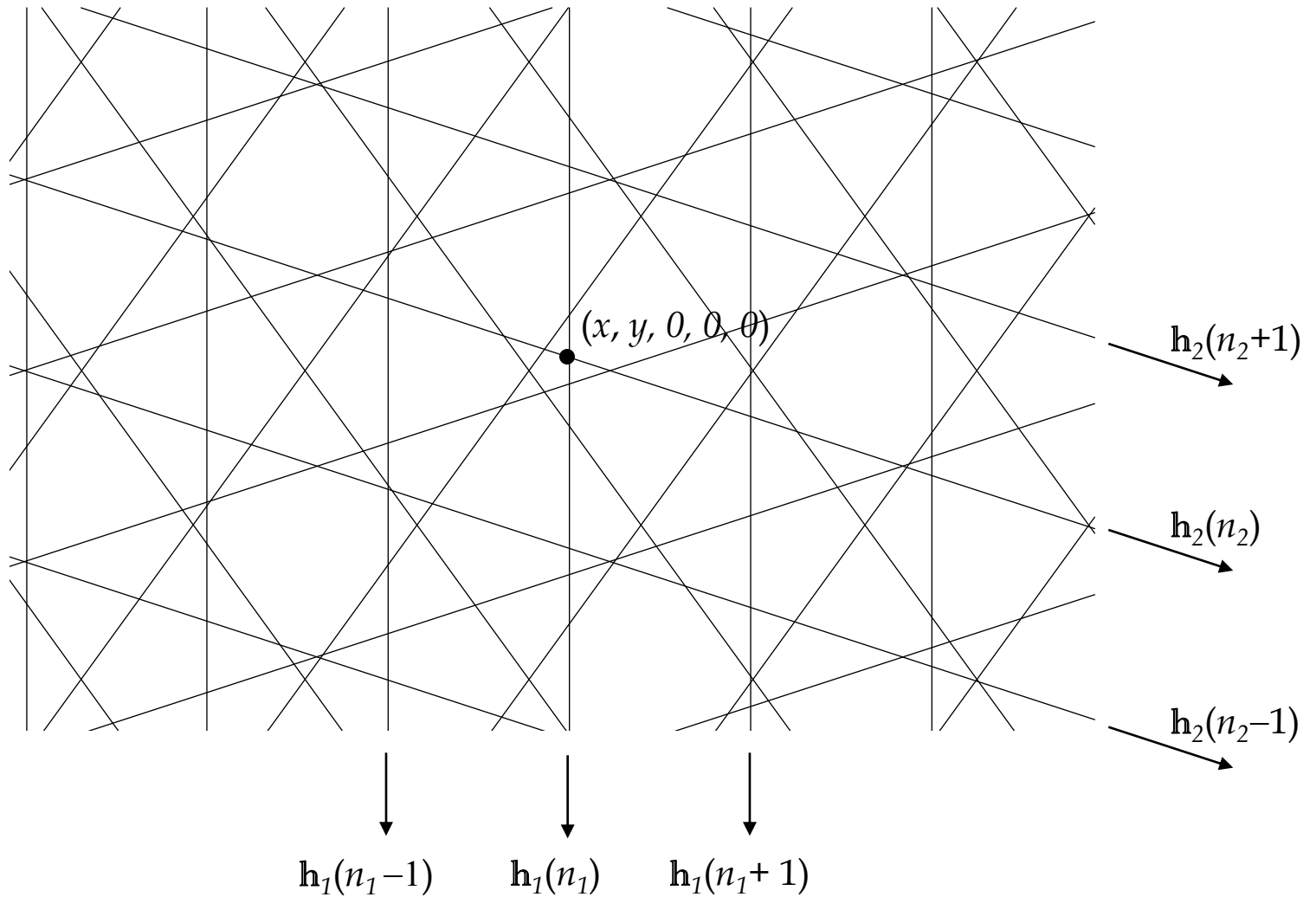
$$\begin{aligned} \mathbf{g}_1(n_1) &= (n_1 + s_1) \mathbf{a}_1 + \{t_2\mathbf{a}_2 + t_3\mathbf{a}_3 + t_4\mathbf{a}_4 + t_5\mathbf{a}_5\} \\ \mathbf{g}_2(n_2) &= (n_2 + s_2) \mathbf{a}_2 + \{t_1\mathbf{a}_1 + t_3\mathbf{a}_3 + t_4\mathbf{a}_4 + t_5\mathbf{a}_5\} \\ \mathbf{g}_3(n_3) &= (n_3 + s_3) \mathbf{a}_3 + \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + t_4\mathbf{a}_4 + t_5\mathbf{a}_5\} \\ \mathbf{g}_4(n_4) &= (n_4 + s_4) \mathbf{a}_4 + \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + t_3\mathbf{a}_3 + t_5\mathbf{a}_5\} \\ \mathbf{g}_5(n_5) &= (n_5 + s_5) \mathbf{a}_5 + \{t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + t_3\mathbf{a}_3 + t_4\mathbf{a}_4\} \end{aligned}$$

