

# Electronic properties of quasicrystals

Single electron properties of tight-binding quasiperiodic models

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# ELECTRONIC PROPERTIES OF QUASICRYSTALS

Under the supervision of Anuradha Jagannathan

In collaboration with : Michel Duneau, Pavel Kalugin, Rémi Mosseri, Frédéric Piéchon.

- Fractal dimensions of wave functions and local spectral measures on the Fibonacci chain

*Macé, Jagannathan, Piéchon, PRB 93 (20), 2016*

- Quantum simulation of a 2D quasicrystal with cold atoms

*Macé, Jagannathan, Duneau, Crystals 6 (10), 124*

- Critical eigenstates and their properties in one-and two-dimensional quasicrystals

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- Gap structure of 1D cut and project Hamiltonians

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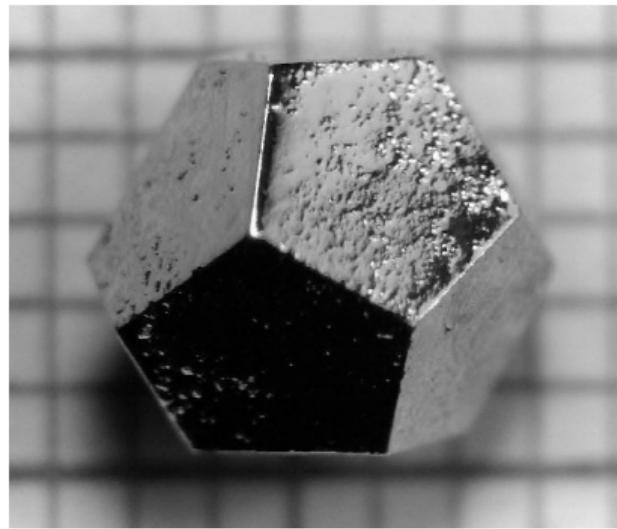
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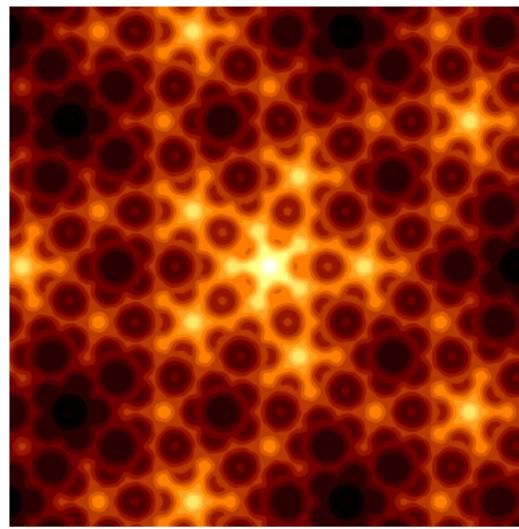
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# ELECTRONIC PROPERTIES OF QUASICRYSTALS



3D HoMgZn quasicrystalline sample  
(doi:10.1038/nmat1244)

Quasicrystals : not periodic yet ordered structures (discovery : 1982).  
 Here : single electron properties of tight-binding quasiperiodic models.

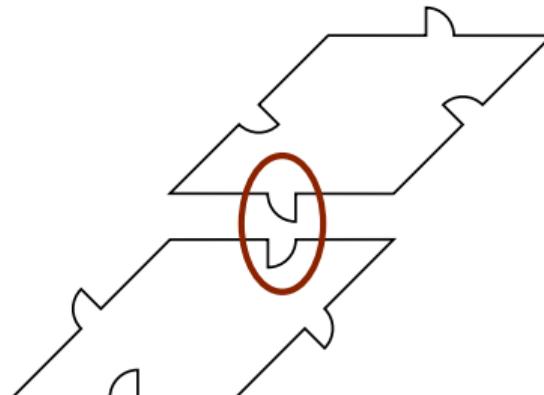


## Groundstate electron density (simple tight-binding model on a 2D tiling)

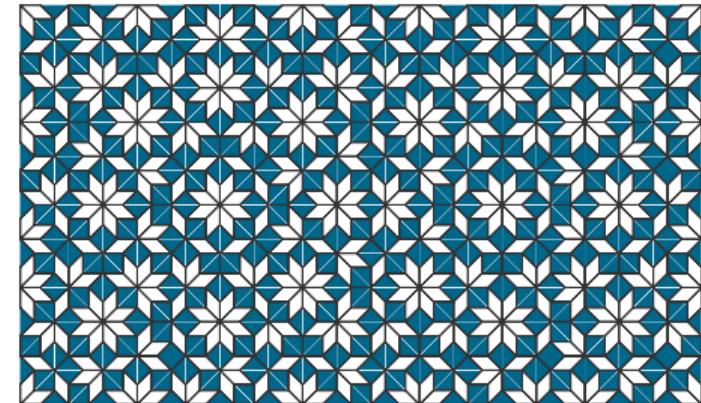
A QUASIPERIODIC PUZZLE [BÉDARIDE *ET AL.* 12]



