Wannier Transform for Quasicrystals

preliminary results

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Outline

[1925-1926] Birth of (modern) Quantum Mechanics:

W. Heisenberg (matrix mechanics) and E. Schrödinger (wave mechanics).

[1928] Birth of modern (or Quantum) Theory of Solids:

F. Bloch (PhD thesis, supervisor Heisenberg).

[1928 - today] Consequence of Bloch's theory:

- conductivity properties: band-gap structure of the energy spectrum, conduction/valence band, Fermi level, etc.;
- Bethe-Sommerfeld conjecture: proved in many cases;
- thermodynamic properties: density of states, absolute continuity of the spectrum, etc.;
- semiclassical models: tight-binding models (Wannier functions), Peierls substitution, etc.;
- topological quantization: QHE, piezoelectricity, de Hass-van Alphen effect, etc.;

[1984] Discovery of the first quasicrystal:

D. Shechtman *et al.*

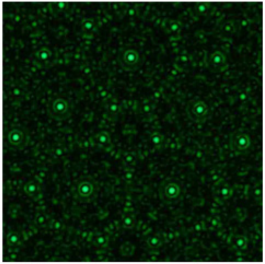
- A Crystal is a d(=3) dimensional periodic arrangement of atoms with translational periodicity along its principal axes.
  - 230 Fyodorov groups (rotations, reflections, inversions, translations)
  - 32 point groups (without translations)
  - 11 Laüe groups (center of symmetry)
  - 5 rotational symmetries (2, 3, 4, 6-fold) $\equiv$ CR-Theorem

Laüe groups $\equiv$ (X-ray, electron, ect.) diffraction patterns.

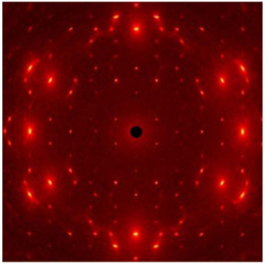
- In 1984, Shechtman, Blech, Gratias and Cahn showed a diffraction patterns (of an Al-Mn alloy) with 10-fold symmetry (forbidden by CR-Th).

- Many stable and meta-stable quasicrystals have been found:
  - pointlike diffraction patterns (like in a perfect crystal),
  - forbidden symmetry (5, 8, 10, 12-fold),
  - Long-range order (*Keyword*).

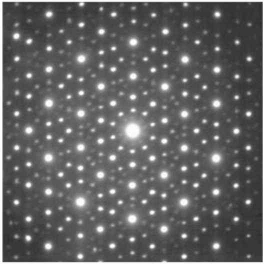
Diffraction Pattern



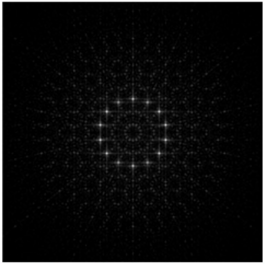
5-fold sym. (arrays of nanoholes)
[F. Huanga et al., Appl. Phys. Lett., 90, 2007]



8-fold sym. (Sc-Zn alloy)
[American Physical Society]

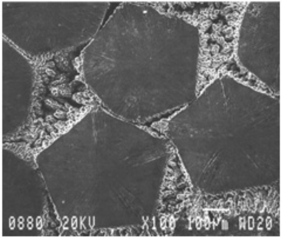


10-fold sym. (Zn-Mg-Ho alloy)
[Wikimedia, Materialscientist]

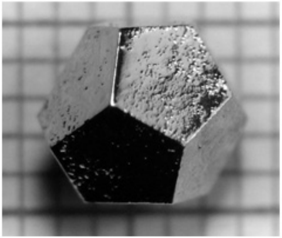


14-fold sym. (simulated patterns, 7 plane waves)
[M. Rule, http://spacecollective.org]

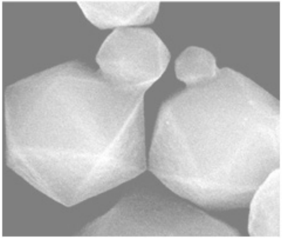
Scanning Electron Micrographs



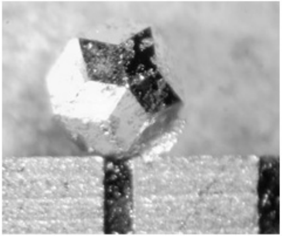
5-fold symmetric-QC (Al-Cu-Ru)
[C. Politis et al., Mod. Phys. Lett. B 3, 1989]



Dodecahedral-QC (Ho-Mg-Zn)
[AMES lab., US Department of Energy]



Icosahedral-QC (composite silica spheres)
[A. van Blaaderen, Nature 461, 2009]



Rhombic triacontahedral-QC (Tb-Mg-Cd)
[T. Huie, JYI 8, 2003]

Modeling of quasicrystals: "D-set" $\mathscr{L} \subset \mathbb{R}^d$

i) Discrete and aperiodic.

$\mathscr{L} + a = \mathscr{L}$ *iff* $\mathbb{R}^d \ni a = 0$;

ii) Delone set:

- *uniformly discrete, i.e. there is $r > 0$ such that every open ball of radius r meets $\mathscr{L}$ at most on one point;*
- *relatively dense, i.e. there is $R > 0$ such that every closed ball of radius R meets $\mathscr{L}$ at least on one point.*

iii) Repetitive:

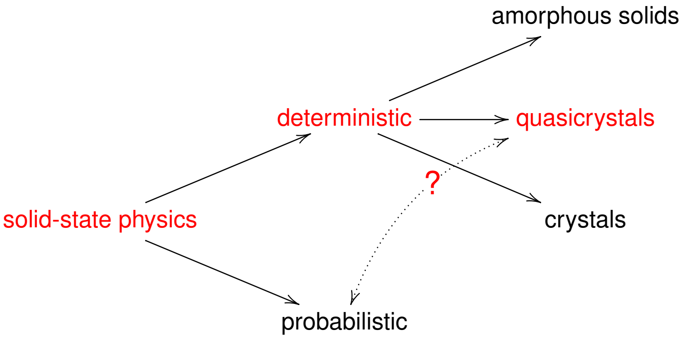
given any patch $\wp \subset \mathscr{L}$, there is a $R > 0$ such that in any ball of radius R there is a patch $\wp' \subset \mathscr{L}$ which differs by $\varepsilon > 0$ (in Hausdorff sense) from $\wp$ up to a translation.

iv) Finite local coplexity (FLC):

for any $R > 0$ the number of patches of radius R is finite. $\Leftrightarrow$ $\mathscr{L} - \mathscr{L}$ is a discrete closed subset of $\mathbb{R}^d$ (finite type).

“Strange” physical properties of quasicrystals:

- mostly insulators at low temperature (even though made of good metals !!);
- mechanically hard and fragile;
- superplastic transition at high temperature (just below the melting temperature);



- Quantum-mechanical description ($\mathscr{L}$ =D-set):

$$H_{qc} := -\frac{\hbar}{2m}\Delta + V_{qc}, \qquad V_{qc} := \sum_{i=1}^{N} \sum_{a \in \mathscr{L}_i} v^{(i)}(\,\cdot\, - a)$$

i =atomic types, $\mathscr{L}_i \subset \mathscr{L}$ positions of i-atoms, $v^{(i)}$ typical potential of an i-atom.

