Gap structure of 1D cut and project Hamiltonians

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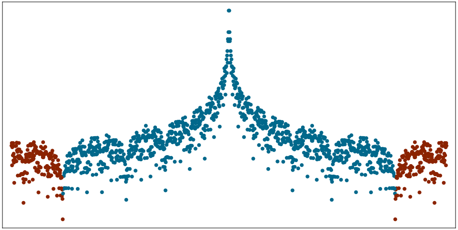
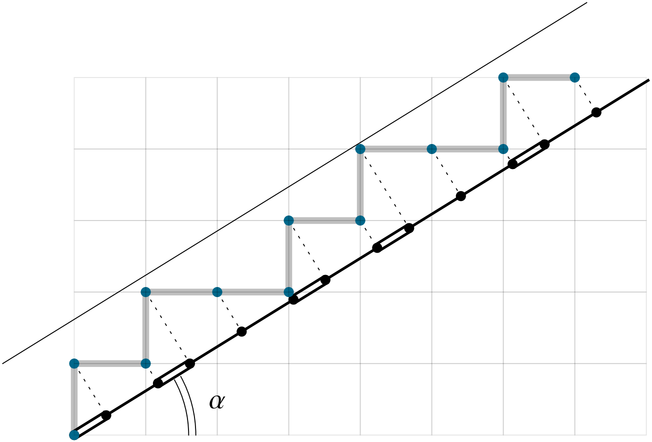


Outline

1. The gap labeling theorem
2. The Fibonacci chain
3. General case
4. Conclusion

Electrons on quasiperiodic chains

Canonical cut-and-project method



Quasiperiodic chain:

$$\alpha \in \mathbb{R}\mathbb{Q}$$

Approximants:

$$\alpha_l = \frac{p_l}{q_l} \in \mathbb{Q}$$

$$\alpha_l \to \alpha$$

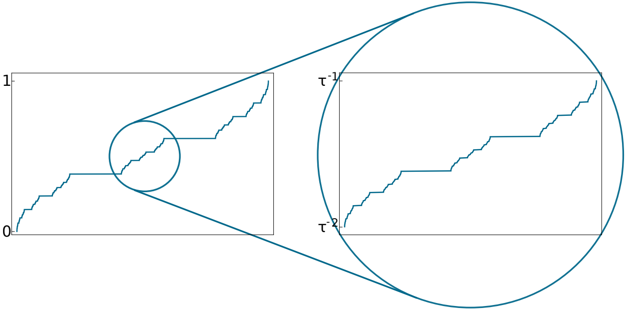
Hamiltonian: $H(\alpha) = \sum_{x \in \mathbf{Z}} t_{x,x+1} |x\rangle \langle x+1| + \text{h.c.}$

2 lengths $\to$ 2 jump amplitudes $t_{x,x+1} = t_1$ or t_2.

The electronic spectrum

A convenient way to plot the spectrum: the integrated density of states (idos).

idos(E) = fraction of states below energy E



idos of the Fibonacci Hamiltonian

- Electronic spectrum of quasiperiodic chains is hard to describe
- Rather: describe the idos in the gaps → **gap labeling theorem**

$$\text{idos}(E \in \text{gap}) = n\tau^{-2} \mod 1$$

The gap labeling theorem

The IDOS inside spectral gaps can be indexed using the irrational involved in the construction of the chain

$$\mathrm{idos}(E \in \mathrm{gap}) = \frac{n}{1+\alpha} \mod 1$$

- Constrains the spectrum... but is not enough to reconstruct it
- Model independent! (while the spectrum is model dependent) $\to$ n is a topological invariant

The gap labeling theorem

$$\mathrm{idos}(E \in \mathrm{gap}) = \frac{n}{1+\alpha} \mod 1$$

- Has the gap label n a physical interpretation?
- Can the theorem be applied to approximants?
- Does it help understanding the quasiperiodic limit?

