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.

1D Tilings

Substitutions and Atomic Distributions

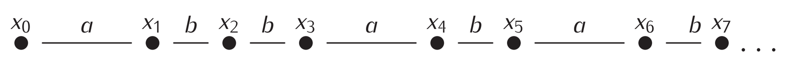
Define a *binary* substitution rule by

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

Associate occurrence matrix: $M = \left(\begin{smallmatrix}\alpha & \beta \\ \gamma & \delta\end{smallmatrix}\right)$
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

$$\rho(x) = \sum_k \delta(x - x_k)$$

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

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

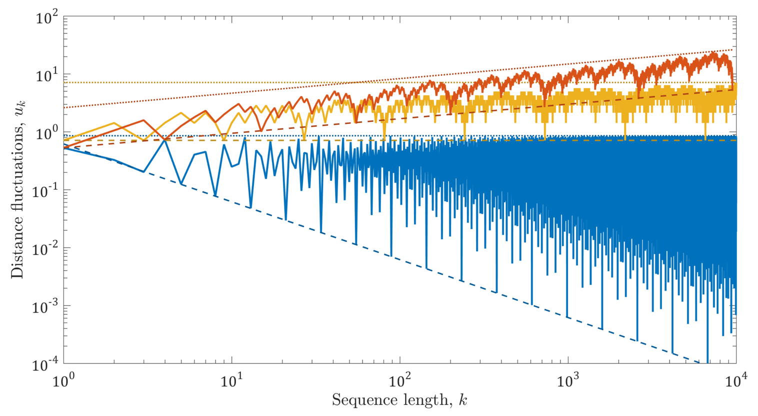
Let $g(\xi) = \sum_k e^{-i\xi x_k}$ be the diffraction pattern, and $S(\xi) = |g(\xi)|^2$ the structure factor. Bragg peaks are located at [1]

$$\xi_{m,N} = \frac{2\pi}{\bar{d}} \frac{m}{\lambda_1^N}.$$

We consider the following families:

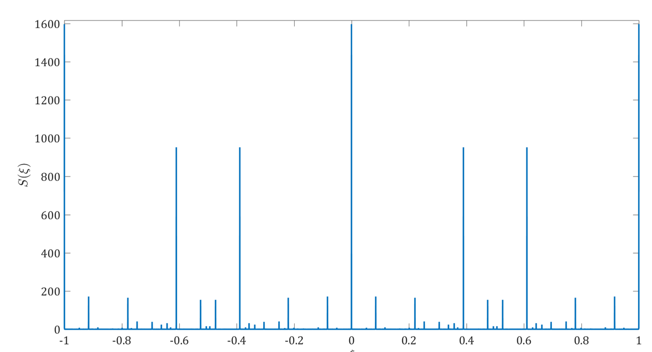
Pisot. The second eigenvalue $|\lambda_2| < 1$.

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



Examples

Fibonacci. $a \mapsto ab$, $b \mapsto a$. It is Pisot, $M = \left(\begin{smallmatrix}1 & 1 \\ 1 & 0\end{smallmatrix}\right)$,
$\lambda_1 = (\sqrt{5}+1)/2 \equiv \tau$ the golden ratio and $\lambda_2 = -\tau^{-1}$.
Bragg peaks: $\xi_{p,q} = (p + q\,\tau)\, 2\pi/\bar{d}$.



Thue-Morse. $a \mapsto ab$, $b \mapsto ba$. Here it is Pisot, $M = \left(\begin{smallmatrix}1 & 1 \\ 1 & 1\end{smallmatrix}\right)$,
$\lambda_1 = 2$ and $\lambda_2 = 0$. Bragg peaks: $\xi_{m,N} = m\, 2^{-N}(2\pi/\bar{d})$.

The Phason – Structural Phase

Another way to define a tiling is by using a characteristic function. We consider the following choice [4, 5]:

$$\chi(n, \phi) = \operatorname{sign}\left[\cos\left(2\pi n \lambda_1^{-1} + \phi\right) - \cos\left(\pi \lambda_1^{-1}\right)\right]$$

with $n = 0 \ldots F_N - 1$ and $[0, 2\pi] \ni \phi \to \phi_\ell = 2\pi F_N^{-1}\,\ell$. The phase ϕ—called a phason—accounts for the freedom to choose the origin.
Let $s_0(n) = \chi(n, 0)$. Let $\mathcal{T}[s_0(n)] = s_0(n+1)$ be the translation operator. Define

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

Consider now a row permuted Σ_1

$$\Sigma_1(n, \ell) = \mathcal{T}^{m(\ell)}[s_0(n)], \qquad m(\ell) = \ell\, F_{N-1}^{-1} \pmod{F_N}.$$

Lemma. For $\phi_\ell = 2\pi\ell/F_N$ with $n, \ell = 0 \ldots F_N - 1$ one has $\chi(n, \phi_\ell) = \Sigma_1(n, \ell)$.

