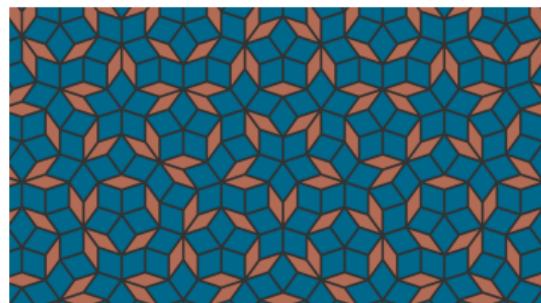


Exact results on electronic wavefunctions of 2D quasicrystals

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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?

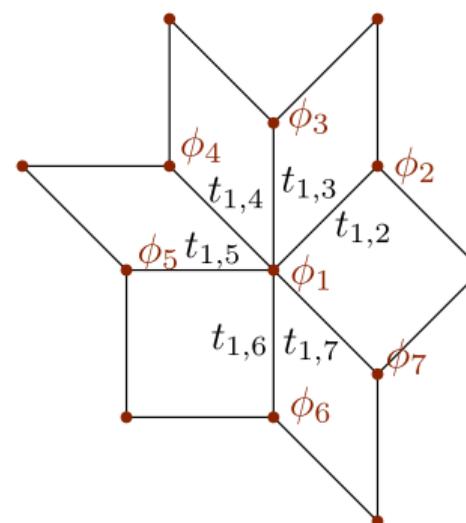
TOY MODELS OF QUASICRYSTALS

We want to model:

- a single electron (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

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

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



Solve for the stationary states (or eigenstates):

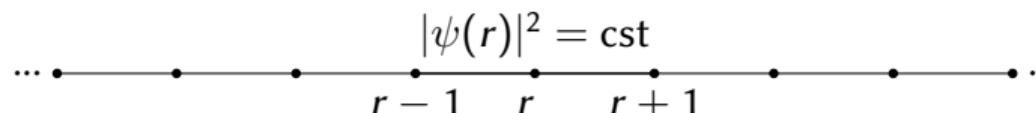
$$E\psi_m = \sum_{n \in V(m)} t_{m,n} \psi_n$$

OUTLINE

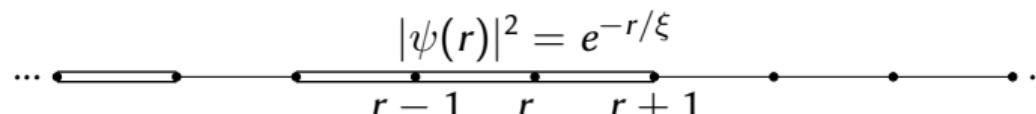
- 1** 1D model (Fibonacci chain): a “baby example”
- 2** 2D models (Penrose and Ammann-Beenker tilings): the “grown-up example”
- 3** Conclusion and perspectives

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 local power law decay, they are **critical**

THE FIBONACCI CHAIN

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

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

$$M^\infty(A) = \dots ABABAABAABABAABABA\dots$$

The corresponding chain of atoms:



The Schrödinger equation for the eigenstate of energy E :

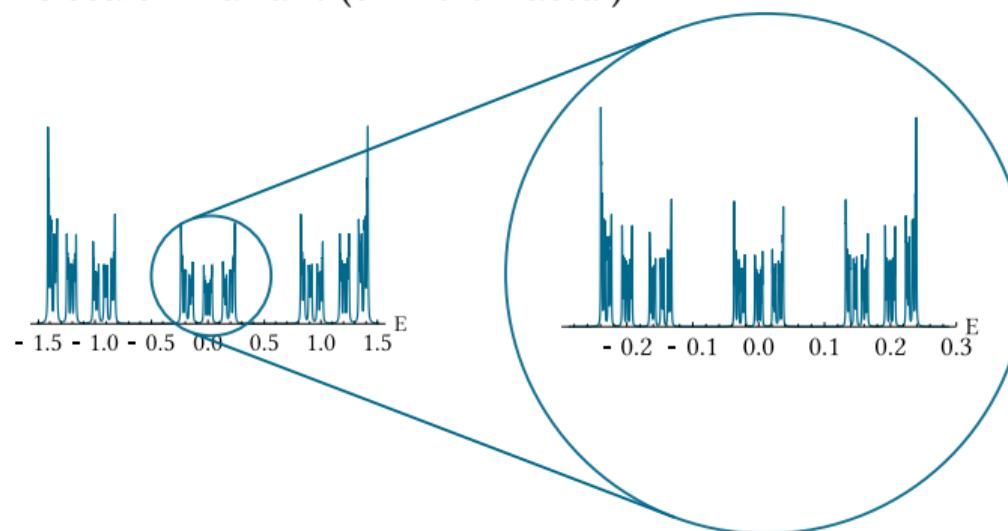
$$t_{m-1,m}\psi_{m-1} + t_{m,m+1}\psi_{m+1} = E\psi_m$$

