Theory of Aperiodic Solids:

from 1980 to present

Sponsoring

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Content

I - Aperiodic Solids

I.1)- Examples

- Periodic metals in a uniform magnetic field: *the magnetic field breaks the translation invariance for electrons due to quantum effect.*

- Doped semiconductors at low temperature (ex: **Si**, **AsGa**,): *the conduction electrons are confined in the impurity band and see only a random lattice.*

- Metallic Alloys: atoms may be located on a periodic lattice but there is some *randomness in the distribution of various species.*

- Amorphous materials, glass: *positive configurational entropy, short range order*.

- Quasicrystals (ex: $\mathbf{Al_{62.5}Cu_{25}Fe_{12.5}}$, $\mathbf{Al_{70}Pd_{22}Mn_{8}}$, $\mathbf{Al_{70}Pd_{22}Re_{8}}$): *long range order, low complexity, pure point diffraction spectrum*.

I.2)- Electronic Properties

- Spectral gaps *suppressed* by lack of order.
- *Incommensurability* in quasicrystal or due to the magnetic field, *creates a lot of gaps* (Cantor spectrum), at least in $1D$ or $2D$.
- Transport can be *anomalous*: at low temperature, the conductivity behaves as a power law in terms of the collision time

$$\langle (X(t) - X(0))^2 \rangle \overset{t\uparrow 0}{\sim} t^{2\beta} \qquad \Rightarrow \qquad \sigma \overset{T\downarrow 0}{\sim} \tau_{col}^{2\beta-1}$$

(Schulz-Baldes, JB '97)

$\beta = 1$ (quantum ballistic motion) $\Rightarrow$ *Drude formula* (normal metals)

$1/2 < \beta < 1$ (subballistic) $\Rightarrow$ *metallic*

$\beta = 1/2$ (quantum diffusion) $\Rightarrow$ *residual conductivity* (weak localization)

$0 = \beta < 1/2$ (subdiffusion) $\Rightarrow$ *insulator* (quasicrystals)

I.3)- Spectral Properties

- For *strong disorder*: dense set of eigenvalues, eigenstates are exponentially localized

  (from Pastur-Mochanov '78, Fröhlich-Spencer '81, to Germinet-Klein '08, via Aizenman, ...)

- For $1D$ *quasiperiodic potentials*: pure point spectrum (large coupling) versus absolutely continuous spectrum (small coupling)

  (Aubry-André '78, JB. et al, Sinai, Chulaevsky, Jitomirskaya, Bourgain,...)

- For $1D$ *quasicrystals and substitution tilings*: no point spectrum, no *a.c* spectrum, pure *s.c.* with positive Hausdorff dimension

  (JB '88-92, Raymond, Damanik, Gorodestki, Liu, Qu Wen ..)

- **Conjecture:** if $D \geq 3$ at *small coupling*, then *a.c* spectrum is expected.

I.4)- Mechanical Properties

- **Metallic crystals** have *no gap* at the Fermi level. *Defects* can be moved *without energy cost* and the periodic crystal structure makes their *propagation* easy. Then *elasticity* theory applies.

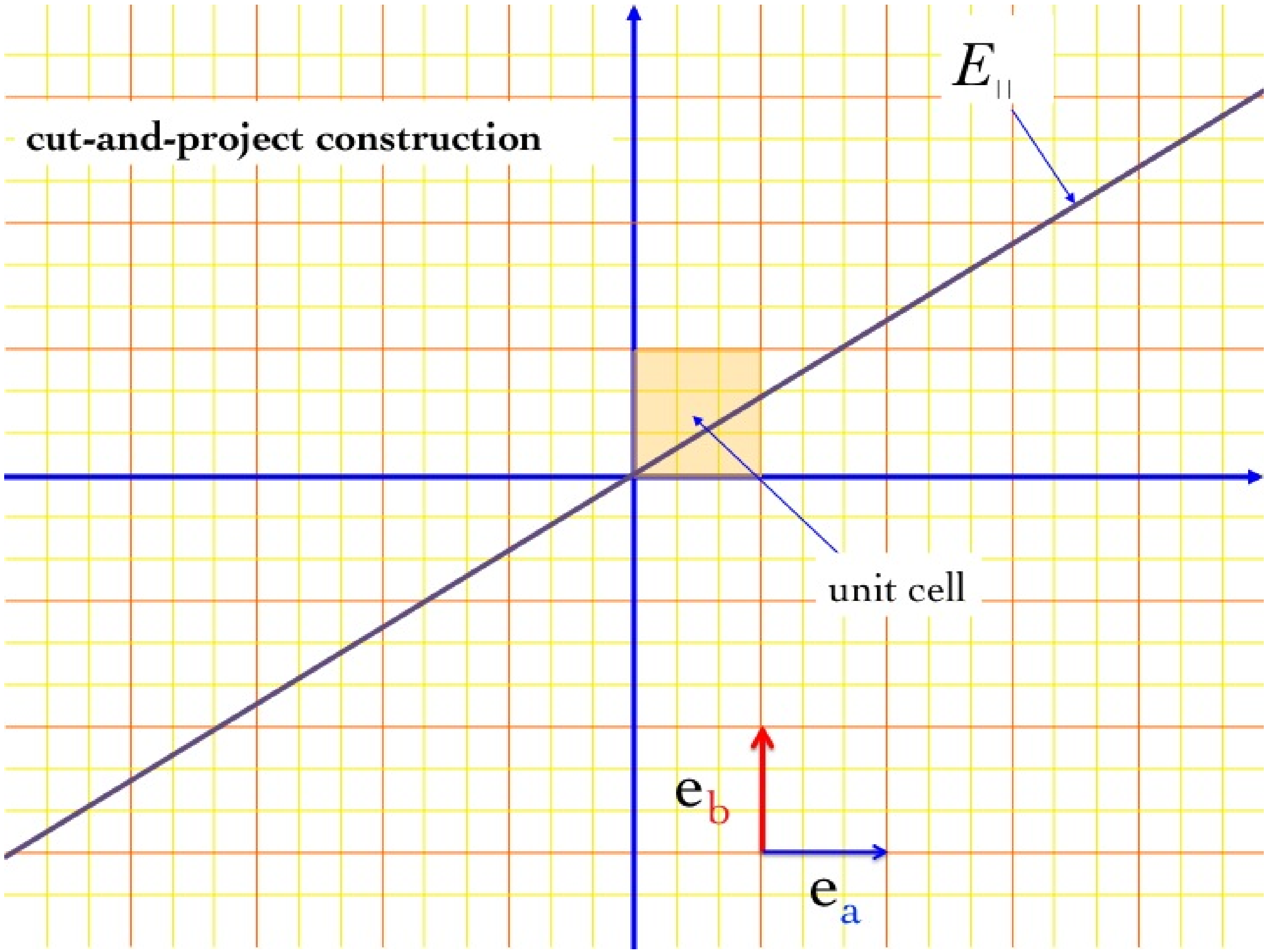
- By contrast, **insulators**, like oxides (ex: silicone oxides in rocks, aluminium oxides in jewelry) have a *large gap* at Fermi level. Moving defects is energetically *costly*. They are *hard* and can be brittle. Elasticity theory *fails* to apply at short wave length.

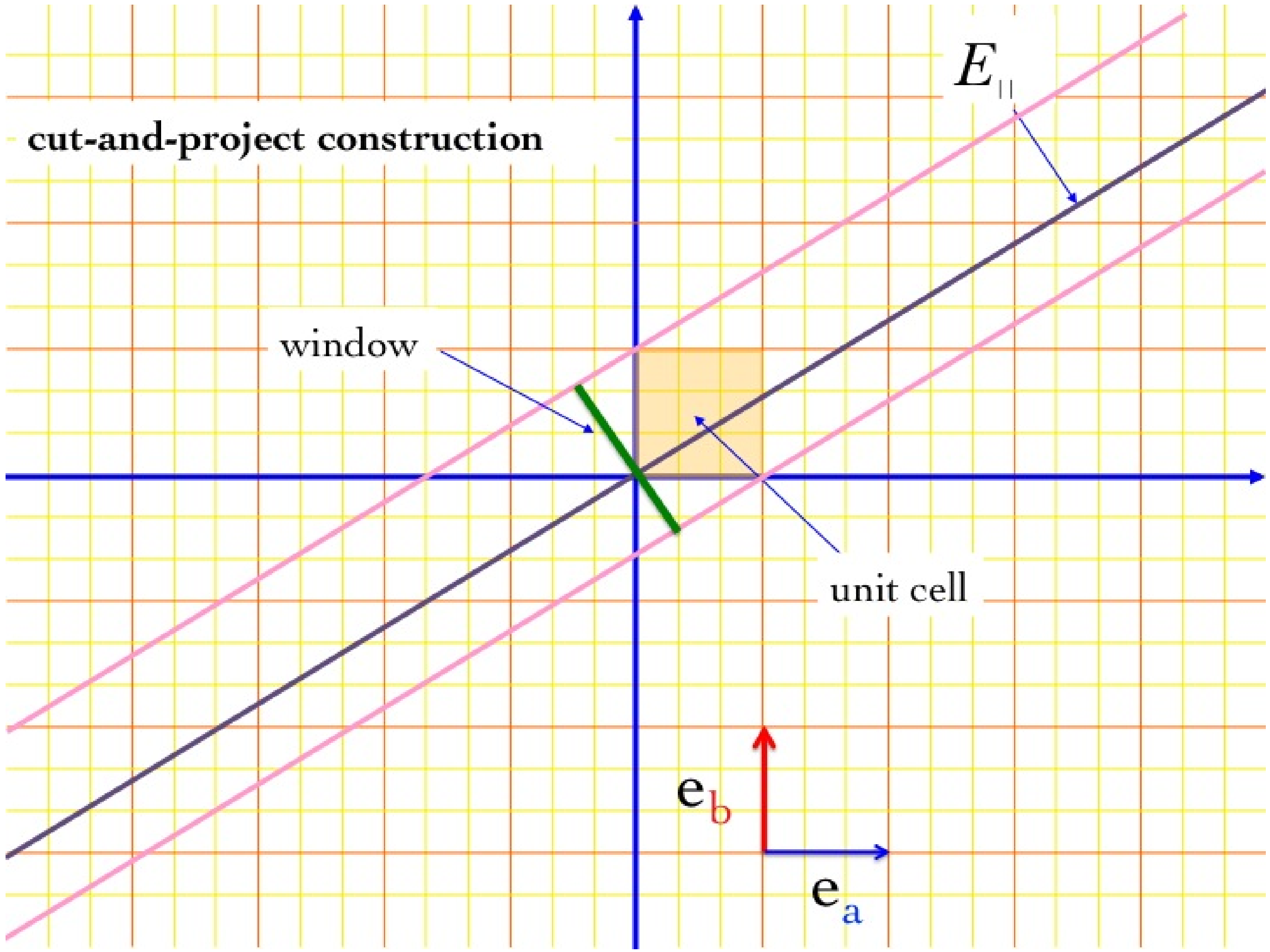
- **Quasicrystals** have no gap but their stability is enforced by a *pseudo gap* at Fermi level. Propagation of defect is *less costly* than in oxides but the atomic structure is an *obstacle* to short wavelength propagation. As a result quasicrystals are *hard and bristle*. Elasticity theory *fails* to apply to short wavelength.