A simple, but incorrect proof

Let $\alpha_l = \frac{p_l}{q_l} \to \alpha$ be a sequence of approximants.
$N_l = p_l + q_l$ is the maximum number of energy bands.

$$\mathrm{idos}(E \in \mathrm{gap}) = \frac{j(E)}{N_l}$$

We can find integers n, k such that $j = nq_l + kN_l$.

$$\mathrm{idos}(E \in \mathrm{gap}) = \frac{nq_l}{p_l + q_l} \mod 1$$

Letting $l \to \infty$,

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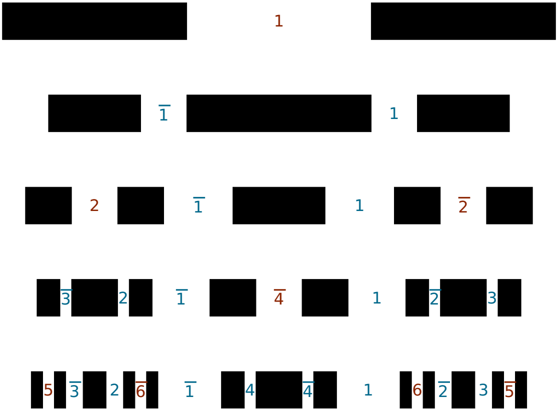
Problem

n may depend on l.

A concrete example

Gaps of successive approximants of the Fibonacci chain.



$\langle E\rangle_l$: mean energy of a gap, $\Delta_l(\langle E\rangle)$: its width.

Identify two gaps if they overlap:

$$0.5\Delta_l(\langle E\rangle) > |\langle E\rangle_l - \langle E'\rangle_{l+1}|$$

A concrete example

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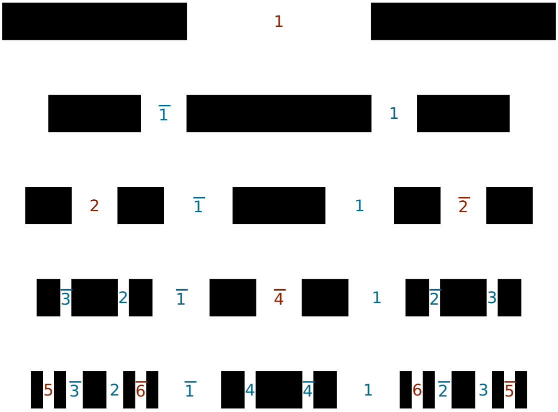

- Blue labeled gaps have a stable label gap label → stable gaps.
- Red labeled do not → transient gaps.

A concrete example

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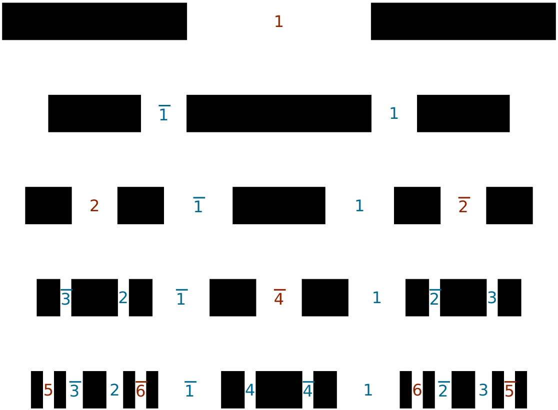
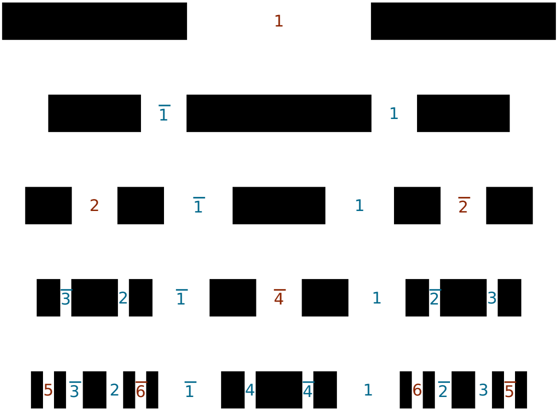


- Transient gaps closes as $l \to \infty$
- Stable gaps stay open.

A concrete example

Gaps of successive approximants of the Fibonacci chain.



- Stable gaps: n independent of l $\to$ naive proof works.
- Transient gaps: n depends on l, but these gaps disappear.

$\to$ the naive proof works and correctly labels the gaps.

Recursive gap labeling

Recursive construction of the spectrum...

...translates into recursive construction of the gaps!

$$
\begin{aligned}
G_l^{\text{left}} &= M^{-2} G_{l-2} \\
G_l^{0} &= M^{-3} G_{l-3} + \mathbf{g}_1 \\
G_l^{\text{right}} &= M^{-2} G_{l-2} + \mathbf{g}_2
\end{aligned}
$$

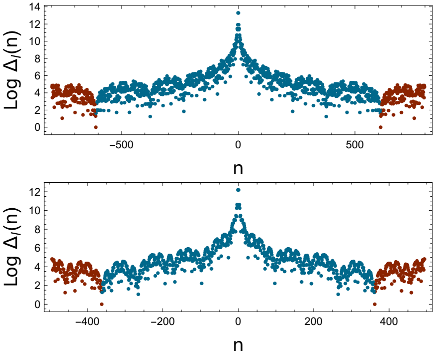
Where G_l is the set of labels:
$G_l = \{(m, n) | \text{ids} = n/(1+\alpha) + m\}$

$$M = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$$

- Stable gaps are the iterates of the 2 main gaps
- Transient gaps are the iterates of the central gap.