- *Numerical calculations extremely hard;*
- *no way of treating the aperiodicity as a perturbation of a periodic structure.*

- For periodic crystals:

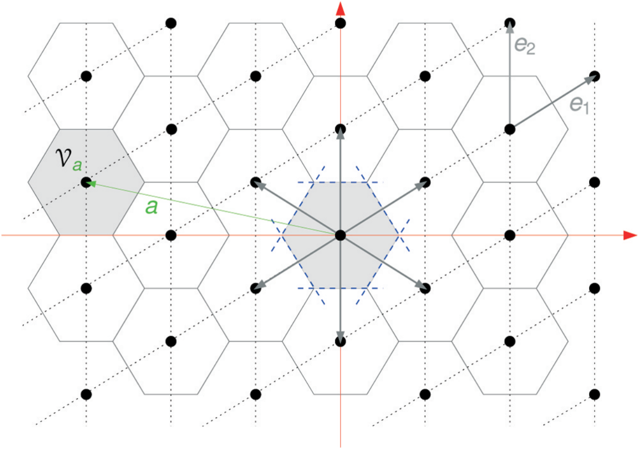
Translation invariance $\Rightarrow$ Wannier transform $\Rightarrow$ Bloch theory.

- Need of new tools to study H_{qc}:

Using the notion of long-range order, is it possible to extend the Wannier transform to quasicrystals ?

- $\mathscr{L}_{\text{per}} \subset \mathbb{R}^d$, discrete

$$0 \in \mathscr{L}_{\text{per}}, \qquad \text{and} \qquad \Gamma_{\text{per}} := \mathscr{L}_{\text{per}} - \mathscr{L}_{\text{per}} \simeq \mathbb{Z}^d.$$



(open) Voronoi cell in $a \in \mathscr{L}_{\text{per}}$

$$\mathcal{V}_a := \left\{ x \in \mathbb{R}^d \ : \ |x - a| < |x - b|, \ \ \forall b \in \mathscr{L}_{\text{per}} \setminus \{a\} \right\}$$

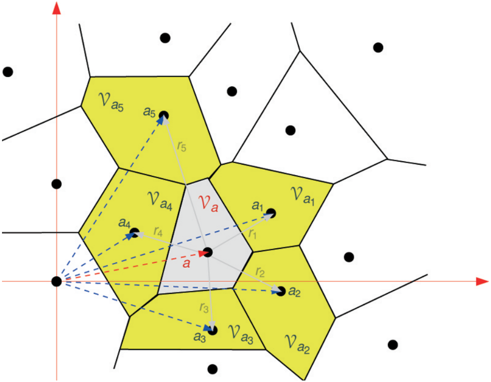
- $\mathscr{L} \subset \mathbb{R}^d$, D-set with $0 \in \mathscr{L}$.

THEOREM (J. C. Lagarias, 1999)

The subgroup of $\mathbb{R}^d$ generated by $\mathscr{L} - \mathscr{L}$ is a finitely generated free group (Lagarias group)

$$\Gamma_{\mathscr{L}} := \langle \mathscr{L} - \mathscr{L} \rangle \simeq \mathbb{Z}^g, \qquad g > d.$$

- Voronoi-tiling of $\mathscr{L}$ ($\mathcal{V}_a =$ *punctured open cells*):



- Voronoi tiles

$$T_a := \overline{\mathcal{V}_a}, \qquad a \in \mathscr{L}.$$

Convex politope with (natural) puncture in a.

- Voronoi-tiling $\{T_a \ : \ a \in \mathscr{L}\}$

$$\bigcup_{a \in \mathscr{L}} T_a = \mathbb{R}^d, \qquad \mathcal{V}_a \cap \mathcal{V}_b = \emptyset \quad \text{if} \quad a \neq b \in \mathscr{L}.$$

- (Open) n-face $\mathcal{F}$ $(\hookrightarrow \mathbb{R}^n)$:

$$\overline{\mathcal{F}_b} := T_{a_1} \cap T_{a_2} \cap \ldots \cap T_{a_{n+1}} \neq \emptyset, \qquad \text{codim.}(\overline{\mathcal{F}_b}) = d - n.$$

$\mathcal{F}_b$ is punctured in $b \in \mathbb{R}^d$ (eg. its barycenter).

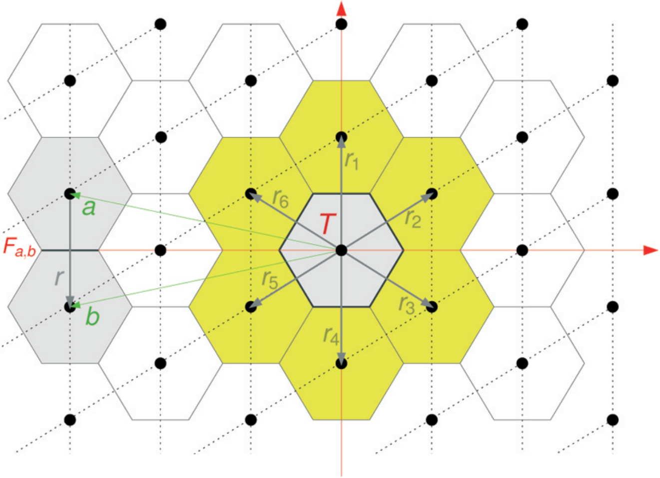
- $\mathscr{F}^{(n)} := \{\mathcal{F}_b \ : \ \text{punctured } n - \text{face of the Voronoi-tiling}\}$.

$\mathscr{F}^{(d)} \equiv$ cells, $\mathscr{F}^{(d-1)} \equiv$ faces, $\mathscr{F}^{(1)} \equiv$ edges, $\mathscr{F}^{(0)} \equiv$ vertices.

Outline

- a and b are nearest-neighbours (n.-n.) if:

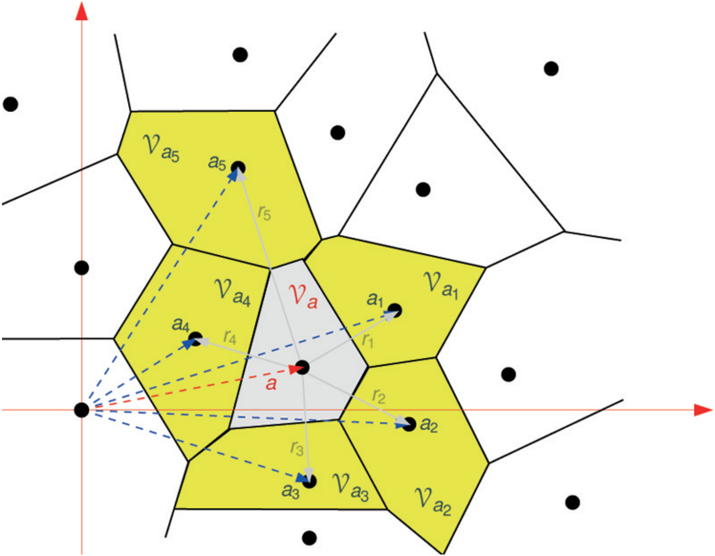
$$\text{codim.}(F_{a,b}) = 1, \qquad F_{a,b} := T_a \cap T_b.$$



- (1-st. order) collar of $\mathcal{V}_a$:

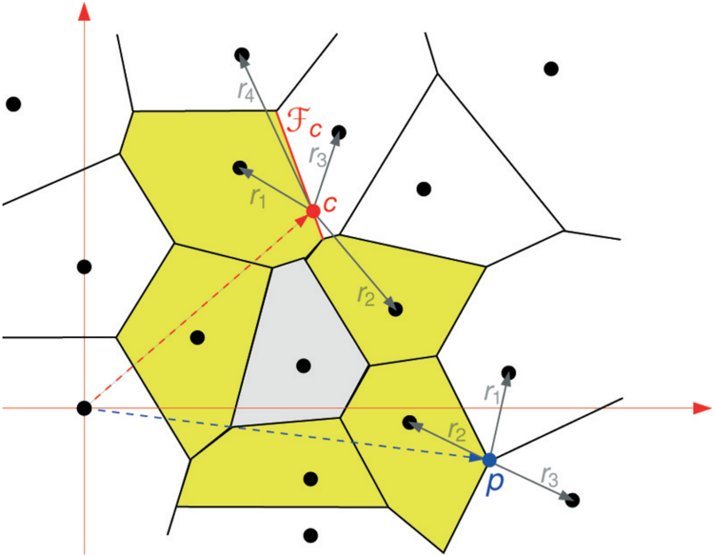
$$\text{Col}(\mathcal{V}_a) := \{r = b - a \ : \ b \text{ is a n.-n. of } a\} \subset \mathscr{L} - \mathscr{L} =: \Gamma_{\mathscr{L}}.$$

- Any Voronoi cell can be endowed with a collar:



$$\mathrm{Col}(\mathcal{V}_a) := \{ r_j = a_j - a \ : \ a_j \text{ is a n.-n. of } a \} \subset \Gamma_{\mathscr{L}}.$$

- Any *n*-face can be punctured (barycenter) and collared:



$$\text{Col}(\mathcal{F}_c) := \{ r_j = a_j - c \ : \ T_{a_j} \cap \mathcal{F}_c \neq \emptyset \} \subset \mathscr{L} - c.$$

Definition

Let $\mathcal{F}_{c_j} \in \mathscr{F}^{(n)}$, with $j = 1, 2$, be a pair of n-faces with punctures in $c_j \in \mathbb{R}^d$. Then

$$\mathcal{F}_{c_1} \sim \mathcal{F}_{c_2} \qquad (\textit{translationary equivalent})$$

iff:

(i) $\mathcal{F}_{c_1} - c_1 = \mathcal{F}_{c_2} - c_2$ *(same geometric support);*

(ii) $\mathrm{Col}(\mathcal{F}_{c_1}) = \mathrm{Col}(\mathcal{F}_{c_2})$ *(same collar).*

- Because of the FLC

$$\mathscr{Q}^{(d)} := \mathscr{F}^{(d)}/\sim\, = \{\mathcal{V}_1, \dots, \mathcal{V}_{N_d}\} \qquad \text{(proto-cells)}$$

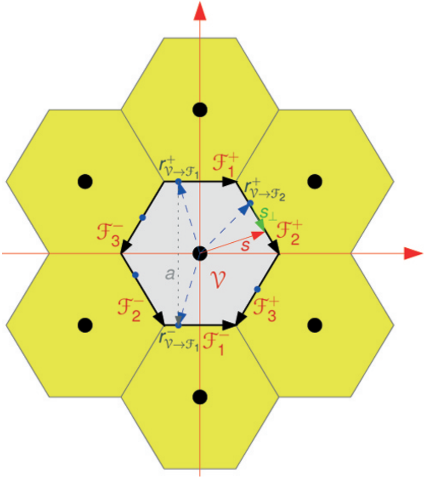
$$\mathscr{Q}^{(d-1)} := \mathscr{F}^{(d-1)}/\sim\, = \{\mathcal{F}_1, \dots, \mathcal{F}_{N_{d-1}}\} \qquad \text{(proto-faces)}$$

$$\vdots \qquad \text{(proto-n-faces)}$$

$$\mathscr{Q}^{(0)} := \mathscr{F}^{(0)}/\sim\, = \{p_1, \dots, p_{N_0}\} \qquad \text{(proto-vertices)}$$

with $N_j < +\infty$, $j = 0, \dots, d$.

Periodic case



1 proto-cell

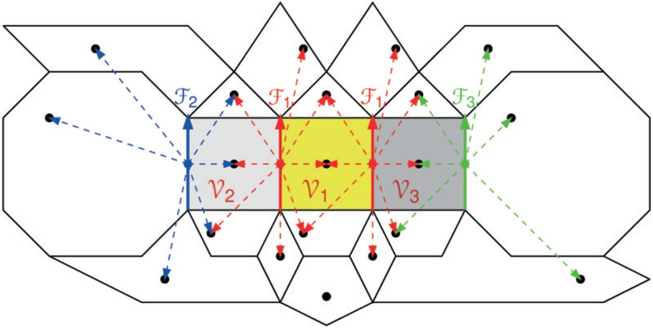
$\mathscr{Q}^{(d)} = \{\mathcal{V}\}$

1 proto-vertex

$\mathscr{Q}^{(0)} = \{p\}$

- $\mathscr{Q}^{(d-1)} = \{\mathcal{F}_1, \ldots \mathcal{F}_N\}$; any proto-faces is a "double" face for $\mathcal{V}$:

$$\partial\mathcal{V} = \underbrace{\overline{\mathcal{F}_1^+} \cup \overline{\mathcal{F}_1^-}}_{\sim\overline{\mathcal{F}_1}} \cup \underbrace{\overline{\mathcal{F}_2^+} \cup \overline{\mathcal{F}_2^-}}_{\sim\overline{\mathcal{F}_2}} \cup \ldots \cup \underbrace{\overline{\mathcal{F}_N^+} \cup \overline{\mathcal{F}_N^-}}_{\sim\overline{\mathcal{F}_N}}.$$



Relative position number

$$\mathscr{N} : \mathscr{Q}^{(n)} \times \mathscr{Q}^{(n-1)} \longrightarrow \{0,1,2\}$$

$$\boxed{\mathscr{N}(\mathcal{F}_j,\mathcal{G}_k) := \sharp\{r = c_k - b_j \ : \ \mathcal{G}_{c_k} \subset \overline{\mathcal{F}_{b_j}}, \ \forall\, \mathcal{G}_{c_k} \sim \mathcal{G}_k \text{ and } \mathcal{F}_{b_j} \sim \mathcal{F}_j\}}.$$

$$\mathscr{N}(\mathcal{F}_j,\mathcal{G}_k) = \begin{cases} 0, & \text{forbidden attachment}, \\ 1, & \text{unique attachment}, \qquad 1 \text{ rel. position } r_{\mathcal{F}_j \to \mathcal{G}_k}, \\ 2, & \text{local periodicity}, \qquad 2 \text{ rel. positions } r^{\pm}_{\mathcal{F}_j \to \mathcal{G}_k}. \end{cases}$$

• Any proto-n-face can be oriented by $\mathcal{F}_j \hookrightarrow \mathbb{R}^n$.

• The orientation of a proto-n-faces $\mathcal{F}_j$ fixes the orientation of all the equivalent "real" n-faces in the Voronoi tiling. A relative orientation between n-faces in the Voronoi tiling is fixed.