... hyper grids in 5D

$$\begin{aligned} \mathbf{g}_1(n_1) \cap \mathbf{E}_{\text{phys}} &= 5/2(n_1 + s_1) \mathbf{a}_{1,\text{phys}} + \{t(\mathbf{a}_{2,\text{phys}} - \mathbf{a}_{5,\text{phys}})\} =: \mathbf{h}_1(n_1) \\ \mathbf{g}_2(n_2) \cap \mathbf{E}_{\text{phys}} &= 5/2(n_2 + s_2) \mathbf{a}_{2,\text{phys}} + \{t(\mathbf{a}_{3,\text{phys}} - \mathbf{a}_{1,\text{phys}})\} =: \mathbf{h}_2(n_2) \\ \mathbf{g}_3(n_3) \cap \mathbf{E}_{\text{phys}} &= 5/2(n_3 + s_3) \mathbf{a}_{3,\text{phys}} + \{t(\mathbf{a}_{4,\text{phys}} - \mathbf{a}_{2,\text{phys}})\} =: \mathbf{h}_3(n_3) \\ \mathbf{g}_4(n_4) \cap \mathbf{E}_{\text{phys}} &= 5/2(n_4 + s_4) \mathbf{a}_{4,\text{phys}} + \{t(\mathbf{a}_{5,\text{phys}} - \mathbf{a}_{3,\text{phys}})\} =: \mathbf{h}_4(n_4) \\ \mathbf{g}_5(n_5) \cap \mathbf{E}_{\text{phys}} &= 5/2(n_5 + s_5) \mathbf{a}_{5,\text{phys}} + \{t(\mathbf{a}_{1,\text{phys}} - \mathbf{a}_{4,\text{phys}})\} =: \mathbf{h}_5(n_5) \end{aligned}$$

... grids in the physical space (intersection with the physical space)

$\mathbf{h}_i(n_i) \cap \mathbf{h}_j(n_j)$  ... intersection of hyper grids (point)



$$(x, y, 0, 0, 0) = (n_1 + s_1) \mathbf{a}_1 + (n_2 + s_2) \mathbf{a}_2 + t_3 \mathbf{a}_3 + t_4 \mathbf{a}_4 + t_5 \mathbf{a}_5$$