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

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

SPECTRUM AND EIGENSTATES

- The spectrum is scale invariant (or multifractal)



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

What is the structure of these critical states?

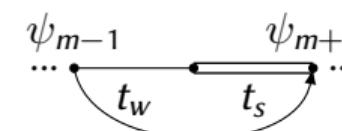
A BABY EXAMPLE: THE EIGENSTATE AT ZERO ENERGY

- 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

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



- There are 4 possible cases:

$$\psi_{m+1} = \frac{t_w}{t_s}\psi_{m-1} = \rho^{+1}\psi_{m-1}$$

$$\psi_{m+1} = \frac{t_s}{t_w}\psi_{m-1} = \rho^{-1}\psi_{m-1}$$

$$\psi_{m+1} = \frac{t_w}{t_w}\psi_{m-1} = \rho^{+0}\psi_{m-1}$$

$$\psi_{m+1} = \frac{t_s}{t_s}\psi_{m-1} = \rho^{+0}\psi_{m-1}$$

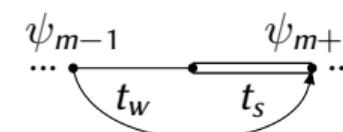
A BABY EXAMPLE: THE EIGENSTATE AT ZERO ENERGY

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

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

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

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

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

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

THE FIELD OF ARROWS AND THE FIELD OF HEIGHTS

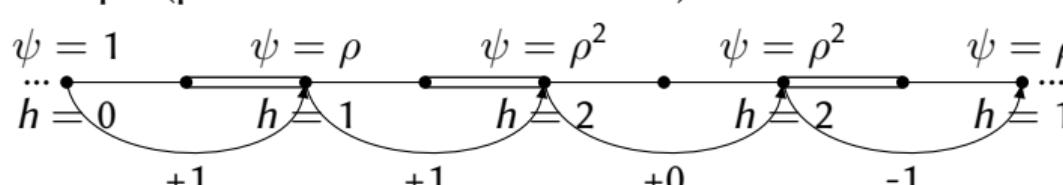
Iterating $\psi_{m+1} = \rho^{A_{m-1,m+1}} \psi_{m-1}$,

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

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**

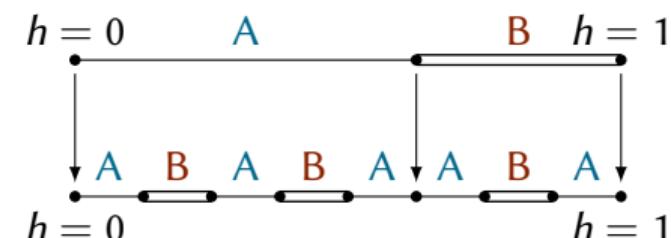
\rightarrow expected behavior in both cases.

What happens for a quasiperiodic chain?

