Gap structure of 1D cut and project Hamiltonians

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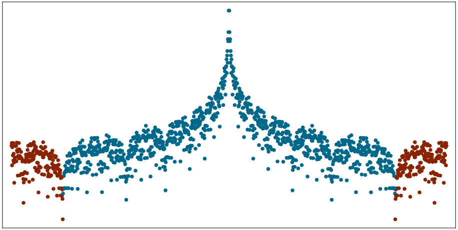


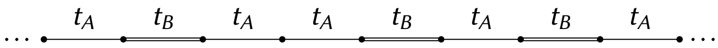
Outline

Electrons on quasiperiodic chains

Canonical cut and project method of slope $\alpha \to$ chain of two letters:

…ABAABABAABAABABAABABA…

Quantum model:

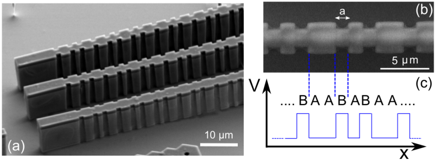


Hamiltonian: $H(\alpha) = \sum_{x\in\mathbb{Z}} t_{x,x+1} |x\rangle \langle x+1| + \text{h.c.}$
where $t_{x,x+1} = t_A$ or t_B.
t_A/t_B is the only parameter of the model.

$$\alpha = \frac{m}{n} \in \mathbb{Q} \implies \text{periodic chain of period } N = m + n$$

$$\alpha \in \mathbb{R} \setminus \mathbb{Q} \implies \text{quasiperiodic chain}$$

Experimental realization with cavity polaritons [Tanese *et al* 2015]



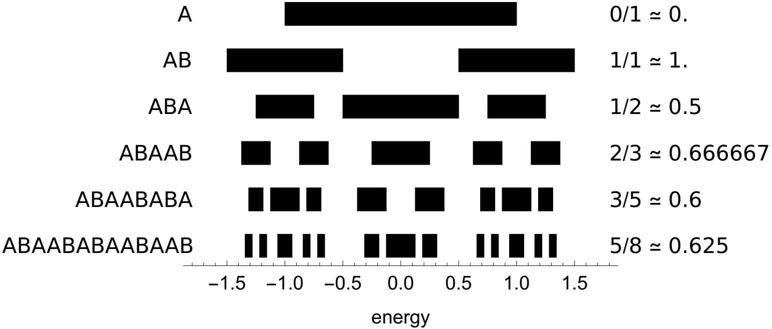
The energy spectrum

Well understood: electrons on *periodic* chains (Bloch's theory)

Idea: approach a QP chain α by a sequence of periodic *approximants*:

$$\alpha_l = \frac{m_l}{n_l} \xrightarrow[l \to \infty]{} \alpha$$

$\rightarrow$ energy spectrum consists of $m_l + n_l$ *energy bands*

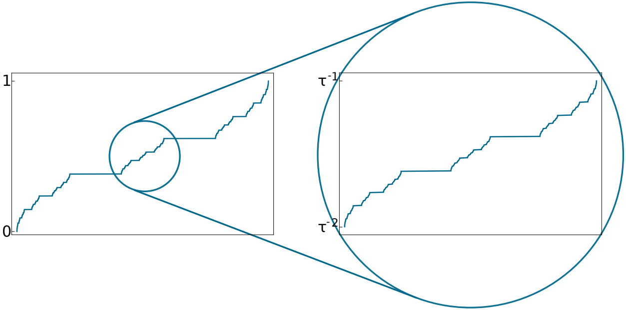


Fibonacci chain: $\alpha_l = F_l / F_{l+1} \xrightarrow[l \to \infty]{} \tau^{-1} = 0.618\ldots$

IDOS AND GAP LABELING

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 $\rightarrow$ **gap labeling theorem**

$$\mathrm{idos}(E \in \mathrm{gap}) = p + q\tau^{-2}$$

The gap labeling theorem

The IDOS inside spectral gaps can be written

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

where $p, q \in \mathbb{Z}$ are the *gap labels*.