$$t_3 = \mathbf{a}_3^* \cdot (x, y, 0, 0, 0) = n_3 + s_3 + \delta$$

$$t_4 = \mathbf{a}_4^* \cdot (x, y, 0, 0, 0) = n_4 + s_4 + \delta'$$

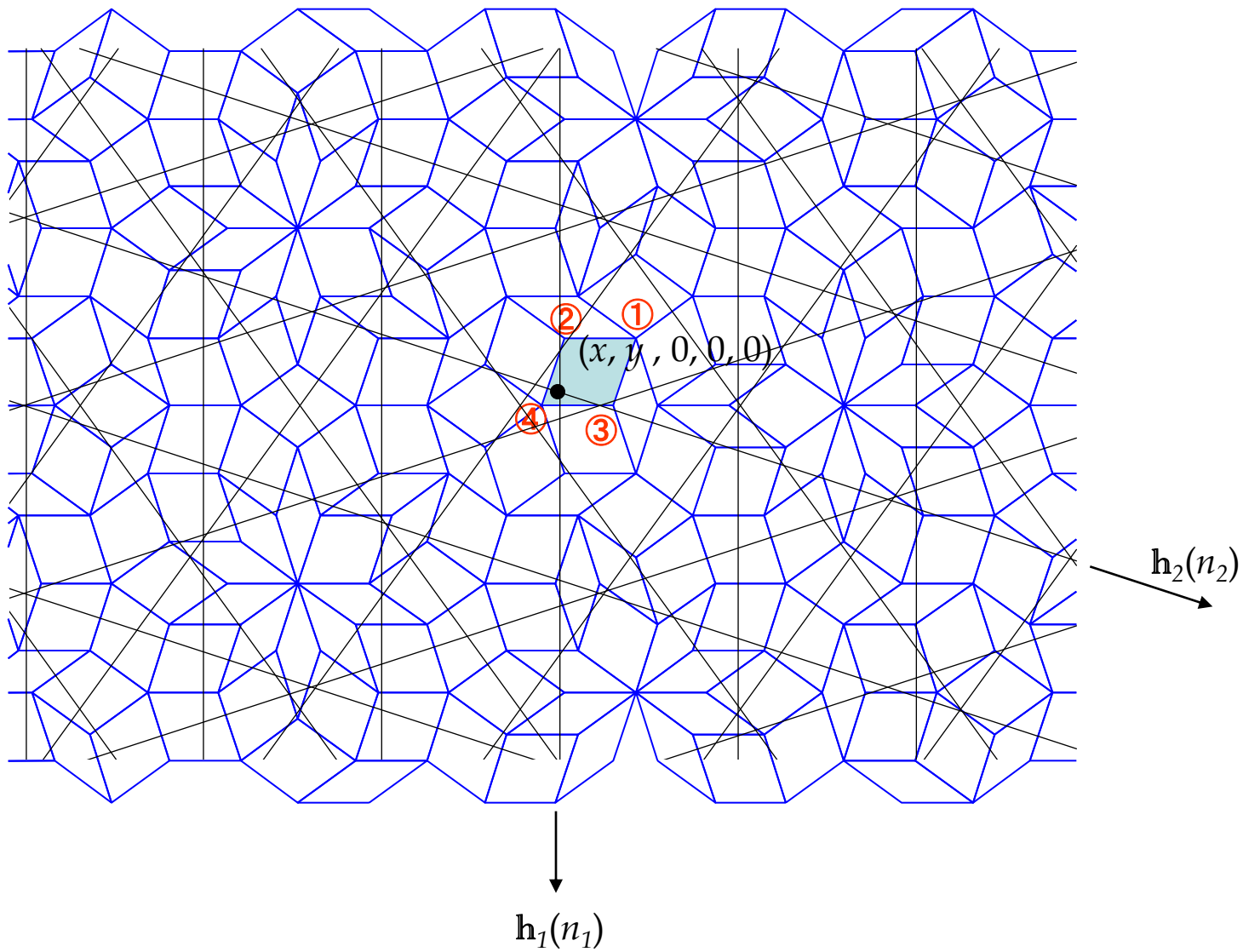
$$t_5 = \mathbf{a}_5^* \cdot (x, y, 0, 0, 0) = n_5 + s_5 + \delta''$$

$$\left( \begin{array}{l} n_3 = [t_3 - s_3], \delta = \text{Frac}(t_3 - s_3) \\ n_4 = [t_4 - s_4], \delta' = \text{Frac}(t_4 - s_4) \\ n_5 = [t_5 - s_5], \delta'' = \text{Frac}(t_5 - s_5) \\ \mathbf{a}_j^* = \mathbf{a}_j \ (j = 1, 2, 3, 4, 5) \\ \dots \text{ the basis vectors of the} \\ \text{reciprocal lattice} \end{array} \right)$$

At the intersection point, the physical space cut through four hypercubic unit cells. The base points of these unit cells are:

- 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  $(n_1 - 1, n_2 - 1, n_3, n_4, n_5)$

For general intersection points,  $\mathbf{h}_i(n_i) \cap \mathbf{h}_j(n_j)$ , the relevant four hypercubes are identified in a similar manner; for  $k \neq i, j$ .



## Summary of Part A

- 1. The hyperspace scheme is the most basic concept for describing aperiodic tilings that are related to quasicrystals.**
- 2. The four techniques for constructing aperiodic tilings are connected with each other through the hyper-space.**
- 3. The dual-grid method is a practical method for constructing the Ammann-Beenker tiling and the rhombic Penrose tiling.**

## Computer programs: drawing quasiperiodic tilings in the plane

PROGRAM 1: 'AmmannBeenker2pov.pl'

PROGRAM 2: 'Penrose2pov.pl'

These programs (written in Perl, approx. 300 lines) generate Ammann-Beenker and rhombic Penrose tilings with the grid method.

