WANNIER TRANSFORM

for

APERIODIC SOLIDS

Sponsoring

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Main References

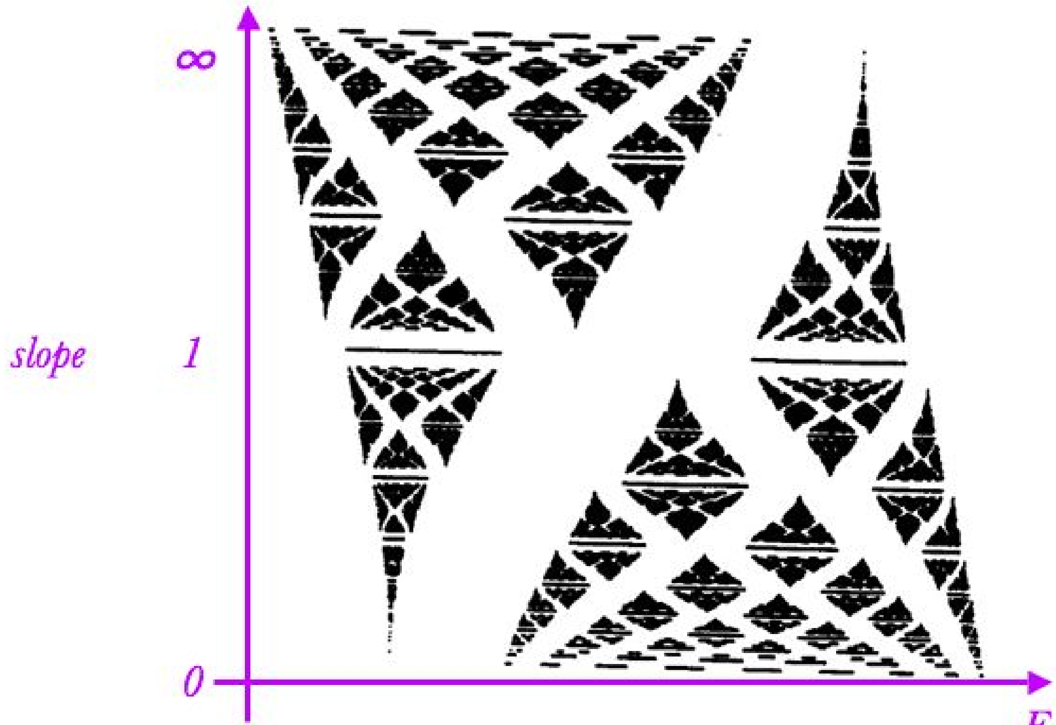
J. E. Anderson, I. Putnam,
Topological invariants for substitution tilings and their associated C^*-algebras,
Ergodic Theory Dynam. Systems, **18**, (1998), 509-537.

J. C. Lagarias,
Geometric models for quasicrystals I. Delone sets of finite type,
Discrete Comput. Geom., **21**, (1999), 161-191.

J. Bellissard, R. Benedetti, J. M. Gambaudo,
Spaces of Tilings, Finite Telescopic Approximations,
Comm. Math. Phys., **261**, (2006), 1-41.

J. Bellissard, G. De Nittis, V. Milani,
Wannier transform for aperiodic tilings,
in preparation, (2010)

Motivation



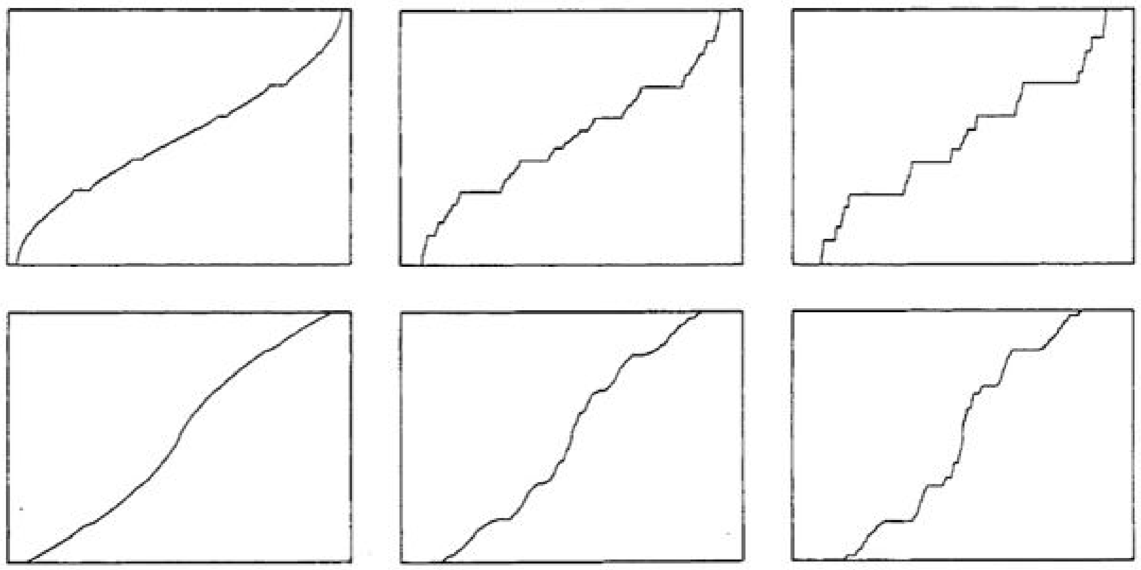
Energy spectrum for particle in a 1D-quasicrystal as a function of the slope in a cut-and-project scheme

Physica Scripta. Vol. T9, 193–198, 1985

Renormalization of Quasiperiodic Mappings

Stellan Ostlund and Seung-hwan Kim

Motivation



a) b) c)

Fig. 3. – We show, respectively, the IDOS of the Octonacci chain (up) and the IDOS of the labyrinth, for *a*) $r = 0.8$ (no gap, finite measure), *b*) $r = 0.6$ (some gaps and finite measure) and *c*) $r = 0.3$ (infinity of gaps and zero measure). The energy varies between -2 and 2, since $r < 1$.

C. SIRE

Electronic Spectrum of a 2D Quasi-Crystal Related to the Octagonal Quasi-Periodic Tiling.

EUROPHYSICS LETTERS

Europhys. Lett., 10 (5), pp. 483-488 (1989)

Motivation

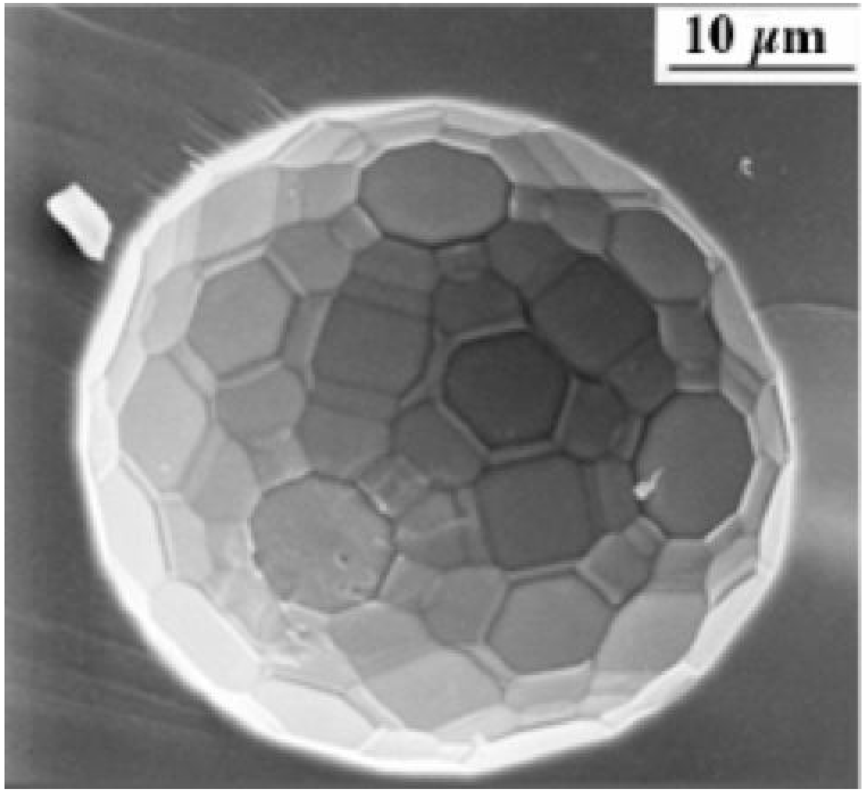
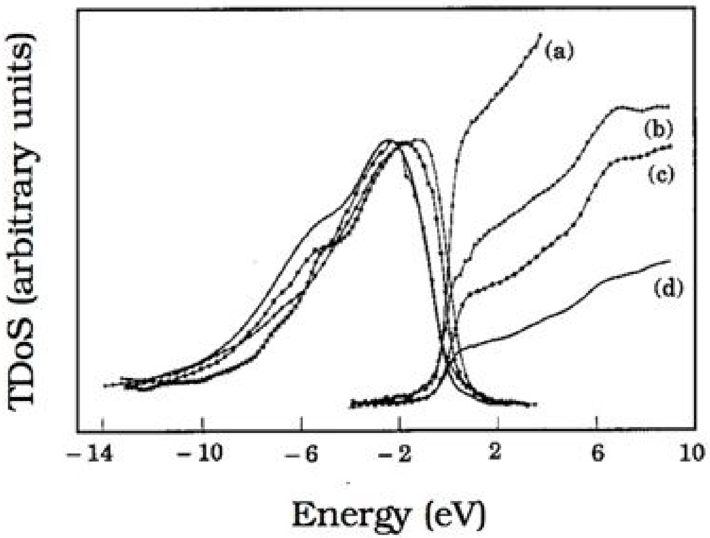