THE $E = 0$ STATE IS NOT LOCALIZED

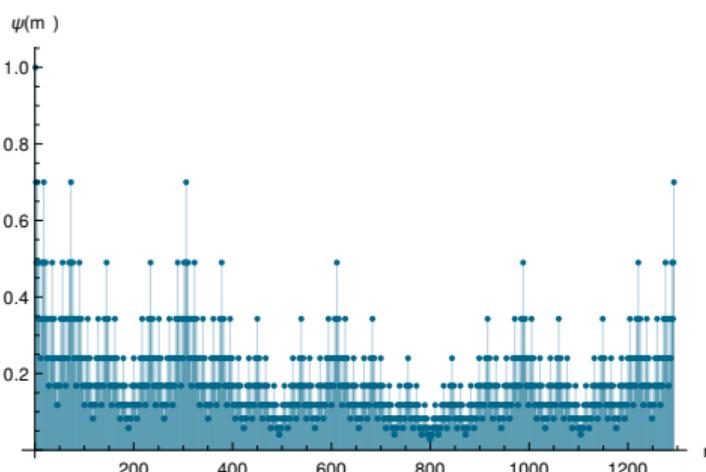
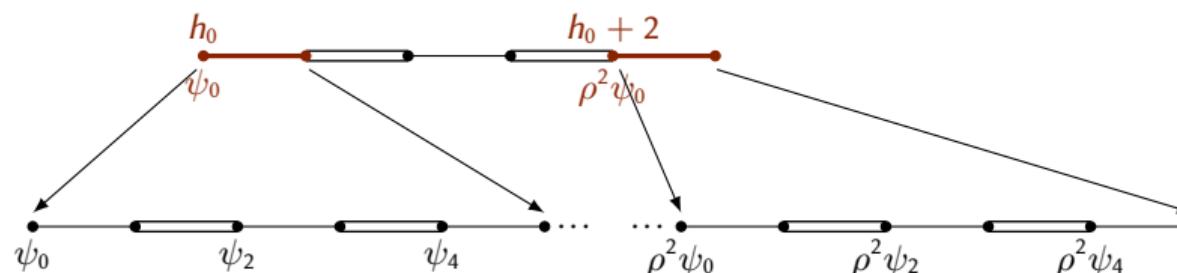
Apply the substitution three times:

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



→ 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 arbitrary 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**

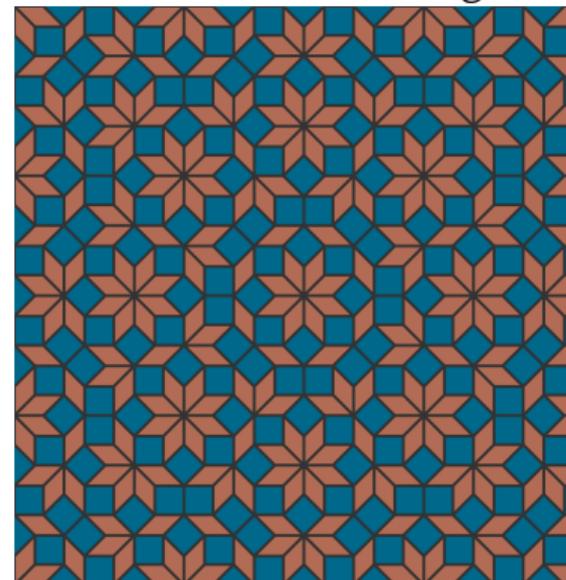
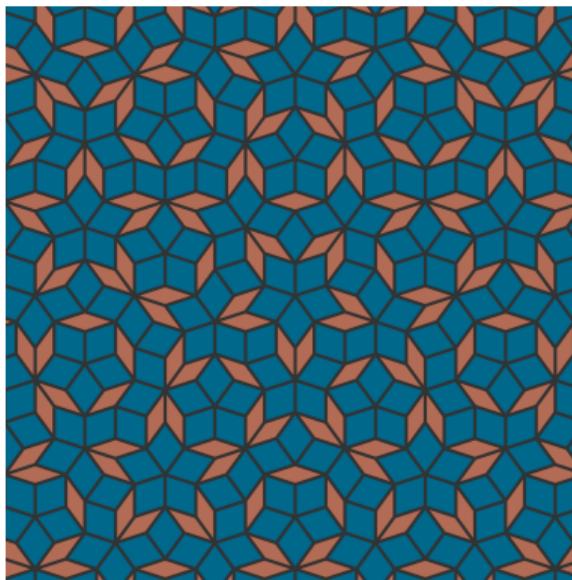
CUT AND PROJECT CHAINS: A SUMMARY

- 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 structural properties of the wavefunction
- → **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.

