Spectral analysis on self-similar graphs, fractals, and groups

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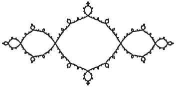

** (part iv) **

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A subset $\boldsymbol{\Lambda} \subset \mathbb{R}^{\boldsymbol{d}}$ is a **Delone set** if it is **uniformly discrete**:

$$\exists \varepsilon > 0 : \ |\vec{x} - \vec{y}| > \varepsilon \quad \forall \vec{x}, \vec{y} \in \Lambda$$

and relatively dense:

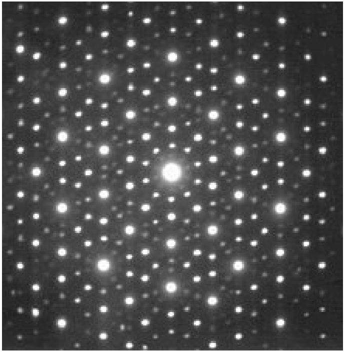
$$\exists R > 0 : \ \Lambda \cap B_R(\vec{x}) \neq \varnothing \quad \forall \vec{x} \in \mathbb{R}^d.$$

A Delone set has **finite local complexity** if $\forall R > 0 \exists$ finitely many clusters $P_1, \ldots, P_{n_R}$ such that for any $\vec{x} \in \mathbb{R}^d$ there is an i such that the set $B_R(\vec{x}) \cap \Lambda$ is translation-equivalent to P_i.

A Delone set Λ is **aperiodic** if $\Lambda - \vec{t} = \Lambda$ implies $\vec{t} = \vec{0}$. It is **repetitive** if for any cluster $P \subset \Lambda$ there exists $R_P > 0$ such that for any $\vec{x} \in \mathbb{R}^d$ the cluster $B_{R_P}(\vec{x}) \cap \Lambda$ contains a cluster which is translation-equivalent to P.

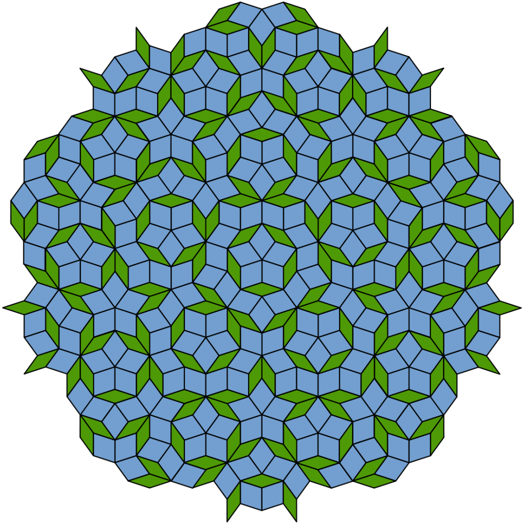
These sets have applications in crystallography (≈ 1920), coding theory, approximation algorithms, and the theory of quasicrystals.

Electron diffraction picture of a Zn-Mg-Ho quasicrystal



Aperiodic tilings were discovered by mathematicians in the early 1960s, and, some twenty years later, they were found to apply to the study of natural quasicrystals (1982 Dan Shechtman, 2011 Nobel Prize in Chemistry).

Penrose tiling



pattern space of a Delone set

Let $\Lambda_0 \subset \mathbb{R}^d$ be a **Delone set**. The **pattern space (hull)** of Λ_0 is the closure of the set of translates of Λ_0 with respect to the metric ϱ, i.e.

$$\Omega_{\Lambda_0} = \overline{\left\{\varphi_{\vec{t}}\,(\Lambda_0) : \vec{t} \in \mathbb{R}^d\right\}}.$$