Figure 1: A sample of the icosahedral quasicrystal *AlPdMn*

Motivation

† = *Density of States*



Partial DoS† measured by SXES* or SXAS*

(a) Pure Al

(b) ω-Al_7Cu_2Fe

(c) Rhombohedral approximant $Al_{62.5}Cu_{26.5}Fe_{11}$

(d) Icosahedral phase $Al_{62}Cu_{25.5}Fe_{12.5}$

* = *Soft X-ray Emission or Absorption Spectroscopy*

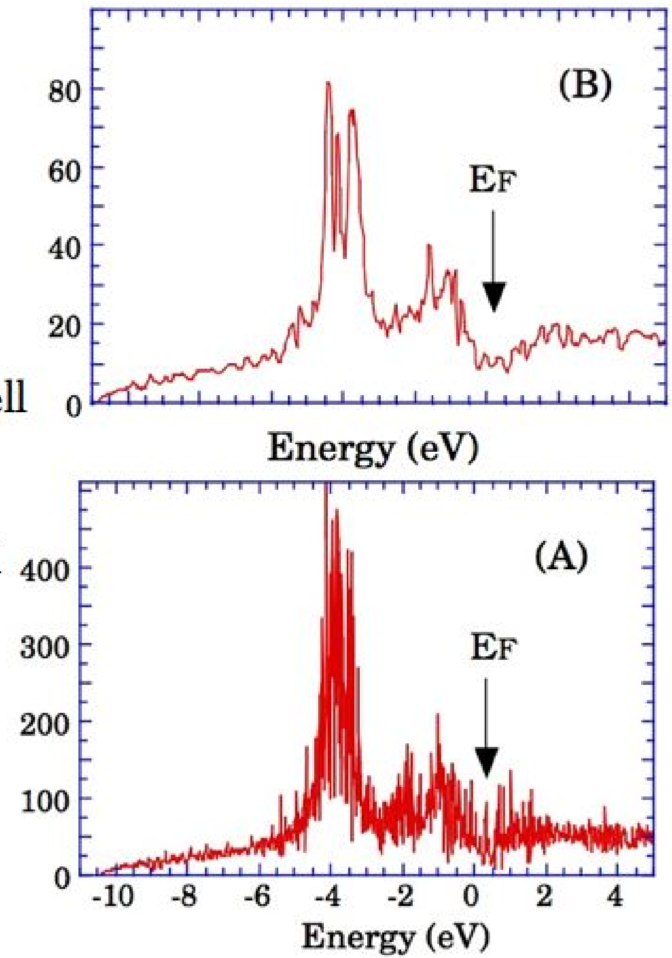
Motivation

DoS† for alloys with close composition

(A) Approximant 1/1
$Al_{62.5}Cu_{25}Fe_{12.5,}$ 128 atom/cell

(B) Non approximant
ω-Al_7Cu_2Fe 40 atom/cell

† = Density of States



Motivation

- For periodic crystals, the *Wannier transform* leads to band spectrum calculation *(Bloch theory)*

- The Wannier transform uses the translation invariance of the crystal

- Is it possible to extend it to *aperiodic solids* ?

Content

1. An example: Fibonacci
2. The Wannier Transform
3. The Schrödinger Operator
4. To conclude

I - An example: Fibonacci

The Fibonacci Sequence

The *Fibonacci sequence* is an infinite word generated by the substitution

$$\hat{\sigma}: \qquad a \longrightarrow ab\,, \qquad\qquad b \longrightarrow a$$

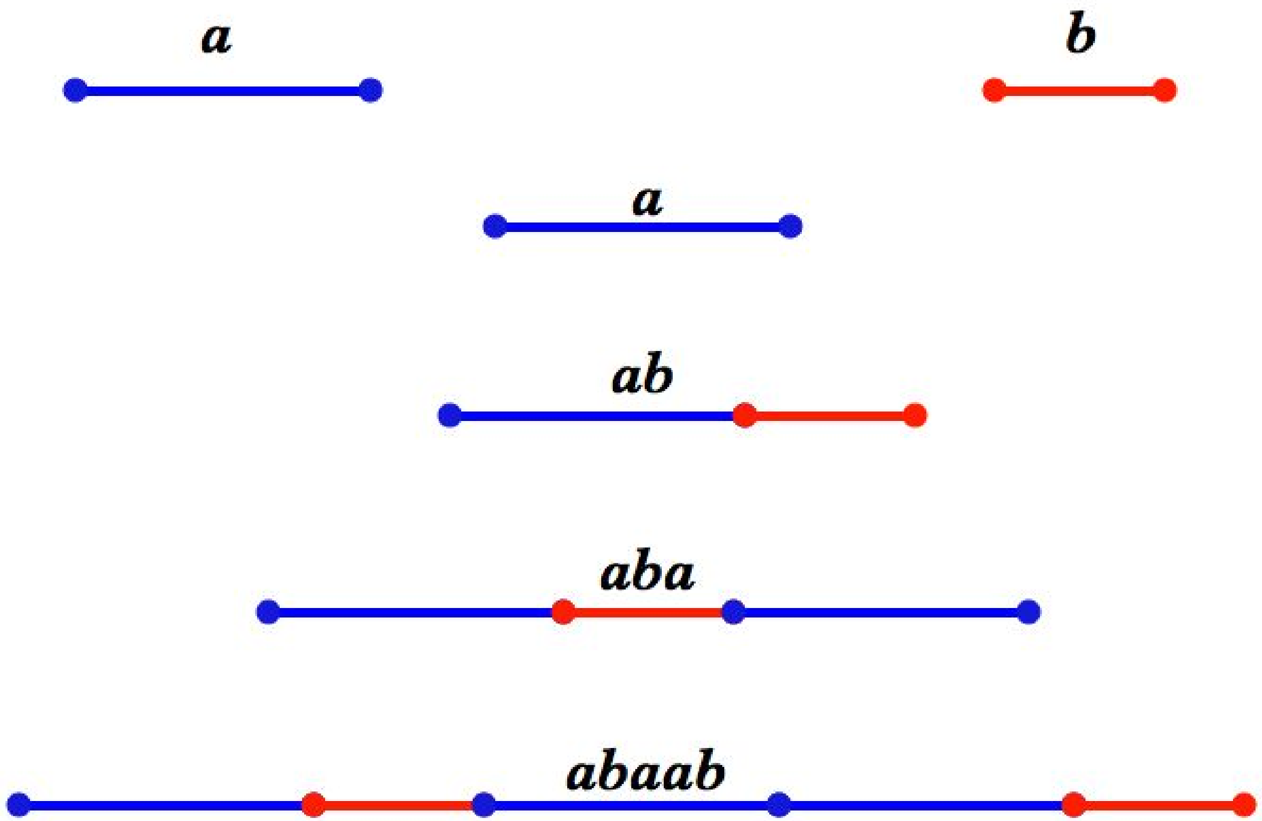
Iterating gives

$$\underbrace{a}_{a_0} \to \underbrace{ab}_{a_1} \to \underbrace{ab|a}_{a_2=a_1a_0} \to \underbrace{aba|ab}_{a_3=a_2a_1} \to \underbrace{abaab|aba}_{a_4=a_3a_2} \to \underbrace{abaababa|abaab}_{a_5=a_4a_3}$$

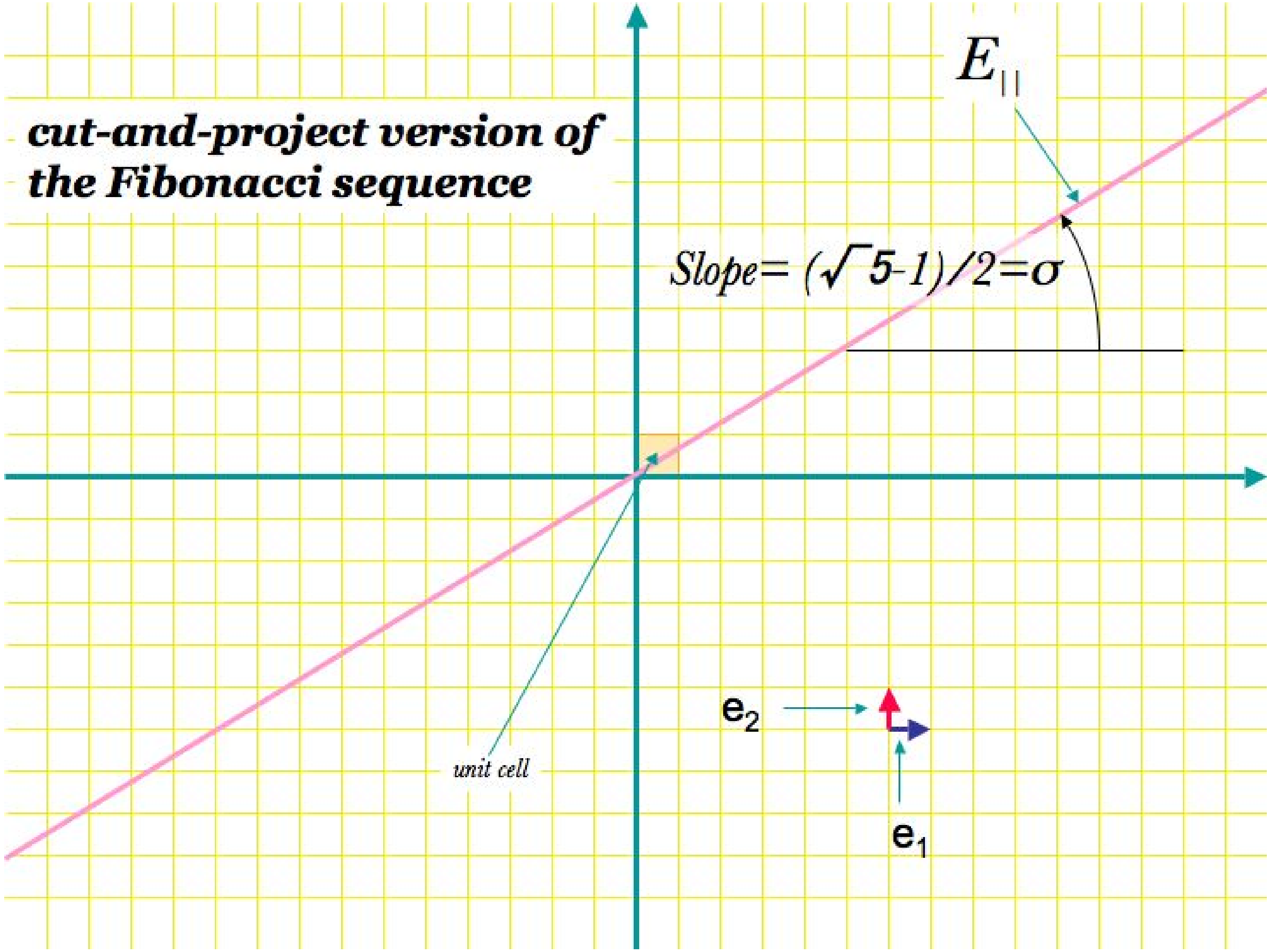
It can be represented by a $1D$*-tiling* if