Incidence Number (I.N.)

$$[\,\cdot\,;\,\cdot\,]_\sim : \mathcal{Q}^{(n)} \times \mathcal{Q}^{(n-1)} \longrightarrow \{-1, 0, 1\}$$

$$[\mathcal{F}_j;\mathcal{G}_k]_\sim = \begin{cases} 0, & \text{if } \mathcal{N}(\mathcal{F}_j,\mathcal{G}_k) = 0 \\ \pm 1 = [\mathcal{F}_{b_j};\mathcal{G}_{c_k}] & \text{if } \mathcal{N}(\mathcal{F}_j,\mathcal{G}_k) = 1 \quad c_k - b_j = r_{\mathcal{F}_j \to \mathcal{G}_k} \\ 0 = \sum_{\sigma \in \{\pm\}} [\mathcal{F}_{b_j};\mathcal{G}_{c_k^\sigma}] & \text{if } \mathcal{N}(\mathcal{F}_j,\mathcal{G}_k) = 2 \quad c_k^\pm - b_j = r^\pm_{\mathcal{F}_j \to \mathcal{G}_k} \end{cases}$$

Short notation:

$$[\mathcal{F}_j, \mathcal{G}_k^\sigma]_\sim := [\mathcal{F}_{b_j};\mathcal{G}_{c_k^\sigma}] \qquad \text{when} \quad \mathcal{N}(\mathcal{F}_j,\mathcal{G}_k) = 2.$$

- Homological relation (S. Eilenberg, 1944):

$$\sum_{\mathcal{F}_j \in \mathcal{Q}^{(n)}} [\mathcal{R}_i, \mathcal{F}_j]_\sim \, [\mathcal{F}_j, \mathcal{G}_k]_\sim = 0, \qquad \forall\, \mathcal{R}_i \in \mathcal{Q}^{(n+1)},\ \mathcal{G}_k \in \mathcal{Q}^{(n-1)}.$$

THEOREM

The graded set

$$\mathcal{Q} := \biguplus_{j=0}^{d} \mathcal{Q}^{(j)}$$

is a CW-complex with (singular) homology induced by the Incidence Number $[\,\cdot\,;\,\cdot\,]_\sim$.

- $\mathcal{Q}$ is the Anderson-Putnam Complex (APC) associated to the D-set $\mathscr{L}$ (cf. J. E. Anderson & I. F. Putnam, 1998).

Wannier decomposition

$$L^2(\mathbb{R}^d) \xrightarrow{\quad \mathrm{I} \quad} L^2(\mathcal{V}) \otimes \ell^2(\mathscr{L}_{\mathrm{per}}) \xrightarrow{\quad \mathrm{II} \quad} L^2(\mathcal{V}) \otimes L^2(\mathbb{B})$$

$$\psi \longmapsto \sum_{a \in \mathscr{L}_{\mathrm{per}}} \delta_a \otimes (\mathcal{T}_{-a}\psi) \restriction_{\mathcal{V}} \longmapsto \sum_{a \in \mathscr{L}_{\mathrm{per}}} \check{\delta}_a \otimes (\mathcal{T}_{-a}\psi) \restriction_{\mathcal{V}}$$

Step I

- $\mathbb{R}^d \ni x \mapsto (s, a) \in \mathcal{V} \times \mathscr{L}_{\mathrm{per}}$ (spatial decomposition),
- $(\mathcal{T}_a \psi)(\,\cdot\,) := \psi(\,\cdot\, - a)$ (translation operators),
- $\{\delta_a\} \subset \ell^2(\mathscr{L}_{\mathrm{per}}) \simeq \ell^2(\Gamma)$ (canonical basis).

Step II

- $\mathrm{Id}_{L^2(\mathcal{V})} \otimes \check{\mathscr{F}}$ (inverse-Fourier transform),
- $\mathbb{B} := \mathbb{R}^d / \Gamma^*$, (Brillouin zone),
- $\check{\delta}_a := \check{\mathscr{F}}(\delta_a) = \mathrm{e}^{-ik\cdot a} \in L^2(\mathbb{B})$.

- **Wannier transform** (periodic set $\mathscr{L}_{\text{per}}$):

$$L^2(\mathbb{R}^d) \ni \psi \stackrel{\mathscr{W}}{\longmapsto} (\mathscr{W}\psi) \in L^2(\mathcal{V}) \otimes L^2(\mathbb{B}), \qquad \mathscr{W} := (\text{step II}) \circ (\text{step I})$$

$$\boxed{(\mathscr{W}\psi)(s;k) := \sum_{a \in \mathscr{L}_{\text{per}}} e^{-ik\cdot a}\, \psi(s+a), \qquad s \in \mathcal{V}, \quad k \in \mathbb{B}}$$

$s \in \mathcal{V}$ the position w.r.t. the puncture 0 !

- **Plancherel's formula** (unitarity):

$$\|\psi\|^2_{L^2(\mathbb{R}^d)} = \int_{\mathbb{B}} \underbrace{\left(\int_{\mathcal{V}} |(\mathscr{W}\psi)(s;k)|^2 \, ds \right)}_{\|(\mathscr{W}\psi)(\cdot;k)\|^2_{L^2(\mathcal{V})}} \underline{dk}.$$

$\underline{dk}$ = normalized Haar measure.

- **Smoothness**:

$$\left(\mathscr{W} \frac{\partial^\alpha \psi}{\partial x^\alpha} \right)(s;k) = \frac{\partial^\alpha}{\partial s^\alpha} (\mathscr{W}\psi)(s;k), \qquad \psi \in C^\infty(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$$

- Wannier transform (D-set $\mathscr{L}$):

$$L^2(\mathbb{R}^d) \ni \psi \overset{\mathscr{W}}{\longmapsto} \begin{pmatrix} (\mathscr{W}^{(1)}\psi) \\ \vdots \\ (\mathscr{W}^{(N_d)}\psi) \end{pmatrix} \in L^2(\mathscr{Q}) \otimes L^2(\mathbb{B})$$

$$\boxed{(\mathscr{W}^{(j)}\psi)(s;k) := \sum_{a\in\mathscr{L}_j} e^{-ik\star a}\, \psi(s+a), \qquad s \in \mathcal{V}_j,\quad k \in \mathbb{B}.}$$

- $\mathscr{L}_j := \{a \in \mathscr{L} \ : \ \mathcal{V}_a \sim \mathcal{V}_j\} \subset \Gamma_{\mathscr{L}}$ where $\mathscr{Q}^{(d)} = \{\mathcal{V}_1, \ldots, \mathcal{V}_{N_d}\}$

$$\mathscr{L} = \mathscr{L}_1 \biguplus \ldots \biguplus \mathscr{L}_{N_d};$$

- $L^2(\mathscr{Q}) := \bigoplus_{j=1}^{N_d} L^2(\mathcal{V}_j)$;
- $\mathbb{B} := \mathbb{R}^g/\Gamma^*_{\mathscr{L}}$, (Brillouin zone or Pontryagin dual of $\Gamma_{\mathscr{L}}$);
- $e^{-ik\star} : \Gamma_{\mathscr{L}} \to \mathbb{S}^1$, (Pontryagin character).

THEOREM (J. V. Bellissard, G. D., V. Milani)

The Wannier transform associated to $\mathscr{L}$ is a unitary map

$$\mathscr{W} : L^2(\mathbb{R}^d) \longrightarrow \Pi_{\mathscr{L}}\Big(L^2(\mathscr{Q}) \otimes L^2(\mathbb{B})\Big).$$

The Plancherel's formula holds true:

$$\|\psi\|^2_{L^2(\mathbb{R}^d)} = \int_{\mathbb{B}} \left(\sum_{j=1}^{N_d} \|(\mathscr{W}^{(j)}\psi)(\cdot;k)\|^2_{L^2(\mathcal{V}_j)} \right) \underline{dk}.$$

- $\mathscr{H}_j \subset L^2(\mathbb{B})$ closed subspace generated by $\left\{\xi_a(k) := e^{-ik\star a} \ : \ a \in \mathscr{L}_j\right\}$.
- The projection $\Pi_{\mathscr{L}}$

$$\Pi_{\mathscr{L}} : L^2(\mathscr{Q}) \otimes L^2(\mathbb{B}) \longrightarrow \bigoplus_{j=1}^{N_d} L^2(\mathcal{V}_j) \otimes \mathscr{H}_j$$

removes “forbidden frequencies”.