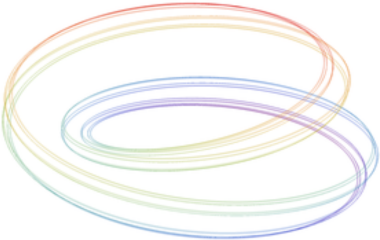
Definition

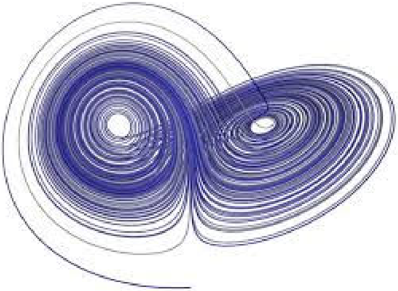
Let $\Lambda_0 \subset \mathbb{R}^d$ be a Delone set and denote by $\varphi_{\vec{t}}\,(\Lambda_0) = \Lambda_0 - \vec{t}$ its translation by the vector $\vec{t} \in \mathbb{R}^d$. For any two translates Λ_1 and Λ_2 of Λ_0 define $\varrho(\Lambda_1, \Lambda_2) = \inf\{\varepsilon > 0 : \ \exists\ \vec{s}, \vec{t} \in B_\varepsilon(\vec{0}) : \ B_{\frac{1}{\varepsilon}}(\vec{0}) \cap \varphi_{\vec{s}}(\Lambda_1) = B_{\frac{1}{\varepsilon}}(\vec{0}) \cap \varphi_{\vec{t}}(\Lambda_2)\} \wedge 2^{-1/2}$

Assumption

The action of $\mathbb{R}^d$ on Ω is uniquely ergodic:
Ω is a compact metric space with the unique $\mathbb{R}^d$-invariant probability measure μ.

Topological solenoids (similar topological features as the pattern space $\mathbf{\Omega}$):





Theorem (P.Alonso-Ruiz, M.Hinz, T., R.Treviño, arXiv:1801.08956)

(i) *If* $\vec{W} = (\vec{W}_t)_{t\geq 0}$ *is the standard Gaussian Brownian motion on* $\mathbb{R}^d$*, then for any* $\Lambda \in \Omega$ *the process* $X_t^\Lambda := \varphi_{\vec{W}_t}(\Lambda) = \Lambda - \vec{W}_t$ *is a conservative Feller diffusion on* (Ω, ϱ)*.*

(ii) *The semigroup* $P_t f(\Lambda) = \mathbb{E}[f(X_t^\Lambda)]$ *is*

self-adjoint on L^2_μ, Feller but not strong Feller.

Its associated Dirichlet form is regular, strongly local, irreducible, recurrent, and has Kusuoka-Hino dimension d*.*

(iii) *The semigroup* $(P_t)_{t>0}$ **does not admit heat kernels with respect to μ**. *It does have Gaussian heat kernel with respect to the not-σ-finite (no Radon-Nykodim theorem) pushforward measure* λ_Ω^d

$$p_\Omega(t, \Lambda_1, \Lambda_2) = \begin{cases} p_{\mathbb{R}^d}(t, h_{\Lambda_1}^{-1}(\Lambda_2)) & \text{if } \Lambda_2 \in \mathrm{orb}(\Lambda_1), \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

(iv) **There are no semi-bounded or L^1 harmonic functions ("Liouville-type")**

no classical inequalities

Useful versions of the Poincare, Nash, Sobolev, Harnack inequalities DO NOT HOLD, except in orbit-wise sense.

spectral properties

Theorem (P.Alonso-Ruiz, M.Hinz, T., R.Treviño, arXiv:1801.08956)

The unitary **Koopman operators** $U_{\vec{t}}$ *on* $L^2(\Omega, \mu)$ *defined by* $U_{\vec{t}} f = f \circ \varphi_{\vec{t}}$ *commute with the heat semigroup*

$$\boxed{U_{\vec{t}} P_t = P_t U_{\vec{t}}}$$

hence commute with the Laplacian Δ, *and all spectral operators, such as the unitary Schrödinger semigroup.*

... hence we may have continuous spectrum (no eigenvalues) under some assumptions even though μ is a probability measure on the compact set Ω.