$$a \to [0,1] \qquad b \to [0,\sigma] \qquad \sigma = \frac{\sqrt{5}-1}{2} \sim .618$$

The Fibonacci Sequence



The Fibonacci Sequence



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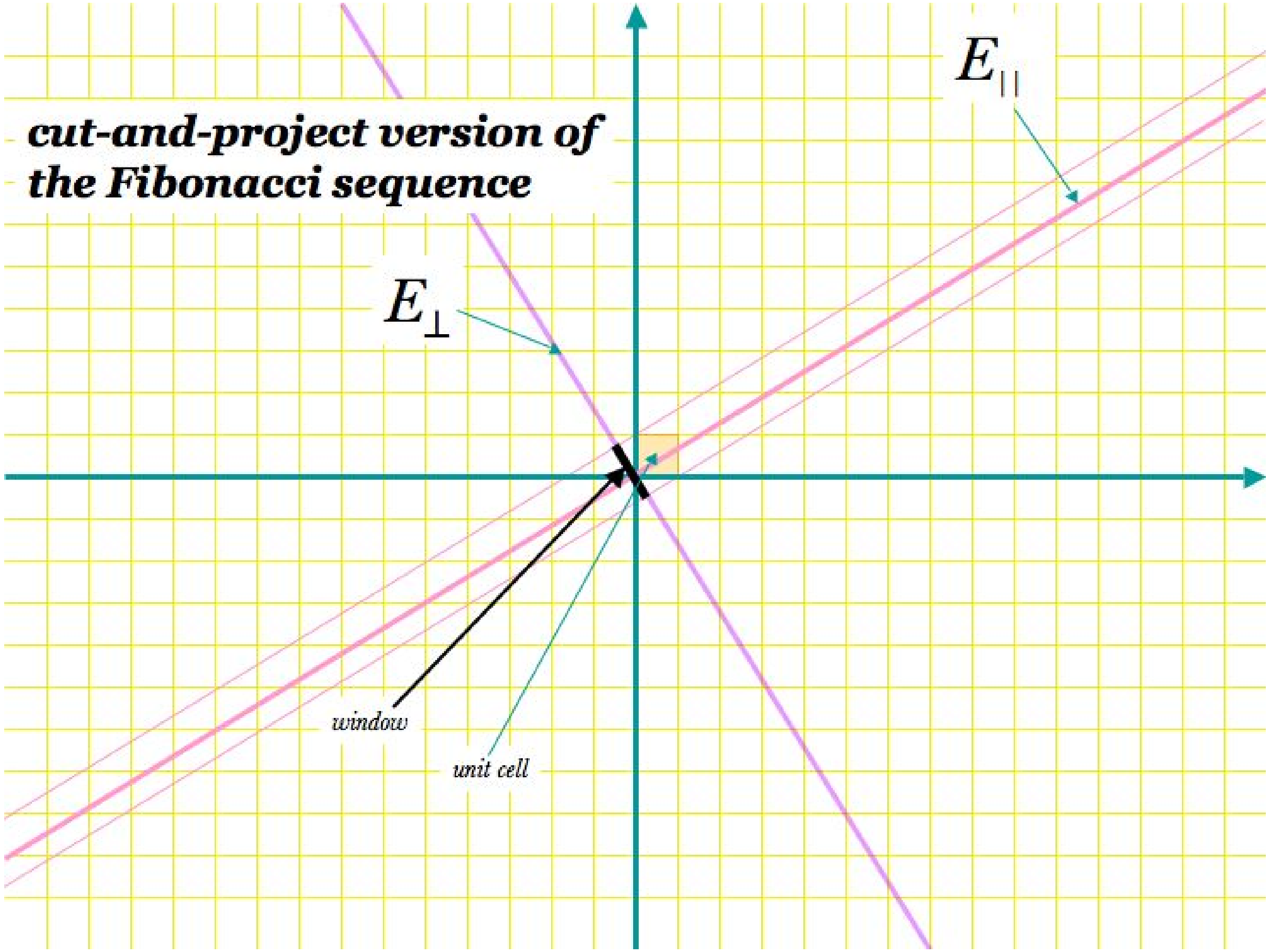

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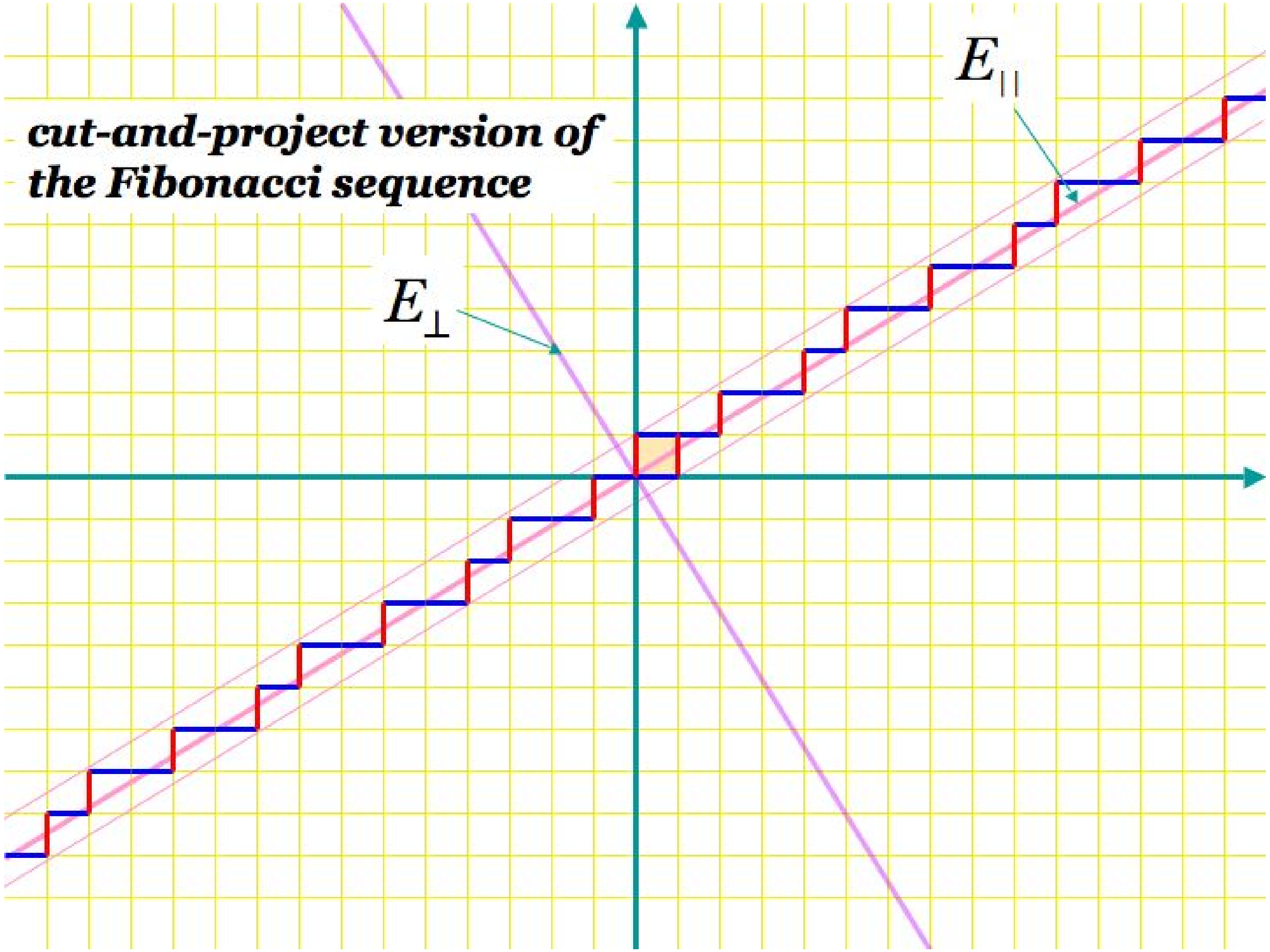