- Quasicrystal-Hamiltonian for the D-set $\mathscr{L}$:

$$H_{qc} := -\Delta + \sum_{j=1}^{N_d} \left(\sum_{a \in \mathscr{L}_j} v^{(j)}(\,\cdot\, - a) \right) = -\Delta + V_{\mathscr{L}}$$

selfadjoint on $H^2(\mathbb{R}^d)$.

- Under the assumption *supp*$(v^{(j)}) \subset \mathcal{V}_j$:

$$\mathscr{W} : (V_{\mathscr{L}}\psi) \longrightarrow \begin{pmatrix} v^{(1)}(\mathscr{W}^{(1)}\psi) \\ \vdots \\ v^{(N_d)}(\mathscr{W}^{(N_d)}\psi) \end{pmatrix}, \qquad \psi \in L^2(\mathbb{R}^d)$$

i.e. $\mathscr{W} V_{\mathscr{L}} \mathscr{W}^{-1} = \left(\bigoplus_j v^{(j)}\right) \otimes \mathrm{Id}_{L^2(\mathbb{B})}$ (diagonal and k-indep.).

- $\mathscr{W} \Delta \mathscr{W}^{-1}$ can be studied by means of the quadratic form

$$\langle \nabla\psi; \nabla\psi \rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{B}} \underbrace{\left(\sum_{j=1}^{N_d} \langle \nabla_s(\mathscr{W}^{(j)}\psi)(\cdot;k); \nabla_s(\mathscr{W}^{(j)}\psi)(\cdot;k) \rangle_{L^2(\mathcal{V}_j)} \right)}_{Q_k^0[(\mathscr{W}\psi)(\cdot;k)]} \underline{dk}.$$

PROBLEM ! Determination of the form domain $\mathscr{D}(Q_k^0)$

- Evidently $\mathscr{D}(Q_k^0) \subset H^1(\mathscr{Q}^{(d)})$

$$H^q(\mathscr{Q}^{(d)}) = \bigoplus_{j=1}^{N_d} H^q(\mathcal{V}_j), \qquad H^q(\mathscr{Q}^{(d-1)}) = \bigoplus_{j=1}^{N_{d-1}} H^q(\mathcal{F}_j), \qquad \ldots \quad \text{(Sobolev spaces)}$$

- The trace operator is a linear bounded:

$$H^1(\mathcal{V}_j) \ni \ \phi \overset{\tau}{\longmapsto} \phi \restriction_{\partial \mathcal{V}_j} \in H^{\frac{1}{2}}(\partial \mathcal{V}_j).$$

$T_j := \overline{\mathcal{V}_j}$ is a polytope hence $\partial \mathcal{V}$ is a Lipschitz boundary.

- $\mathscr{W}$ induces boundary conditions on $H^1(\mathscr{Q}^{(d)})$ for any $k \in \mathbb{B}$:

$$\boxed{\mathscr{D}(Q_k^0) := \left\{ \phi \in H^1(\mathscr{Q}^{(d)}) \ : \ \phi \text{ verifies the } k-\text{boundary condition.} \right\}}$$

THEOREM (J. V. Bellissard, G. D., V. Milani)

The quadratic form

$$Q_k^0[\phi] = \sum_{j=1}^{N_d} \langle \nabla_s \phi_j ; \nabla_s \phi_j \rangle_{L^2(\mathcal{V}_j)}$$

has domain $\boxed{\mathscr{D}(Q_k^0) = \{\phi \in H^1(\mathscr{Q}^{(d)}) \ : \ \eth_k \phi = 0\}.}$

Let $\tilde{\Delta}_k$ *be the selfadjoint operator defined by* Q_k^0 *on* $L^2(\mathscr{Q}^{(d)})$, *then*

$$\mathscr{W} \, \Delta \, \mathscr{W}^{-1} = \Pi_{\mathscr{L}} \, \tilde{\Delta} \, \Pi_{\mathscr{L}}, \qquad \text{with} \qquad \tilde{\Delta} := \int_{\mathbb{B}}^{\oplus} \tilde{\Delta}_k \, \underline{dk}.$$

! REMARK ! The rôle of the projection $\Pi_{\mathscr{L}}$ is not innocent.

$$\mathscr{W} \, H_{qc} \, \mathscr{W}^{-1} = \Pi_{\mathscr{L}} \, \tilde{H} \, \Pi_{\mathscr{L}}, \qquad \text{with} \qquad \tilde{H} := \tilde{\Delta} + \left(\bigoplus_{j=1}^{N_d} v^{(j)} \right) \otimes \mathrm{Id}_{L^2(\mathbb{B})}.$$

- $\tilde{H}$ has band spectrum (standard facts!) but H_{qc} may have Cantor spectrum (eg. in the one-dimensional cases).
- $\Pi_{\mathscr{L}}$ reduces the band spectrum and opens gaps.

Boundary operator:

$$H^1(\mathcal{Q}^{(d)}) \ni \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{N_d} \end{pmatrix} \stackrel{\eth_k}{\longmapsto} \begin{pmatrix} (\eth_k \phi)_1 \\ \vdots \\ (\eth_k \phi)_{N_{d-1}} \end{pmatrix} \in H^{\frac{1}{2}}(\mathcal{Q}^{(d-1)})$$

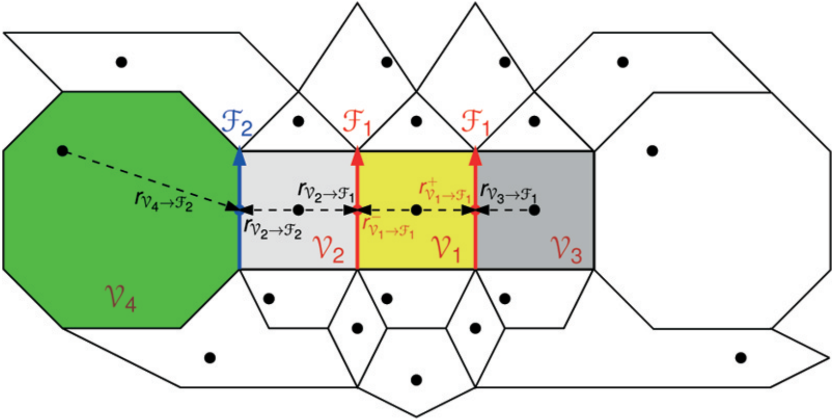
$$\boxed{(\eth_k \phi)_\ell := \sum_{j=1}^{N_d} \left(\sum_{\sigma \in I_{j,\ell}} [\mathcal{V}_j ; \mathcal{F}_\ell^\sigma]_\sim \ e^{-ik \star r^\sigma_{\mathcal{V}_j \to \mathcal{F}_\ell}} \ \phi_j \restriction_{\mathcal{F}_\ell^\sigma} \right)}$$

where $$I_{j,\ell} = \begin{cases} \{0\} & \text{if } \mathcal{N}(\mathcal{V}_j, \mathcal{F}_\ell) = 1 \\ \{+,-\} & \text{if } \mathcal{N}(\mathcal{V}_j, \mathcal{F}_\ell) = 2. \end{cases}$$

Theorem (J. V. Bellissard, G. D., V. Milani)

