FBS-complexes: a versatile language for description of aperiodic structures of finite local complexity

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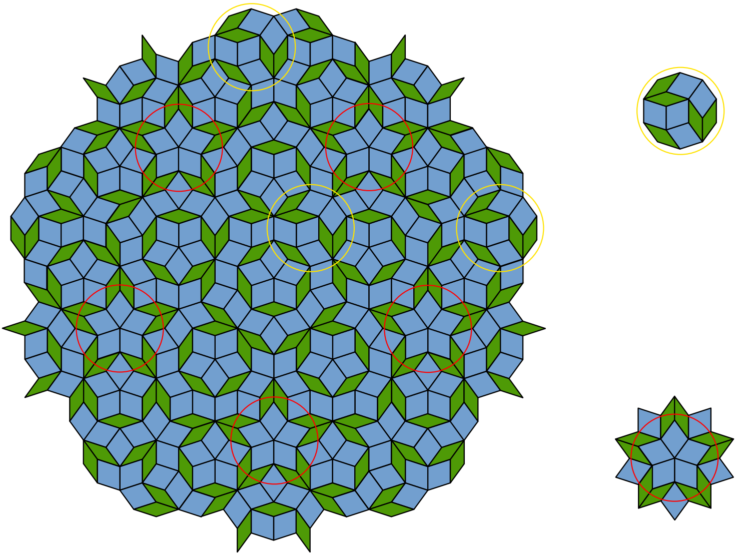
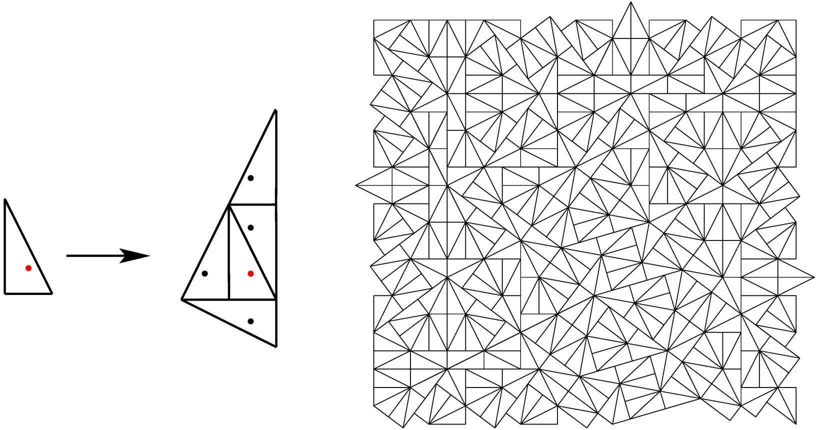
Finite local complexity



Finite local complexity: a non-example

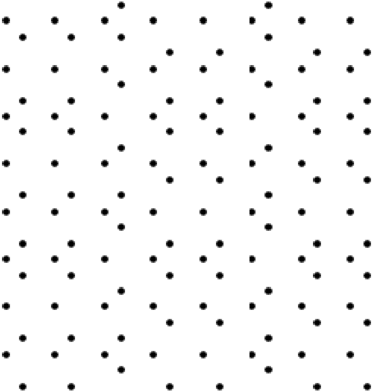
Tiles in the pinwheel tiling come in an infinite number of orientations:

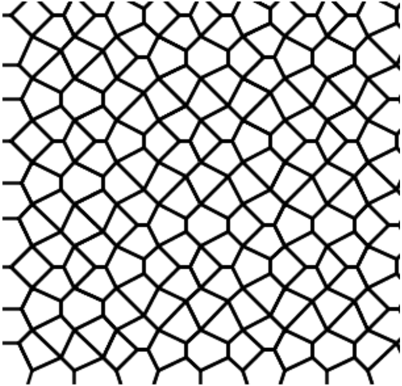


(Image: Baake and Grimm (2012))