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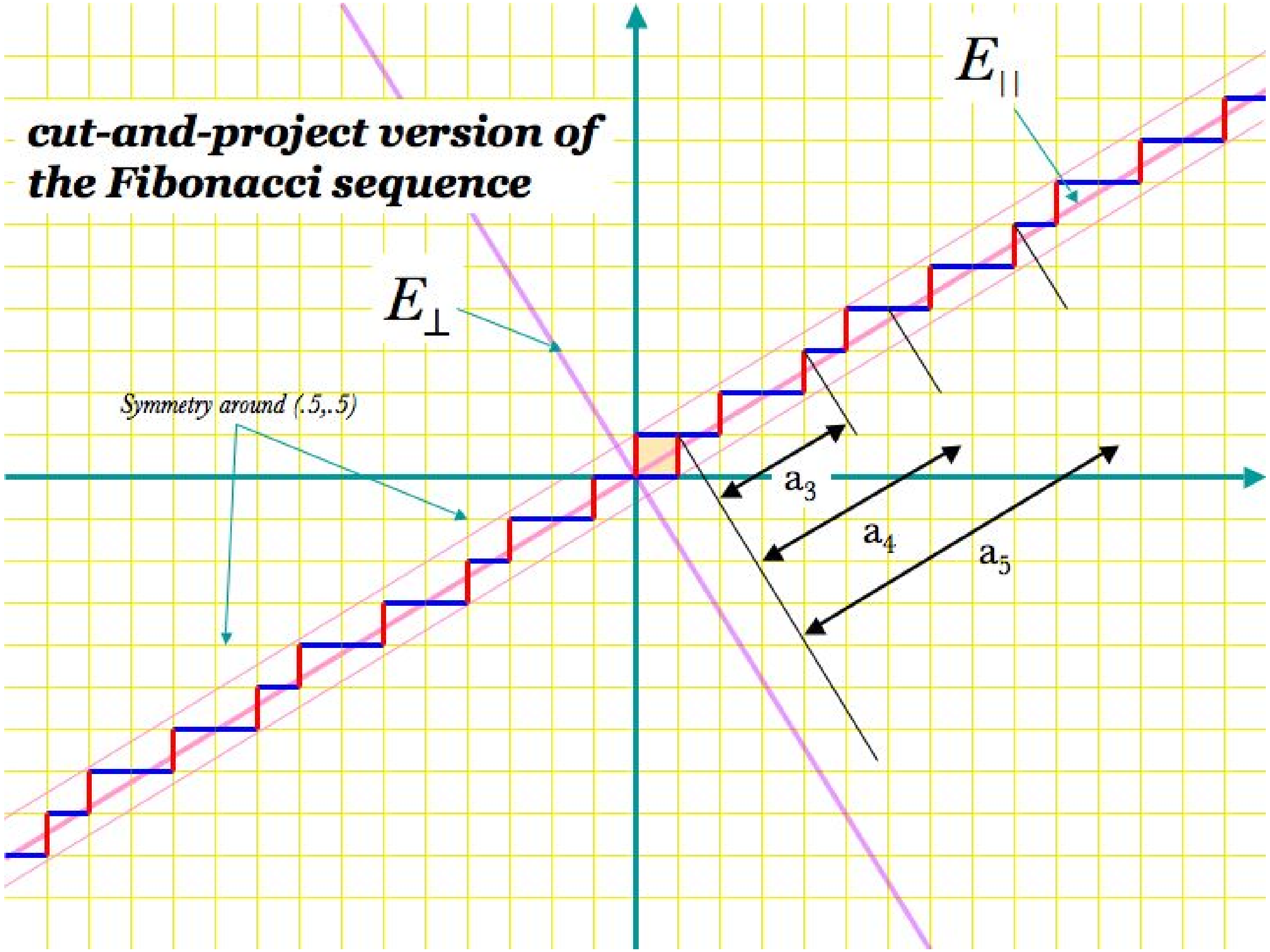
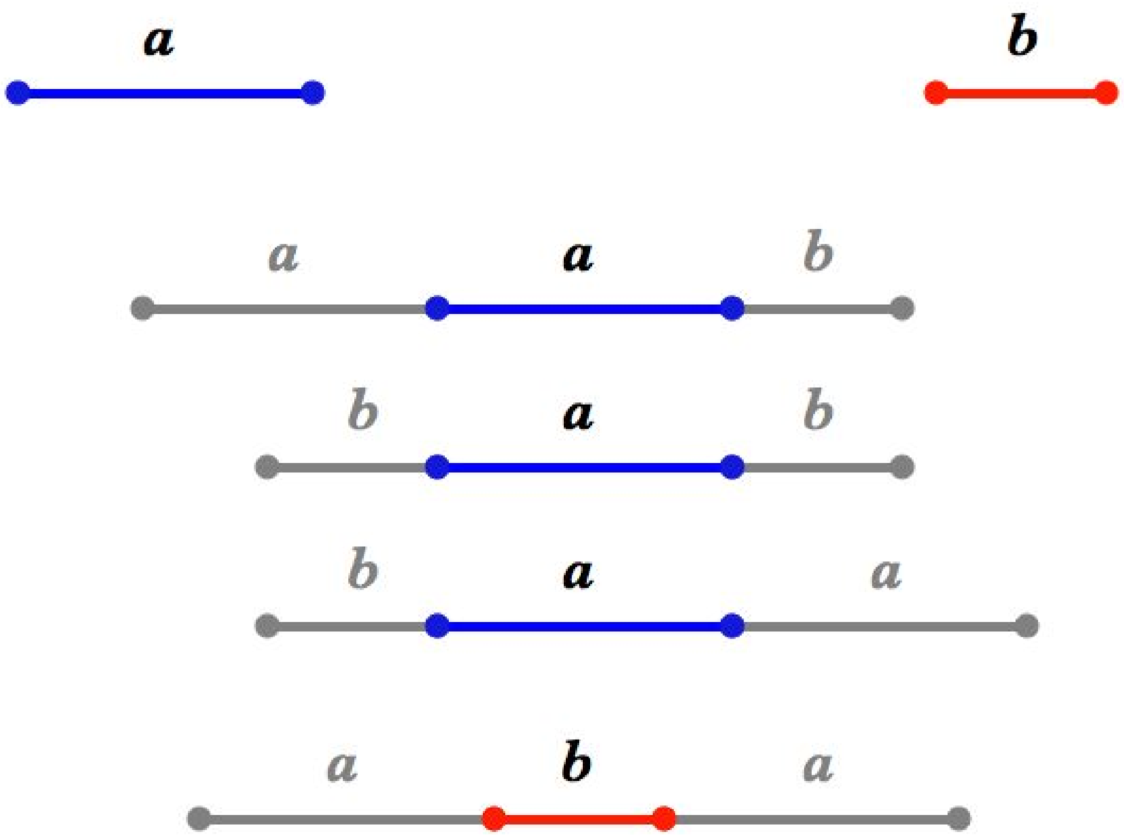
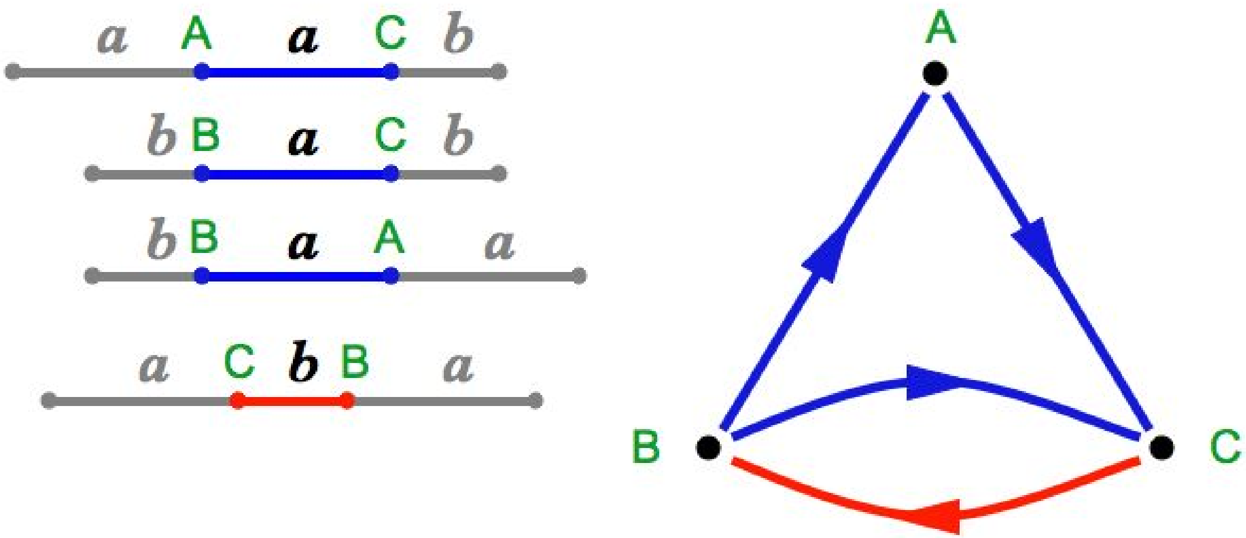