Under special conditions P_t is connected to the evolution of a **Phason**: "Phason is a quasiparticle existing in quasicrystals due to their specific, quasiperiodic lattice structure. Similar to phonon, phason is associated with atomic motion. However, whereas phonons are related to translation of atoms, phasons are associated with atomic rearrangements. As a result of these rearrangements, waves, describing the position of atoms in crystal, change phase, thus the term "phason" (from the wikipedia)".

Phason evolution

Corollary (P.Alonso-Ruiz, M.Hinz, T., R.Treviño, arXiv:1801.08956)

The unitary **Koopman operators** $U_{\vec{t}}$ *on* $L^2(\Omega, \mu)$ *defined by* $U_{\vec{t}} f = f \circ \varphi_{\vec{t}}$ *commute with the heat semigroup*

$$\boxed{U_{\vec{t}} P_t = P_t U_{\vec{t}}}$$

hence commute with the Laplacian Δ*, and all spectral operators, including the unitary* **Schrödinger semigroup** $e^{i\Delta t}$

$$\boxed{U_{\vec{t}} e^{i\Delta t} = e^{i\Delta t} U_{\vec{t}}}$$

Recent physics work on phason ("accounts for the freedom to choose the origin"):
Topological Properties of Quasiperiodic Tilings
(Yaroslav Don, Dor Gitelman, Eli Levy and Eric Akkermans
Technion Department of Physics)
`https://phsites.technion.ac.il/eric/talks/`
J. Bellissard, A. Bovier, and J.-M. Chez, Rev. Math. Phys. 04, 1 (1992).

Topological Properties of Quasiperiodic Tilings

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Abstract

Topological properties of finite quasiperiodic tilings are examined. We study two specific physical quantities: (a) the structure factor related to the Fourier transform of the structure; (b) spectral properties (using scattering matrix formalism) of the corresponding quasiperiodic Hamiltonian. We show that both quantities involve a phase, whose windings describe topological numbers. We link these two phases, thus establishing a "Bloch theorem" for specific types of quasiperiodic tilings.

Substitution Rules – 1D Tilings

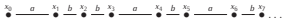
Define a *binary* substitution rule by

$$\begin{matrix}\sigma(a)=a^\alpha b^\beta \\ \sigma(b)=a^\gamma b^\delta\end{matrix} \iff \begin{matrix} a\mapsto a^\alpha b^\beta \\ b\mapsto a^\gamma b^\delta .\end{matrix}$$

Associate occurrence matrix: $M=\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}$ Consider only primitive matrices:

- Largest eigenvalue $\lambda_1>1$ (Perron-Frobenius)
- Left and right first eigenvectors are strictly positive

Distribution of letters underlies distribution of atoms:



Define atomic density

$$\rho(x)=\sum\nolimits_k \delta(x-x_k),$$

with distances for a and b given by $\delta_k=x_{k+1}-x_k=d_{a,b}$.
Let $\bar{d}$ be the mean distance and u_k the deviations from the mean. Define

$$x_k=\bar{d}\,k+\delta u_k,\qquad \delta\equiv d_a-d_b.$$

Let $g(\xi)=\sum_k e^{-i\xi x_k}$ be the diffraction pattern, and $S(\xi)=|g(\xi)|^2$ the structure factor. Using $\xi_0=2\pi/\bar{d}$, the Bragg peaks are located at [1]

$$\xi_{m,N}=m\,\lambda_1^{-N}\,\xi_0,\quad m,N\in\mathbb{Z}.$$

We consider the following families:

Pisot. The second eigenvalue $|\lambda_2|<1$.
Non-Pisot. The second eigenvalue $|\lambda_2|\geq 1$.
Fluctuations u_k are unbounded [2]; there are no Bragg peaks [3].