From FLC patterns to FLC polyhedral tilings

Voronoi tessellation of a point set yields polyhedral cells:

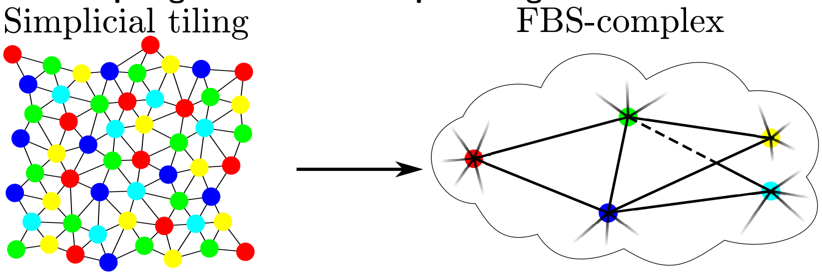




Next step: triangulate each cell to produce a simplicial tiling.
Alternatively: use Delaunay triangulation right away.

From a simplicial tiling to an FBS complex

The recipe: glue all similar simplices together:



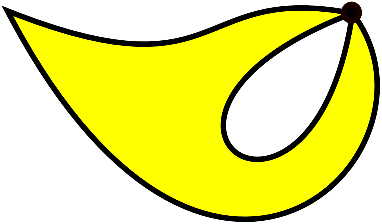
Define "similar simplices":

- Their shapes *must* agree (up to a translation, no rotation allowed!)
- *If* the tiling is decorated, the decorations should also agree.

N.B.: the decoration may encode anything: types of atomic species, local environment up to some range etc. The only condition is: there *must* be a finite number of possible decorations for a given shape.

FBS = "flat-branched semi-simplicial"

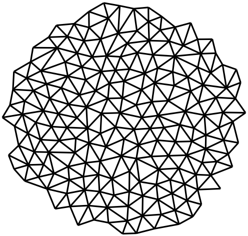
- **Why flat?** Because each simplex inherits a Euclidean structure from the tiling, and because these structures on neighboring simplices agree.
- **Why branched?** Because the underlying tiling may be aperiodic.
- **Why semi-simplicial?** Because vertices of one simplex may be glued together in the complex:



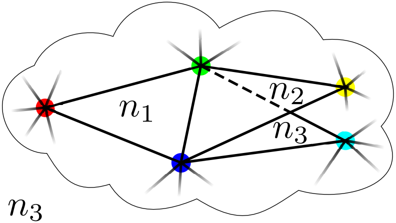
(this is not allowed in *simplicial* complexes!)

From local to global: density and stoichiometry

Take a large "round-shaped" patch of the tiling and count occurrences of each tile species:



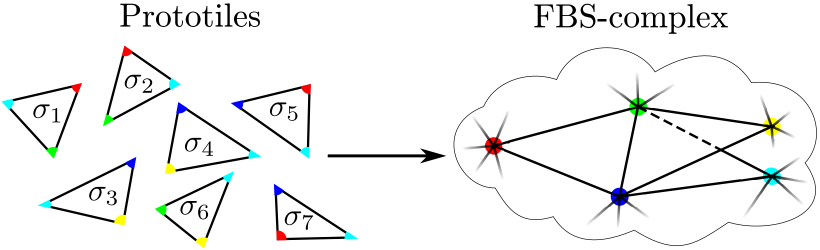
$$n_1 \approx n_2 + n_3$$



The equality is approximate because of the finite size of the patch. In the limit of infinite volume of the patch, it leads to a system of linear equations on the densities of different tile species.
This system must admit non-negative solutions! (What if it does not?)