- The set of labels constrains the spectrum... but is not enough to reconstruct it
- The labels are model independent!
  - In particular, independent of t_A and t_B
  - Gap labels are topological invariants

The gap labeling theorem

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

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

Gap labeling from Bloch's theory

Let $\alpha_l = \frac{m_l}{n_l} \to \alpha$ be a sequence of approximants.
Bloch's theorem: there are $N_l = m_l + n_l$ energy bands.

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

We can find integers p, q such that $j = pN_l + qn_l$.

$$\mathrm{idos}(E \in \mathrm{gap}) = \frac{qn_l}{m_l + n_l} \mod 1$$

Letting $l \to \infty$,

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

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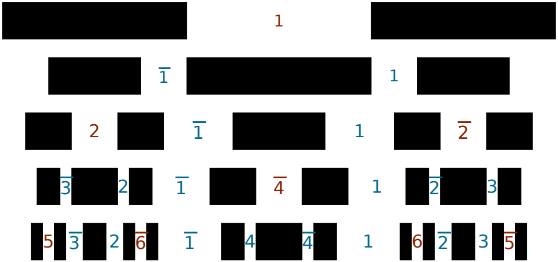
Proof incorrect!
q may depend on l.

Transient and stable gaps

Gaps of successive approximants of the Fibonacci chain.

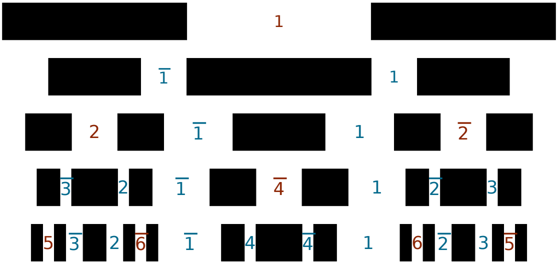


$\langle E\rangle_l$: mean energy of a gap, $\Delta_l(\langle E\rangle)$: its width.
Identify two gaps if they overlap:

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

Transient and stable gaps

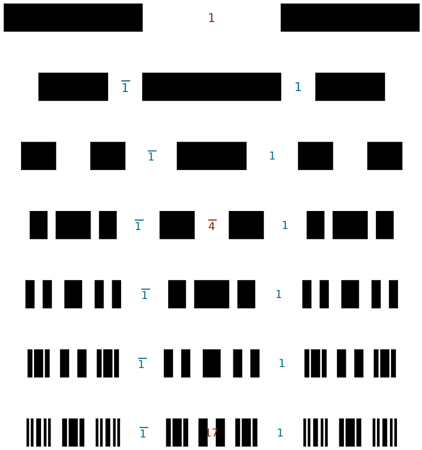
Gaps of successive approximants of the Fibonacci chain.



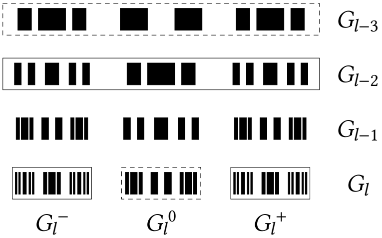
- Blue labeled gaps have a fixed label, that does not depend on l $\rightarrow$ stable gaps.
- Red labeled gaps have a label that is l-dependent $\rightarrow$ transient gaps.