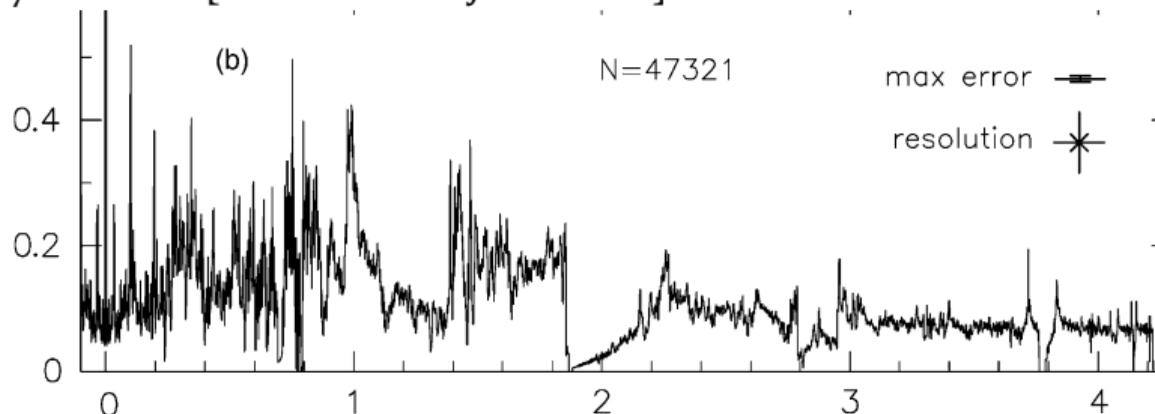


Model for the electron:

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

WHAT IS KNOWN

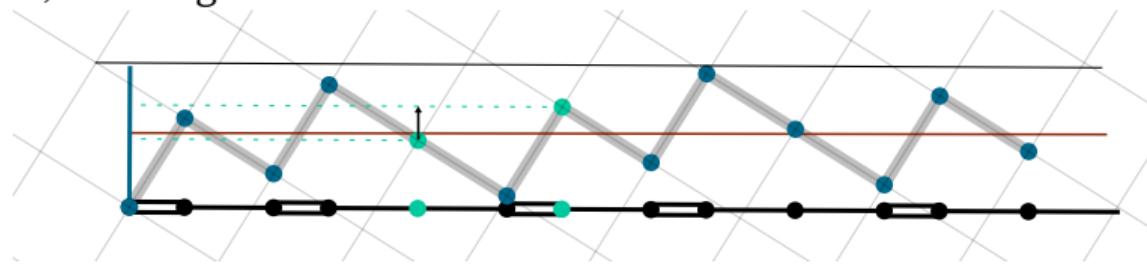
Local density of states [taken from Zijlstra 2014]:



- 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?

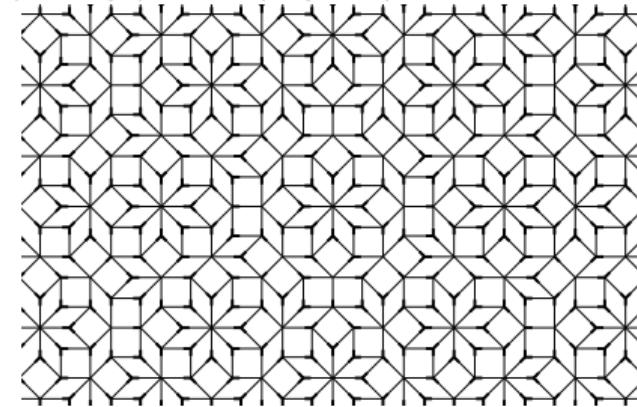
A NATURAL FIELD OF ARROWS

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



- Define arrows in the same way for 2D tilings
- Consider again the height:
$$h(m) = \sum A$$

Can we describe states with this arrow field? $\psi_m = \rho^{h(m)}$



THE GROUNDSTATE WAVEFUNCTION

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

- Idea [Sutherland 1986]: tune the potential

$$E\psi_m = V_m\psi_m + t \sum_{n \in V(m)} \psi_n \iff V_m = E - t \sum_n \beta^{A_{m,n}}$$

Obtain a groundstate which is an arrowed state.