To run with Windows, you need ActivePerl (ver 5.12) and Povray (v.3.6) installed on your computer. These can be downloaded from

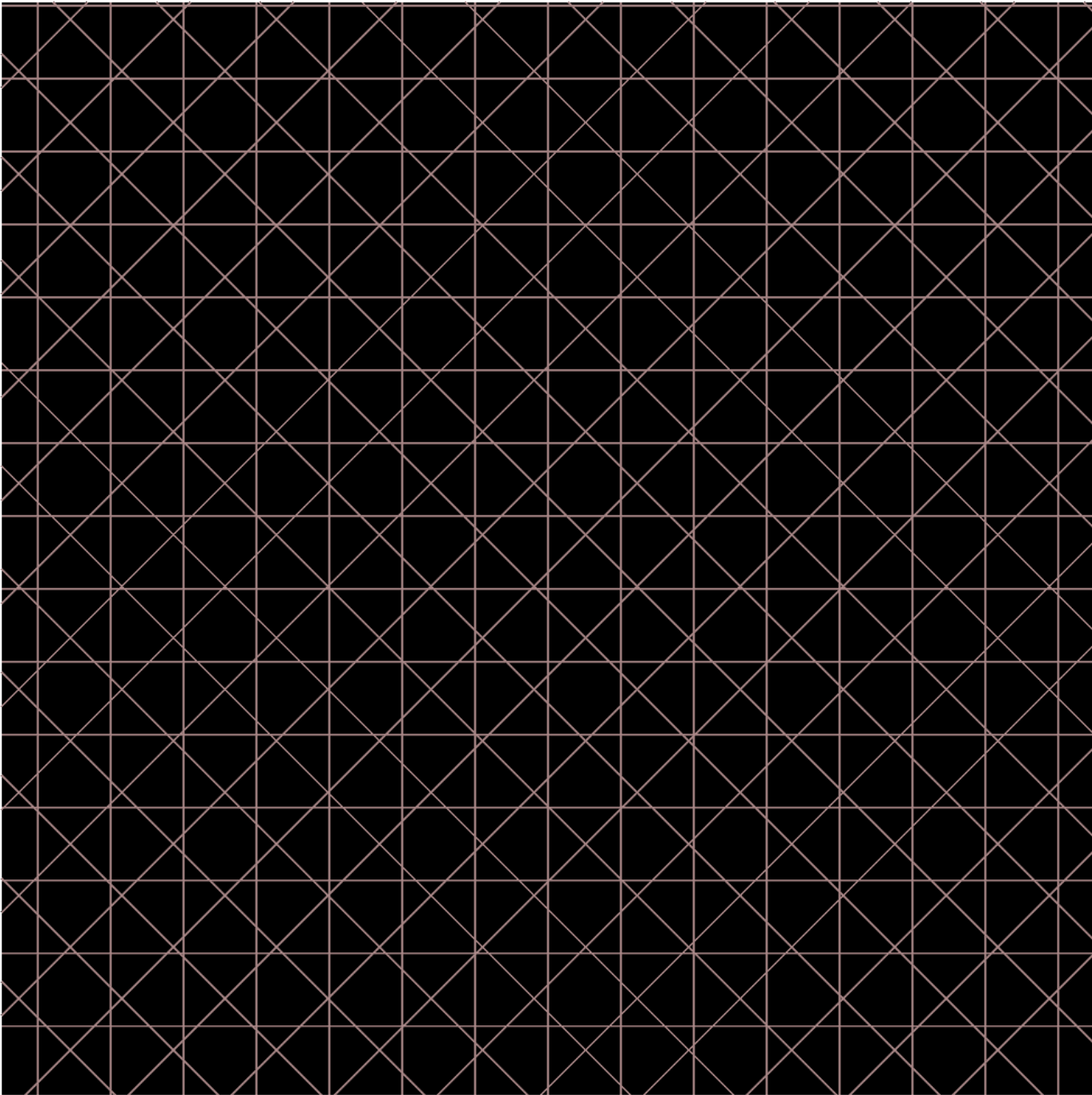
<http://www.activestate.com/activeperl/downloads>