From local to global: encoding matching rules

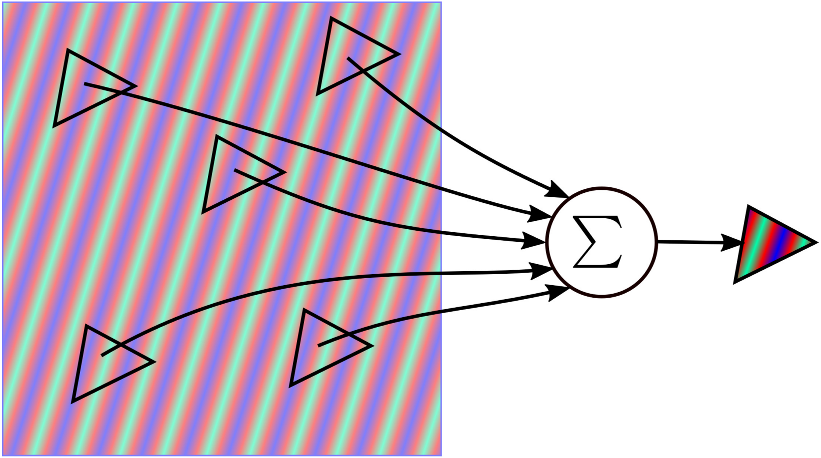
An FBS complex can also be constructed directly from prototiles and the matching rules:



Isometric windings

Tilings respecting the matching rules are in one-to-one correspondence with the special sort of continuous maps from the physical space E to the FBS-complex, called "isometric windings".

From local to global: constraints on coherent diffraction



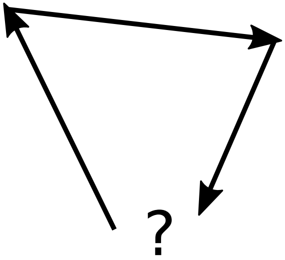
For the wave corresponding to a Bragg peak, the sum should grow asymptotically linearly with the size of the patch.
The results should agree on faces of all simplices of the FBS-complex. This leads to constraints on the contributions of different sites to the coherent diffraction.

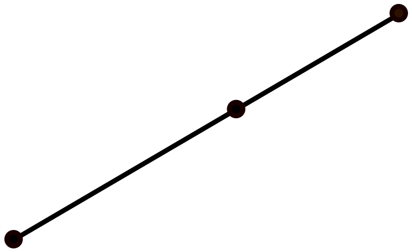
Defining an FBS complex (the first attempt)

A d-dimensional FBS-complex B is a finite d-dimensional semi-simplicial complex equipped with a map

$$\rho : \{\text{edges of } B\} \to E$$

Problems with this definition: non-closed faces and degenerate simplices.





Defining an FBS complex

A d-dimensional FBS-complex B is a finite connected d-dimensional semi-simplicial complex equipped with a homomorphism of the group of 1-chains

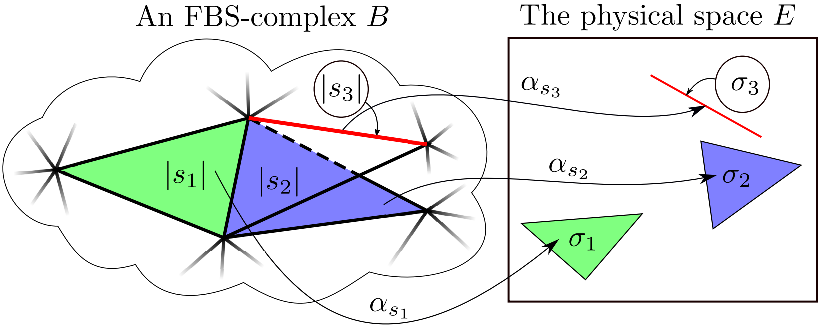
$$\rho : C_1(B, \mathbb{Z}) \to E$$

vanishing on boundaries:

$$\rho \circ \partial = 0$$

and such that for any d-simplex $s \in B$ and the set $\{e_1, \ldots, e_d\}$ of edges of s originating at the same vertex, the vectors $\rho(e_1), \ldots, \rho(e_d)$ are linearly independent.