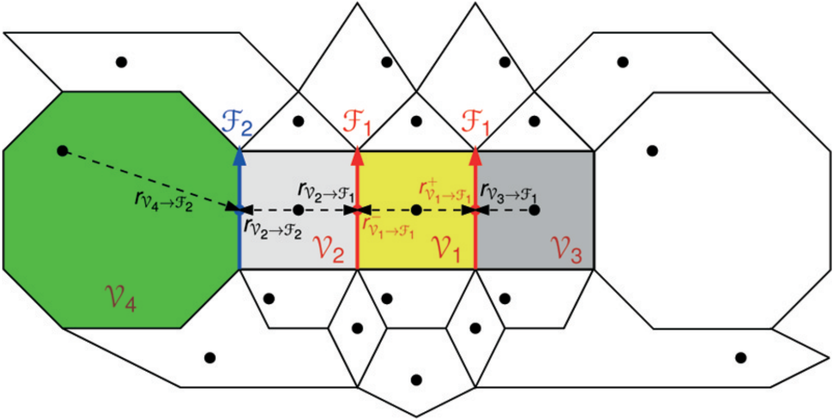
$$H^1(\mathbb{R}^d) =: H^1(\mathcal{Q}^{(d+1)}) \stackrel{\mathcal{W}_k}{\longrightarrow} H^1(\mathcal{Q}^{(d)}) \stackrel{\eth_k}{\longrightarrow} H^{\frac{1}{2}}(\mathcal{Q}^{(d-1)}) \longrightarrow \dots$$

$$\boxed{\eth_k \circ \mathcal{W}_k = 0, \qquad \forall\, k \in \mathbb{B}.}$$



- $\mathcal{N}(\mathcal{V}_j, \mathcal{F}_2) = \delta_{j,2} + \delta_{j,4}$

$$(\eth_k \phi)_2 = \sum_{j=\{2,4\}} [\mathcal{V}_j; \mathcal{F}_2]_\sim \ e^{-ik\star r_{\mathcal{V}_j\to\mathcal{F}_2}} \ \phi_j \restriction_{\mathcal{F}_2}$$



- $\mathcal{N}(\mathcal{V}_j,\mathcal{F}_1) = \delta_{j,2}+\delta_{j,3}+2\,\delta_{j,1}$

$$(\eth_k\phi)_1 = \sum_{j=\{2,3\}} [\mathcal{V}_j;\mathcal{F}_1]_\sim \; e^{-ik\star r_{\mathcal{V}_j\to\mathcal{F}_1}} \; \phi_j \upharpoonright_{\mathcal{F}_1} \qquad \text{(aperiodic)}$$

$$+ \sum_{\sigma=\{+,-\}} [\mathcal{V}_1;\mathcal{F}_1^\sigma]_\sim \; e^{-ik\star r^\sigma_{\mathcal{V}_1\to\mathcal{F}_1}} \; \phi_j \upharpoonright_{\mathcal{F}_1^\sigma} \qquad \text{(loc. periodic)}$$

Proof of the boundary conditions: periodic case

- 1 proto-cell of $\mathcal{V}$. $\mathscr{N}(\mathcal{V},\mathcal{F}_j) = 2$ for any proto-face $\mathcal{F}_j$.

- Let $r^{\pm}_{\mathcal{V}\to\mathcal{F}_j}$ be the relative positions of $\mathcal{F}_j$ w.r.t $\mathcal{V}$.

$$\partial\mathcal{V} = \overline{\mathcal{F}_1^+} \cup \overline{\mathcal{F}_1^-} \cup \overline{\mathcal{F}_2^+} \cup \overline{\mathcal{F}_2^-} \cup \ldots \cup \overline{\mathcal{F}_N^+} \cup \overline{\mathcal{F}_N^-}.$$

- If $s \in \mathcal{F}_j^{\pm}$ then $s = r^{\pm}_{T\to F_j} + s_\perp$.

$$\psi\restriction_{\mathcal{F}_j^{\pm}}(s_\perp) := \psi(r^{\pm}_{\mathcal{V}\to\mathcal{F}_j} + s_\perp)$$

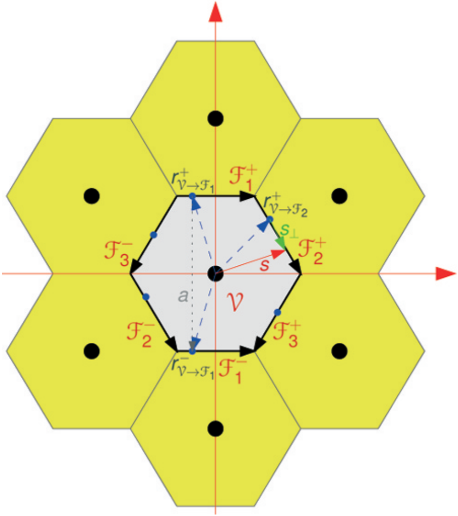
$s_\perp$ is an “affine coordinate” for $\mathcal{F}_j^{\pm}$.

- Let $\psi \in H^1(\mathbb{R}^d)$. A simple computation shows

$$\begin{aligned}(\mathscr{W}\psi)\restriction_{\mathcal{F}_j^-}(s_\perp;k) :&= (\mathscr{W}\psi)(r^-_{\mathcal{V}\to\mathcal{F}_j} + s_\perp;k)\\ &= (\mathscr{W}\psi)(r^-_{\mathcal{V}\to\mathcal{F}_j} - r^+_{\mathcal{V}\to\mathcal{F}_j} + r^+_{\mathcal{V}\to\mathcal{F}_j} + s_\perp;k)\\ &=: e^{ik\cdot(r^-_{\mathcal{V}\to\mathcal{F}_j} - r^+_{\mathcal{V}\to\mathcal{F}_j})}(\mathscr{W}\psi)\restriction_{\mathcal{F}_j^+}(s_\perp;k)\end{aligned}$$

where $r^-_{\mathcal{V}\to\mathcal{F}_j} - r^+_{\mathcal{V}\to\mathcal{F}_j} \in \Gamma_{\text{per}}$.

- $\mathcal{F}_i^{\pm} \hookrightarrow \mathbb{R}^{d-1}$ induces a relative orientation w.r.t. $\mathcal{V}$.



Incidence number:

$$[\mathcal{V};\mathcal{F}_j^{\pm}] = \pm 1.$$

- k-boundary condition induced by $\mathscr{W}$: $k \in \mathbb{B}$, $j = 1, 2, \ldots$

$$\sum_{\sigma\in\{+,-\}} [\mathcal{V};\mathcal{F}_j^{\sigma}]\, e^{-ik\cdot r^{\sigma}_{\mathcal{V}\to\mathcal{F}_j}} \, (\mathscr{W}\psi)\restriction_{\mathcal{F}_j^{\sigma}} (\cdot;k) = 0.$$

Conclusions and Remarks

• D-sets $\mathscr{L}$ models the long-range order of quasicrystals.

• The Lagarias group $\Gamma_{\mathscr{L}}$ plays the role of $\mathbb{Z}^g$ ($g > d$) in general. The Brillouin zone $\mathbb{B}$ is the Pontryagin dual of $\Gamma_{\mathscr{L}}$.

• The classification of the proto-cells by means of the (1-st deg.) collar leads to the Anderson-Putnam complexes $\mathscr{Q}$. The Wannier transform $\mathscr{W}$ identifies vectors in $L^2(\mathbb{R}^d)$ with a proper subspace of $L^2(\mathscr{Q}) \otimes L^2(\mathbb{B})$.

• The Schrödinger operators are represented via $\mathscr{W}$ as the compression of a Bloch-type operators depending on $k \in \mathbb{B}$ by means of the boundary conditions (cohomoogical description).

• Using n-th deg. collars one obtains a sequence of AP-complexes $\{\mathscr{Q}_n\}$ together with the maps $\mathscr{Q}_{n+1} \to \mathscr{Q}_n$. This gives rise to the notion of an inverse limits. The cohomogical description of the boundary conditions seems to be the appropriate language in this framework.

