

# Exact results on electronic wavefunctions of 2D quasicrystals

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# ELECTRONS ON QUASICRYSTALS

- In 1D (quasiperiodic chains): electronic spectrum and wavefunctions are well known.
- In 2D and 3D: many numerical investigations, but almost no exact results.  
→ recent (big!) improvement: Kalugin, Katz (2014) guessed the groundstate of a large class of 2D models.
  - What does this groundstate look like?
  - Which new insights does it bring us?

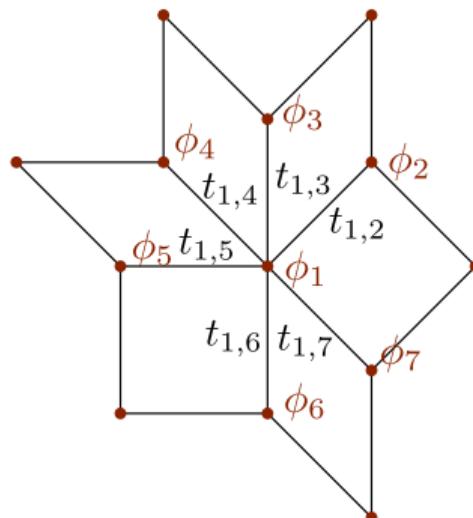
# TOY MODELS OF QUASICRYSTALS

We want to model:

- a single electron (i.e. **no interactions**)
- on a **quasiperiodic tiling**, in 1D or in 2D
- in the simplest possible way : **tight-binding model** with nearest neighbors hoppings

$$i \frac{\partial \phi_m(t)}{\partial t} = \sum_{n \text{ NN } m} t_{m,n} \phi_n(t)$$

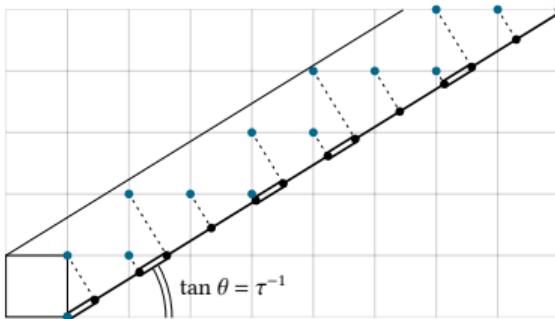
$|\phi_m(t)|^2$  = proba to be on atom  $m$  at time  $t$ .



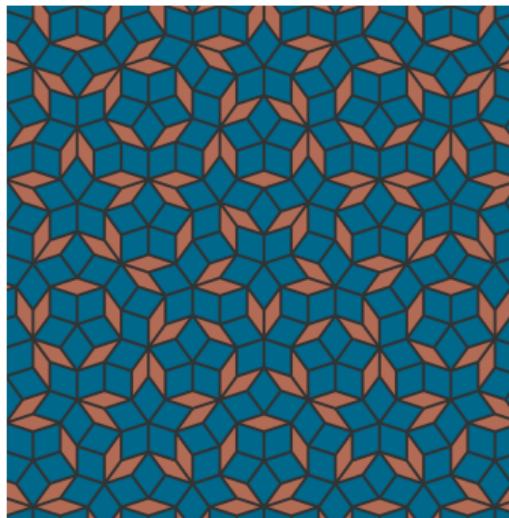
Solve for the eigenstates:

$$E\psi_m = \sum_{n \text{ NN } m} t_{m,n} \psi_n$$

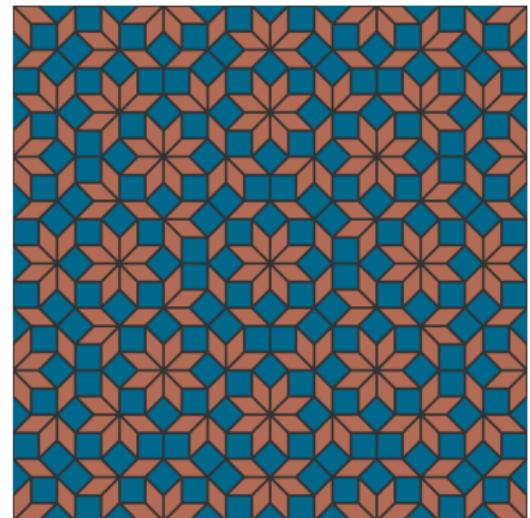
# THE QUASIPERIODIC MODELS



The Fibonacci chain  
constructed by cut and project.



The Penrose tiling.



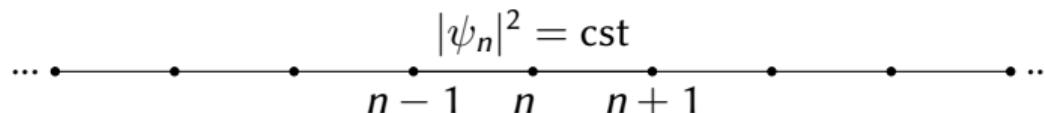
The Ammann-Beenker tiling.