The Fibonacci Sequence



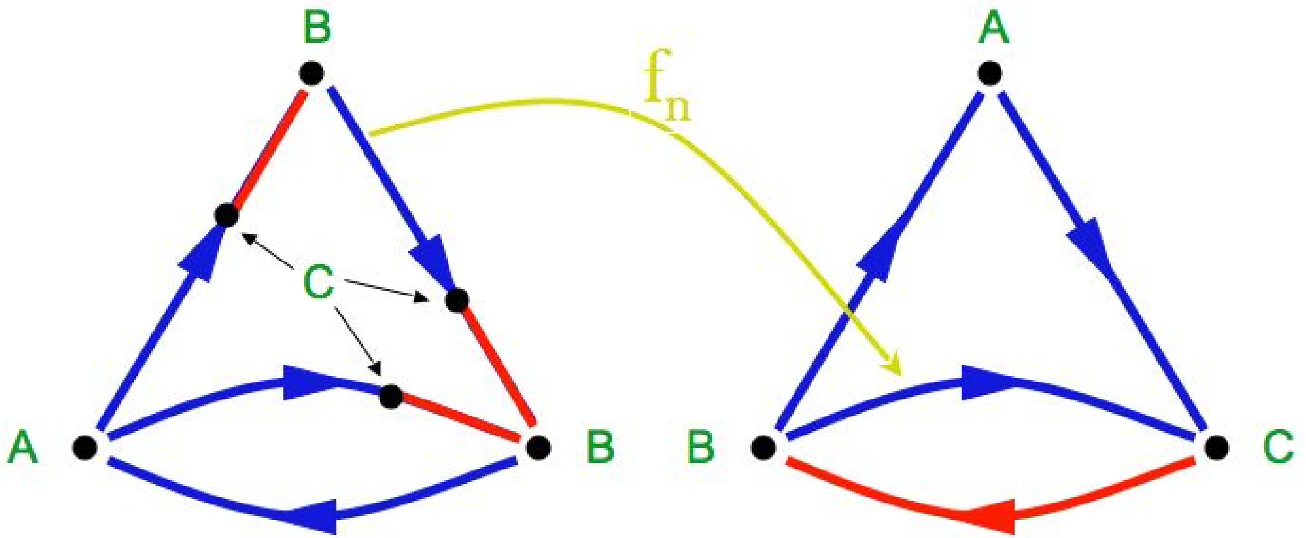
- Collared tiles in the Fibonacci tiling -

The Fibonacci Sequence



- The Anderson-Putnam complex for the Fibonacci tiling -

The Fibonacci Sequence



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

- The substitution map -

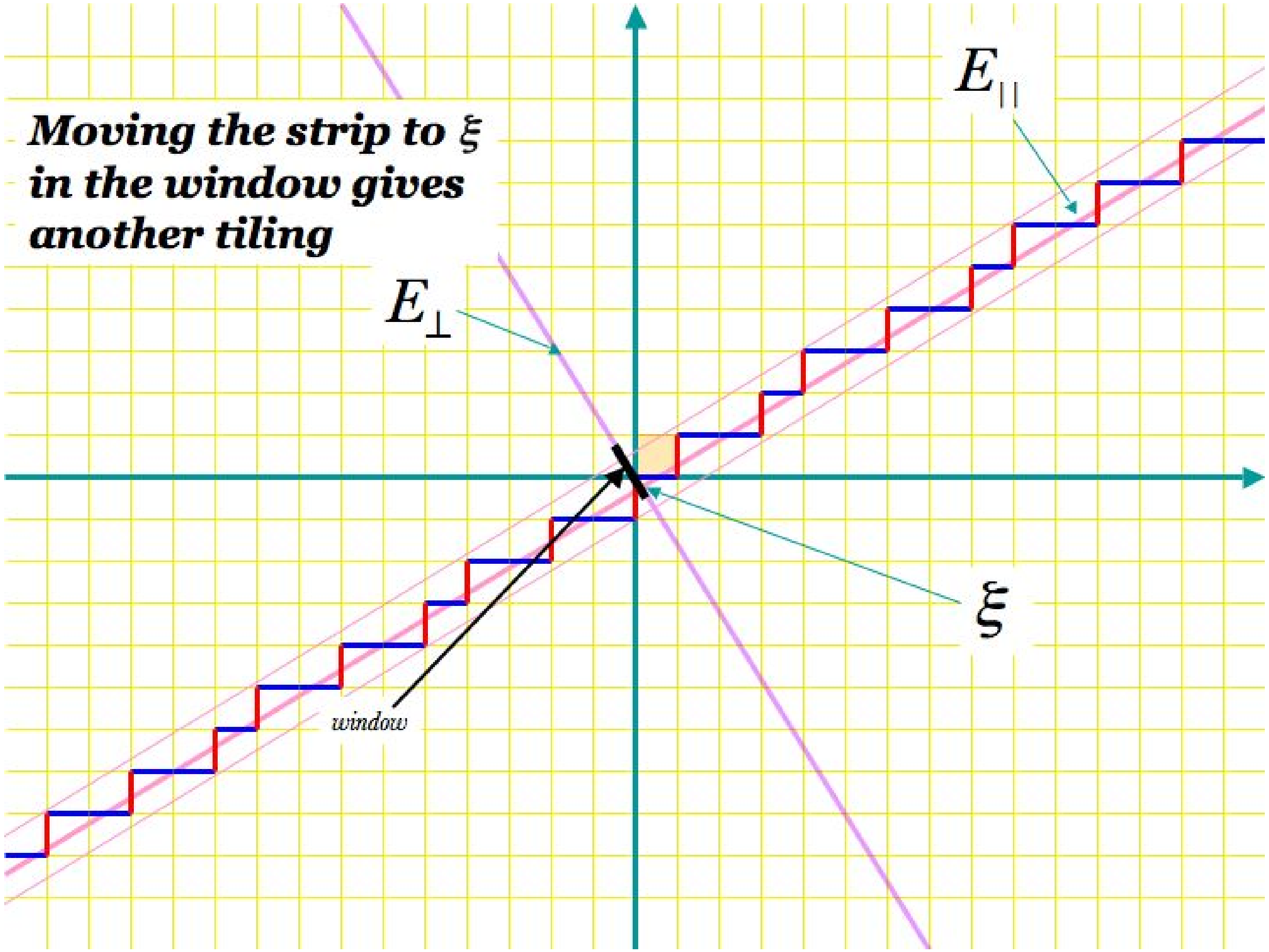
The Fibonacci Sequence

Let $\Xi_n \subset X_n$ be the set of *tile endpoints* (0-cells). The sequence of complexes $(X_n)_{n\in\mathbb{N}}$ together with the maps $f_n : X_{n+1} \mapsto X_n$ gives rise to inverse limits

$$\varprojlim(X_n, f_n) = \Omega \qquad \varprojlim(\Xi_n, f_n) = \Xi$$

- The space Ω is *compact* and is called the *Hull*.
- It is endowed with an *action* of $\mathbb{R}$ generated by infinitesimal translation on the X_n's
- The space Ξ is a Cantor set and is called the *transversal*
- Ξ parametrizes a the set of all tilings sharing the same words as the Fibonacci sequence with one tile endpoint at the origin.
- There is a *two-to one* correspondence between Ξ and the window.