Examine the following examples:

Fibonacci. $a\mapsto ab$, $b\mapsto a$. It is Pisot, $M=\begin{pmatrix}1&1\\1&0\end{pmatrix}$, $\lambda_1=(\sqrt{5}+1)/2\equiv\tau$ the golden ratio and $\lambda_2=-\tau^{-1}$. Bragg peaks are located at $\xi_{p,q}=(p+q/\tau)\,\xi_0$.
In C&P language, $s=1/\tau$ and

$$\boxed{\xi_{p,q}/\xi_0=p+qs}\quad p,q\in\mathbb{Z}.$$

Thue–Morse. $a\mapsto ab$, $b\mapsto ba$. Here it is Pisot, $M=\begin{pmatrix}1&1\\1&1\end{pmatrix}$,
$\lambda_1=2$ and $\lambda_2=0$. Bragg peaks: $\xi_{m,N}=m\,2^{-N}\,\xi_0$, $m,N\in\mathbb{Z}$.

Spectral Properties of Tilings

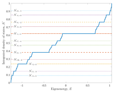
Consider a 1D tight-binding equation,

$$-(\psi_{k+1}+\psi_{k-1})+V_k\psi_k=2E\psi_k.$$

The gaps in the integrated density of states are given by the gap labeling theorem [4],

$$\mathcal{N}_{m,N}=\frac{1}{c}m\,\lambda_1^{-N}\quad(\mathrm{mod}\ 1),\quad m,N\in\mathbb{Z}.$$

Here, c is the gcd of λ_1 and its corresponding eigenvectors in both M and the collared M_2.



In C&P sequences,

$$\boxed{\mathcal{N}_{p,q}=p+qs\quad(\mathrm{mod}\ 1)}\quad p,q\in\mathbb{Z}.$$

Structural Phase – Phason as a Gauge Field

Another way to define a tiling is by using a characteristic function. We consider the following choice [5, 6]:

$$\chi(n,\phi)=\mathrm{sign}[\cos(2\pi n s+\phi)-\cos(\pi s)].$$

with $s\to s_N=c_N/d_N$ the slope of the C&P scheme, and $n=0\ldots d_N-1$.

The phase ϕ, called a phason, accounts for the gauge freedom to choose the origin. It is taken discretely as $\phi\to\phi_\ell=2\pi\ell/d_N$.

Let $s_0(n)=\chi(n,0)$. Let $\mathcal{T}[s_0(n)]=s_0(n+1)$ be the translation operator. Define

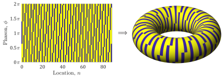
$$\Sigma_0=\begin{pmatrix}s_0\\ \mathcal{T}[s_0]\\ \cdots\\ \mathcal{T}^{d_N-1}[s_0]\end{pmatrix}\implies\Sigma_0(n,\ell)=\mathcal{T}^\ell[s_0(n)].$$

Consider now the row permuted Σ_1

$$\Sigma_1(n,\ell)=\mathcal{T}^{m(\ell)}[s_0(n)],\qquad m(\ell)=\ell\,c_N^{-1}\quad(\mathrm{mod}\ d_N).$$

Lemma. For $\phi_\ell=2\pi\ell/d_N$ with $n,\ell=0\ldots d_N-1$ one has $\chi(n,\phi_\ell)=\Sigma_1(n,\ell)$.
This defines a *discrete* phason ϕ_ℓ for the structure.

The structure of Σ_1 ($d_N\times d_N$) is that of a torus:



The discrete Fourier transform of Σ_1 about n reads

$$G(\xi,\ell)\equiv\sum\nolimits_{n=0}^{d_N-1}\omega^{-\xi n}\,\Sigma_1(n,\ell)=\omega^{m(\ell)\xi}\,\varsigma_0(\xi).$$

- The structure factor $S(\xi,\phi)=|\varsigma_0(\xi)|^2$ is ϕ-independent.
- The phase of $G(\xi,\ell)$ reads

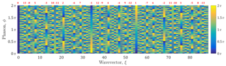
$$\boxed{\Theta(\xi,\ell)\equiv\arg\omega^{m(\ell)\xi}=\phi_\ell\,\xi/c_N\quad(\mathrm{mod}\ 2\pi).}$$

Corollary. For any diffraction peak (discrete Bragg peak) $\xi_{p,q}=q c_N$ one has the (discrete) winding number at $\xi_{p,q}$,

$$\Theta(\xi_{p,q})=\frac{2\pi}{d_N}\ell\,q,$$

hence

$$\boxed{W_{\xi_{p,q}}=\frac{1}{2\pi}\int_0^{2\pi}\frac{\partial\Theta(\xi=\xi_{p,q},\phi)}{\partial\phi}\,\mathrm{d}\phi=q.}$$



Here we used the Fibonacci sequence ($s=1/\tau$) with $d_N=89$ sites. The winding numbers are indicated by the red numbers above.