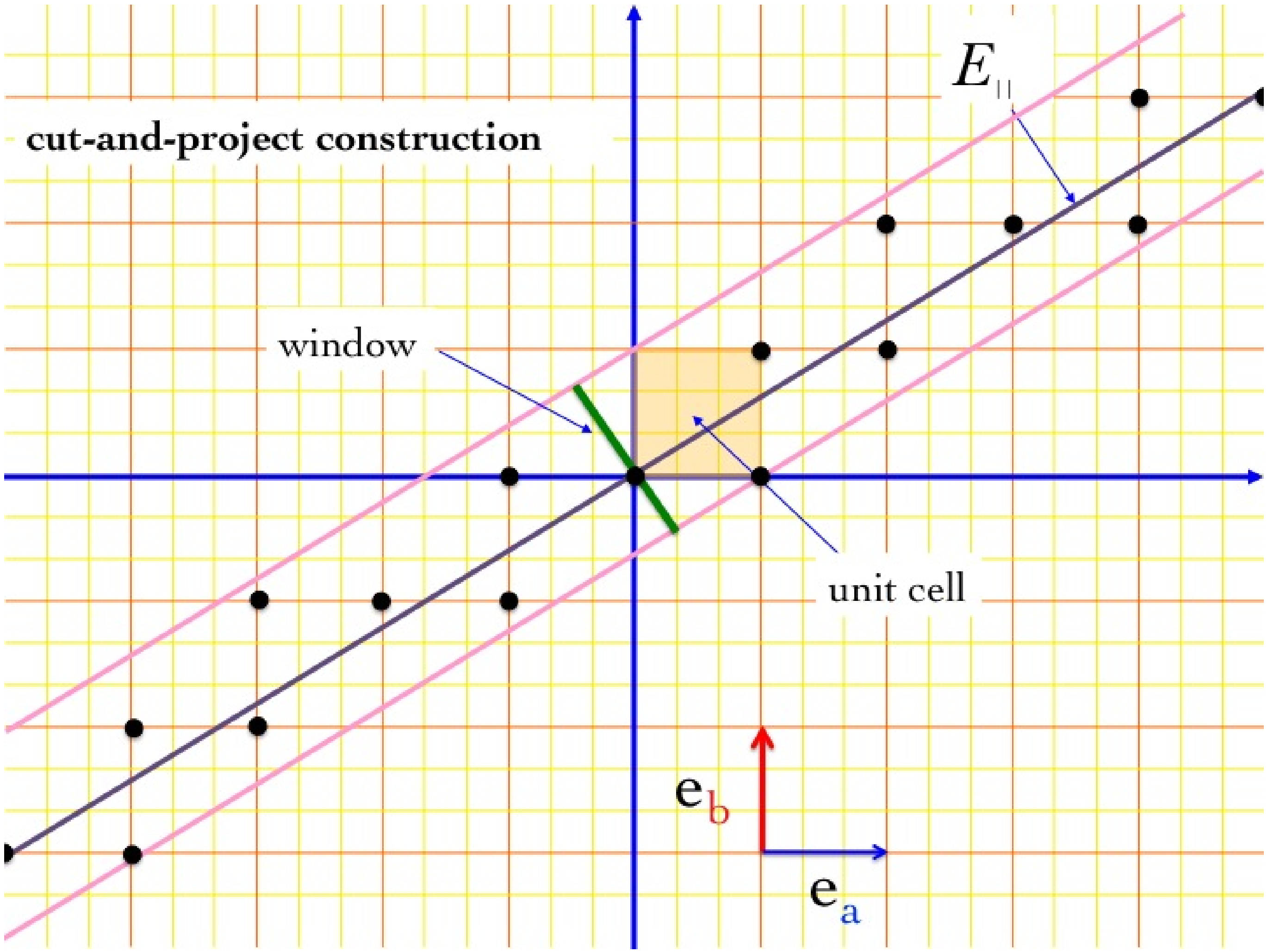
II - Atomic Structure

II.1)- Examples

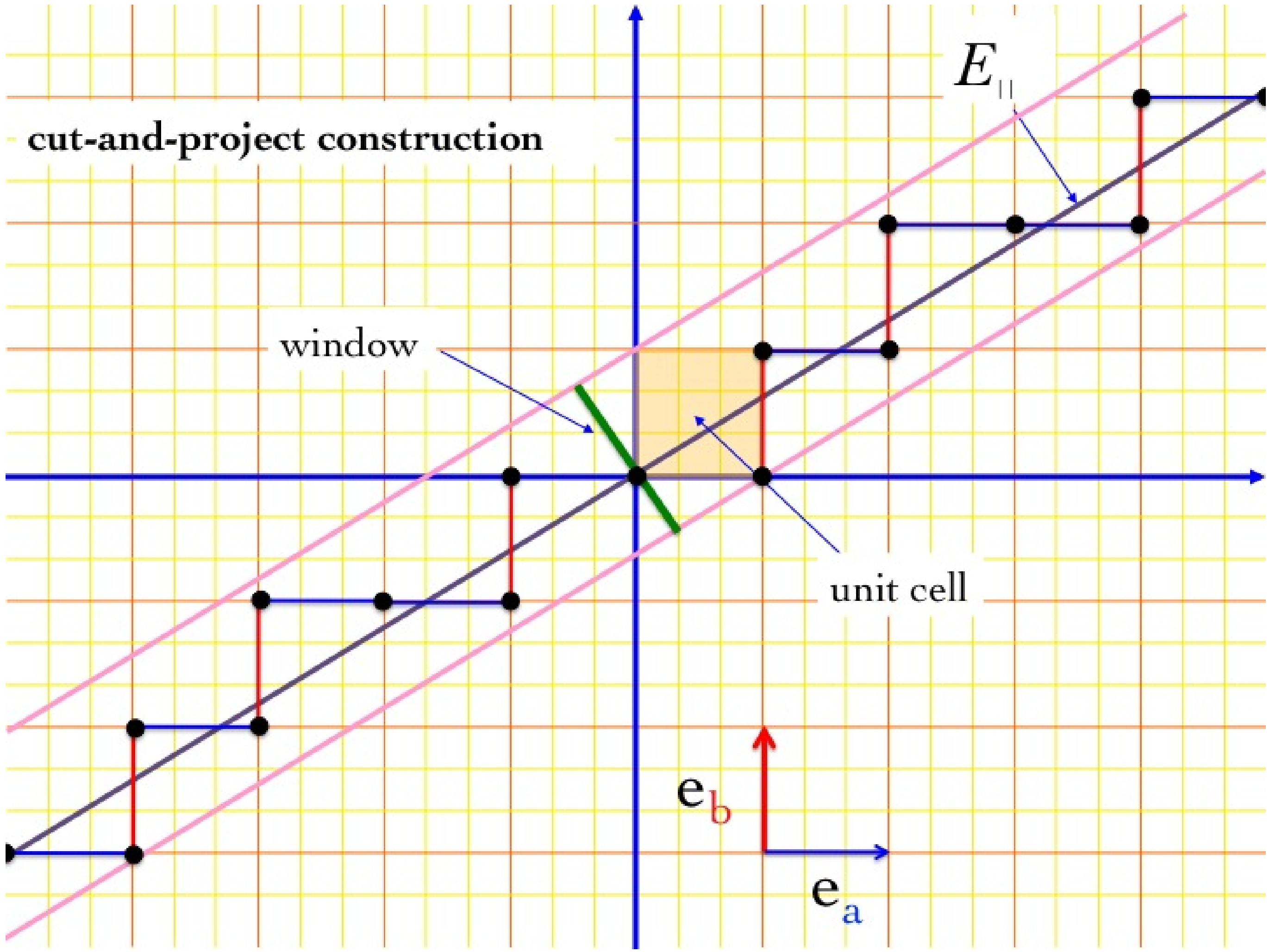
- **Periodic Crystal**: the atoms are located on a *periodic lattice*.
- **Impurities in a semiconductor**: scattered *randomly* on the sites of the silicon diamond lattice
- **Quasicrystals**: atoms are located on a *quasiperiodic lattice*, obtained by a *cut-and-project* construction.