The Fibonacci Sequence



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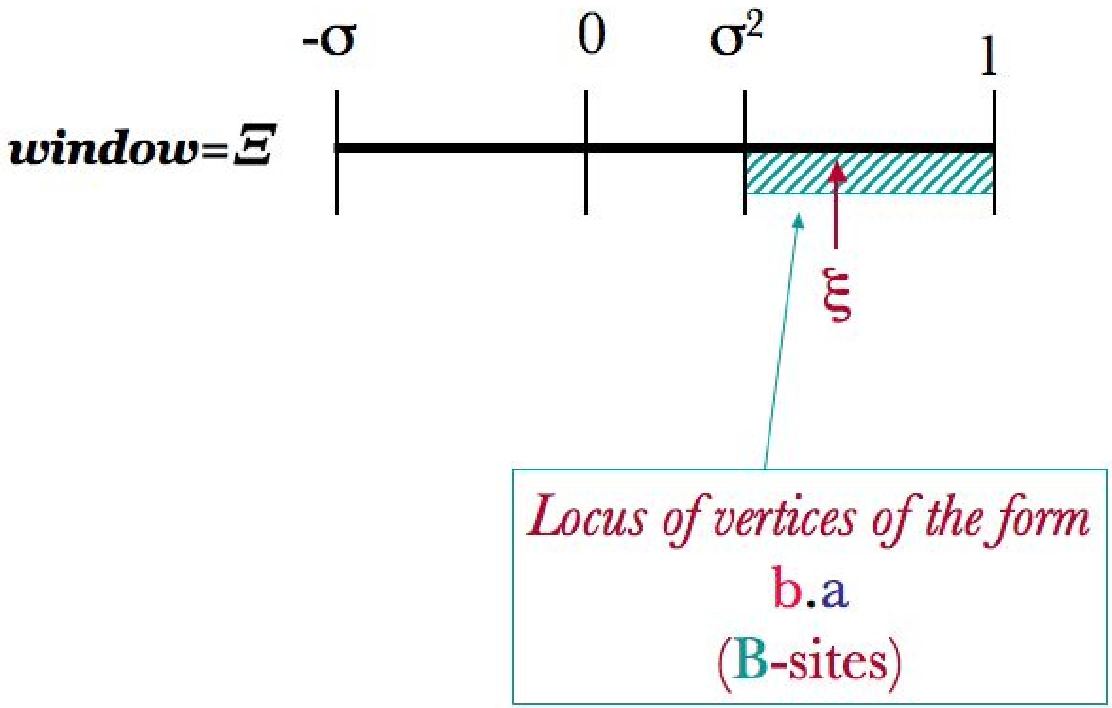
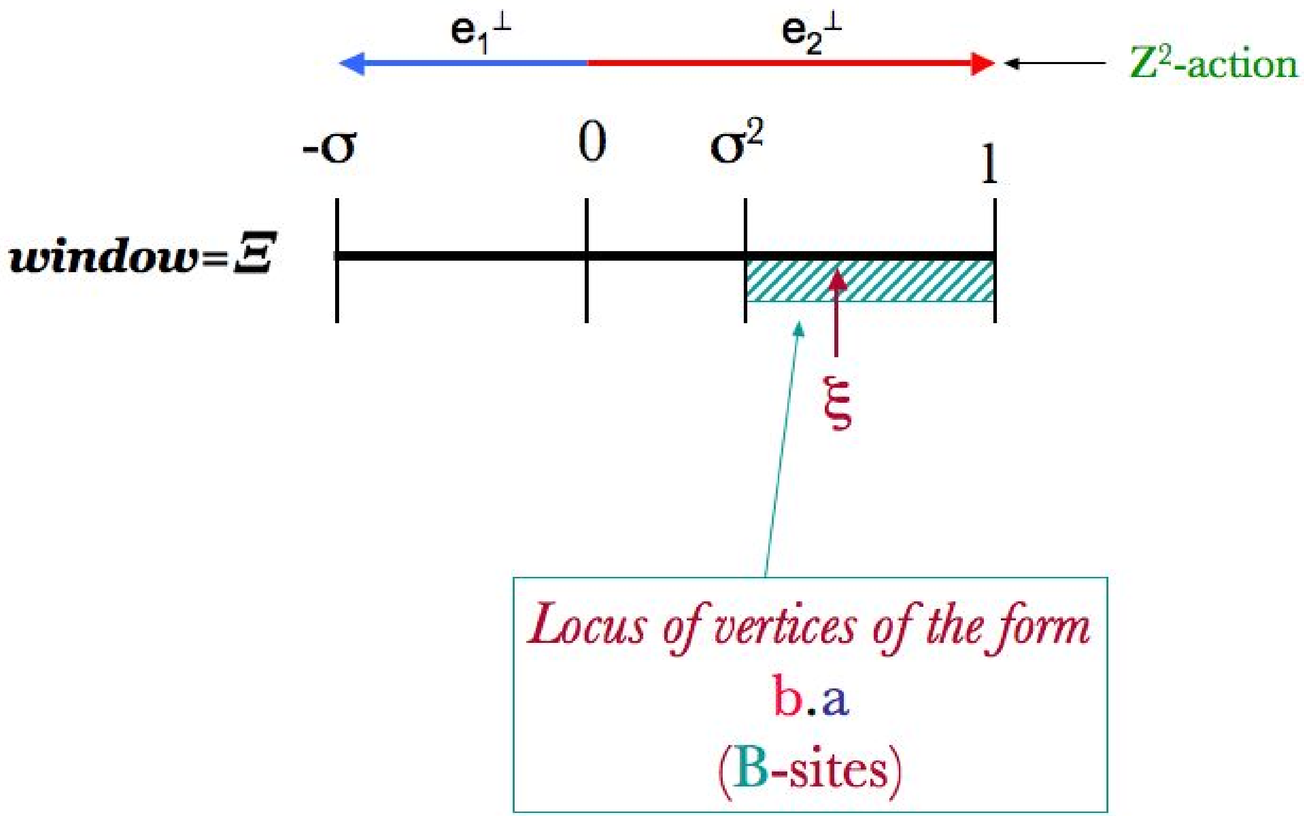
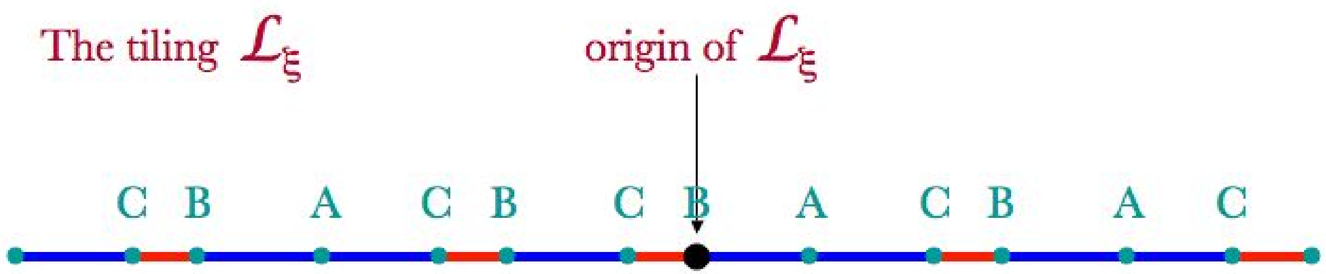


