Exact results on electronic wavefunctions of 2D quasicrystals

Nicolas Macé, Anuradha Jagannathan, Frédéric Piéchon

Laboratoire de Physique des Solides
Université Paris-Saclay

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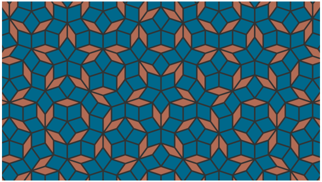


Electronic properties of quasicrystals

We can we do to access the electronic properties of quasicrystals?

- Experiments
  - Measure of physical properties.
- “Realistic” simulations
  - Direct access to the electronic states
- Toy models
  - More managable (sometimes exactly solvable) $\rightarrow$ easier to see the consequences of quasiperiodicity
  - Simple states can be seen as “building block” for more realistic ones (like Bloch’s states for periodic materials)

Toy models of quasicrystals

We want to model:

- a single electron (ie we do not consider interactions)
- on a quasiperiodic tiling, in 1D or in 2D
- in the simplest possible way : tight-binding model with nearest neighbors hoppings only

$$i\frac{\partial \phi_m}{\partial t}(t) = \sum_{n \in V(m)} t_{m,n}\phi_n(t) \text{ with } |\phi_m(t)|^2 = \text{Prob}\,(\text{on atom } m \text{ at time } t)$$

[Picture of the hoppings on a tiling]
We solve for the stationary states (or eigenstates):

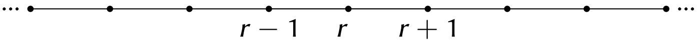
$$E\psi_m = \sum_{n \in V(m)} t_{m,n}\psi_n$$

Challenge: find a proper description of these eigenstates...

What is known: periodic and disordered models

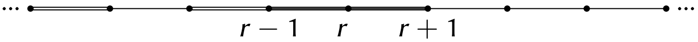
- Eigenstates on periodic materials:
  - Plane waves
  - **constant** amplitude → **extended states**

$$\psi(r) = e^{ikr}$$



- Eigenstates on disordered materials:
  - Evanescent waves
  - **exponentially decreasing** amplitude → **localized states**

$$\psi(r) = e^{-r/\xi}$$



What about quasiperiodic materials?

We will see on examples their electrons are somewhat **in between**: the wavefunctions have local power law decay, they are **critical**

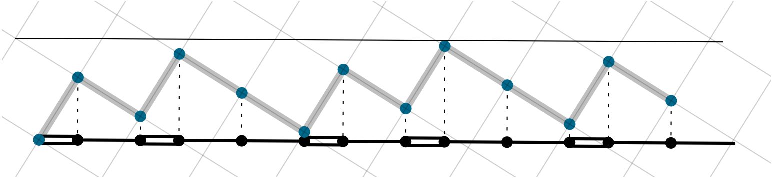
Outline

1 Quasiperiodic chains

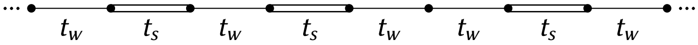
2 2D case

Cut and project chains

The geometrical model:



The corresponding chain of atoms:



The Schrödinger equation for the eigenstate of energy E:

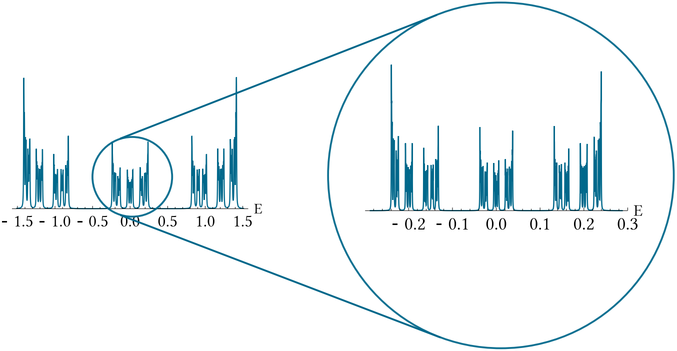
$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = E\psi_m$$

$$t_{m-1,m} = t_s \text{ or } t_w \text{ and we set } t_s = 1,\ t_w = \rho$$

What can be say about the spectrum/eigenstates of this model?

Spectrum/eigenstates of cut and project chains

- The spectrum is scale invariant (or multifractal)



- The eigenstates are generically critical (all of them are for the Fibonacci chain [reference])

What is the structure of these critical states?