cut-and-project construction
$E_{||}$
unit cell
e_b
e_a

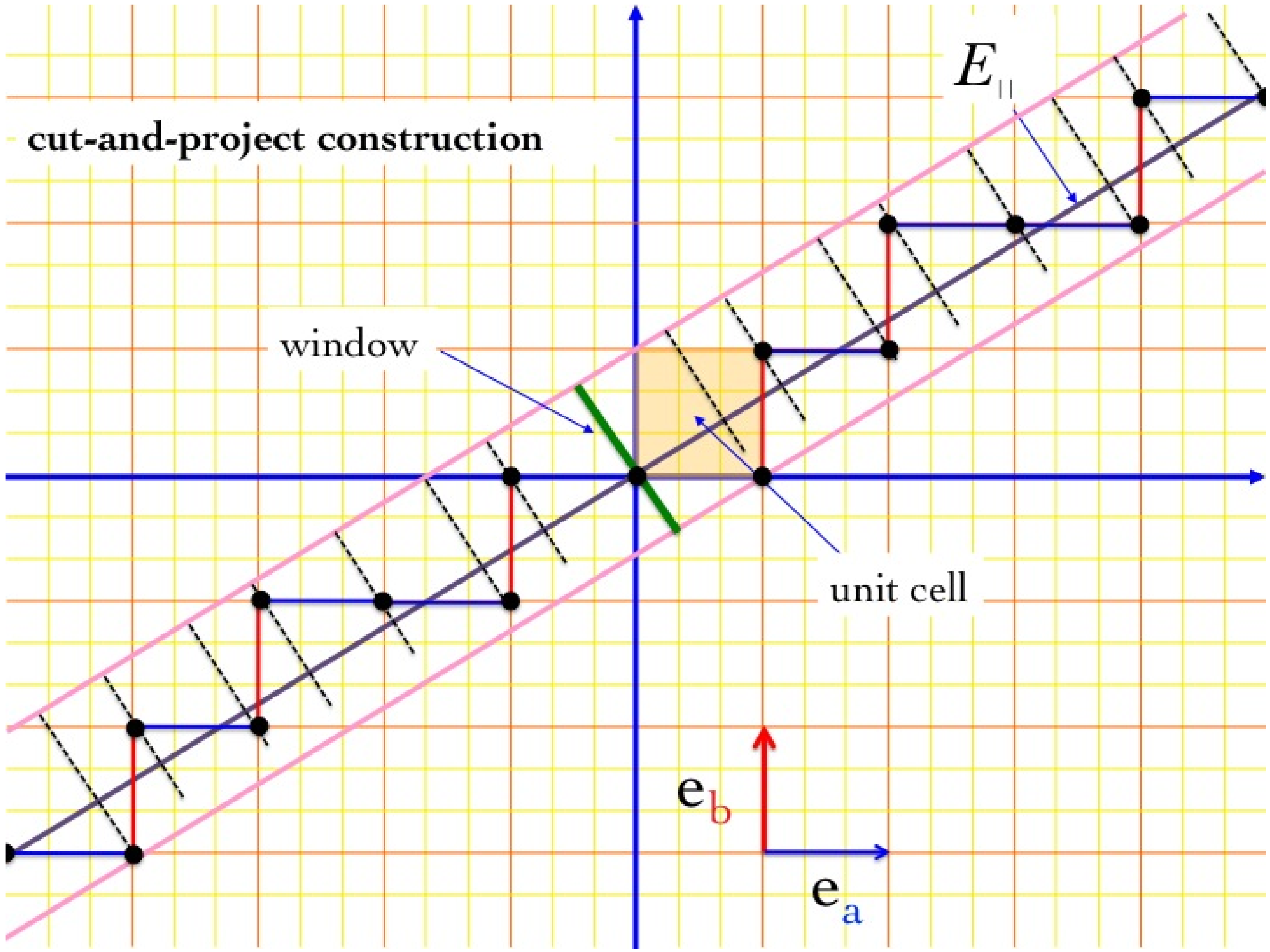

cut-and-project construction
$E_{||}$
window
unit cell
e_b
e_a



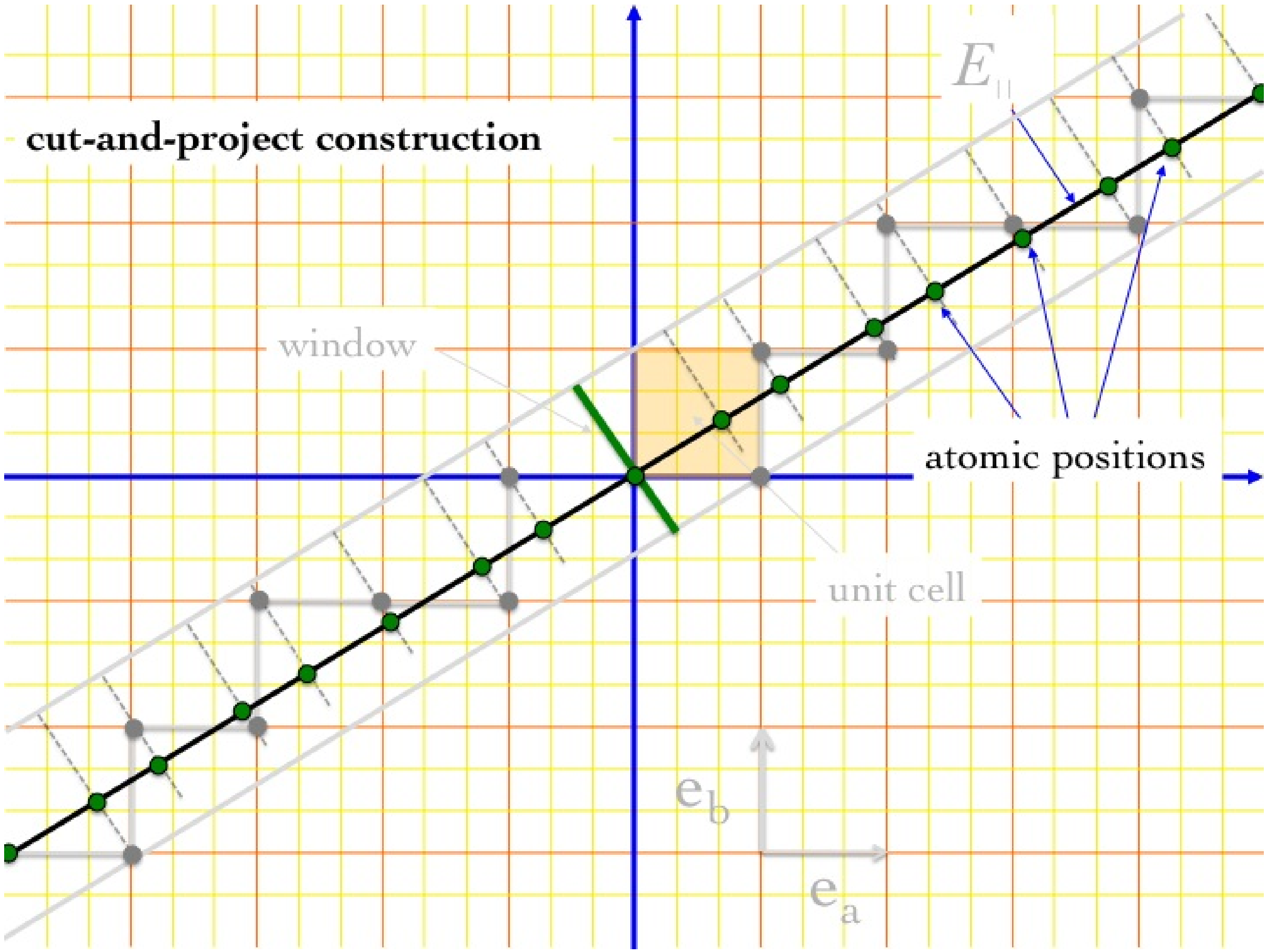
cut-and-project construction
$E_{||}$
window
unit cell
e_b
e_a



cut-and-project construction
$E_{||}$
window
unit cell
e_b
e_a



cut-and-project construction
$E_{||}$
window
unit cell
e_b
e_a


cut-and-project construction
$E_{||}$
window
atomic positions
unit cell
e_b
e_a

II.2)- The Fibonacci Chain

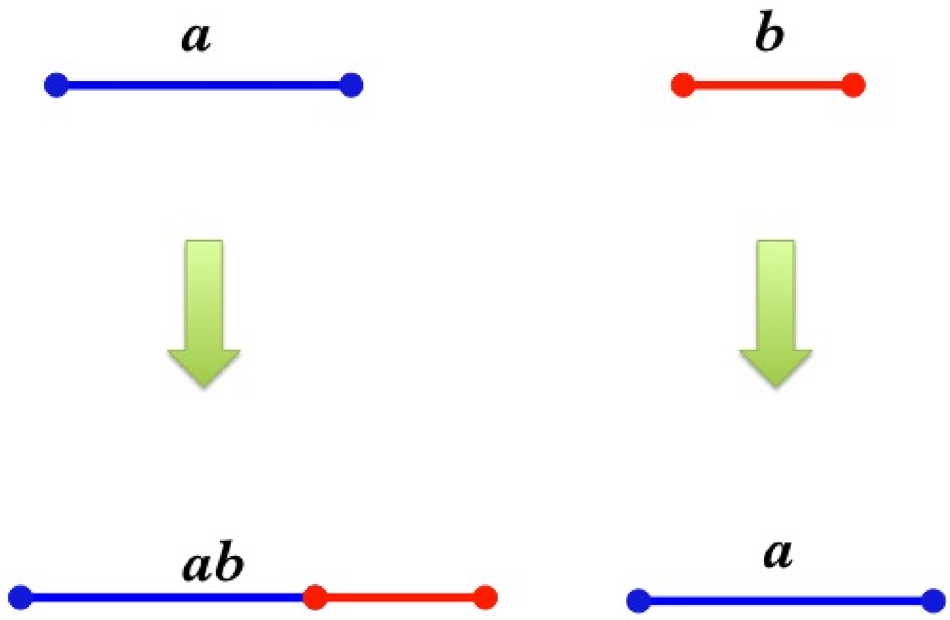
- The *Fibonacci Chain* is obtained by cut-and-project