Remark. The analysis above for the winding numbers is done for rational approximations $s_N=c_N/d_N$. It holds by construction for the irrational case $s_N\to s$.

Spectral Phase: Scattering Matrix Approach

Spectral properties are also accessible from the continuous wave equation,

$$-\psi''(x)-k_0^2\,v(x)\,\psi(x)=k_0^2\,\psi(x),$$

with scattering boundary conditions.

The scattering $\mathcal{S}$-matrix is defined by $\begin{pmatrix}\overleftarrow{o}\\ \overrightarrow{o}\end{pmatrix}=\begin{pmatrix}\overleftarrow{\tau}(k) & \overrightarrow{r}(k)\\ \overleftarrow{r}(k) & \overrightarrow{\tau}(k)\end{pmatrix}\begin{pmatrix}\overrightarrow{\imath}\\ \overleftarrow{\imath}\end{pmatrix}\equiv\mathcal{S}\begin{pmatrix}\overrightarrow{\imath}\\ \overleftarrow{\imath}\end{pmatrix}$, with $\overrightarrow{\tau}=\overrightarrow{R}\,e^{i\overrightarrow{\vartheta}}$ and $\overleftarrow{\tau}=\overleftarrow{R}\,e^{i\overleftarrow{\vartheta}}$. It is unitary and can be diagonalized to $\mathcal{S}\mapsto\begin{pmatrix}e^{i\gamma_1}&0\\0&e^{i\gamma_2}\end{pmatrix}$ so that $\det\mathcal{S}=e^{2i\delta(k)}$ with the total phase shift $\delta(k)=(\gamma_1(k)+\gamma_2(k))/2$ independent of ϕ. We are interested in the chiral phase,

$$\boxed{\alpha(k,\phi)=\overrightarrow{\vartheta}(k,\phi)-\overleftarrow{\vartheta}(k,\phi).}$$

Using the Krein-Schwinger formula [7] allows to relate the change of density of states to the scattering data,

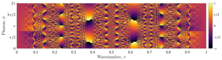
$$\varrho(k)-\varrho_0(k)=\frac{1}{2\pi}\,\mathrm{Im}\,\frac{\mathrm{d}}{\mathrm{d}k}\ln\det\mathcal{S}(k).$$

So that the integrated density of states is

$$\mathcal{N}(k)-\mathcal{N}_0(k)=\delta(k)/\pi.$$

The total phase shift $\delta(k)$ is independent of the phason ϕ unlike the *chiral* phase $\alpha(k,\phi)$, whose winding for values of k inside the gaps is given by [8],

$$\boxed{W_{\alpha_q}=\frac{1}{2\pi}\int_0^{2\pi}\frac{\partial\alpha\,(k=k_{p,q},\phi)}{\partial\phi}\,\mathrm{d}\phi=2q.}$$



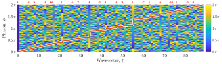
Here we used the Fibonacci sequence ($s=1/\tau$) with $d_N=233$ sites.

Relation between both Phases: a "Bloch Theorem"

In 1D C&P structures, The locations of Bragg peaks for a diffraction spectrum correspond to the spectral density of states,

$$\boxed{\xi_{p,q}/d_N=p+qs=\mathcal{N}_{p,q}}\quad p,q\in\mathbb{Z}.$$

Drawing the integrated density of states $\mathcal{N}$ (red line) on top the structural phase $\Theta(\xi,\phi)$, shows numerically the relation between $\xi_{p,q}$ and $\mathcal{N}_{p,q}$.