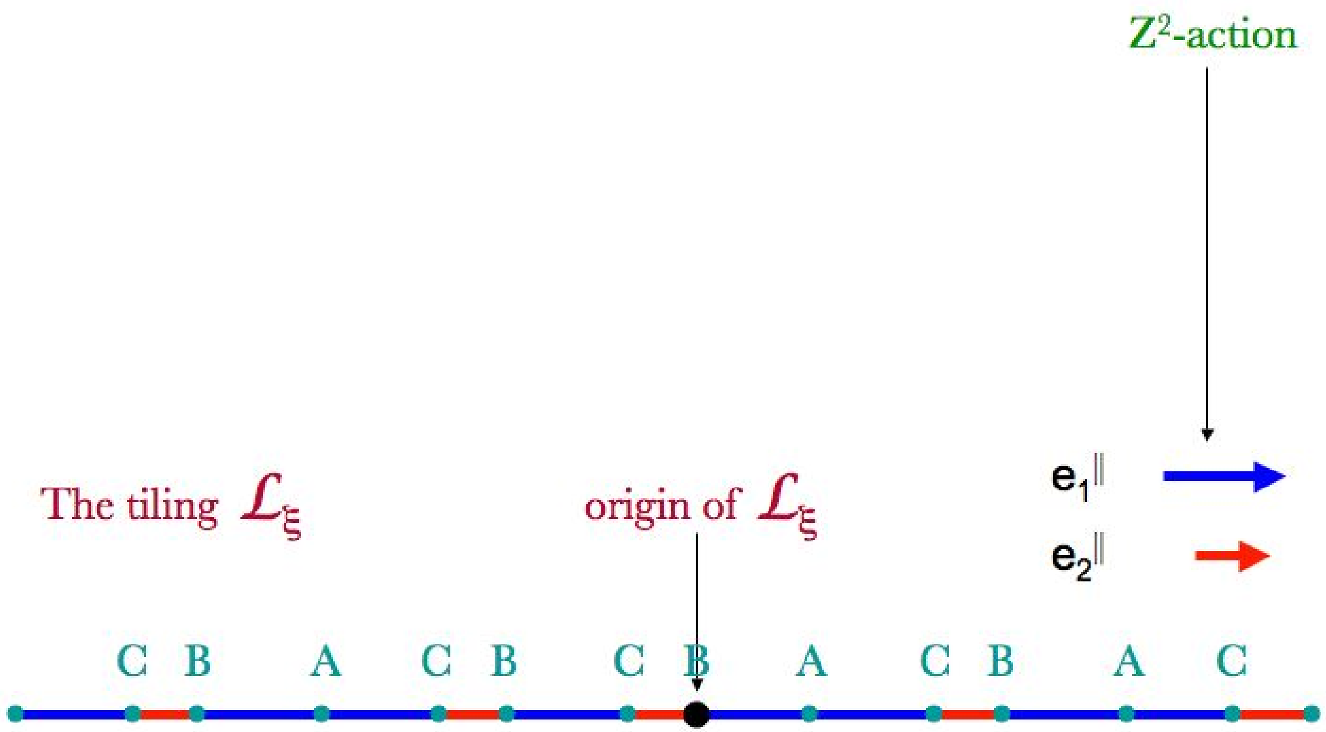
The Fibonacci Sequence



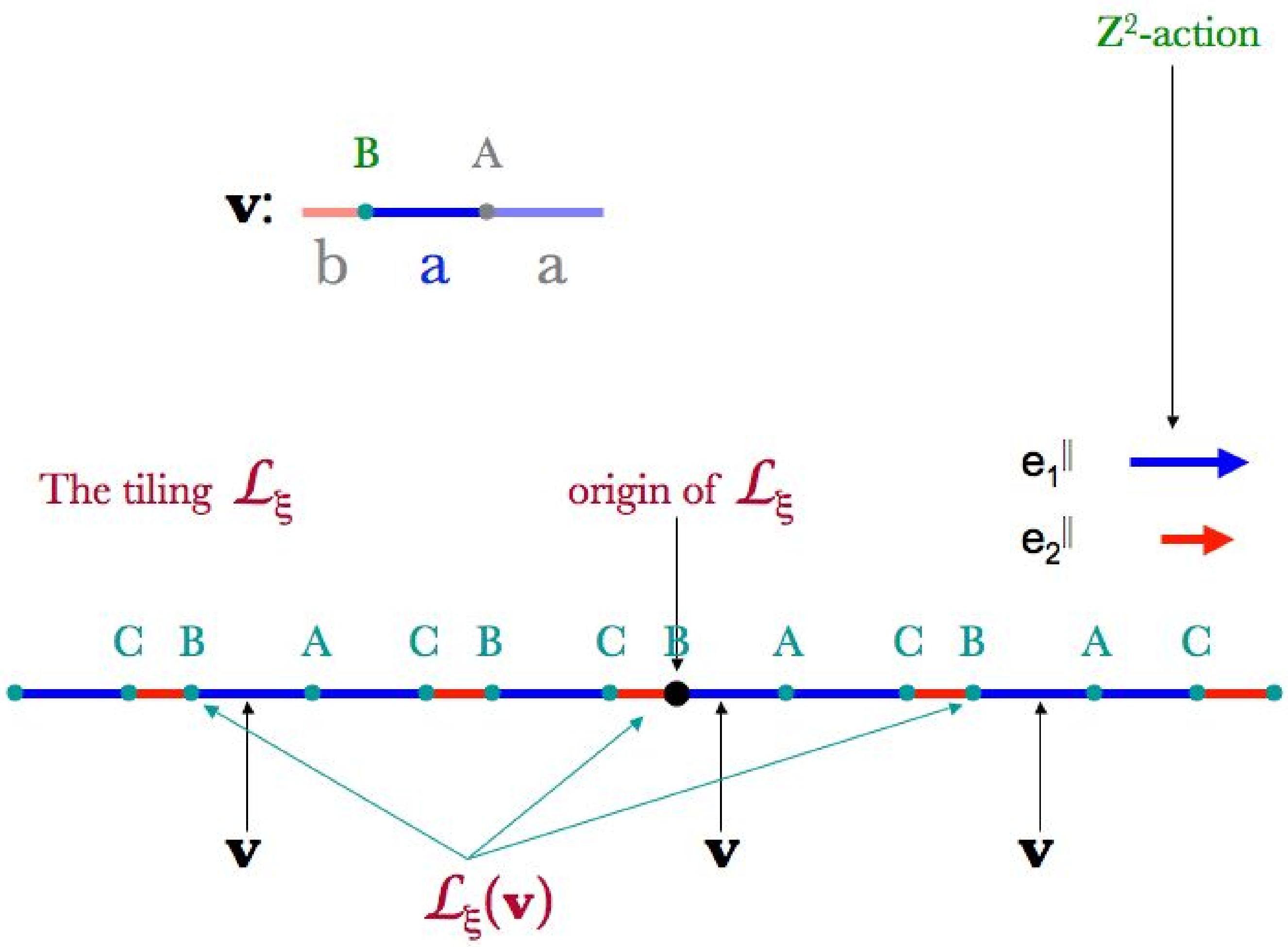
The Fibonacci Sequence



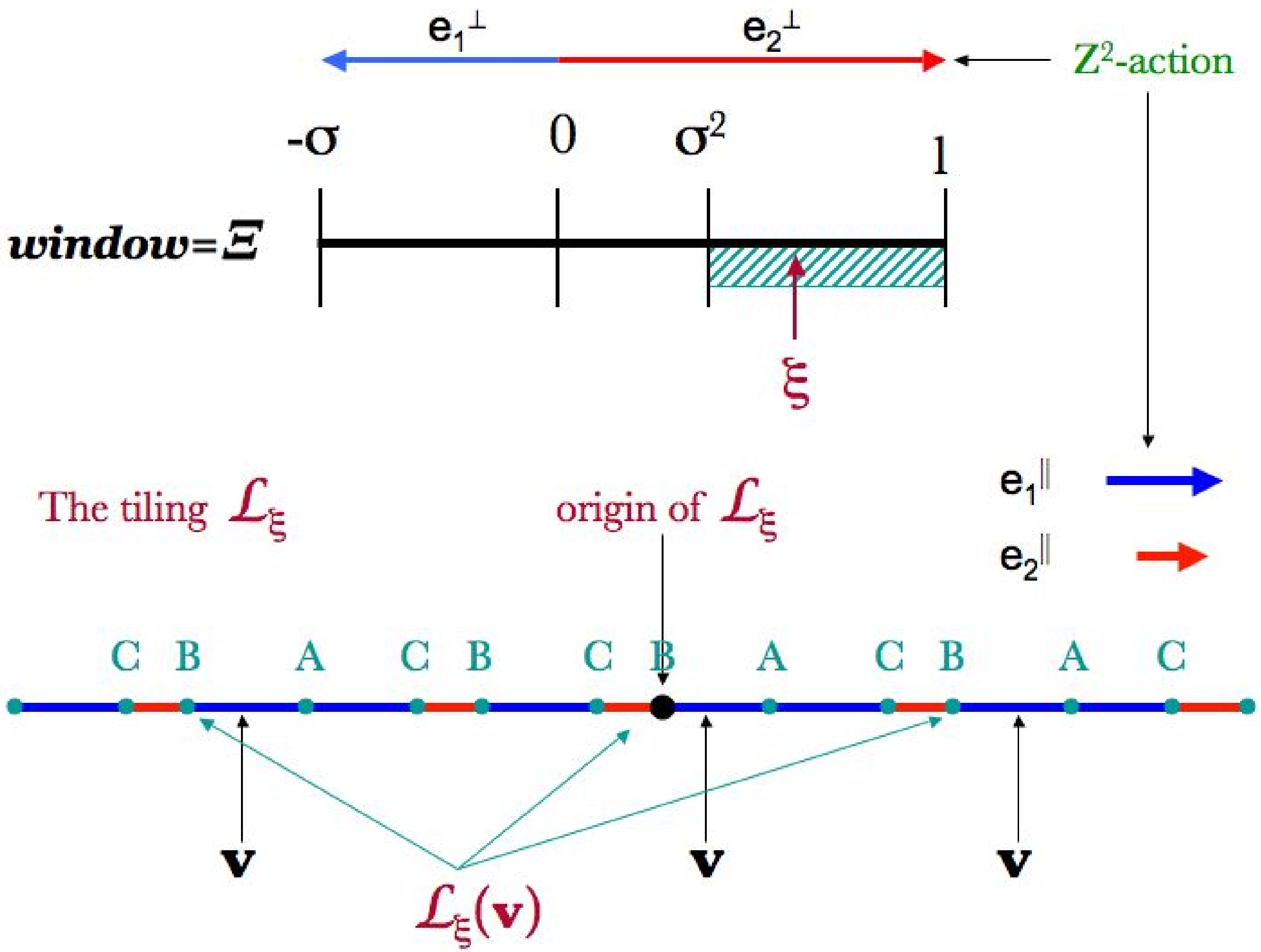
The Fibonacci Sequence



The Fibonacci Sequence



The Fibonacci Sequence



The Fibonacci Sequence: Groupoid

Γ_Ξ is the set of pairs (ξ, a) with $\xi \in \Xi$ and $a \in \mathcal{L}_\xi$.

It is a *locally compact groupoid* when endowed with the following structure

- **Units:** Ξ,
- **Range and Source maps:** $r(\xi, a) = \xi$, $s(\xi, a) = \mathrm{T}^{-a}\xi$
- **Composition:** $(\xi, a) \circ (\mathrm{T}^{-a}\xi, b) = (\xi, a+b)$
- **Inverse:** $(\xi, a)^{-1} = (\mathrm{T}^{-a}\xi, -a)$
- **Topology:** induced by $\Xi \times \mathbb{R}$

II - Wannier Transform

J. Bellissard, G. De Nittis, V. Milani,
Wannier transform for aperiodic tilings,
in preparation, (2010)

Wannier Transform: Periodic Case

If $\mathbb{Z} \subset \mathbb{R}$ is a one dimensional lattice the Wannier transform is defined for a *function* $f \in C_c(\mathbb{R})$ by

$$g(s;k) = \mathscr{W} f(s;k) = \sum_{a \in \mathbb{Z}} f(s+a)\, e^{-\imath k \cdot a}$$

Here k belongs to the dual group of $\mathbb{Z}$, called *Brillouin zone*

$$\mathbb{B} \sim \mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$$

- **Bloch boundary conditions:** $g(s+a;k) = g(s;k)e^{\imath k \cdot a}$ whenever $a \in \mathbb{Z}$.
- **Plancherel's formula:**

$$\int_0^1 ds \int_{\mathbb{T}} \frac{dk}{2\pi}\, |g(s;k)|^2 = \int_{\mathbb{R}} dx\, |f(x)|^2$$

.

- **Unitarity:** $\mathscr{W} : L^2(\mathbb{R}) \mapsto L^2([0,1]) \otimes L^2(\mathbb{T})$ is a *unitary operator*.

Wannier Transform: Definition

In the case of the Fibonacci sequence: $\xi \in \Xi$, $\mathcal{L}_\xi$ being the corresponding Delone set, $v = \hat{\sigma}^n(w)$ the n-th substitute of a *collared tile*. Denote by $\mathbb{B} \simeq \mathbb{T}^2$ the dual group of $\mathbb{Z}^2$.