$$\mathbb{Z}^2 \to E_{||} \simeq \mathbb{R}$$

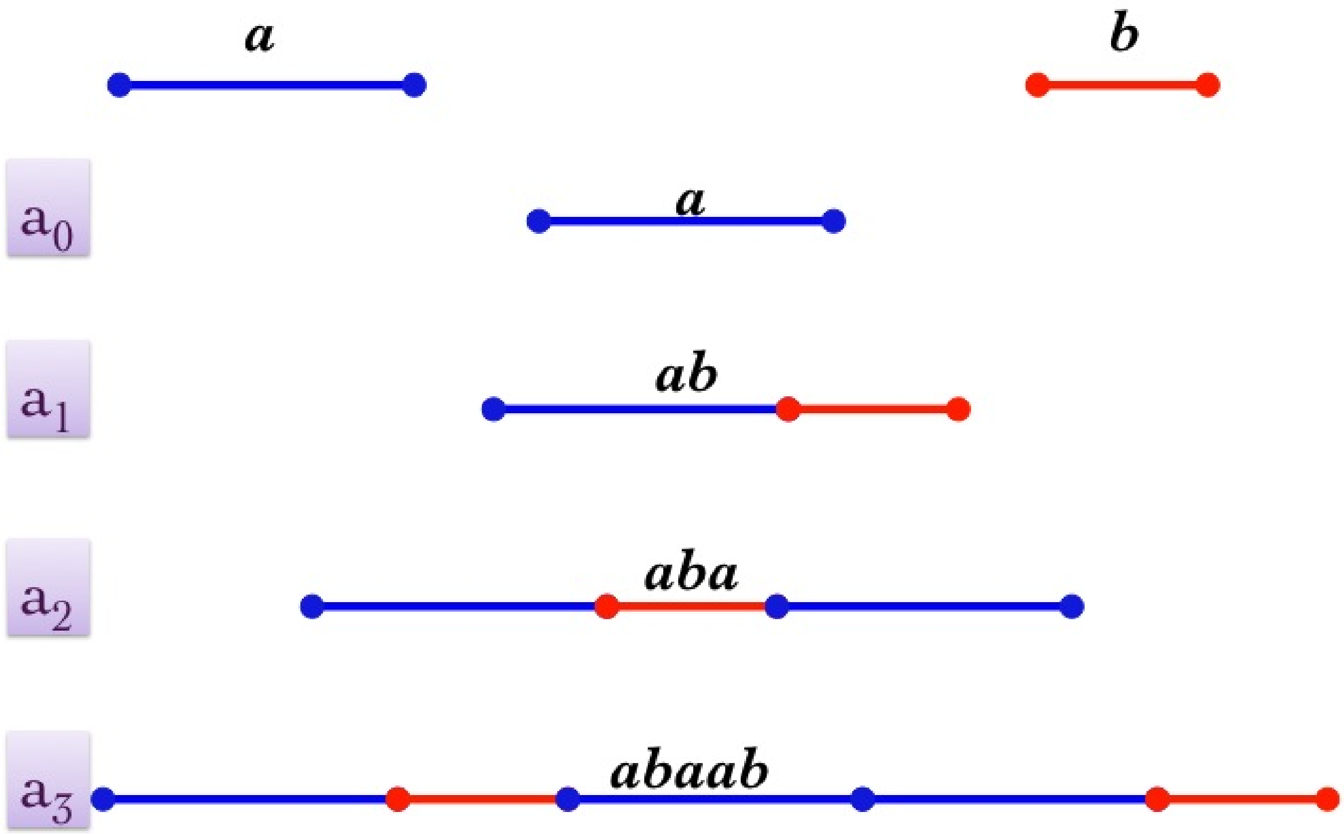
- The slope of $E_{||}$ is the golden mean

$$\sigma = \frac{\sqrt{5}-1}{2}$$

- It is a *substitution sequence* with inflation rate σ which is irrational.



The Fibonacci Substitution


a
b
a0
a
a1
ab
a2
aba
a3
abaab

II.3)- The Octagonal Lattice

- The *octagonal lattice* is obtained by cut-and-project

$\mathbb{Z}^4 \to \mathbb{R}^2$ $\{e_1, e_2, e_3, e_4\}$ = **standard basis of** $\mathbb{Z}^4$

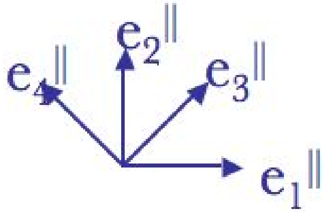
- The projection respects the 8-fold symmetry generated by the rotation

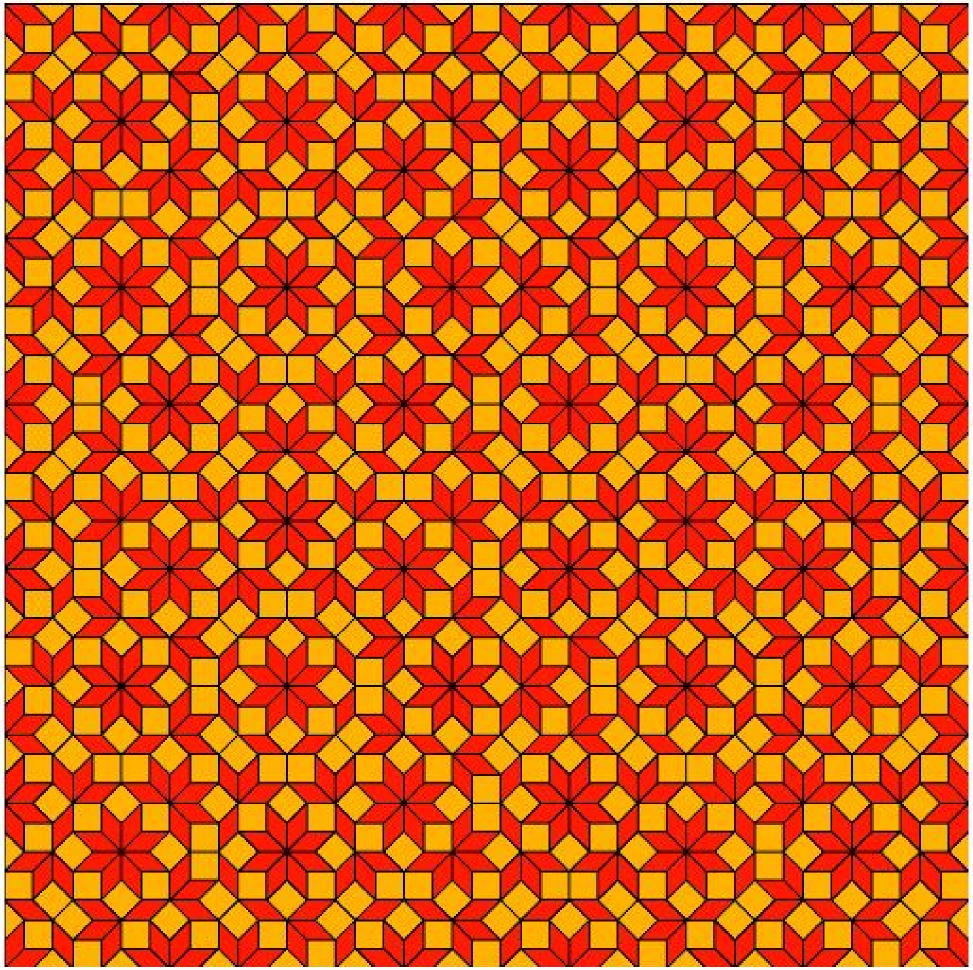
$$R : e_1 \to e_3 \to e_2 \to e_4 \to -e_1$$

- It is a *substitution lattice* with inflation rate $\sqrt{2} + 1$ which is irrational.

Octagonal Lattice

$Z^4 \rightarrow R^2$





Octagonal Lattice

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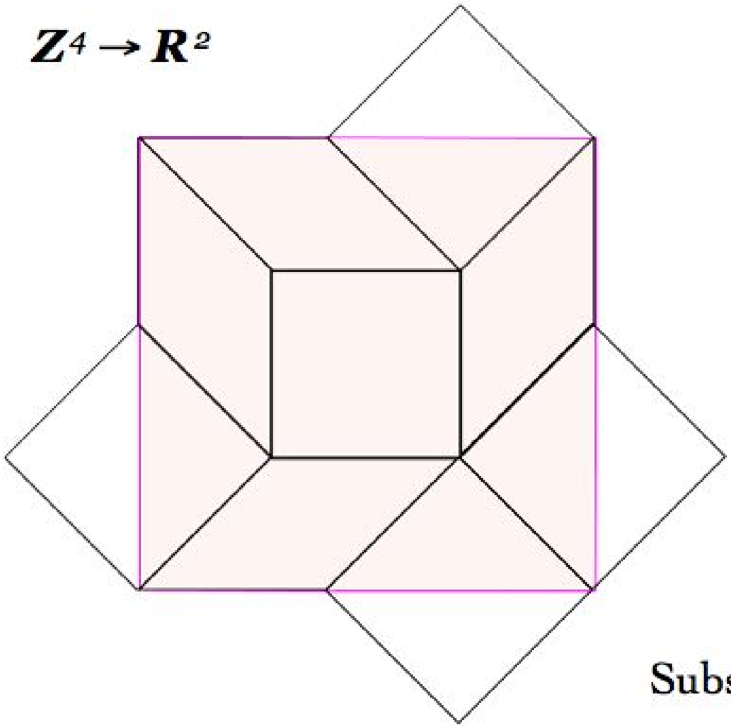
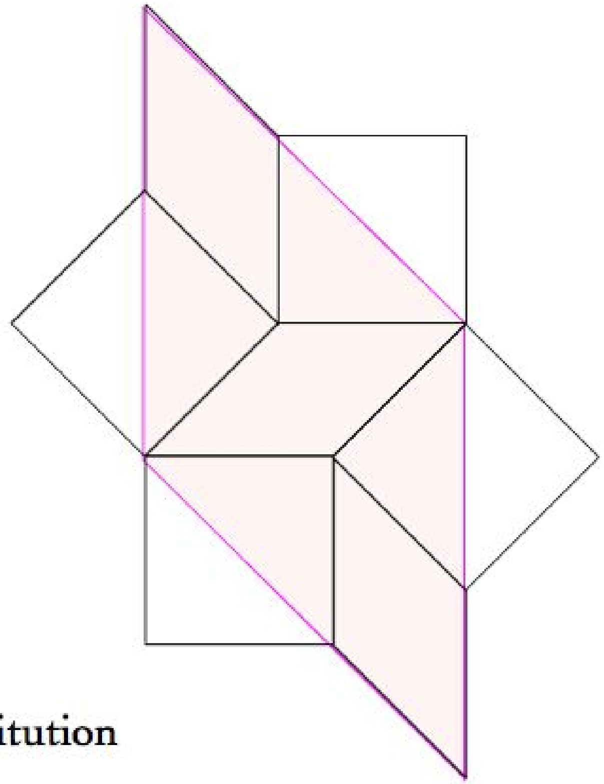
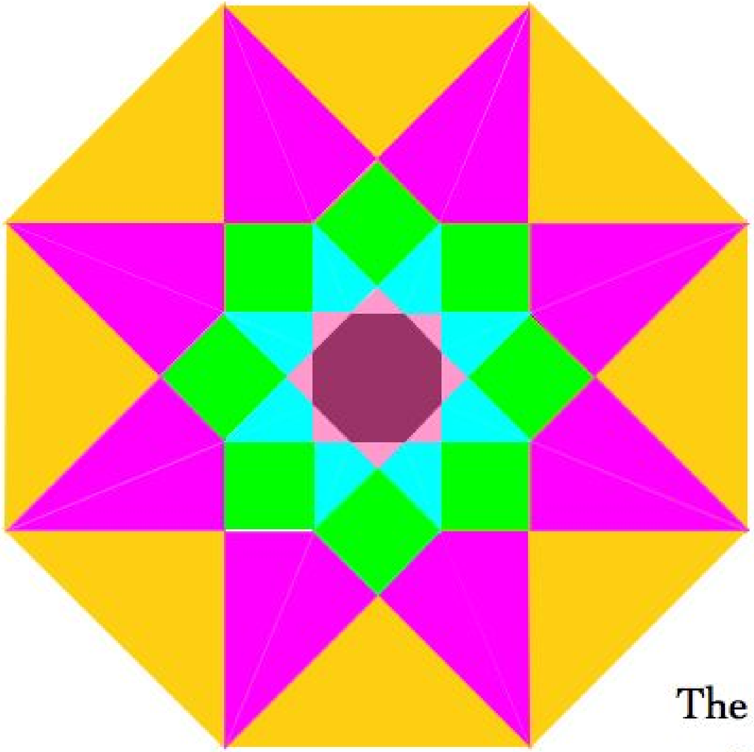