Corollary. This defines a *discrete* phason ϕ_ℓ for the structure.

The discrete Fourier transform of Σ_1 reads

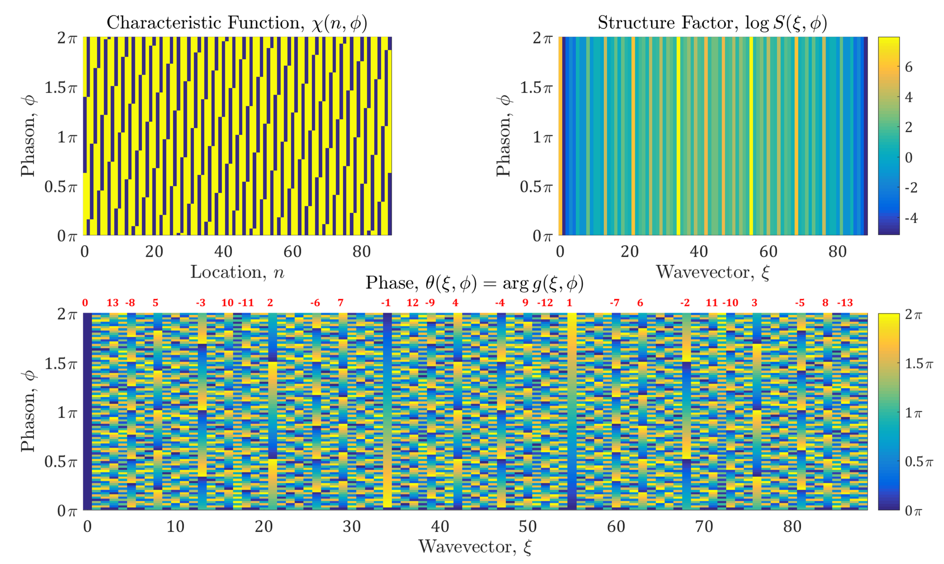
$$G(\xi, \ell) \equiv \sum_{n=0}^{F_N - 1} \omega^{-\xi n}\, \Sigma_1(n, \ell) = \omega^{m(\ell)\xi}\, \varsigma_0(\xi).$$

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

$$\Theta(\xi, \ell) \equiv \arg \omega^{m(\ell)\xi} = \phi_\ell\, \xi / F_{N-1} \pmod{2\pi}.$$

Corollary. For any $\xi_q = q F_{N-1}$ one has the (discrete) winding number at ξ_q,

$$\Theta(\xi_q) = \frac{2\pi}{F_N}\ell\, q \implies W_{\xi_q} = \frac{1}{2\pi}\int_0^{2\pi} \frac{\partial\Theta(\xi = \xi_q, \phi)}{\partial\phi}\, d\phi = q.$$



Spectral Properties of Tilings

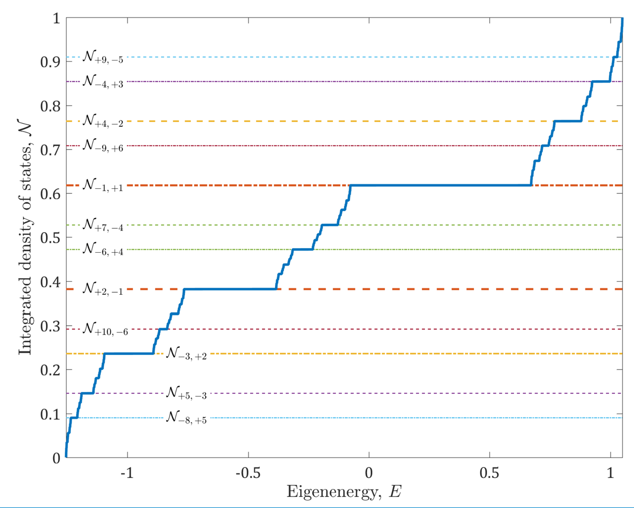
Consider a 1D discrete tight-binding equation,

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

The gaps in the integrated density of states are given by [6]

$$\mathcal{N}_{m,N} = \frac{1}{c}\frac{m}{\lambda_1^N} \pmod 1, \quad m, N \in \mathbb{Z}.$$

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



Scattering Matrix

Spectral properties are also accessible from the continuous wave equation,

$$-\frac{d^2\psi}{dx^2} - k_0^2 v(x)\,\psi(x) = k_0^2 \psi(x)$$

with scattering boundary conditions.