Recovering the tile shapes



Let $\{e_1, \ldots, e_k\}$ be the edges of a k-simplex $s \in B$ having a common vertex. Identification of the barycentric coordinates yields a homeomorphism of $|s|$ onto an open affine simplex in E:

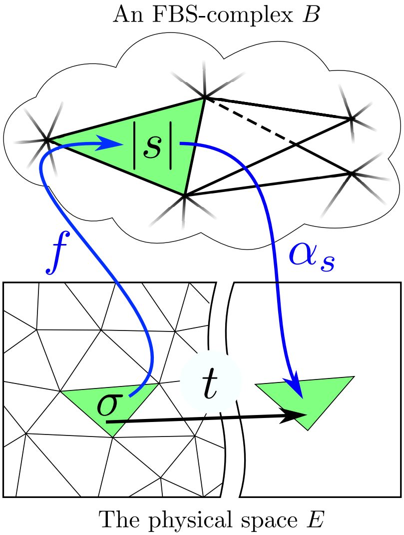
$$\alpha_s : |s| \to \left\{ \sum_{i=1}^{k} c_i \rho(e_i) \;\middle|\; \sum_{i=1}^{k} c_i < 1,\ c_i > 0 \right\} + t$$

defined up to a translation $t \subset E$.

Isometric windings

A continuous map $f : E \to |B|$ is called isometric winding if

- Over each simplex $|s| \subset |B|$ (of any dimension) f is a covering map.
- For each connected component σ of $f^{-1}(|s|)$, the composition $\alpha_s \circ f\big|_\sigma$ is a translation by some vector $t \in E$.



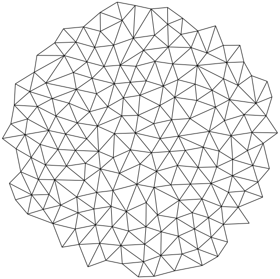
Density and stoichiometry revisited

Let $f : E \to B$ be an isometric winding. Suppose that for all $s \in B$ the spatial density ν_s of tiles in $f^{-1}(|s|)$ is well defined (either as a natural density, or by averaging over a transitionally invariant measure on the Hull of the tiling). Then

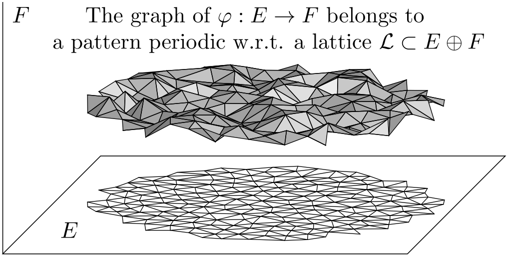
$$c = \sum_{\substack{s \in B \\ \dim s = d}} \nu_s s$$

is a d-cycle in $C_d(B, \mathbb{R})$. That is, possible values of densities are determined by the homology group $H_d(B, \mathbb{R})$.

Quasiperiodic tilings: lifting and matching rules



$\dim(E) = d$



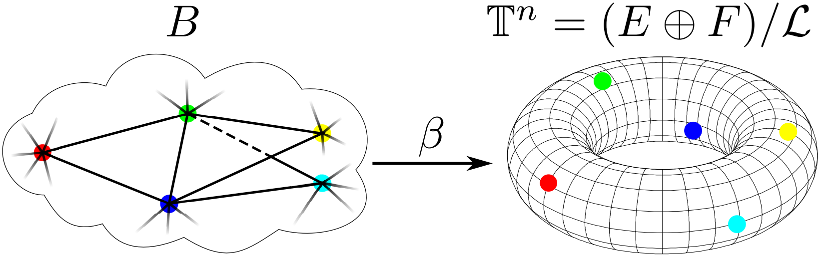
$\dim(E \oplus F) = n$

Matching rules

For tilings obtained by the cut-and-project method, the *phason coordinate* φ is globally bounded. It is generally believed that this is the case for real quasicrystals; if this condition is enforced by the underlying FBS-complex B, we say that B represents *weak matching rules*. If φ grows slower than linearly, we say that B represents *minimal matching rules*.