Substitution

Octagonal Lattice

$Z^4 \rightarrow R^2$



The Transversal or Window

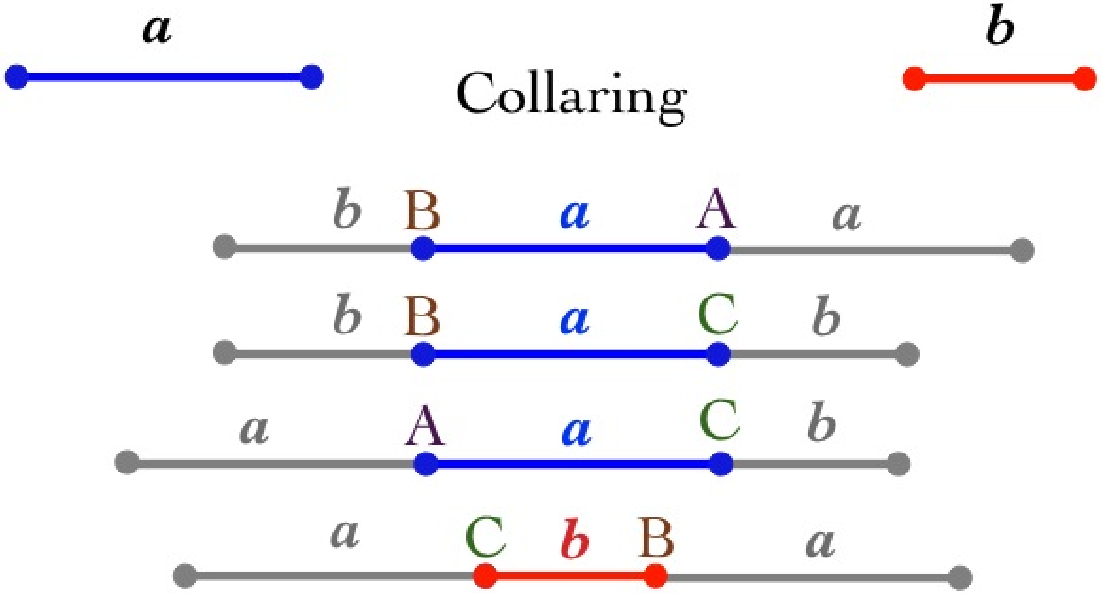
II.4)- The Anderson-Putnam Complex

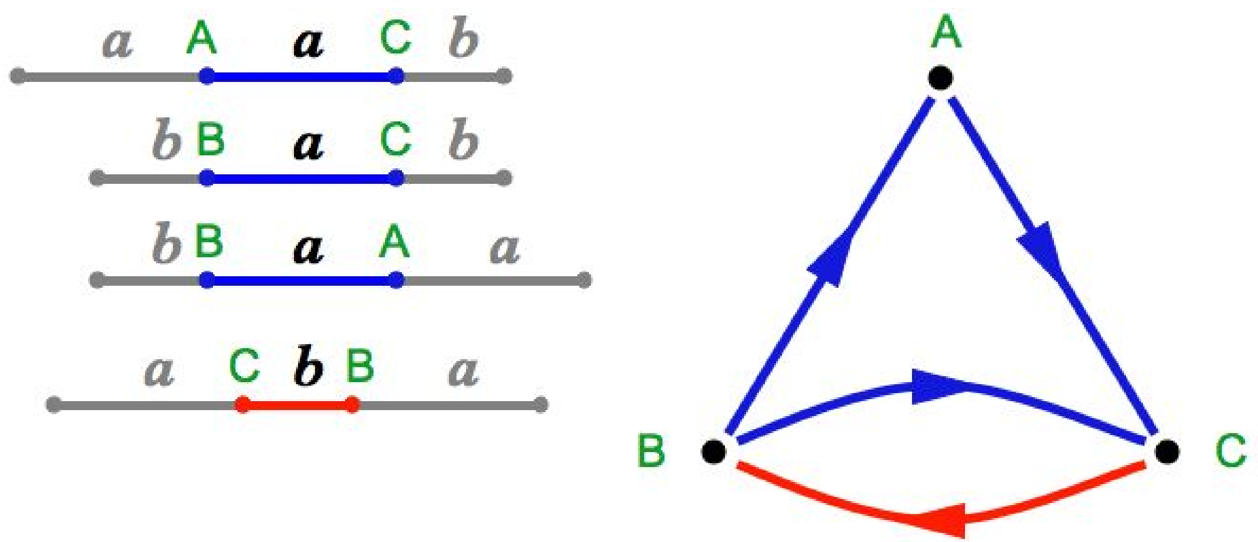
- Each tile T is *decorated*. For example by its *collar* $\Rightarrow (T, c)$ (c is the collar and is just a label)

- A *prototile* is a decorated tile *modulo translations*. Their disjoint union is called $\tilde{X}$.

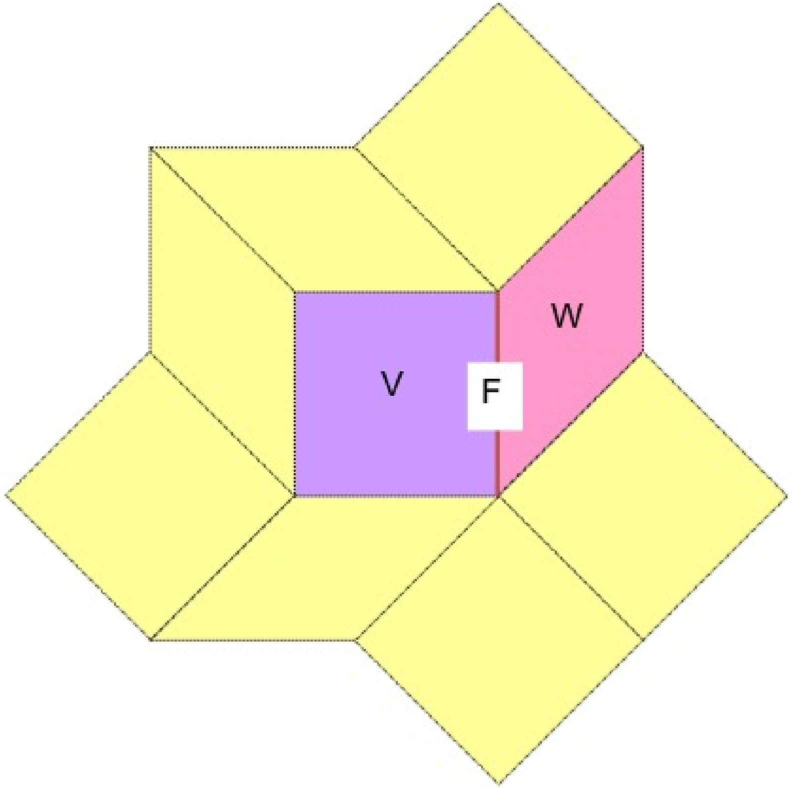
- Two points in the boundary of two distinct prototiles in $\tilde{X}$ are *identified* if somewhere in the tiling the corresponding tiles touch at these positions.