Thank you for your attention

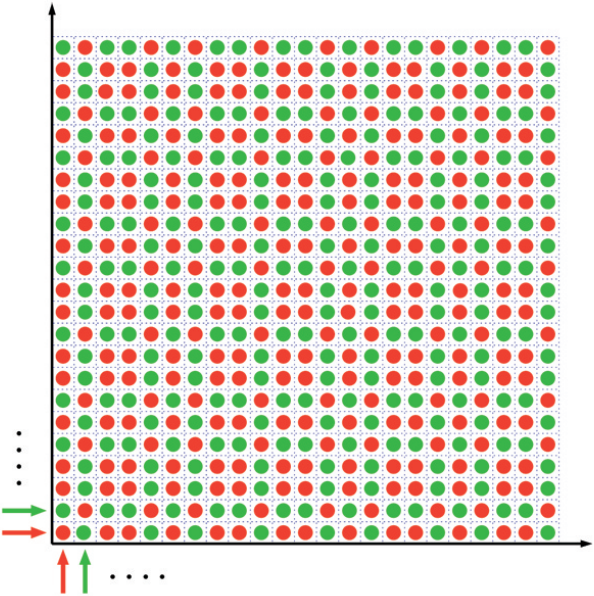
&

Joyeux anniversaire
Prof. Bellissard

"Tout l'art réside dans le fait de devenir adulte sans devenir vieux".

Frank Lloyd Wright

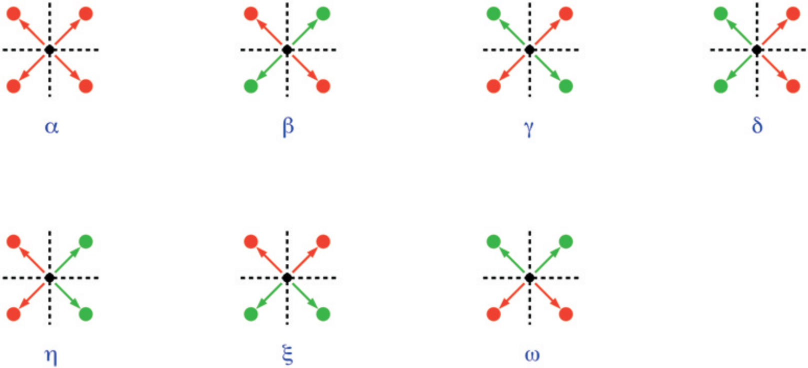
Fibonacci tiling of the plane



red–type substitution rule

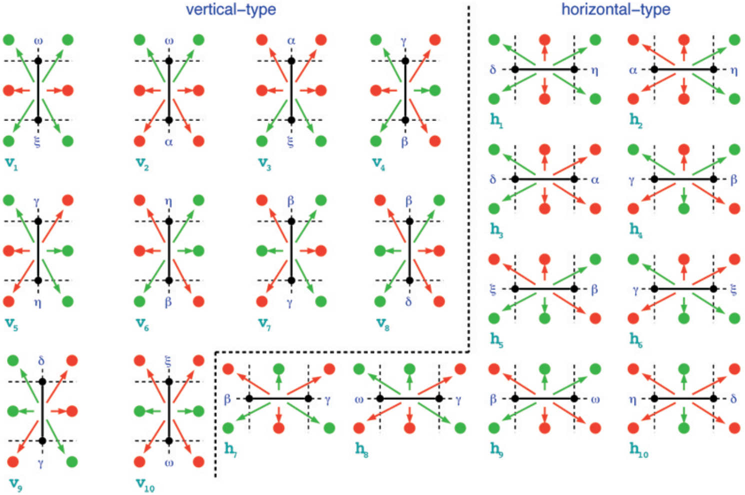
green–type subtitution rule

Classification of the collared vertices



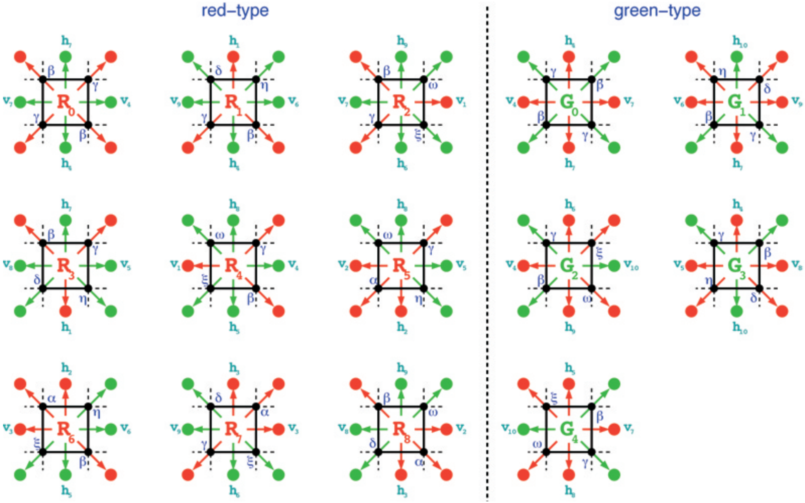
proto-vertices: $N_0 = 7$.

Classification of the collared edges



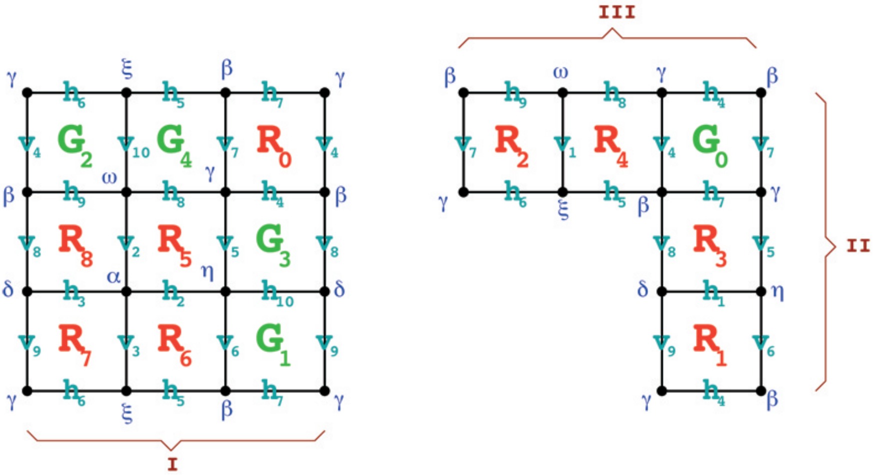
proto-edges: $N_1 = 20.$

Classification of the collared cells

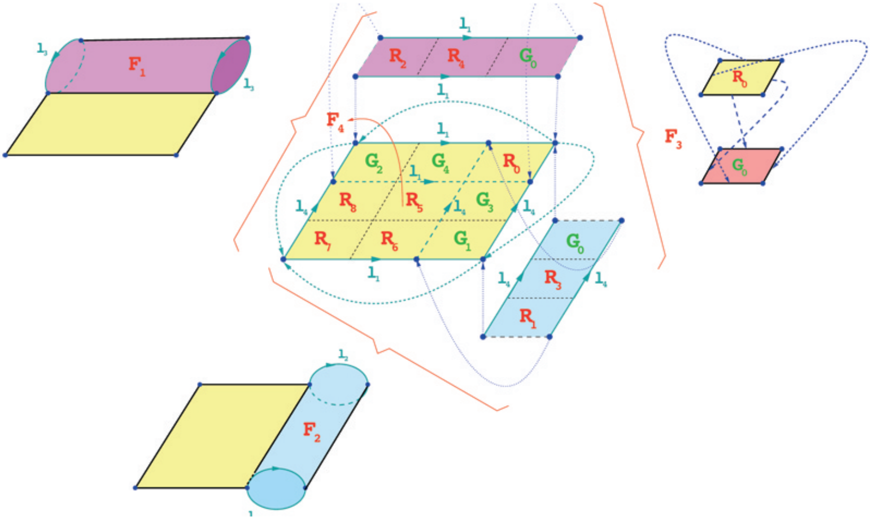


proto-cells: $N_2 = 14.$

The Anderson-Putnam Complex



Euler characteristic: $\chi_E := N_0 - N_1 + N_2 = 1.$



F_1
1_3
1_3
1_1
R_2 R_4 G_0
1_1
F_4
1_1
G_2 G_4 R_0
1_1
R_8 R_5 G_3
1_4
1_4
1_4
R_7 R_6 G_1
1_1
G_0
R_3
1_4
1_4
R_1
F_3
R_0
G_0
1_2
F_2