Quasiperiodic tilings: the lifting map β

Factoring the lifted tiling w.r.t. the lattice $\mathcal{L}$ yields this:

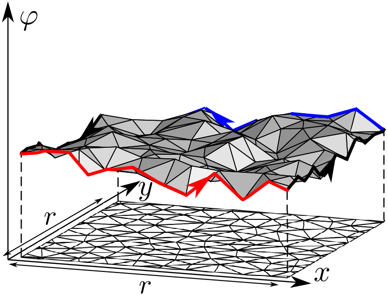


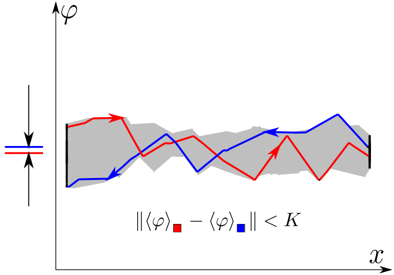
The map β emerges in two different contexts:

- If we start with an existing tiling model, then the FBS-complex is known, but the lifting is to be constructed.
- If we start with the phased data, then the lifting dimension n and the positions of the lifted vertices of B in $\mathbb{T}^n$ are known, but B itself is to be constructed.

Quasiperiodic tilings: slope locking property

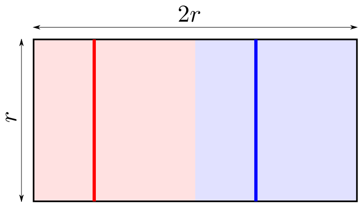
The map $\beta : B \to \mathbb{T}^n$ is called *slope locking* if the image of every d-cycle on B annihilates the space of mixed forms $T = \left(\bigwedge^{d-1} E^*\right) \wedge F^*$.





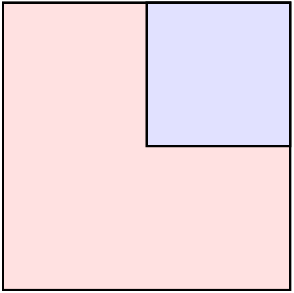
The consequence of the slope locking: since $dx \wedge d\varphi$ is a mixed form, its integral over the lifted tiling patch within a cube of edge length r evaluates to a boundary term and is bounded by Kr^{d-1} for some global constant K independent on r.

Quasiperiodic tilings: order propagation

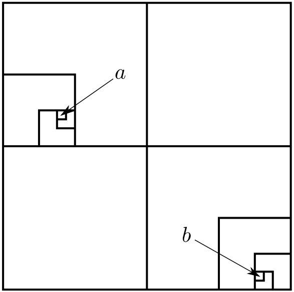


$\forall r \in \mathbb{R}_+$

$\|\langle\varphi\rangle_{\square} - \langle\varphi\rangle_{\square}\| < K$

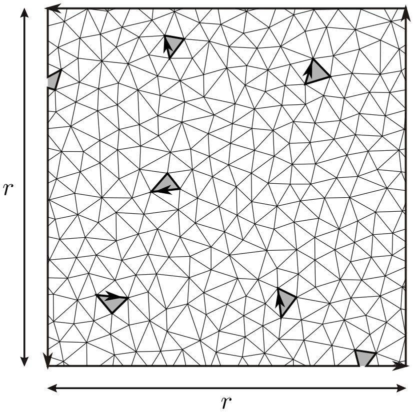


$\|\langle\varphi\rangle_{\square} - \langle\varphi\rangle_{\square}\| < Kd$



$\|\varphi(a) - \varphi(b)\| < Kd\log_2(r) + \text{const}$

Quasiperiodic tilings: defects and robustness



Defects can be modeled by tiles originating from a larger FBS-complex $\check{B} \supset B$ (shaded triangles). The length of the boundary of the defect-free part of this patch scales with r as