- The resulting space is the *Anderson-Putnam complex* $X = \tilde{X}/\sim$

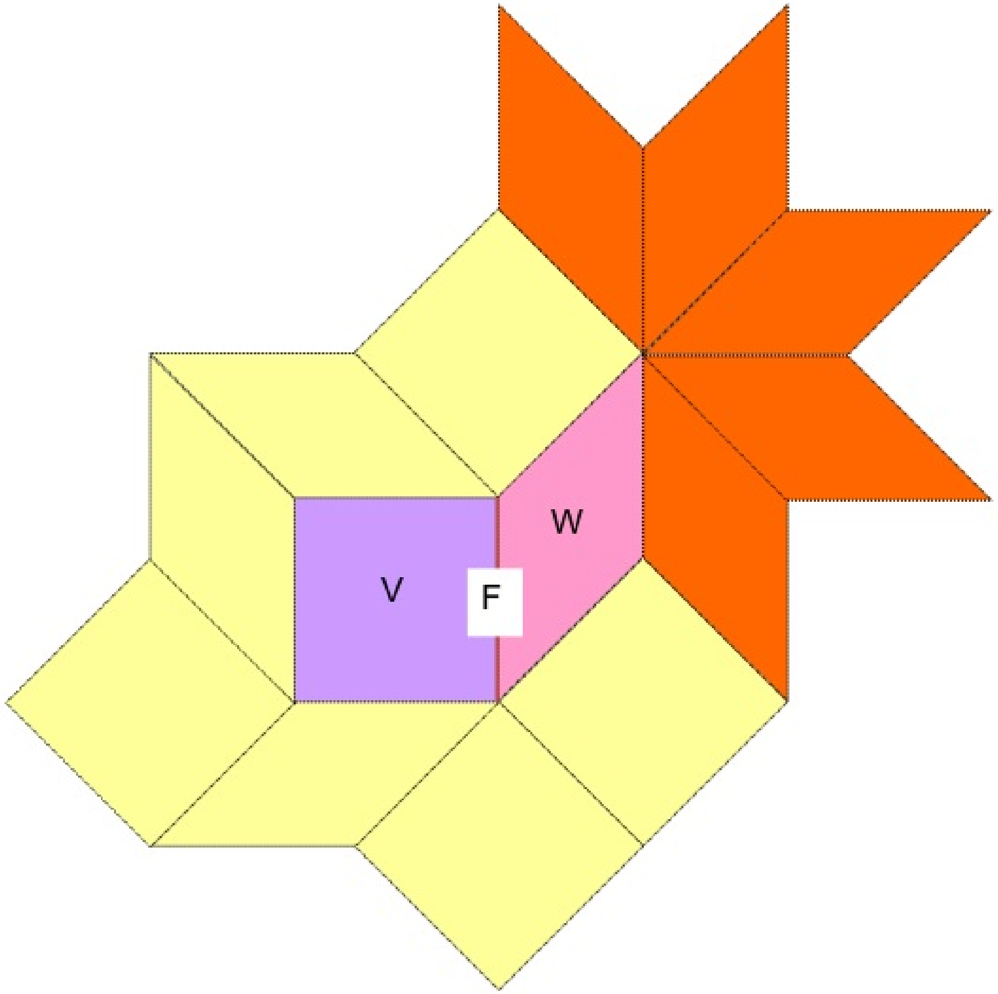

a
b
Collaring
b B a A a
b B a C b
a A a C b
a C b B a

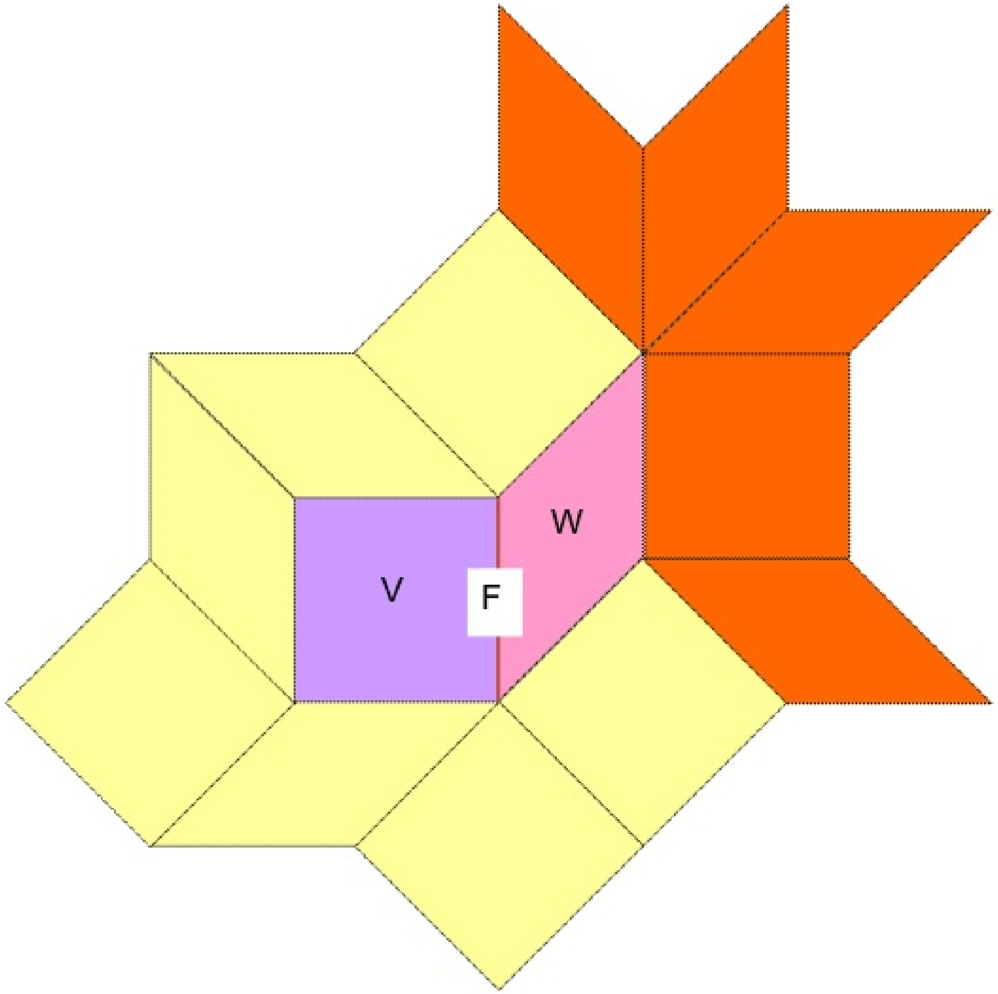


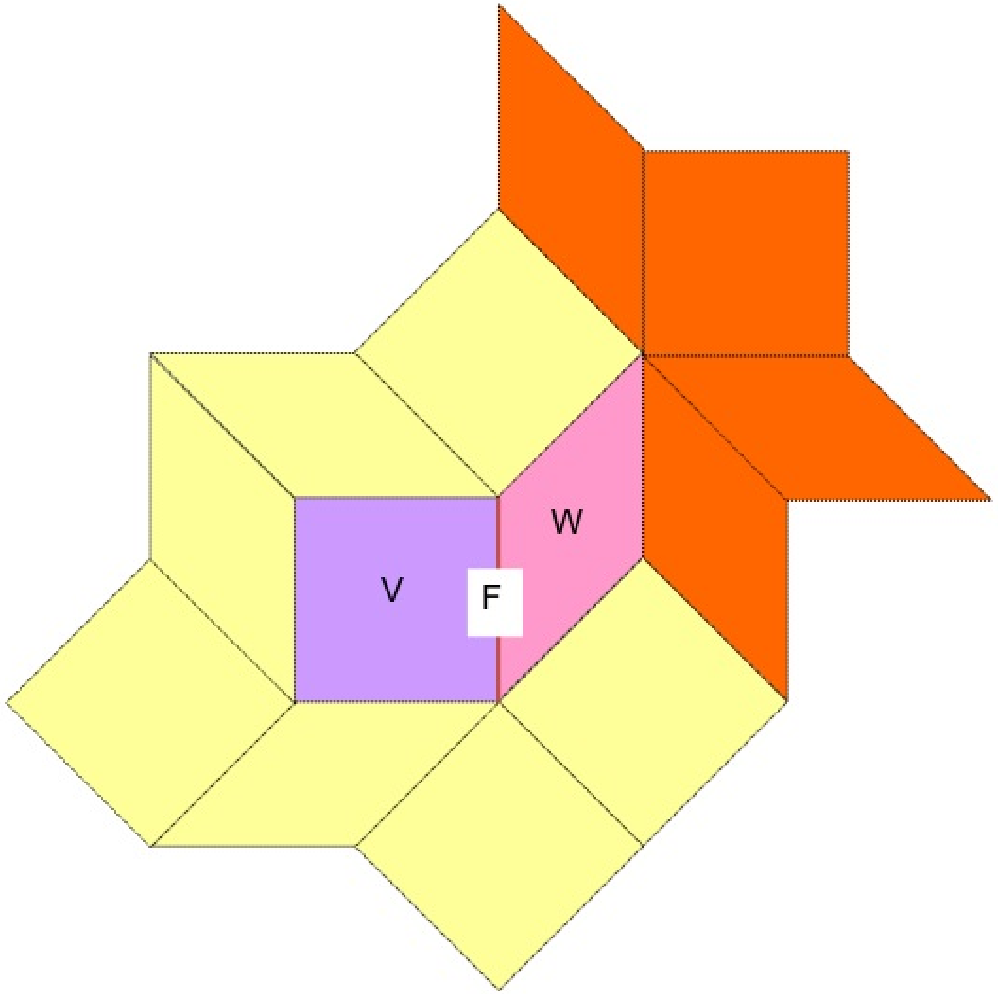
a A a C b
b B a C b
b B a A a
a C b B a
A
B
C

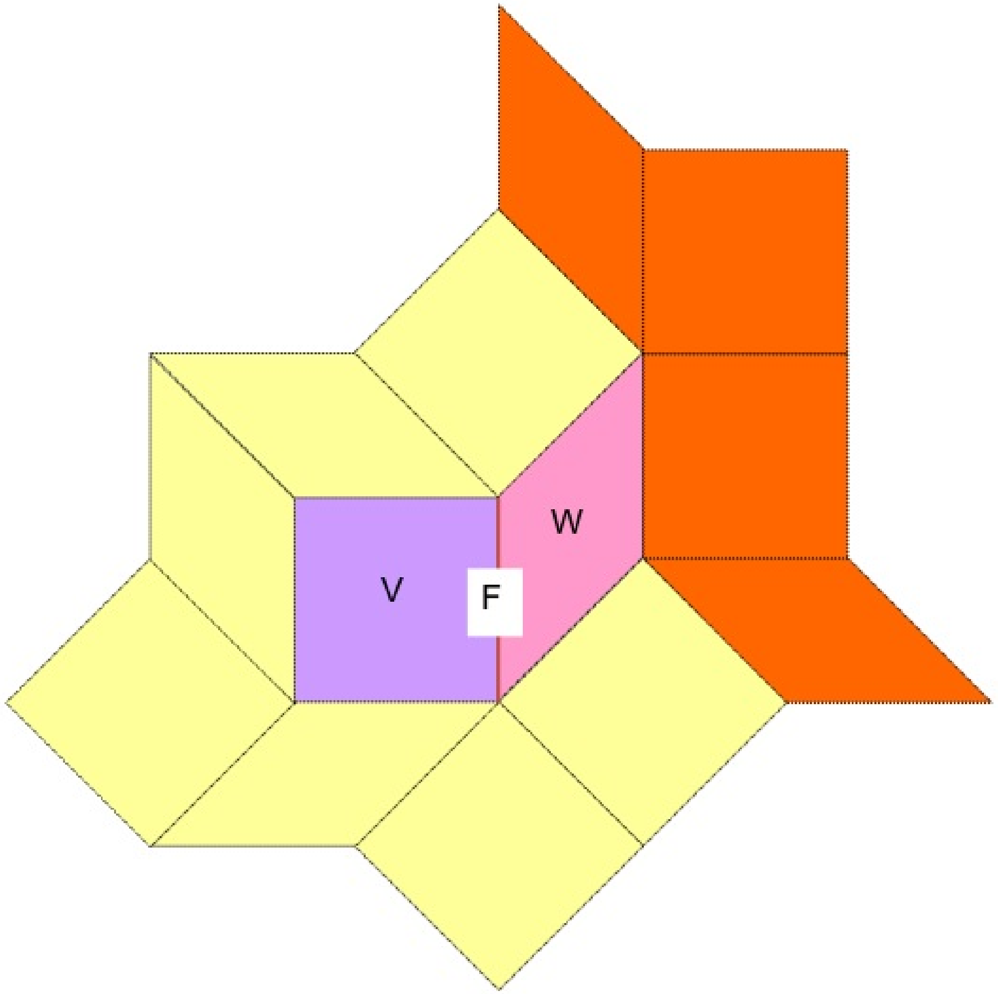


W
V
F


V
F
W


W
V
F


W
V
F



W
V
F

II.5)- Substituting

- Replace each collared prototile (T, c) in X by its *substitute* $(\hat{\sigma}(T), \hat{\sigma}(c))$, which is a *patch*. This gives X_1.