<http://www.povray.org/download/>

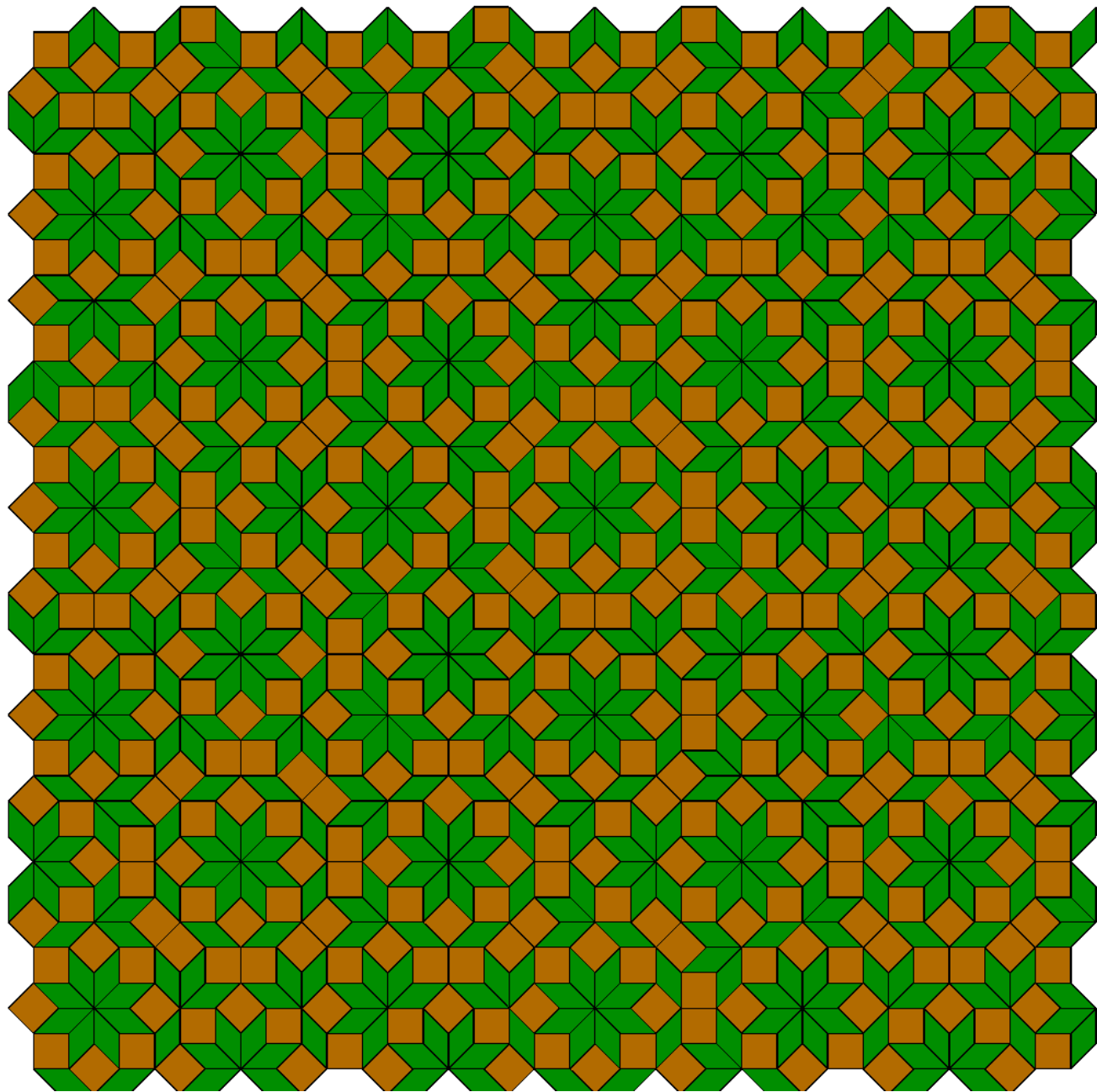
The installation is very simple.