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

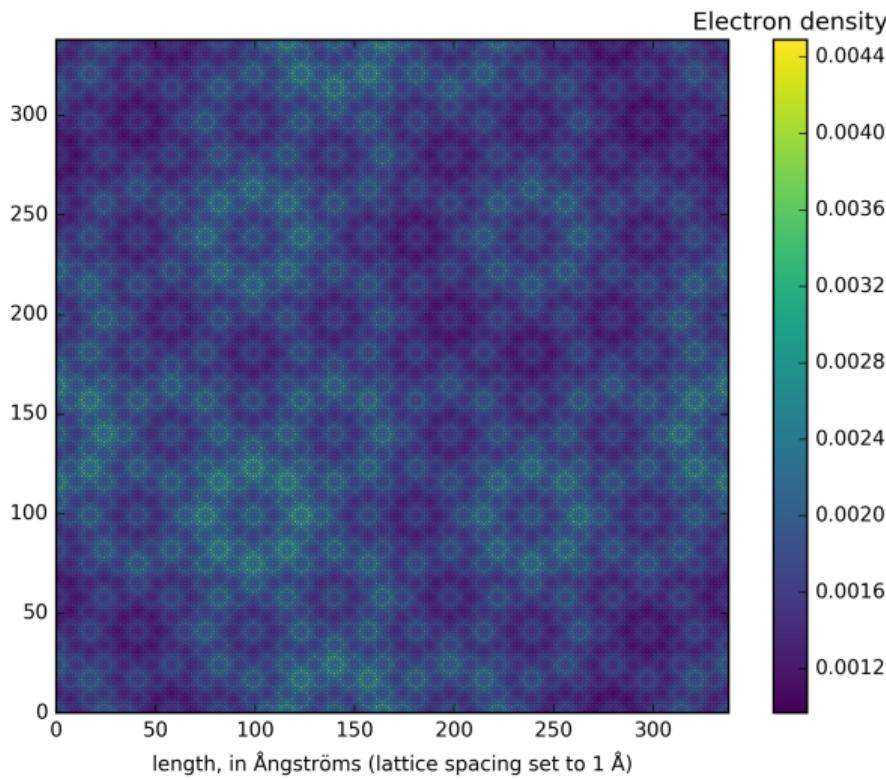
- [Kalugin, Katz 2014] conjecture: state still arrowed, but with a local modulation:

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

where C_m is local:

$C_m \simeq C_n$ if the tiling looks the same around m and n

ROBUSTNESS OF THE STRUCTURE



- 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.

→ what can we do now?

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

We can compute the scaling analytically for the groundstate:

$$D(\psi) = \log \left(\frac{\omega(\rho^2)^2}{\omega(\rho^4)} \right) / \log \omega(1)$$

with (for Ammann-Beenker)

$$\omega(z) = \frac{a(z) + \sqrt{a(z)^2 - z^2}}{z}$$
$$a(z) = 4z^2 + 9z + 4$$

Scaling only depends on the arrow distribution, only on the **geometry** of the tiling.

CONCLUSION

- Examples of generic **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 quantities.

Perspectives:

- For Penrose and Ammann-Beenker, the arrow field is not enough to describe excited states. Extra ingredients?
- Other 2D quasicrystals: generalized Penrose, dodecagonal ...

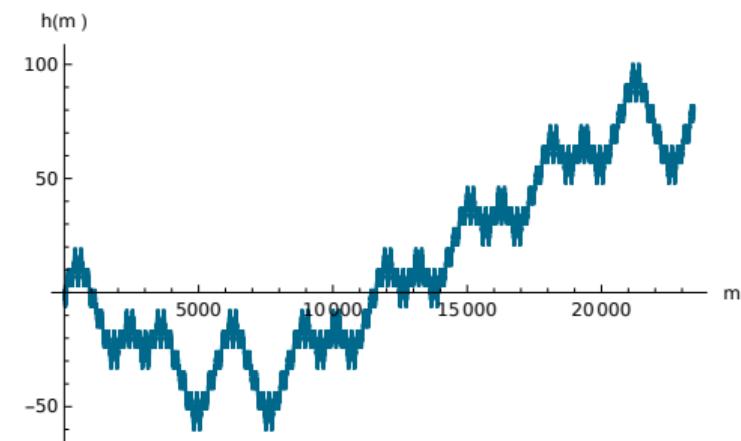
CUT AND PROJECT CHAINS ARE SPECIAL!