The scattering $\mathcal{S}$-matrix is defined by $\left(\begin{smallmatrix}\vec{o} \\ \overleftarrow{o}\end{smallmatrix}\right) = \left(\begin{smallmatrix}\vec{r}(k) & t(k) \\ t(k) & \overleftarrow{r}(k)\end{smallmatrix}\right)\left(\begin{smallmatrix}\vec{\imath} \\ \overleftarrow{\imath}\end{smallmatrix}\right) \equiv \mathcal{S}\left(\begin{smallmatrix}\vec{\imath} \\ \overleftarrow{\imath}\end{smallmatrix}\right)$, with $\vec{r} = \vec{R}\, e^{i\vec{\vartheta}}$ and $\overleftarrow{r} = \vec{R}\, e^{i\overleftarrow{\vartheta}}$. It is unitary and can be diagonalized to

$$\mathcal{S} \mapsto \begin{pmatrix} e^{i\varphi_1} & 0 \\ 0 & e^{i\varphi_2}\end{pmatrix}$$

so that $\det\mathcal{S} = e^{2i\delta(k)}$ with $\delta(k) = (\varphi_1(k) + \varphi_2(k))/2$ and $\alpha(k) = \vec{\vartheta}(k) - \overleftarrow{\vartheta}(k)$.
Using the Krein-Schwinger formula [7] allows to relate the change of density of states to the scattering data,

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

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],

$$W_{\alpha_q} = \frac{1}{2\pi}\int_0^{2\pi} \frac{\partial\alpha(\nu = \nu_{p,q}, \phi)}{\partial\phi}\, d\phi = 2q.$$

Both the winding numbers W_{ξ_q} previously found and W_{α_q} are *topological*. As such, they are robust against perturbations.

Cut and Project Scheme

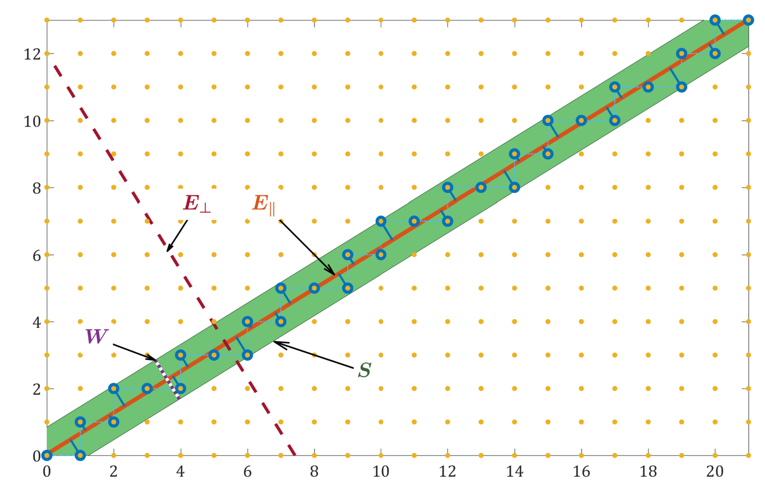
Yet another method to build quasiperiodic tilings is by the Cut & Project. The procedure is as follows [9].

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 $\rho(\boldsymbol{x}) \equiv \rho_c(\boldsymbol{x}) = \sum_{\boldsymbol{y} \in Y} \delta(\boldsymbol{x} - \boldsymbol{y})$ with $\boldsymbol{x} \in E$. Note the implicit dependency of Y on $\boldsymbol{c}$.



For the 1D systems we consider all along, 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 $1/s = 1 + \cot\alpha$.