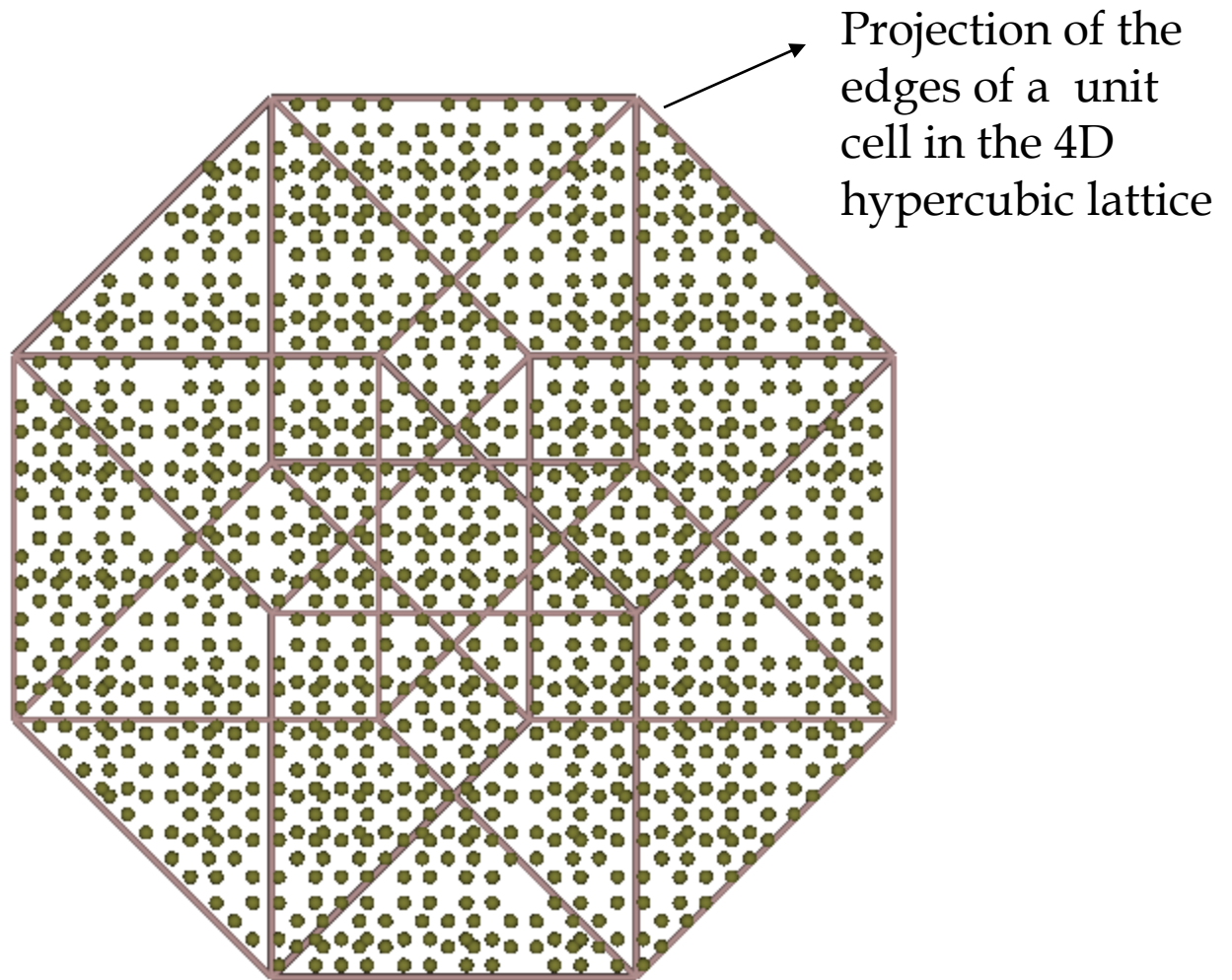
Put each of the .pl files into an empty folder. Double clicking the file to run. Then three output files are generated. (The '.pl' extension should be associated with perl command. But usually it is done automatically when you install ActivePerl.)