Consider the chain constructed by the substitution

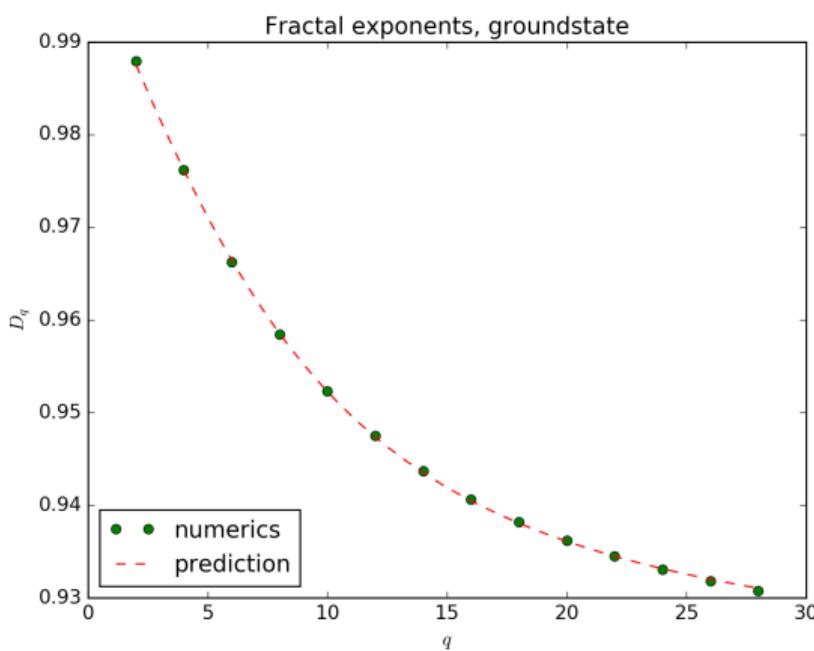
$$\begin{aligned} A &\rightarrow ABBB \\ B &\rightarrow A \end{aligned}$$

- 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!

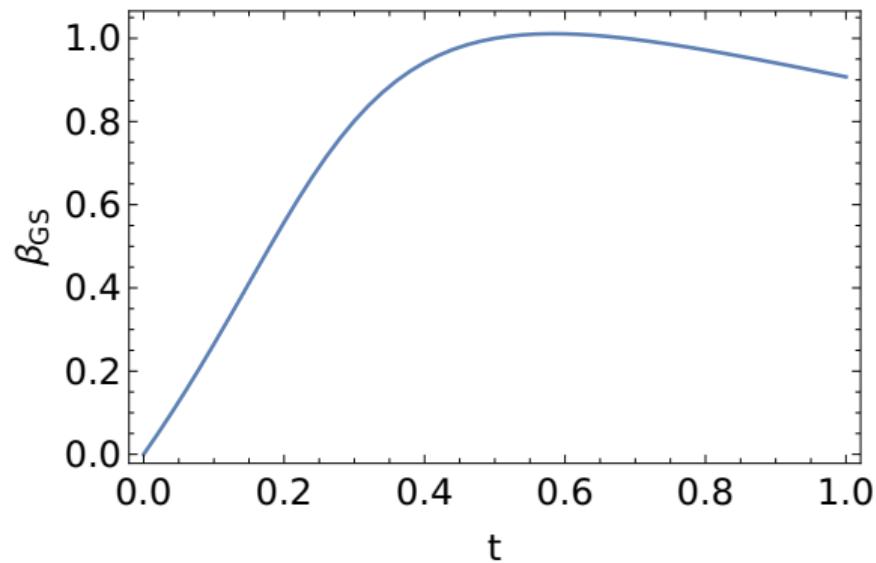
→ criticality is sensitive to the **complexity** of the tiling



THEORY/NUMERICS ON THE 2D GROUNDSTATE



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



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

COMPUTATION OF A LOCAL OBSERVABLE

Compute the local observable \hat{O} , in the ψ 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: $\psi_m = C_m \rho^{h(m)}$

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

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