General case

We plot the gapwidth Δ_l as a function of the label for various quasiperiodic chains:



- The width decreases as a power-law of the label
- Above a critical label, all gaps are transient
- Recursive gap labeling using the Hofstadter rules? [Rüdinger, Piéchon 98]

Conclusion and perspectives

- The gap labeling theorem can be extended to approximants
- The price to pay is the introduction of transient gaps, absent in the quasiperiodic case
- Gap labels have a physical meaning:
  - It orders gap by decreasing width
  - It separates stable from transient gaps
  - It can be interpreted as a Chern number [Levy *et al* 2015]

Perspectives:

- Understand the gap width behavior with the gap label
- Investigate to 2D quasicrystals, which also have gaps [Prunelé *et al* 2002]

The gap labeling theorem: precise statement

Let w be a cut-and-project word. Consider the Hamiltonian:

$$H(w) = \sum_{x,y} t(T^{-y}w, x-y) \left|x\right\rangle \left\langle y\right|$$

Interactions must be local:

$$\sup_{u \in \mathrm{Hull}(w)} \sum_{x} |t(u,x)| < \infty$$

Gap labeling theorem:
The idos in a gap is a linear combination of frequencies of local environments of w.

taken from *The non-commutative geometry of aperiodic solids*, Bellissard 2003.

Cases where the naive proof fails

Consider approximants to the Fibonacci chain. Gaps are labeled by

$$\mathrm{idos}(n) = \frac{n}{1+\alpha_l} \mod 1$$

Consider the sequence of gap labels

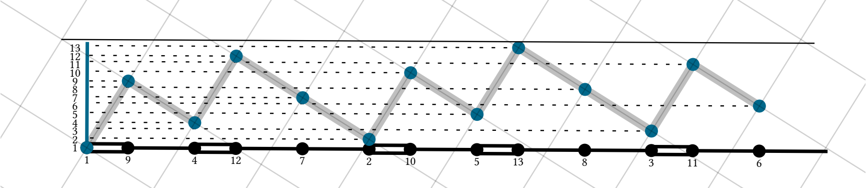
$$n_{l=3k} = \left[\frac{(2+\sqrt{5})^k}{2\sqrt{5}} \right]$$

We have $\mathrm{idos}(n_l) = 1/2$ (it labels the $E = 0$ gap). Taking $l \to \infty$, we could – incorrectly – conclude that $1/2$ is a gap.
However, there is no finite n such that

$$\frac{1}{2} = n\tau^{-2} \mod 1$$

Conumbering and gap labeling

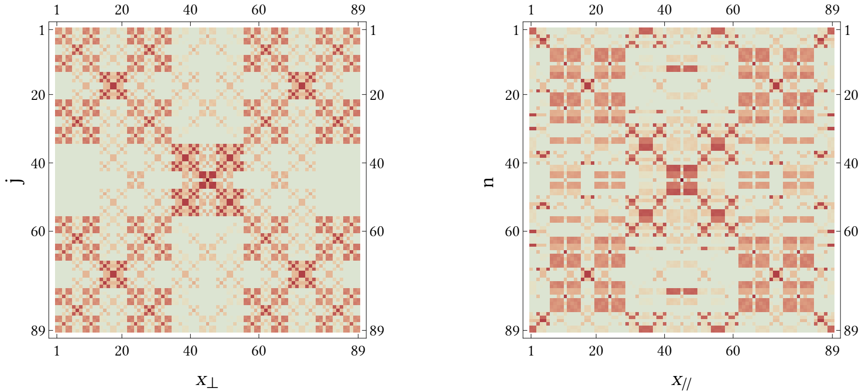
Conumbering: labeling of the atoms according to their internal space position.



see Mosseri & Sire 1990.

$$\text{idos} = \frac{j}{N_l} \quad \xleftarrow{\text{conumbering}} \quad \xrightarrow[\text{normal numbering}]{} \quad \text{idos} = \frac{n}{1+\alpha_l} \mod 1$$

Conumbering and gap labeling



Plotting the local density of states makes the symmetry between gap labels and atomic labels evident.