Relation between Phases: A "Bloch theorem"

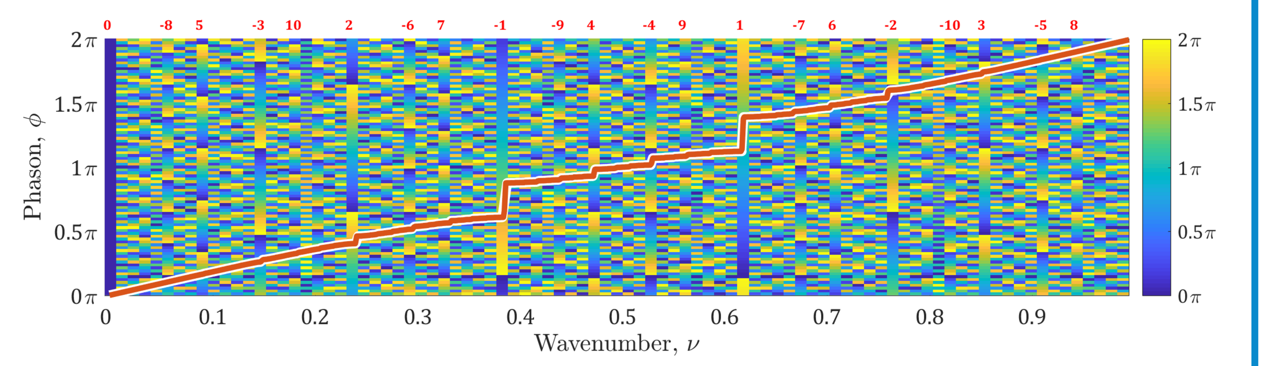
The windings of the *structural* phase $\Theta(\nu, \phi)$, where $\nu = \xi/F_N$ the normalized wavenumber, correspond to the Bragg peak locations given by

$$\nu_{p,q} = p + q\lambda_1 \implies W_{\nu_{p,q}} = q.$$

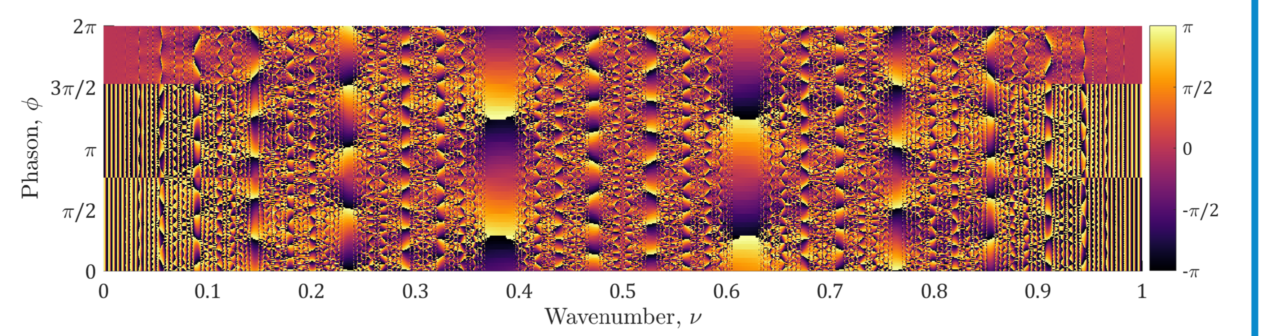
Note also, that the integrated density of states of the corresponding Hamiltonian has gap locations given by the Gap-labeling theorem [6] expressed by

$$\tau_*[K_0(\Omega_T)] = \mathcal{N}_{p,q} = p + q\lambda_1 \pmod 1.$$

Drawing the integrated density of states on top the structural phase shows the relation between the winding $\Theta(\nu, \phi)$ and the integer q in the integrated density of states (red line),



Now, consider the *spectral* (chiral) phase $\alpha(\nu, \phi)$. Its winding $W_{\alpha_q} = 2q$ can be directly read by the following graph, which is analogous to the figure above. It directly shows the relation between the two phases $\Theta(\nu, \phi)$ and $\alpha(\nu, \phi)$.



Here, we used $F_N = 233$ sites, $n_A = 1$ and $n_B = 1.15$ for better discernment.

We view this result as a Bloch-like theorem for quasiperiodic tilings [10].

Useful Tools

Unlike the case of periodic structures, for aperiodic tilings topological numbers cannot be simply expressed as Chern numbers, since the notion of Brillouin zone does not exist any longer. We are thus led to use other set of tools.

- Tiling space T (dependent on λ_1) and its hull Ω_T.
- Čech cohomology $\check{H}^1(\Omega_T)$, simplicial cohomology $H^1(\Gamma_n)$ and Bratteli graphs [11, 12].
- K-theory, $K_0(\Omega_T)$ group and the abstract Gap-labeling theorem [6, 13]

$$\mu_*[K_0(\mathcal{C}(\Omega_T))] = \tau_*[K_0(\mathcal{C}^*(\Omega_T, \mathbb{R}^n))].$$

- Pattern-equivariant functions f_{PE} and cohomology $H^1_{\mathrm{PE}}(\Omega_T)$ [14].

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* [4, 5].

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