Examples of transient and stable gaps

- The $E = 0$ gap
  - reappears every 3 iterations
  - has the label $q_l = \left\lfloor \frac{(2+\sqrt{5})^{l/3}}{2\sqrt{5}} + \frac{1}{2} \right\rfloor$
  - is transient
  - has vanishing width in the quasiperiodic limit. **True for all transient gaps**
- The two largest gaps
  - have label $q = \pm 1$
  - are stable
  - have a nonzero width in the quasiperiodic limit **True for all stable gaps**



Recursive gap labeling



Recursive construction of the spectrum

Let G_l be the set of gap labels:
$G_l = \{(p, q) | \text{ids} = p + q/(1+\alpha)\}$
G_l obeys the recursive relation:

$$\begin{aligned} G_l^{\text{left}} &= M^{-2} G_{l-2} \\ G_l^0 &= M^{-3} G_{l-3} + (1, -1) \\ G_l^{\text{right}} &= M^{-2} G_{l-2} + (0, 1) \end{aligned}$$

M is the *inflation matrix*:

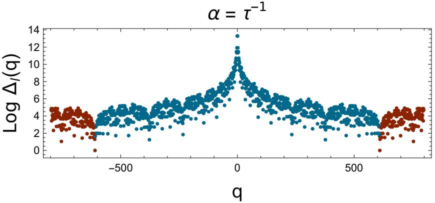
$$M = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$$

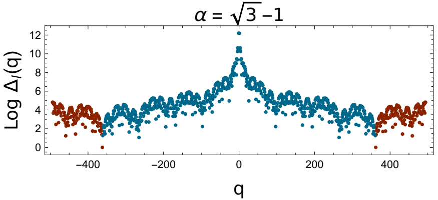
- Geometrical interpretation of the Fibonacci gap labeling
- Stable and transient gap are better understood:
  - Stable gaps are the iterates of the 2 largest gaps
  - Transient gaps are the iterates of the $E = 0$ gap.

General case

We can still distinguish (numerically) stable and transient gaps for various cut and project chains.

We plot the gapwidth Δ_l as a function of the label:





- The width decreases as a power-law of the label
- Above a critical label, all gaps are transient

$\rightarrow$ gap labels are physically meaningful for this model!

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 winding number of edge states inside the gaps [Levy *et al* 2015]

Perspectives:

- Recursive gap labeling using the Hofstadter rules [Rüdinger, Piéchon 98]
- 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

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

Consider the sequence of gap labels

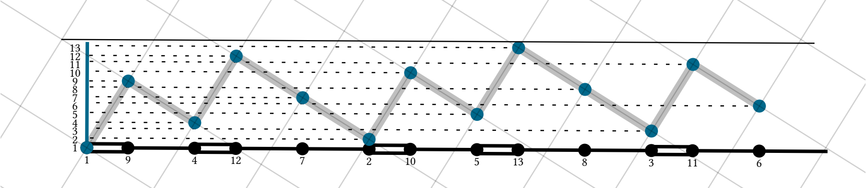
$$q_{l=3k} = \left[\frac{(2+\sqrt{5})^k}{2\sqrt{5}} \right]$$

We have $\mathrm{idos}(q_l) = 1/2$ (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 q such that

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

Conumbering and gap labeling

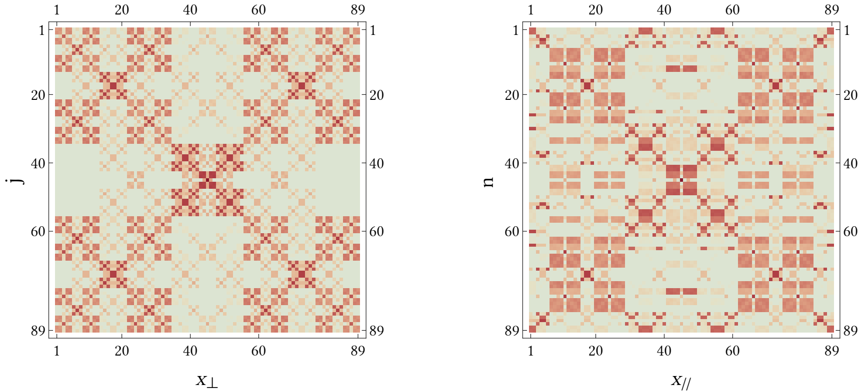
Conumbering: labeling of the atoms according to their internal space position.



see Mosseri & Sire 1990.

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

Conumbering and gap labeling



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