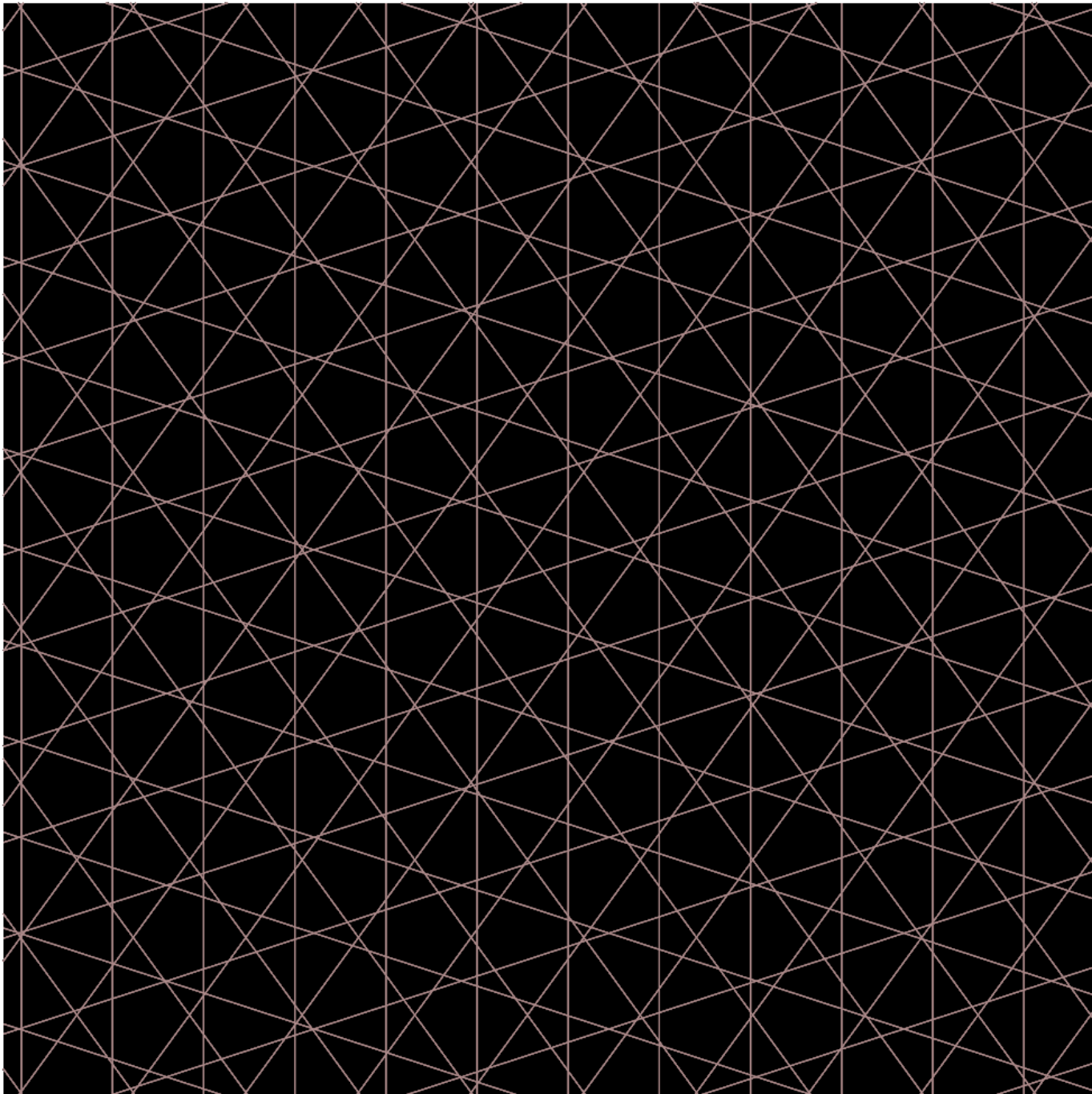
The output files are (1) the tiling, (2) grid lines (3) mapping of the vertices to the internal space. If you open them in Povray and run, each of these objects can be displayed.