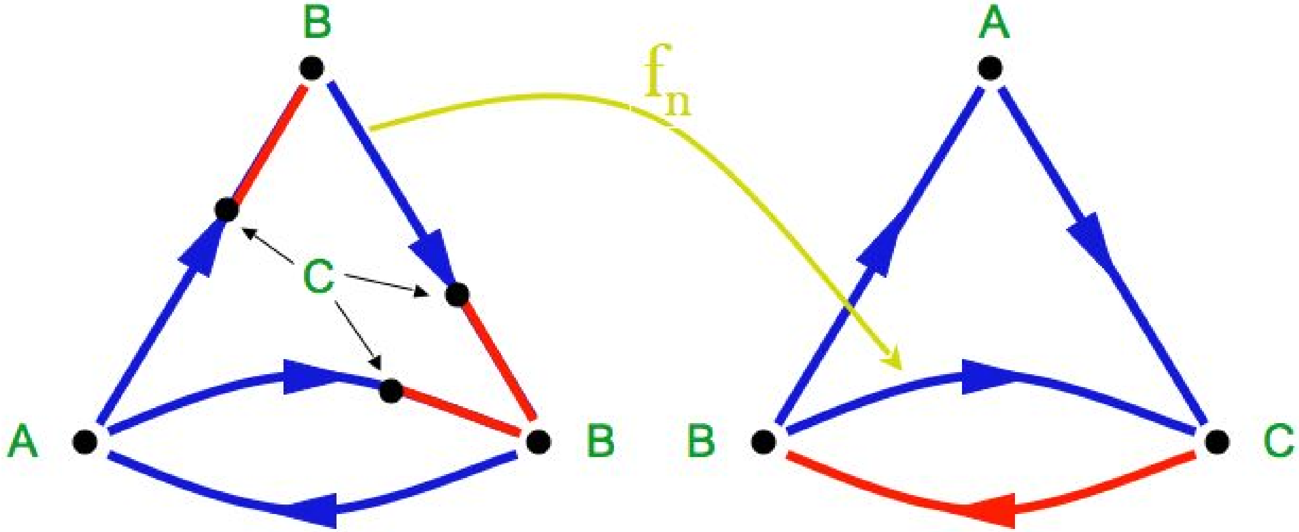
- *Topologically* $X_1 \sim X_0 = X$ again, but the *length scale is stretched* by the inflation rate.

- Then *identify* each collared tiles in these *substituted* patches into the corresponding collared tile in X: this gives a smooth map $f_1 : X_1 \to X_0$ with $Df = \mathbf{1}$ which is *finite-to-one*.

- *Iterating* the substitution gives a sequence $(X_n)_{n\in\mathbb{N}}$ of Anderson-Putnam complexes and maps

$$f_{n+1} : X_{n+1} \to X_n$$

.



$$X_{n+1} \xrightarrow{f_n} X_n$$

II.6)- The Hull

- The *Hull* Ω of a distribution of atoms, or of a tiling, is the *closure* of the family of its *translate* in space, with respect to a *suitable topology*.

- The Hull is a *compact metrizable* space on which the *translation group acts* by homeomorphisms. The orbits of the translation group makes the Hull a *foliated space*.

- Equivalently, the Hull can also be seen as the set of all possible atomic distributions or tiling, sharing the same *atlas* of *local patches* (local indistinguishability).

- An important result is that the Hull is the *inverse limit*

$$\Omega = \varprojlim (X_n, f_n)$$

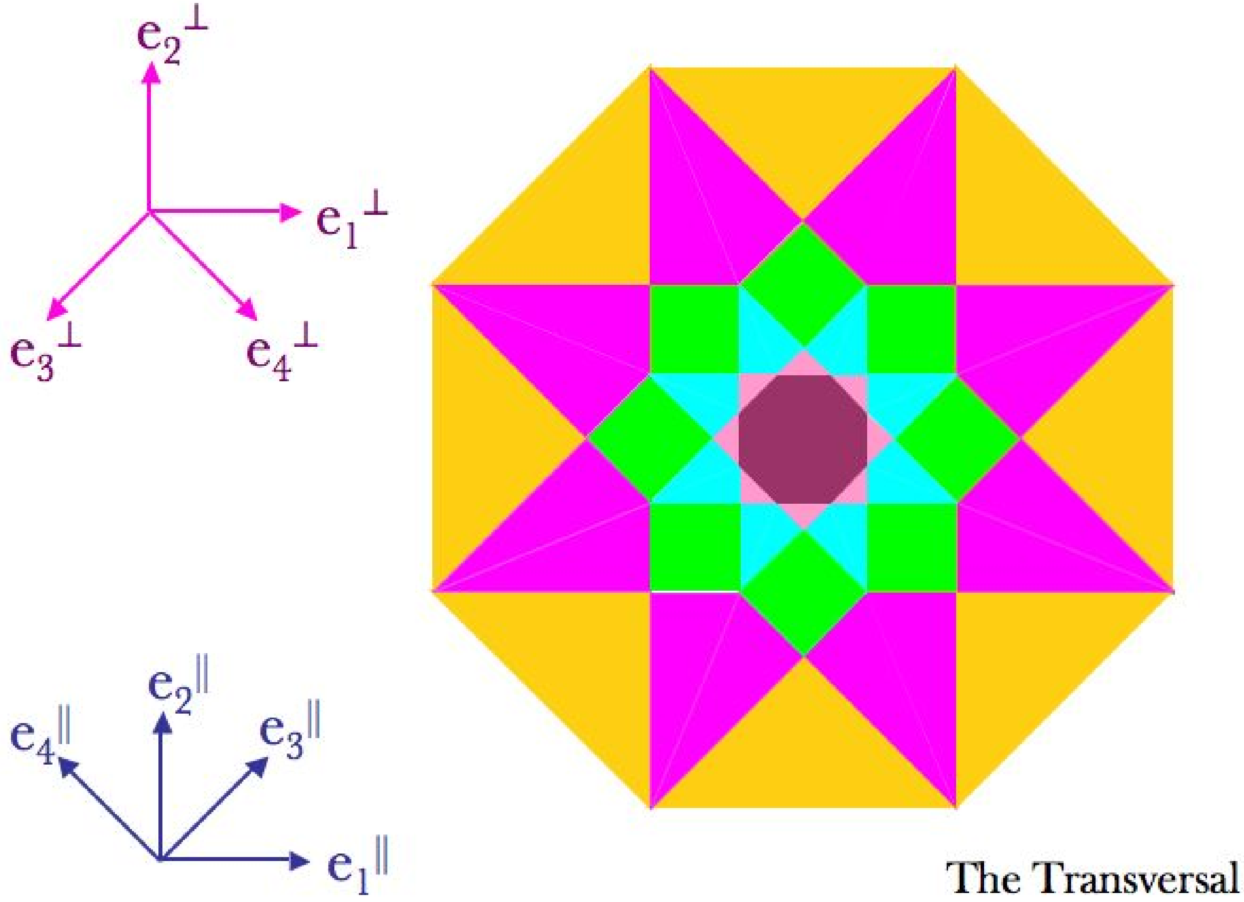
II.7)- Tiling Space and Transversal

- The *transversal* is the set of atomic distribution in the Hull with one atom *located at the origin* of the space.

- The *tiling space* is the set of all atomic distributions with *one atom at the origin* sharing the *same atlas* of local patches. Hence

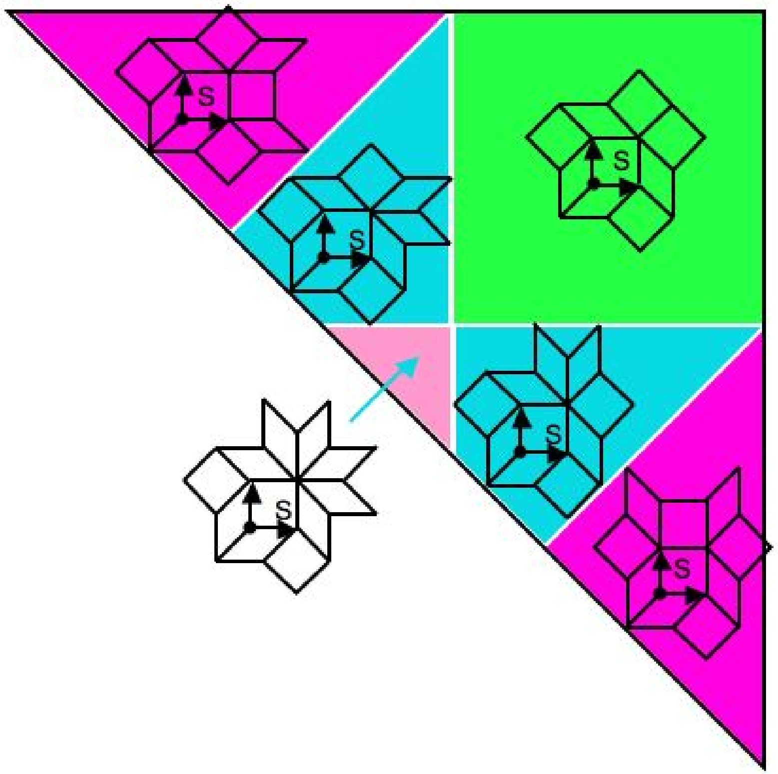
  tiling space= *transversal*.

- For quasicrystals obtained by the *cut-and-project* construction, the transversal is homeomorphic to the *window* with a dense set of *cuts*.