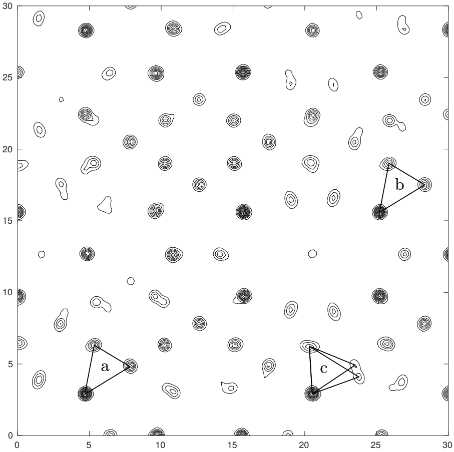
$$\mathcal{O}(\max(\varepsilon r^d, r^{d-1})),$$

where ε is the density of defects. The difference of the average vallues of φ on the opposite faces is then bounded by $K_1' + \varepsilon K_2' r$.

The arguments above then leads to the following upper bound for the phason coordinate:

$$\|\varphi(x)\| < K_1 \log(\|x\|) + K_2 \varepsilon \|x\| + \mathrm{const}$$

Real quasicrystals: constructing $\mathcal{T}_0$ and B_0



The cut through the phased density of $\mathrm{Cd}_{5.7}\mathrm{Yb}$ by the two-fold symmetry plane. Triangles (a) and (b) are $\mathcal{L}$-equivalent.

- Label each peak by the type of its atomic surface and a translation $\ell \in \mathcal{L}$.
- Eliminate some peaks to avoid short distances (making random choice).
- Construct the simplicial tiling $\mathcal{T}_0$ by Delaunay triangulation.
- Construct the FBS-complex B_0 by factoring $\mathcal{T}_0$ with respect to the $\mathcal{L}$-equivalence.

N.B.: Both of the triangles labeled (c) will appear in $\mathcal{T}_0$.

Real quasicrystals: reduction and refinement

Reduction

The "raw" FBS-complex B_0 contains too many simplices for $\beta_0 : B_0 \to \mathbb{T}^n$ be slope locking. When constructing $\mathcal{T}_0$, we know already that some simplices are uncertain (those with vertices at the peaks of small amplitude, or those occurring rarely in $\mathcal{T}_0$). We try to construct the working FBS-complex B by gradually eliminating such simplices from B_0.

Refinement

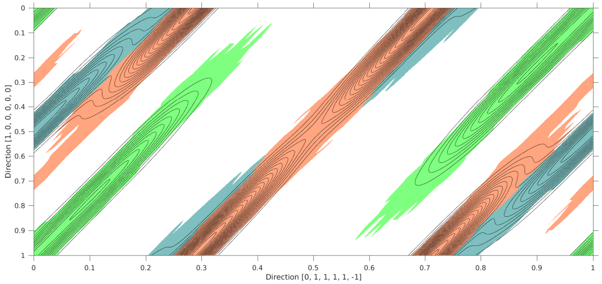
Initially, the $\mathcal{L}$-equivalence in $\mathcal{T}_0$ is defined w.r.t. the labeling of the vertices by atomic surfaces. To extend the range of the matching rules, we can refine the labeling by the labels of the nearest neighbors. This procedure can be repeated, each time encoding into B_0 the information about larger local configurations.