Then, for $s \in \mathbb{R}$ and $k \in \mathbb{B}$ the *Wannier transform* of a *function* $f \in C_c(\mathbb{R})$ is

$$\boxed{\mathcal{W}_\xi f(v, s; k) = \sum_{a \in \mathcal{L}_\xi(v)} f(s+a) e^{-\imath k \cdot a}}$$

Wannier Transform: Properties

- **Smoothness:** if f is *smooth*, then

$$\mathscr{W}_\xi\left(\frac{d^k f}{dx^k}\right) = \frac{\partial^k \mathscr{W}_\xi f}{\partial s^k}$$

- **Covariance:** if $g = \mathscr{W} f$ then

$$g_\xi(v, s+b; k) = g_{\mathrm{T}^b \xi}(v, s; k)\, e^{\imath k \cdot b} \qquad b \in \mathcal{L}_\xi$$

- **Inversion:** if dk denotes the *normalized Haar measure* on $\mathbb{B}$

$$f(s+a) = \int_{\mathbb{B}} dk g_\xi(v, s; k)\, e^{\imath k \cdot a} \qquad a \in \mathcal{L}_\xi, s \in \mathbb{R}$$

Wannier Transform: Momentum Space

Let $\mathcal{E}_\xi(v) \subset L^2(\mathbb{B})$ be the closed subspace generated by

$$\{e_a : k \in \mathbb{B} \mapsto e^{-\imath k\cdot a} \; ; \; a \in \mathcal{L}_\xi\}$$

- $\mathcal{E}(v) = \big(\mathcal{E}_\xi(v)\big)_{\xi\in\Xi}$ is a *continuous field* of Hilbert spaces.
- If $W_v(\xi, a) : \mathcal{E}_{T^{-a}\xi}(v) \mapsto \mathcal{E}_\xi(v)$ is defined by

$$W_v(\xi, a)e_b = e_{a+b}$$

  then the family $(W_v(\gamma))_{\gamma\in\Gamma_\Xi}$ defines a *strongly continuous unitary representation* of the groupoid Γ_Ξ.

Wannier Transform: Momentum Space

- Define $\mathcal{H}_\xi = \bigoplus_v L^2(v) \otimes \mathcal{E}_\xi(v) \subset L^2(X_n) \otimes L^2(\mathbb{B})$ where v varies among the *d-cells* of the Anderson-Putnam complex.

- Let $\Pi_\xi : L^2(X_n) \otimes L^2(\mathbb{B}) \mapsto \mathcal{H}_\xi$ be the corresponding *orthogonal projection*.

- $\mathcal{H} = \left(\mathcal{H}_\xi\right)_{\xi \in \Xi}$ is a continuous field of Hilbert spaces.

- Similarly $U(\gamma) = \bigoplus_v \mathbf{1}_v \otimes W_v(\gamma)$ defines a strongly continuous unitary representation of the groupoid Γ_Ξ on $\mathcal{H}$.

Wannier Transform: Plancherel

- The Wannier transform is a *strongly continuous field of unitary operators* defined on the constant field $L^2(\mathbb{R})$ with values in $\mathcal{H}$

$$\int_{\mathbb{R}} dx\, |f(x)|^2 = \sum_{v} \int_{v} ds \int_{\mathbb{B}} dk\, |\mathscr{W}_{\xi} f(v, s; k)|^2$$

- The Wannier transform is *covariant*:

$$U(\xi, a)\, \mathscr{W}_{\mathrm{T}^{-a}\xi} = \mathscr{W}_{\xi}\, U_{\mathrm{reg}}(a)$$

where U_{reg} is the usual action of the translation group $\mathbb{R}$ in $L^2(\mathbb{R})$.

III - Schrödinger's Operator

J. Bellissard, G. De Nittis, V. Milani,
Wannier transform for aperiodic tilings,
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The Schrödinger Operator: Model

As an example let an *atomic nucleus* be placed is each tile, namely sites in $\mathcal{L}_\xi$. The atomic species are labeling the tiles. The corresponding *atomic potential* has compact support small enough to be contained in one tile

$$V_\xi(x) = \sum_{v} \sum_{a \in \mathcal{L}_\xi(v)} v_{\mathrm{at}}^{(v)}(x - a)$$

The *Schrödinger operator* describing the electronic motion is then a covariant family

$$H_\xi(x) = -\Delta + V_\xi$$

The Schrödinger Operator: Form

If $f \in C_c^1(\mathbb{R})$ then, like in the *Bloch Theory* for periodic potentials

$$Q_\xi(f,f) = \langle f | H_\xi f \rangle_{L^2(\mathbb{R})}$$

$$= \sum_v \int_v ds \int_{\mathbb{B}} dk \left(\left| \nabla_s \mathscr{W}_\xi f(v,s;k) \right|^2 + v_{\text{at}}^{(v)}(s) \left| \mathscr{W}_\xi f(v,s;k) \right|^2 \right)$$

$$= \int_{\mathbb{B}} dk \, \hat{Q}_k \left((\mathscr{W}_\xi f)_k, (\mathscr{W}_\xi f)_k \right)$$

with

$$\hat{Q}_k(g,g) = \sum_v \int_v ds \left(|\nabla_s g(v,s)|^2 + v_{\text{at}}^{(v)}(s) |g(v,s)|^2 \right)$$

The Schrödinger Operator: Form

A function g belongs to the *form domain* of $\hat{Q}_k$ if and only if

1. both $g(v, s)$ and its derivative are in $L^2(v)$ for all $(d = 1)$-*cell* v

2. g satisfies the following *cohomological equation*:
   at each $(\{d - 1\} = 0)$-*cell* u of the Anderson-Putnam complex

$$\sum_{v:\partial_0 v = u} g(v, u) e^{\imath k \cdot a_{\hat{v} \to v}} = \sum_{w:\partial_1 v = u} g(w, u) e^{\imath k \cdot a_{\hat{v} \to w}}$$

   where $a_{v \to w}$ is the *translation* vector sending the initial point of v the initial point of w, and $\hat{v}$ is one tile touching u.

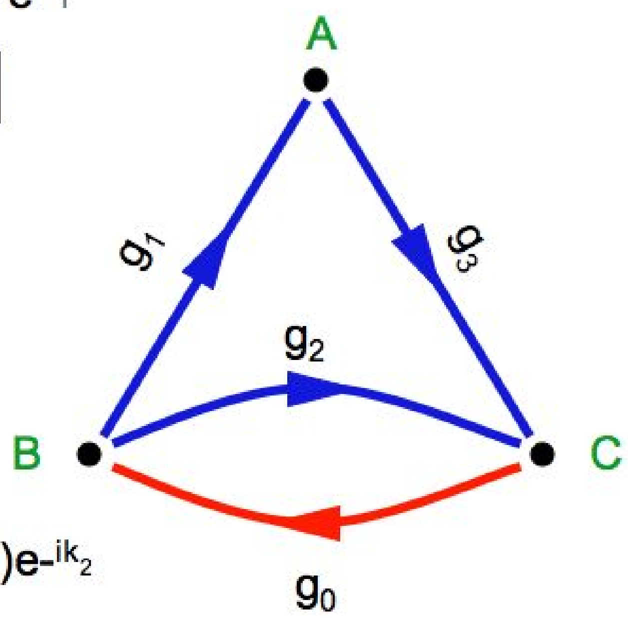
The Schrödinger Operator: Form

A : $g_3(s=0) = g_1(s=1)\, e^{ik_1}$

B : $g_1(s=0)+ g_2(s=0) = g_0(s=\sigma)e^{ik_2}$

C : $g_0(s=0) = (g_2(s=1)+ g_3(s=1))\, e^{ik_1}$

$$\boxed{-g''_j(s)+v_j(s)\, g_j(s) = E(k)\, g_j(s)}$$



A : $g'_3(s=0) = g'_1(s=1)\, e^{i\text{-}k_1}$

B : $g'_1(s=0) = g'_2(s=0) = g'_0(s=\sigma)e\text{-}^{ik_2}$

C : $g'_0(s=0) = g'_2(s=1)\, e^{-ik_1}$

$= g'_3(s=1))\, e^{-ik_1}$

The Schrödinger Operator: Bands

The form $\hat{Q}_k$ generates a selfadjoint operator $\hat{H}_k$ defined by

$$\langle g|\hat{H}_k\, g\rangle_{L^2(X_n)} = \hat{Q}_k(g,g)$$

On each d-cell v, $\hat{H}_k = -\Delta_s + v_{\mathrm{at}}^{(v)}$, with *k-dependent boundary conditions*.

Since a cell is *compact* it follows that $\hat{H}_k$ is *elliptic*, thus it has *compact resolvent*. In particular its spectrum is *discrete* with finite multiplicity, namely its eigenvalues are

$$E_0(k) \leq E_1(k) \leq \cdots \leq E_r(k) \leq \cdots$$

with each $E_r(k)$ a *smooth function* of $k \in \mathbb{B}$.

The Schrödinger Operator: Bands

What is the connection with the original operator ?

Theorem *The Schrödinger operator H_ξ is given by*

$$H_\xi = \Pi_\xi \int_{\mathbb{B}}^{\oplus} dk \, \hat{H}_k \, \Pi_\xi$$

if Π_ξ is the orthogonal projection from $L^2(X_n) \otimes L^2(\mathbb{B})$ onto $\mathcal{H}_\xi$.

The restriction to the subspace $\mathcal{H}_\xi$ is NOT INNOCENT and reduces the band spectrum to produce a Cantor spectrum in the one-dimensional cases.

IV - To Conclude

1. The Fibonacci sequence can be replaced by *aperiodic, repetitive tilings* on $\mathbb{R}^d$ with *finite local complexity*. The Hull and the transversal are well-defined.
2. The *Lagarias group* $\mathbb{L}$ plays the role of $\mathbb{Z}^2$ in general. It is always free with finite rank. Then $\mathbb{B}$ is the group dual to $\mathbb{L}$.
3. The definition of the *Wannier transform* can be extended to this case
4. The sequence of *Anderson-Putnam complexes* $(X_n)_{n\in\mathbb{N}}$ can be defined in this general case as well.
5. The Wannier transform identifies wave functions in $L^2(\mathbb{R}^d)$ with a *proper subspace* of $L^2(X_n) \otimes L^2(\mathbb{B})$
6. The Schrödinger operator can be written in terms of this new representation as the *compression* of a Bloch-type operator exhibiting band spectrum.