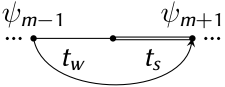
A special case: the eigenstate at zero energy

- Schrödinger equation for the $E = 0$ state:

$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = 0$$

- If we know the wavefunction on one site we know it on the next

$$\psi_{m+1} = -\frac{t_{m-1,m}}{t_{m,m+1}}\psi_{m-1}$$



- Introduce $A_{m-1,m+1}$, the **arrow** from $m-1$ to $m+1$:

$A_{m-1,m+1} = +1$

$A_{m-1,m+1} = -1$

$A_{m-1,m+1} = +0$

$A_{m-1,m+1} = +0$

Remember that $\rho = t_s/t_w$. Then,

$$\boxed{\psi_{m+1} = -\rho^{A_{m-1,m+1}}\psi_{m-1}}$$

The field of arrows and the field of heights

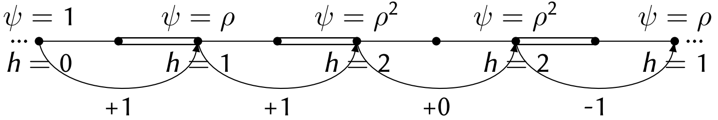
Iterating $\psi_{m+1} = -\rho^{A_{m-1,m+1}} \psi_{m-1}$ we can compute the wavefunction on any site:

$$\psi_{2m} = (-1)^m \psi_0 \rho^{h(m)}$$

Where h is **the field of heights**, the integral of the field of arrows:

$$h(m) = \sum_{n=0}^{m} A_{n,n+2}$$

Example (piece of the Fibonacci chain):



Back to the special cases, with arrows!

- Periodic chain:

  - Arrows $= 0 \implies h(m) = 0 \implies \psi_m = \text{cst}$
  - **constant** amplitude $\rightarrow$ **extended states**

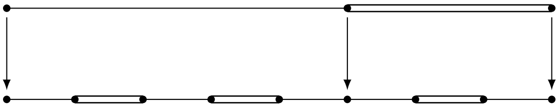
- Disordered chain:

  - Arrows randomly distributed $\implies h(m) \sim \langle A \rangle \times m \implies \psi_m \sim e^{-m/\xi}$ with $\xi^{-1} = |\log \rho| \langle A \rangle$
  - **exponentially decreasing** amplitude $\rightarrow$ **localized states**

The arrows give another interpretation to these well known results.
What happens for a quasiperiodic chain?

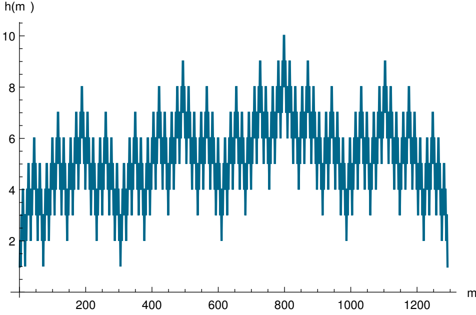
Fibonacci chain and the inflation

The Fibonacci chain can be constructed by cut and project, but also by **inflation**



Properties of the height under inflation:

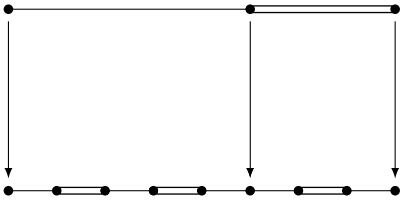
- On the old sites, **height remains constant**
- On newly created sites **height increases at most linearly** $\Longrightarrow$ on a region of size L, height increases at most as $\log L$, typically as $\sqrt{\log L}$.

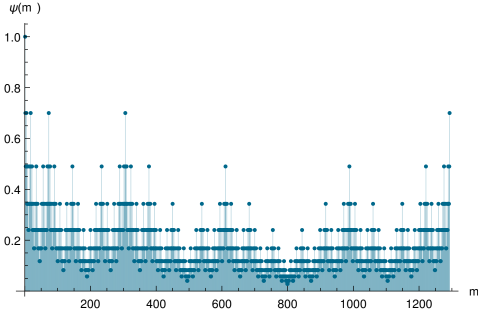


The Fibo arrows and the Fibo wf

- On old sites the height/ the wavefunction stays constant, and old sites can be arbitrarily far away $\rightarrow$ **the wavefunction cannot be localized**
- The height is scale invariant, and so is the wavefunction: $\psi(b \times r) = b^{\alpha}\psi(r) \rightarrow$ **the wavefunction cannot be extended**: is behaves locally as a power law

Conclusion: **the wavefunction is critical.**





Cut and project chains: a summary

- The $E = 0$ wavefunction of cut and project chains can be described by a **height field**
- The height field is the integral of an **arrow field**, which is quasiperiodic
- As a result, **the wavefunction is critical**: it behaves locally as a power law
- On a patch of the tiling of size L, maximal height scales as $\log L$, typical height as $\sqrt{\log L}$

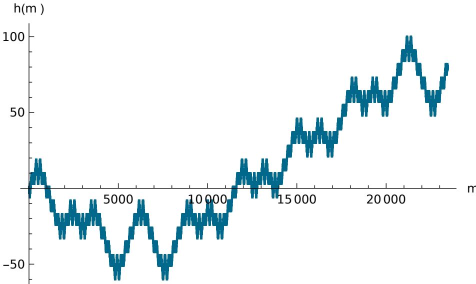
We will find again all these features in 2D!