Both $\xi_{p,q}$ and $\mathcal{N}_{p,q}$ are isomorphic to $\mathbb{Z}\oplus s\mathbb{Z}$. The second $\mathbb{Z}$, corresponding to q, can be derived independently from the windings of both the structural phase $\Theta(\phi)$ and the chiral phase $\alpha(\phi)$. Since these phases account for windings, they are isomorphic

$$\boxed{\Theta(\phi)\cong\alpha(\phi).}$$

The winding gives a topological interpretation to these phases. This result can be viewed as a Bloch theorem for quasiperiodic tilings [9].

Cut and Project Scheme

An alternative method to build quasiperiodic tilings is the Cut & Project scheme. The procedure is as follows [10].

Cut.

1. Start with an n-dimensional space $R=\mathbb{R}^n$.
2. Insert "atoms" on the integer lattice $Z=\mathbb{Z}^n$.
3. Divide R into the *physical space* E and the *internal space* $E_\perp$ such that $E\oplus E_\perp=R$ and $E\cap E_\perp=\emptyset$.
4. To resolve ambiguity for E, choose an initial location $\boldsymbol{c}\in R$ such that E passes through $\boldsymbol{c}$. There is no such requirement for $E_\perp$.

Project.

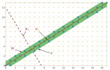
1. Inspect the hypercube $\mathbb{I}_n=[-0.5,0.5)^n$.
2. The *window* is its projection on the internal space $W=\pi_\perp(\mathbb{I}n)$.
3. The *strip* is the product with the physical space $S=W\otimes E$.
4. Choose only the points inside the strip $S\cap Z$, and project them onto the physical space, $Y=\pi(S\cap Z)$.
5. The *atomic density* is given by $\rho(x)\equiv\rho_c(x)=\sum_{y\in Y}\delta(x-y)$ with $x\in E$. Note the implicit dependency of Y on $\boldsymbol{c}$.

For 1D systems, define the phason

$$\phi=2\pi\,b/W\qquad b\in E_\perp,$$

where W is the window above.
The slope s is given by

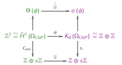
$$1/s=1+\cot\beta.$$



Useful Tools

In periodic structures, topological numbers are described as Chern numbers. This does not happen in quasiperiodic tilings, since there exists no notion of a Brillouin zone. But alternative tools exist to describe topological properties of quasiperiodic tilings. We now enumerate some of them.

- Tiling space $\mathcal{T}$ (dependent on λ_1 or s) and its hull $\Omega_\mathcal{T}$.
- Čech cohomology $\check{H}^1(\Omega_\mathcal{T})$, simplicial cohomology $H^1(\Gamma_n)$ and Bratteli graphs [11, 12].
- K-theory, $K_0(\Omega_\mathcal{T})$ group and the abstract gap labeling theorem [4, 13].
- The Bloch theorem described before can be given an interpolation for 1D C&P tilings (for an irrational slope $s\notin\mathbb{Q}$) by means of the "commutative diagram":



The topological features are contained in $\check{H}^1$ or K_0 groups.

Conclusions

- We have defined two types of phases—a structural and spectral one—whose windings unveil topological features of quasiperiodic tilings.
- We found a relation between these two phases, which can be interpreted as a Bloch-like theorem.
- We have considered here a subset of tilings, which are known as Sturmian (C&P) words. Our results can be extended to a broader families of tilings in one dimension, and to tiles in higher dimensions ($D>1$).
- All these features have been observed experimentally [5, 6].

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Helmholtz, Hodge and de Rham

Theorem

Assume $\boldsymbol{d = 1}$*. Then the space* $\boldsymbol{L^2(\Omega, \mu, \mathbb{R}^1)}$ *admits the orthogonal decomposition*

$$\boldsymbol{L^2(\Omega, \mu, \mathbb{R}^1) = \mathrm{Im}\,\nabla \oplus \mathbb{R}(dx).} \tag{2}$$

In other words, the $\boldsymbol{L^2}$-cohomology is 1-dimensional, which is surprising because the **de Rham cohomology is not one dimensional**.

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