# OUTLINE

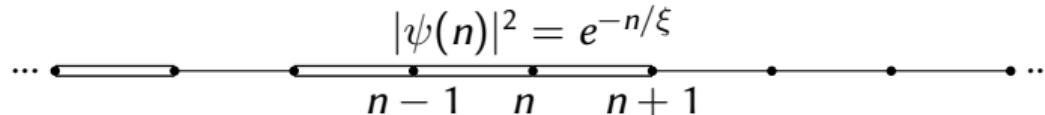
- 1** 1D model (Fibonacci chain)
- 2** 2D models (Penrose and Ammann-Beenker tilings): the “grown-up example”
- 3** Conclusion and perspectives

## PERIODIC AND DISORDERED MODELS

- Eigenstates on periodic materials:
  - Plane waves
  - **uniform probability** → **extended states**



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



## What about quasiperiodic materials?

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

# THE FIBONACCI CHAIN

The geometrical model: a chain of two letters generated by the substitution

$$M : \begin{cases} A \rightarrow AB \\ B \rightarrow A \end{cases}$$

$$M^\infty(A) = ABAABABAABABAABABA\ldots$$

The corresponding chain of atoms:



The Schrödinger equation for the eigenstate of energy  $E$ :

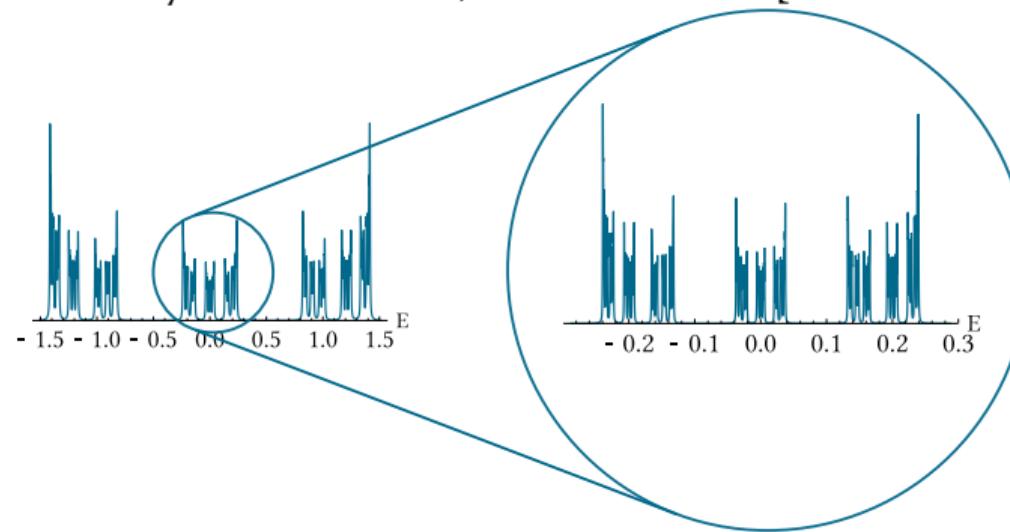
$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = E\psi_m$$

$t_{m-1,m} = t_s$  or  $t_w$  we introduce the ratio  $\rho = t_w/t_s < 1$

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

## SPECTRUM AND EIGENSTATES

- The spectrum is locally scale invariant, or **multifractal** [Kohmoto *et al* 1983]



(Spectrum computed for  $\rho = 0.5$ )

- The eigenstates are all critical (neither localized nor extended)

What is the structure of these critical states?

# 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  $m + 1$ :

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

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

$$A_{m-1,m+1} = +0 \quad \psi_{m+1} = \rho^{+0}\psi_{m-1}$$

$$A_{m-1,m+1} = +0 \quad \psi_{m+1} = \rho^{+0}\psi_{m-1}$$

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

## THE FIELD OF ARROWS AND THE FIELD OF HEIGHTS

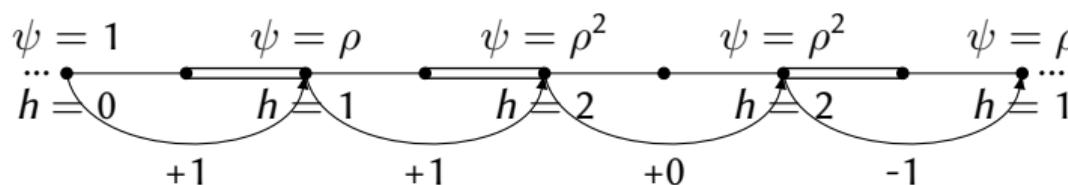
Iterating  $\psi_{m+1} = \rho^{A_{m-1,m+1}} \psi_{m-1}$ ,

$$\psi_m = \psi_0 \rho^{h(m)}$$

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

$$h(m) = \sum_{n=1}^{m/2} A_{2n-2, 2n}$$

Example (piece of the Fibonacci chain):