Atomic density and partial validation

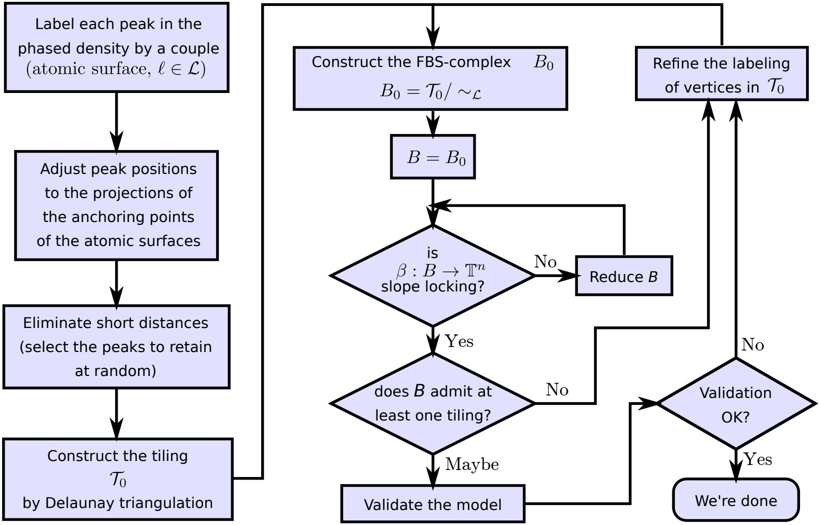
Under some mild "matter conservation" conditions, the model predicts the exact value of the density of atoms belonging to a given atomic surface:

$$\sum_{1 \leq i_1 < \cdots < i_d \leq n} \frac{m_{i_1,\ldots,i_d}}{M} |\mathbf{k}_{i_1} \wedge \cdots \wedge \mathbf{k}_{i_d}|, \text{ where } M, m_{i_1,\ldots,i_d} \in \mathbb{Z}.$$

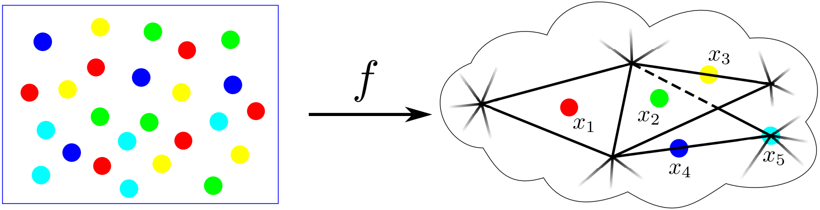
This prediction can be compared with the total density and the volumes of individual atomic surfaces obtained e.g. by the watershed algorithm:



Matching rules exploration: Flow chart



Diffraction revisited: the model



The diffracting density is a tempered distribution:

$$\varrho = \sum_{i=1}^{m} \left(\sum_{y \in f^{-1}(x_i)} w_i \delta_y \right)$$

with the diffraction measure

$$\eta = \sum_{i,j=1}^{m} \overline{w_i} w_j \zeta_{ij},$$

where ζ_{ij} are complex-valued tempered measures on E^*.

Diffraction: some results

If $k \subset E^*$ belongs to the pure point part of the matrix-valued measure ζ, then

$$\zeta_{ij}(\{k\}) = \overline{a_k(x_i)} a_k(x_j),$$

where $a_k : |B| \to \mathbb{C}$ over open d-simplices of $|B|$ are sections of the locally constant sheaf $\mathcal{F}_{(k)}$ of complex spaces, defined by the homomorphism of the fundamental groupoid $\Pi(|B|)$ to $GL(1, \mathbb{C})$:

$$\gamma \mapsto \exp\left(-2\pi \mathrm{i} k \cdot \check{\rho}(\gamma)\right),$$

where $\check{\rho}$ extends ρ from homotopy classes of edge-paths to those of arbitrary paths. Moreover,

$$z_k = \sum_{\substack{s \in B \\ \dim(s) = d}} \left(a_k \big|_{|s|} \right) s$$

is a cycle of $C_d(B, \mathcal{F}_{(k)})$.

References

- Baake, M. and Grimm, U. On the Notions of Symmetry and Aperiodicity for Delone Sets *Symmetry* (2012), **4**, pp. 566-580
- Kalugin, P. and Katz, A. Robust minimal matching rules for quasicrystals *Acta Cryst A*. **75** (2019) pp. 669-693
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