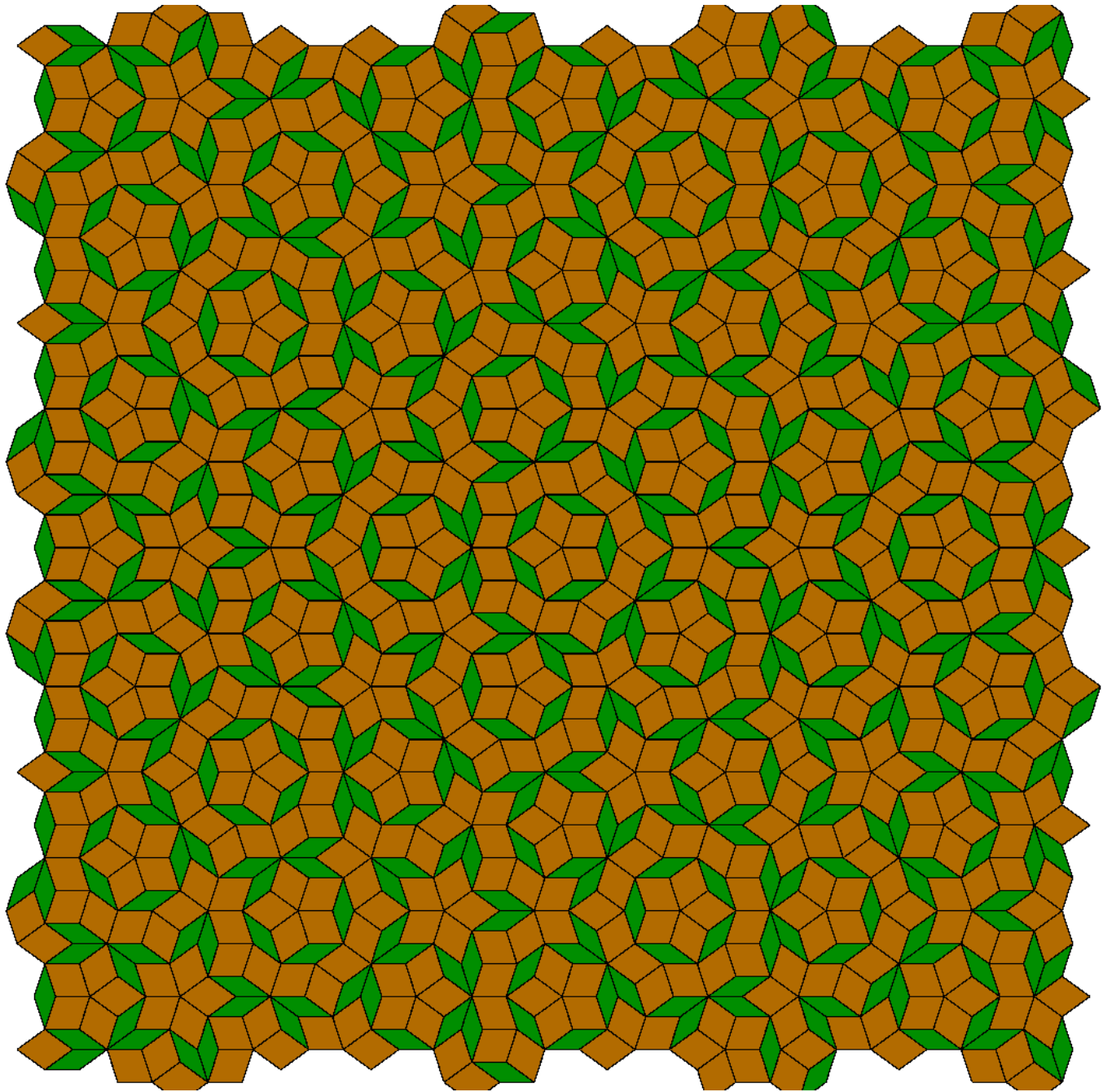


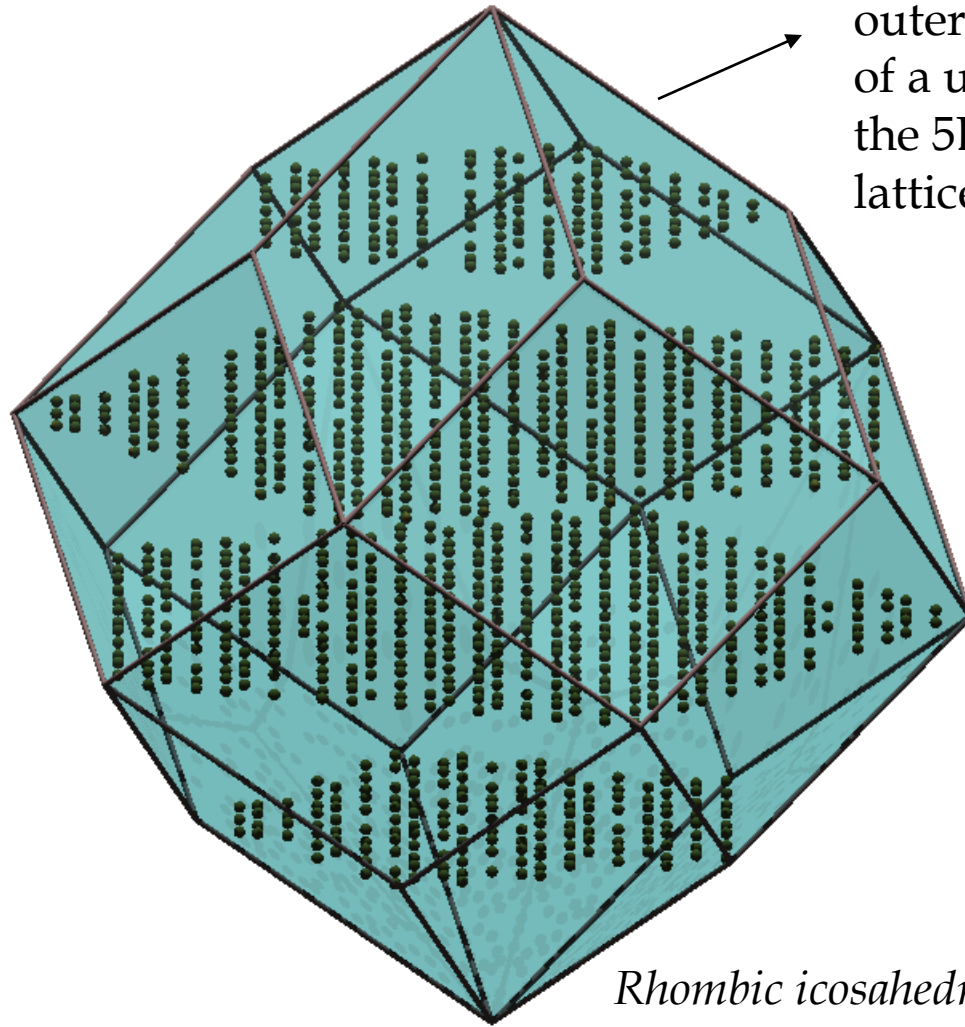












Projection of the  
outer boundaries  
of a unit cell in  
the 5D hypercubic  
lattice

*Rhombic icosahedron*