# BACK TO THE SPECIAL CASES, WITH ARROWS!

## ■ Periodic chain:



- Arrows = 0  $\Rightarrow h(m) = 0 \Rightarrow \psi_m = \psi_0 \rho^0 = \text{cst}$
- **uniform probability**  $\rightarrow$  **extended states**

## ■ Disordered chain:



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

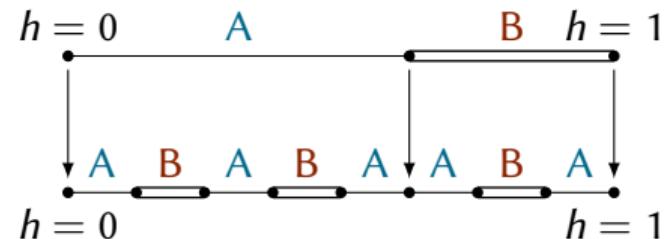
$\rightarrow$  expected behavior in both cases.

What happens for a quasiperiodic chain?

# THE $E = 0$ STATE IS NOT LOCALIZED

Apply the substitution three times:

$$M^3 : \begin{cases} A \rightarrow ABABA \\ B \rightarrow ABA \end{cases}$$

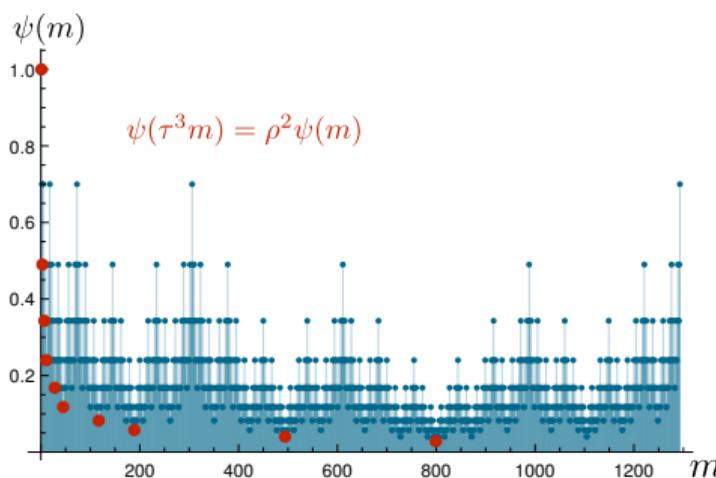
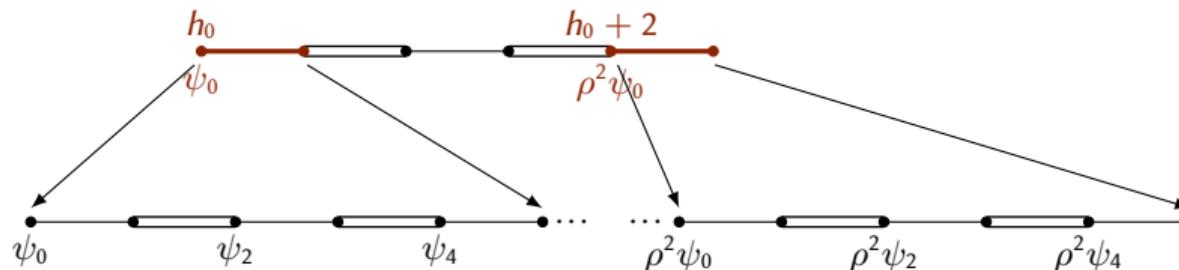


→ the height is invariant under the substitution  $M^3$ : it doesn't change on the preexisting sites

- the wavefunction doesn't change on the preexisting sites
- these preexisting sites get arbitrarily far apart as we iterate the substitution

→ we can find the electron with high probability arbitrarily far from the origin: **the wavefunction is not localized.**

# THE $E = 0$ STATE IS NOT EXTENDED



Local scale invariance:

$$\psi_{a \times m} = b \times \psi_m$$

→ local **power law decay**

$$\psi_{r_n} \sim r_n^\alpha, (\alpha = \log b / \log a)$$

→ **wavefunction is not extended**

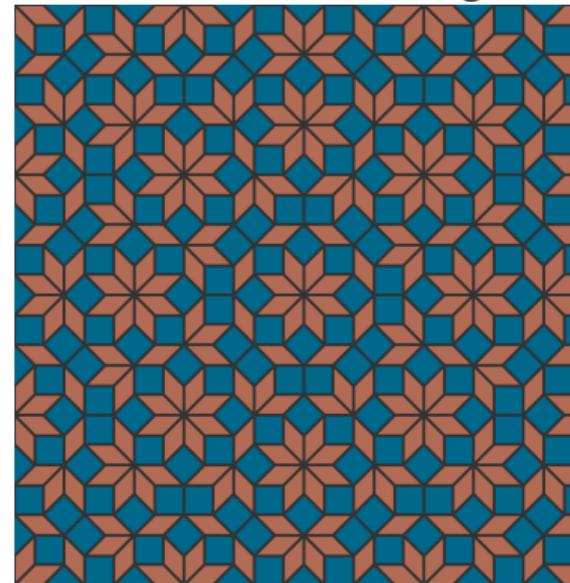
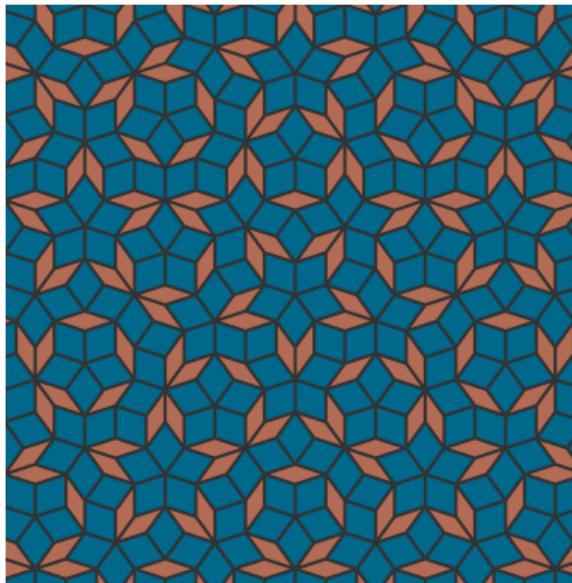
## CUT AND PROJECT CHAINS: A SUMMARY

- The  $E = 0$  wavefunction of cut and project chains is described by a **height field**
- The height field is the integral of an **arrow field**, which is quasiperiodic
- Geometry of the tiling  $\implies$  structure of the wavefunction
- $\rightarrow$  **the wavefunction is critical**: neither localized nor extended, behaves locally as a power law

We will find again all these features in 2D!

# 2D TILINGS

We consider the Penrose and the Ammann-Beenker tilings.



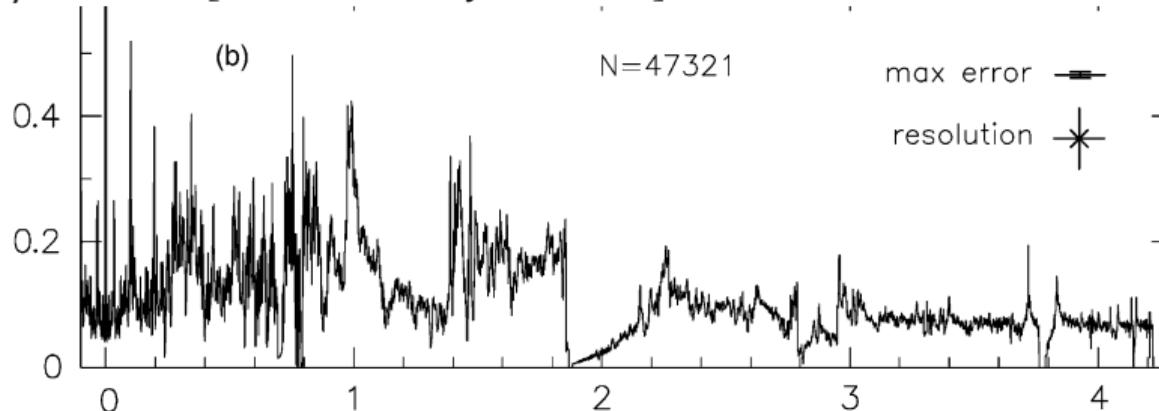
Model for the electron:

$$E\psi_m = V_m\psi_m + \sum_{n \text{ NN } m} t\psi_n$$

Quasiperiodicity  
encoded in the  
adjacency of the vertices

# WHAT IS KNOWN

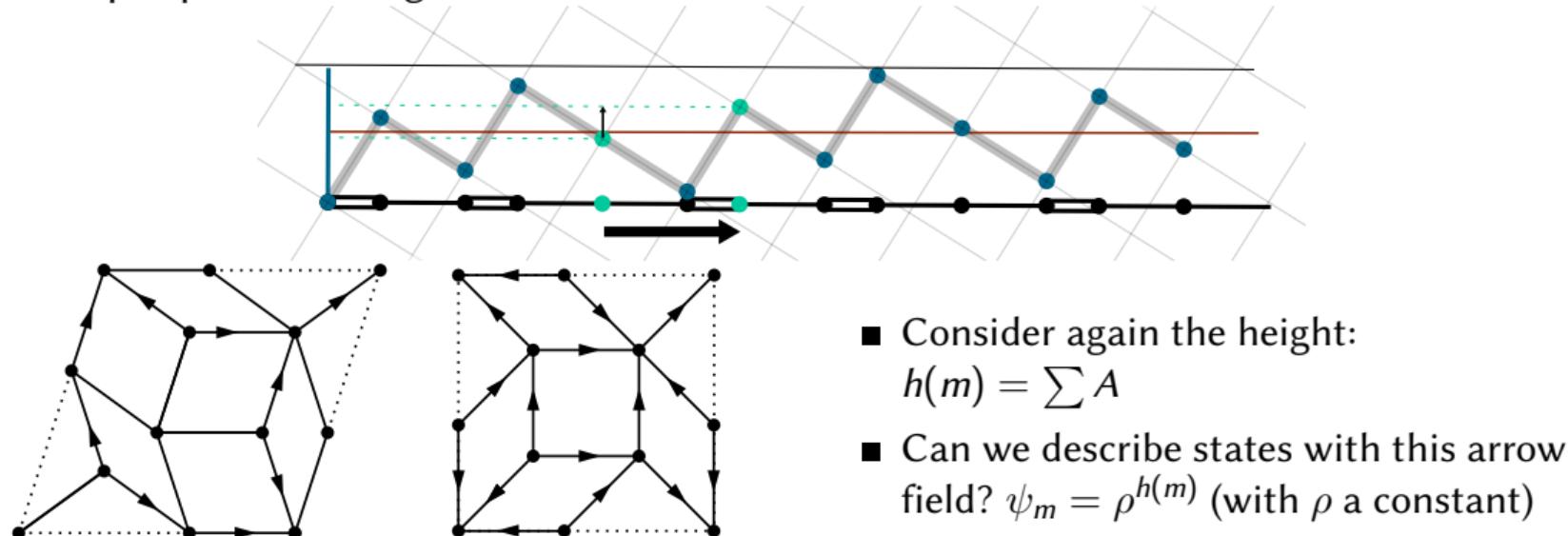
Local density of states [taken from Zijlstra 2014]:



- Spectrum: no apparent fractal structure
  - States are critical (numerical result, eg [Rieth, Schreiber 1998])
- can we introduce a field of arrows to describe some of these critical wavefunctions?

## A NATURAL FIELD OF ARROWS

In superspace, arrows go from the center to the border of the slice:



# THE GROUNDSTATE WAVEFUNCTION

Can we find an “arrowed state”  $\psi_m = \rho^{h(m)}$  ? (with  $\rho$  a constant)

- Idea [Sutherland 1986]: tune the potential

$$E\psi_m = V_m\psi_m + t \sum_{n \text{ NN } m} \psi_n \iff V_m = E - t \sum_n \rho^{A_{m,n}}$$

Obtain a groundstate which is an arrowed state.

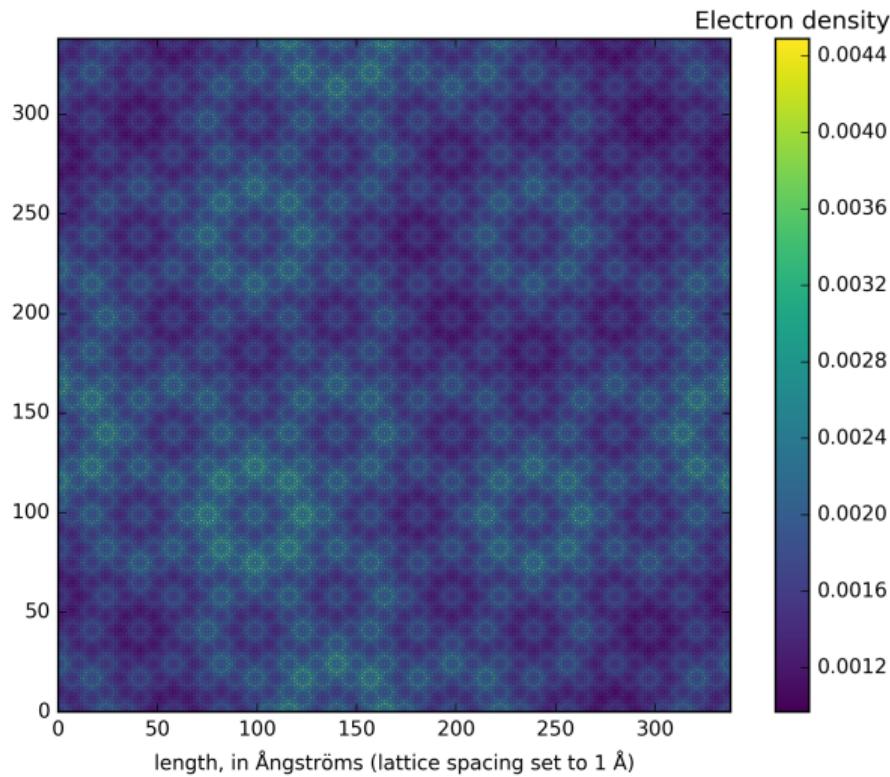
Not very physical! Generically, potential is not finely tuned.

- [Kalugin, Katz 2014]: add a **local modulation**:

$$\psi_m = C(m)\rho^{h(m)}$$

$|C(m) - C(n)| \leq \epsilon$  if the patterns around  $m$  and  $n$  matches on a distance  $1/\epsilon$ .