Hmology of the Anderson-Putnam Complex

- Free Abelian groups generated by celles

$$C_0 = \mathrm{Span} < \alpha, \beta, \gamma, \delta, \eta, \xi, \omega > = \mathbb{Z}^7$$

$$C_1 = \mathrm{Span} < h_1, \dots, h_{10}, v_1, \dots, v_{10} > = \mathbb{Z}^{20}$$

$$C_2 = \mathrm{Span} < R_0, \dots, R_8, G_0, \dots, G_4 > = \mathbb{Z}^{14}$$

- Chain - complex

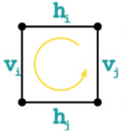
$$0 \longrightarrow C_2 \xrightarrow{\Delta^{(2)}} C_1 \xrightarrow{\Delta^{(1)}} C_0 \longrightarrow 0$$

$\Delta^{(1)}\Big($ 

$\Big) = \alpha - \beta$

$\Delta^{(1)}\Big($ 

$\Big) = \alpha - \beta$

$\Delta^{(2)}\Big($ 

$\Big) = h_j - h_i + v_j - v_i$

$$\Delta^{(1)} \circ \Delta^{(2)} = 0$$

orientation induced by $\mathbb{R}^2$

- Matrix expresions for $\Delta^{(2)}$ and $\Delta^{(1)}$

$\Delta^{(1)} =$

	h_1	h_2	h_3	h_4	h_5	h_6	h_7	h_8	h_9	h_{10}	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	v_{10}
α	0	−1	1	0	0	0	0	0	0	0	0	−1	1	0	0	0	0	0	0	0
β	0	0	0	1	1	0	−1	0	−1	0	0	0	0	−1	0	−1	1	1	0	0
γ	0	0	0	−1	0	−1	1	1	0	0	0	0	0	1	1	0	−1	0	−1	0
δ	−1	0	−1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	−1	1	0
η	1	1	0	0	0	0	0	0	0	−1	0	0	0	0	−1	1	0	0	0	0
ξ	0	0	0	0	−1	1	0	0	0	0	−1	0	−1	0	0	0	0	0	0	1
ω	0	0	0	0	0	0	0	−1	1	0	1	1	0	0	0	0	0	0	0	−1

$\Delta^{(2)} =$

	R_0	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	G_0	G_1	G_2	G_3	G_4
h_1	0	−1	0	1	0	0	0	0	0	0	0	0	0	0
h_2	0	0	0	0	0	1	−1	0	0	0	0	0	0	0
h_3	0	0	0	0	0	0	0	−1	1	0	0	0	0	0
h_4	1	1	0	0	0	0	0	0	0	−1	0	0	−1	0
h_5	0	0	0	0	1	0	1	0	0	0	0	0	0	−1
h_6	0	0	1	0	0	0	0	1	0	0	0	−1	0	0
h_7	−1	0	0	−1	0	0	0	0	0	1	1	0	0	0
h_8	0	0	0	0	−1	−1	0	0	0	0	0	0	0	1
h_9	0	0	−1	0	0	0	0	0	−1	0	0	1	0	0
h_{10}	0	0	0	0	0	0	0	0	0	0	−1	0	1	0
v_1	0	0	1	0	−1	0	0	0	0	0	0	0	0	0
v_2	0	0	0	0	0	−1	0	0	1	0	0	0	0	0
v_3	0	0	0	0	0	0	−1	1	0	0	0	0	0	0
v_4	1	0	0	0	1	0	0	0	0	−1	0	−1	0	0
v_5	0	0	0	1	0	1	0	0	0	0	0	0	−1	0
v_6	0	1	0	0	0	0	1	0	0	0	−1	0	0	0
v_7	−1	0	−1	0	0	0	0	0	0	1	0	0	0	1
v_8	0	0	0	−1	0	0	0	0	−1	0	0	0	1	0
v_9	0	−1	0	0	0	0	0	−1	0	0	1	0	0	0
v_{10}	0	0	0	0	0	0	0	0	0	0	0	1	0	−1

- Rank and kernel of $\Delta^{(2)}$ and $\Delta^{(1)}$

$\Delta^{(1)}: \mathbb{Z}^{20} \longrightarrow \mathbb{Z}^{7}$ $\quad$ $\mathrm{Rk}(\Delta^{(1)}) = 6$ $\quad$ $\dim \mathrm{Ker}(\Delta^{(1)}) = 14$

$\Delta^{(2)}: \mathbb{Z}^{14} \longrightarrow \mathbb{Z}^{20}$ $\quad$ $\mathrm{Rk}(\Delta^{(2)}) = 10$ $\quad$ $\dim \mathrm{Ker}(\Delta^{(2)}) = 4$

- 0 – Homology group

$$H_0 = \frac{C_0}{\mathrm{Im}\,(\Delta^{(1)})} = \mathrm{Span}\langle p \rangle = \mathbb{Z}$$

$$p = [\,\alpha\,] = [\,\beta\,] = [\,\gamma\,] = [\,\delta\,] = [\,\eta\,] = [\,\xi\,] = [\,\omega\,]$$

- 1 – Homology group

$$H_1 = \frac{\mathrm{Ker}\,(\Delta^{(1)})}{\mathrm{Im}\,(\Delta^{(2)})} = \mathrm{Span}\langle l_1, l_2, l_3, l_4 \rangle = \mathbb{Z}^4$$

$$l_1 = [\,\Gamma_{11}\,] = [h_4 + h_8 + h_9] = [h_5 + h_6 + h_7] = [h_2 + h_3 + h_{10}]$$

$$l_2 = [\,\Gamma_{12}\,] = [h_4 + h_7] = [h_1 + h_{10}]$$

$$l_3 = [\,\Gamma_4 + \Gamma_7\,] = [v_4 + v_7] = [v_1 + v_{10}]$$

$$l_4 = [\,\Gamma_1 + \Gamma_8\,] = [v_2 + v_3 + v_{10}] = [v_5 + v_6 + v_7] = [v_4 + v_8 + v_9]$$

- 2 – Homology group

$$H_2 = \mathrm{Ker}\,(\Delta^{(2)}) = \mathrm{Span}\langle F_1, F_2, F_3, F_4 \rangle = \mathbb{Z}^4$$

$$F_1 = S_1 + S_3 = R_2 + R_4 + G_2 + G_4 + R_0 + G_0$$

$$F_2 = S_2 + S_3 = R_1 + R_3 + G_1 + G_3 + R_0 + G_0$$

$$F_3 = S_3 = R_0 + G_0$$

$$F_4 = S_1 + S_2 + S_4 = R_0 + G_1 + G_2 + G_3 + G_4 + R_5 + R_6 + R_7 + R_8$$