Cut and project chains are special!

Consider the chain constructed by the substitution

$$A \to ABBB$$
$$B \to A$$

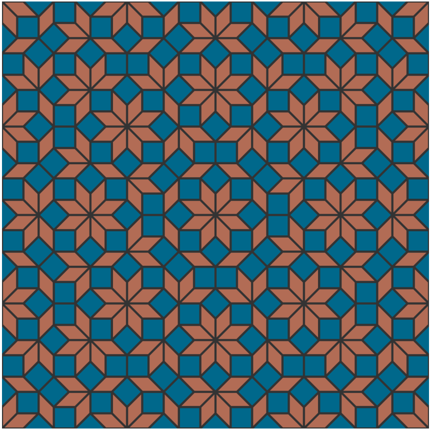
- This substitution cannot be built by cut and project (because it is non-Pisot).
- Height resembles a random walk, and typical height $\sim \sqrt{L}$
- As a result, the wavefunction is localized!



$\to$ criticality is sensitive to the **complexity** of the tiling

2D cut and project tilings

Results stated in this part will be valid for 2 cut and project 2D tilings: the Penrose and the Ammann-Beenker tilings.

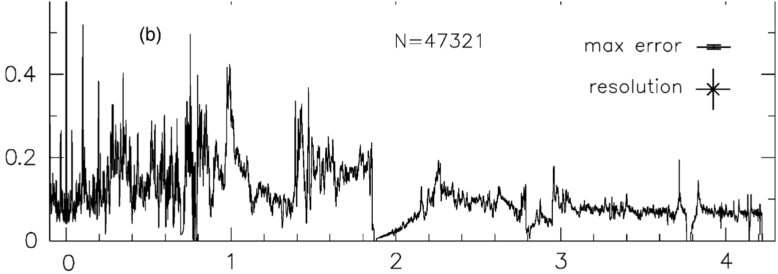


We consider start with the model:

$$E\psi_m = t \sum_{n \in V(m)} \psi_n$$

The quasiperiodic features are encoded in the adjacency of the vertices.

What is known



- Spectrum is more regular: only a few gaps, no apparent fractal structure
- $E = 0$ eigenstates are localized: cannot hope to describe them with arrows.
- The other states are critical (numerical result)

$\rightarrow$ can we introduce a field of arrows to describe some of these critical wavefunctions?

A natural field of arrows

- Sutherland's idea: introduce local potentials to make the construction of the grounstate simpler.
- Sutherland's groundstates on Penrose and AB tilings is constructed via the introduction of a field of arrows, exactly like the 1D ones

$\rightarrow$ what are the properties of this field of arrows?

Inflation and the field of arrows

Here we focus on the AB example, but everything works the same for Penrose.

- Arrows $\leftrightarrow$ matching rules for the tiles
- Matching rules are enforced by the inflation rules $\rightarrow$ we should be able to study the properties of the arrows via the inflation (just like in 1D)
- From the inflation rules, we deduce the maximal height $\sim \log L$
- Statistics of the heights $P_\mu^l(h)$ obeys a diffusion-like equation where l plays the role of time and h the role of space
- $\rightarrow$ typical height is $\sim \sqrt{\log L}$

So we understand everything about Stutherland's wavefunction, but the model has been built for this wavefunction to exist. Can we use this field of arrows to describe wavefunctions on more realistic models? Yes: Pavel.

Characterization of the groundstate wavefunction

- We go back to the model with no local potentials.
- From the plot of the groundstate: we see a complicated local structure (role of the local environment) and the phason line (role of the arrow field)
- Indeed, the wf decomposes into a local part and an arrow part (this was guessed from involved algebraic arguments).
- Computation of the IPR scaling and the multifractal exponents: the local part doesn't play any role $\rightarrow$ exponents only sensitive to the arrow part, ie to the quasiperiodicity!
- Remains valid for a larger class of models $H = \sum_{\langle i,j \rangle} |i\rangle \langle j| + V_i |i\rangle \langle i|$

Conclusion

- Non-interacting eigenstates on quasicrystals are generically critical: here we were able to understand it for some specific states, both in 1D and 2D.
- On our examples, wavefunction construction involves a geometrical quasiperiodic function, the field of arrows.
- Its integral, the height function, has logarithmic growth,
- As a result, the wavefunction is critical: it has a local power law behavior.

Perspectives:

- What happens for the grounstate of other quasicrystals, like the dodecagonal ones?
- For Penrose and AB, the arrow field cannot be used to describe other states. What extra ingredients are required?

More perpsectives!

- A plot of the state just below the gap, with its quasiperiodic array of lines of zeros, that remain to be understood!