## ROBUSTNESS OF THE ARROWED STATES



- The groundstate is **very robust**:  
For any model of the form

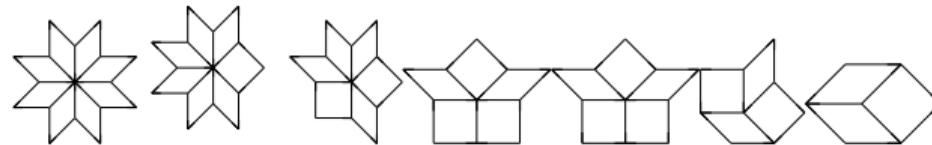
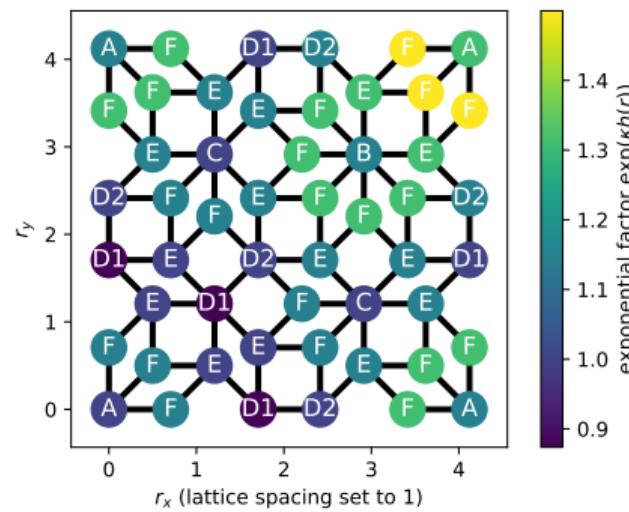
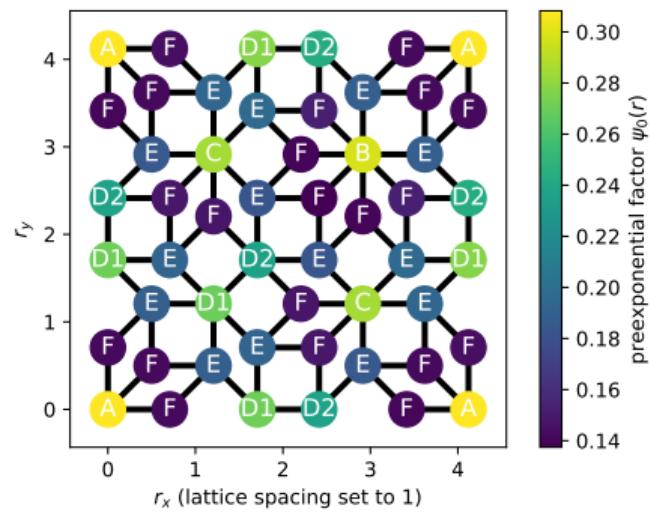
$$E\psi_m = V_m\psi_m + t \sum_n \psi_n$$

the groundstate is an “arrowed state”

$$\psi(m) = C(m)\rho^{h(m)}$$

- Same arguments as in 1D: the state has power law decay, and is critical.

$$\psi(m) = C(m) \times \rho^{h(m)} \text{ UNDER SCRUTINY}$$



## SCALING OF THE GROUNDSTATE

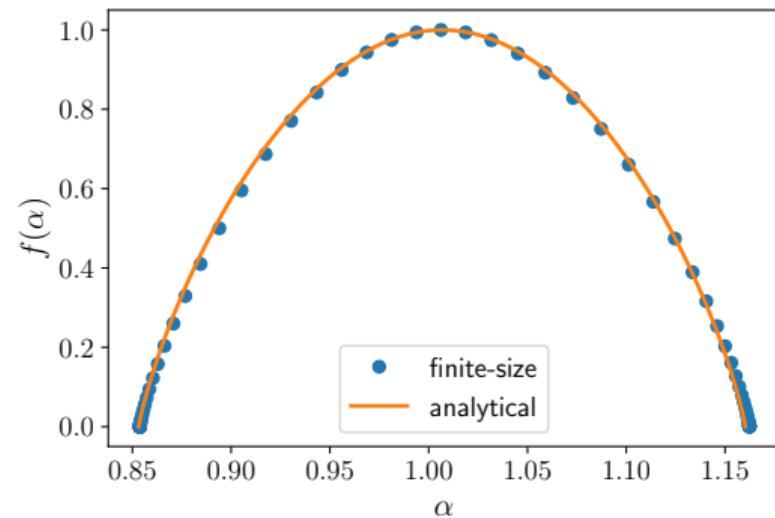
- Participation ratio over a region  $\mathcal{R}$ :

$$\text{PR}(\psi, \mathcal{R}) = \frac{\left(\sum_{m \in \mathcal{R}} |\psi_m|^2\right)^2}{\left(\sum_{m \in \mathcal{R}} |\psi_m|^4\right)^4}$$

- Scaling with the region volume  $\text{Vol}(\mathcal{R})$ :

$$\text{PR}(\psi, \mathcal{R}) \sim \text{Vol}(\mathcal{R})^{D(\psi)}$$

- $D(\psi) = 0 \implies \psi$  localized
- $D(\psi) = 1 \implies \psi$  extended
- $0 < D(\psi) < 1 \implies \psi$  critical



Multifractal spectrum of the groundstate  
(parameters:  $V = 0.5$ ,  $t = 1$ ) on the Penrose tiling.