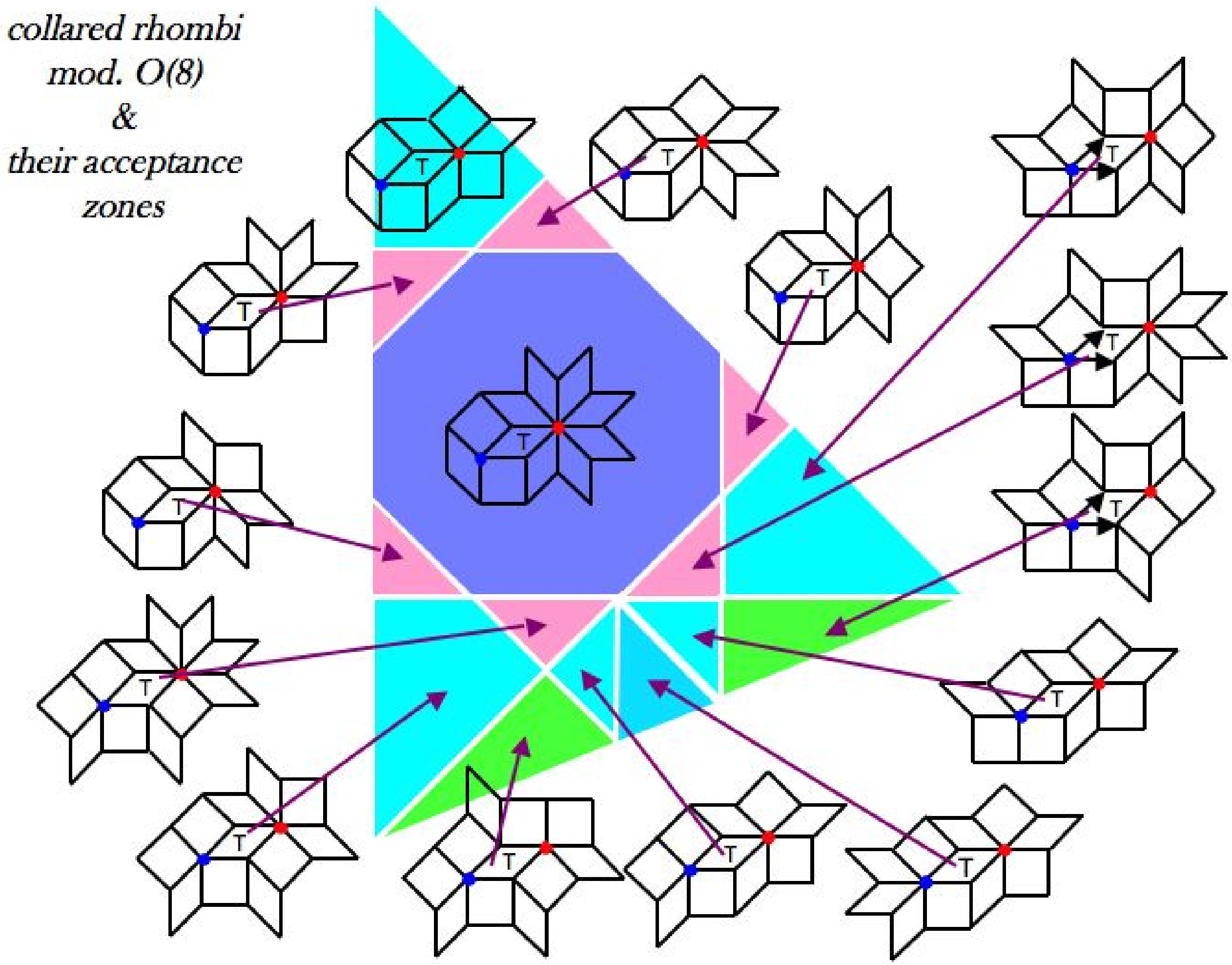


-Transversal of the octagonal lattice-
-with cuts along the boundaries of the acceptance domains-
-marked in color-

collared squares
mod. O(8)
&
their acceptance
zones



-Detail of the transversal of the octagonal lattice-



-Another detail of the transversal of the octagonal lattice-

III - Using the Transversal

III.1)- Stoichiometry

- Each local patch gives rise to a set of atomic distribution in the transversal, called its *acceptance domain*, admitting this patch at the origin.

- There is a *probability* distribution on the transversal such that the density of *occurrences* of a given patch is given by the probability of its *acceptance domain*.

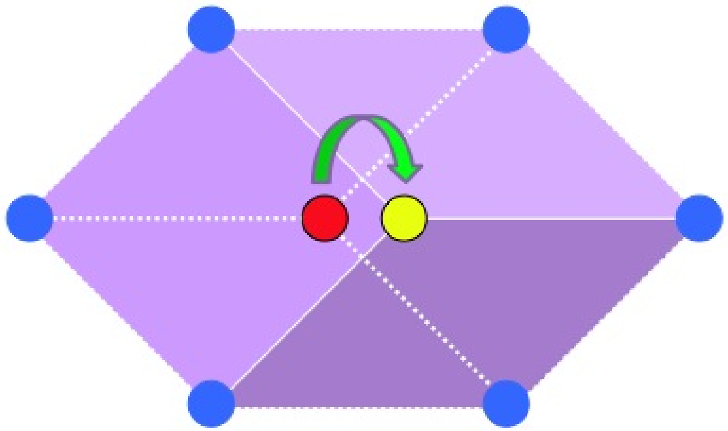
- Hence if a local patch corresponds to some *atomic species*, or to some local assembly of various atoms, the acceptance domain permits to measure its *stoichiometry*.

III.2)- Atomic Motion

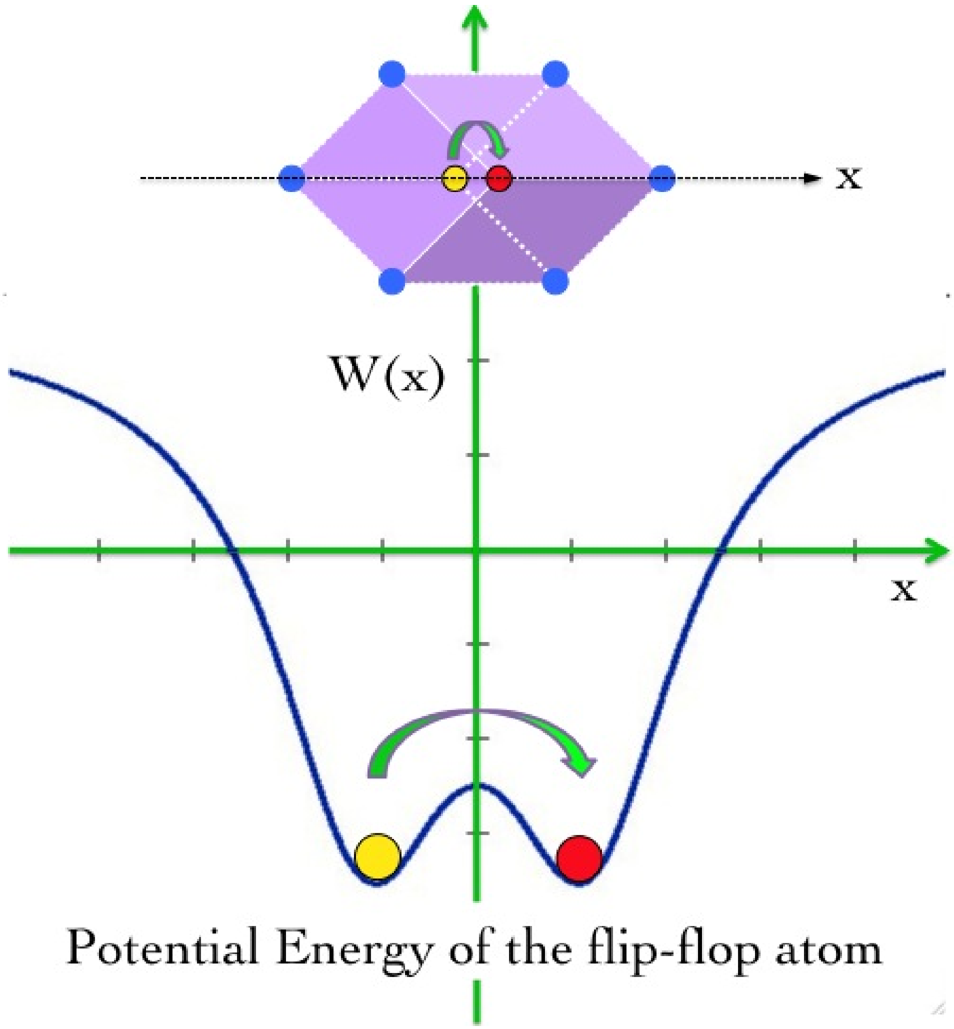
- In the limit of zero temperature, the tiling space represents the exact structure. Still atoms may move because of *flip-flops*.

Octagonal Lattice

$\boldsymbol{Z^4 \rightarrow R^2}$



Flip-Flops



Potential Energy of the flip-flop atom

III.2)- Atomic Motion

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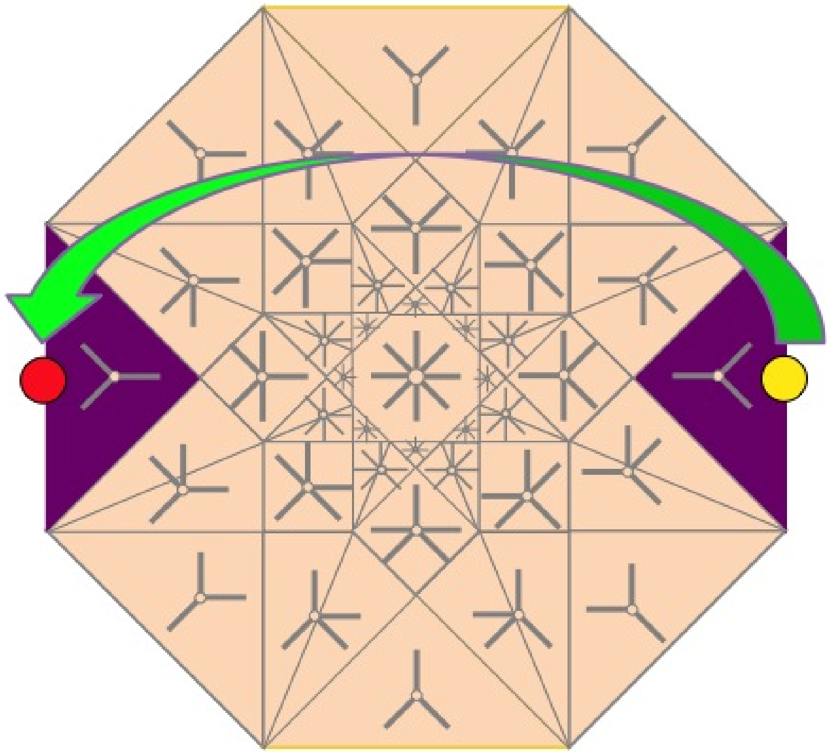
- This *atomic motion* in space corresponds to a motion in the *tiling space*.



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Under development !

Thanks for Listening !