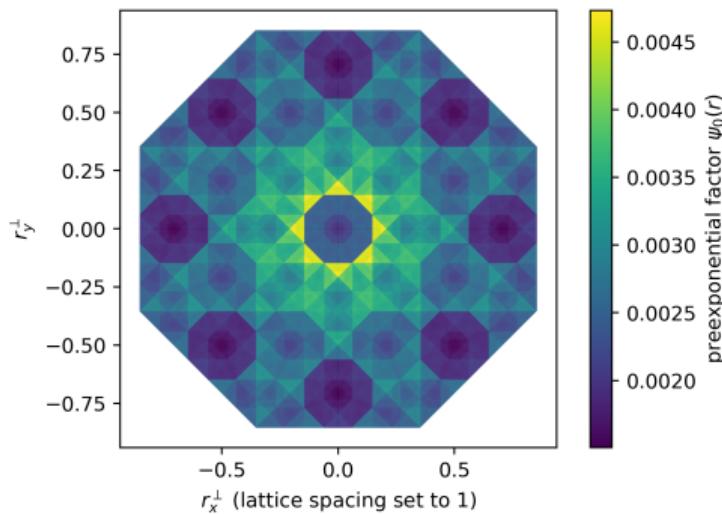
# CONCLUSION

- Arrowed states are examples of **critical** eigenstates.
  - 1D (Fibonacci): the  $E = 0$  state
  - 2D (Penrose and Ammann-Beenker): the groundstate.
- Geometry  $\rightarrow$  quasiperiodic **arrow function**  $\rightarrow$  structure of the state.
- In 2D, structure **robust to changes in the model** (varying potential, hopping)
- Using this description, we can easily compute physical observables.

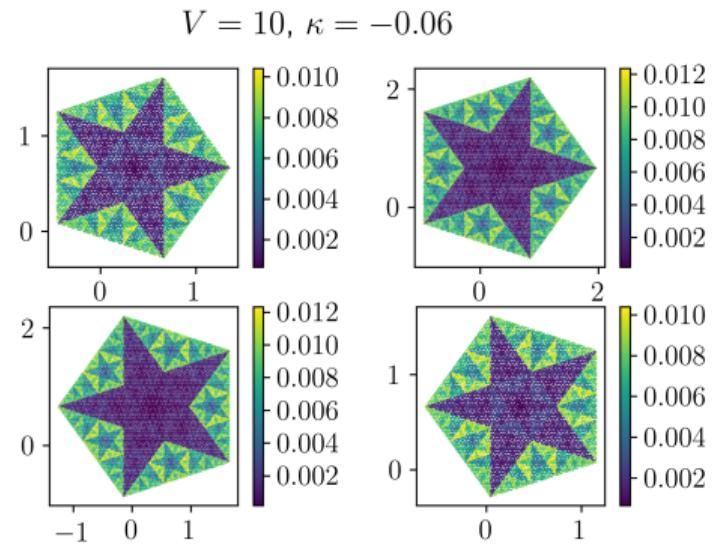
Perspectives:

- For Penrose and Ammann-Beenker, the arrow field is not enough to describe excited states. Extra ingredients?
- Other quasiperiodic tilings: generalized Penrose, dodecagonal ...

# THE LOCAL PART IN PERPENDICULAR SPACE



The local part of a groundstate on the Ammann-Beenker tiling.



The same for the Penrose tiling.

# CUT AND PROJECT CHAINS ARE SPECIAL!

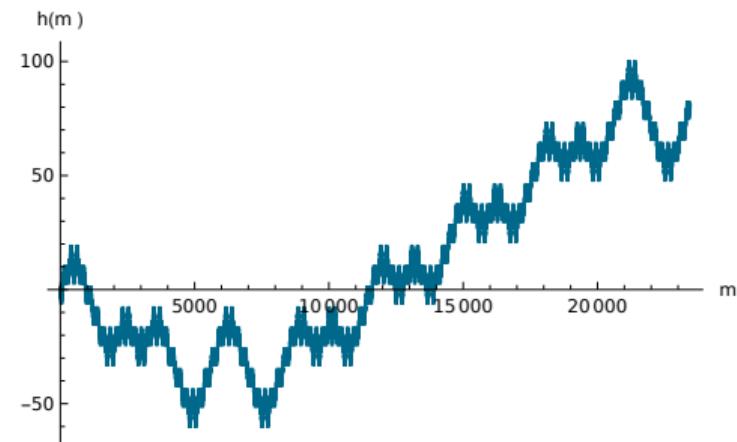
Consider the chain constructed by the substitution

$$A \rightarrow ABBB$$

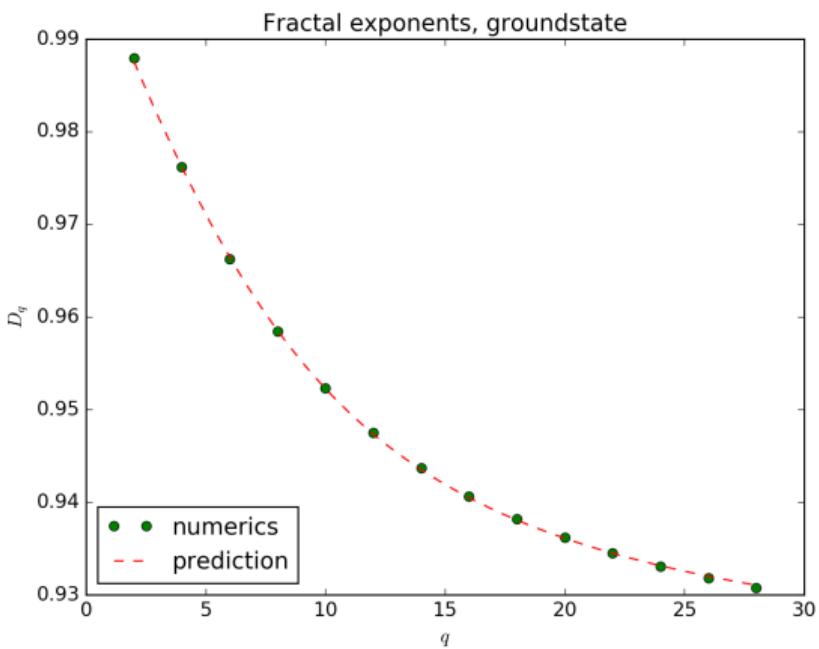
$$B \rightarrow A$$

- 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!

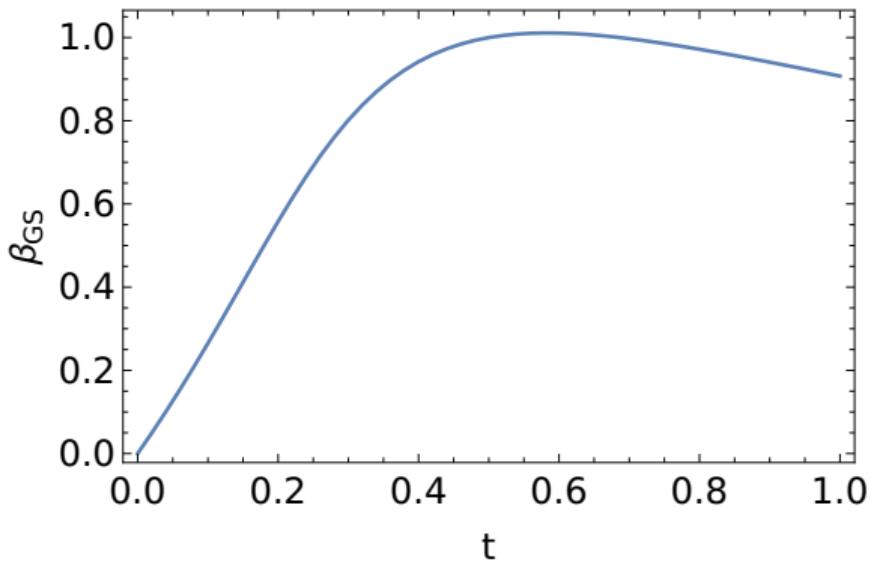
→ criticality is sensitive to the **complexity** of the tiling



# THEORY/NUMERICS ON THE 2D GROUNDSTATE



$$t \sum_{n \text{ NN } m} \psi_n + (t - 1) z_m \psi_m = E \psi_m$$



$$\psi_m = C_m \beta^{h(m)}$$

## COMPUTATION OF A LOCAL OBSERVABLE

Compute the local observable  $\hat{O}$ , in the  $\psi$  state:  $\langle \psi | \hat{O} | \psi \rangle$

Assumptions:

- The observable only depends on the local configuration of the atoms.
- The state is described by an arrow field and a local variation:  $\psi_m = C_m \rho^{h(m)}$

$$\langle \psi | \hat{O} | \psi \rangle = \sum_{m,n} \psi_m^* \hat{O}_{m,n} \psi_n$$

$$\boxed{\langle \psi | \hat{O} | \psi \rangle = \sum_{\mu,\nu} C_\mu^* \hat{O}_{\mu,\nu} C_\nu \sum_{h,h'} f(\mu, h; \nu, h') \rho^{h+h'}}$$