Pay the squares, get the rhombuses for free!



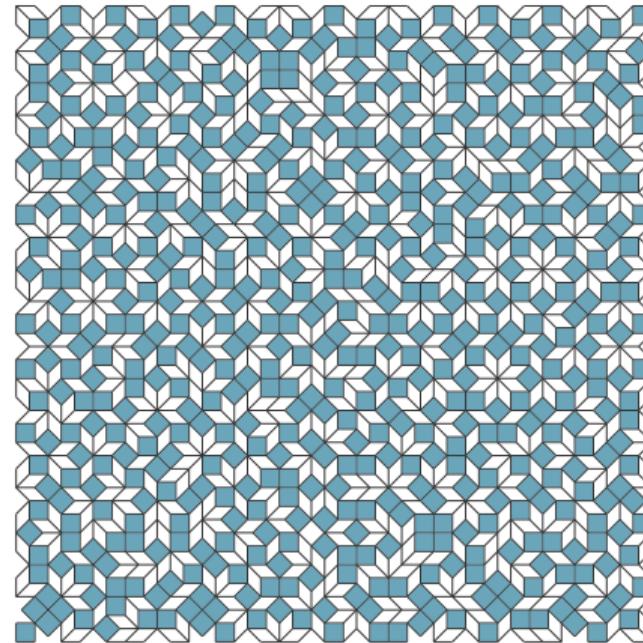
Forbidden configuration.



## Patch of the Ammann-Beenker tiling.

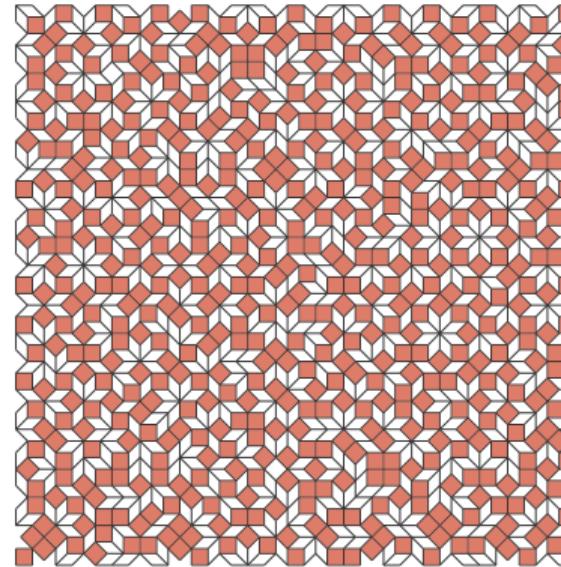
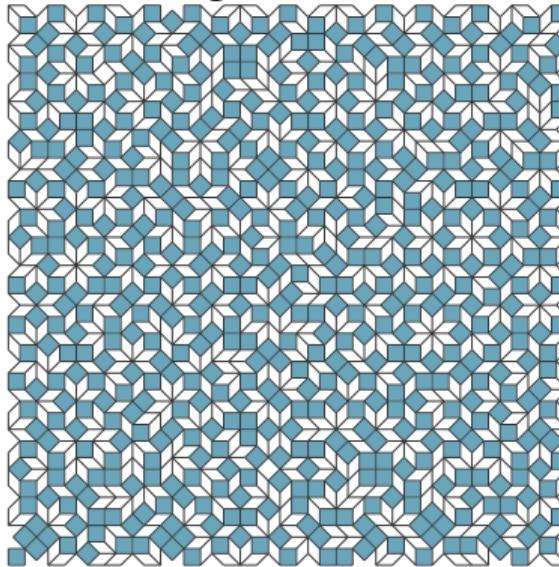
# PERIODIC, QUASIPERIODIC AND RANDOM

## A random tiling :

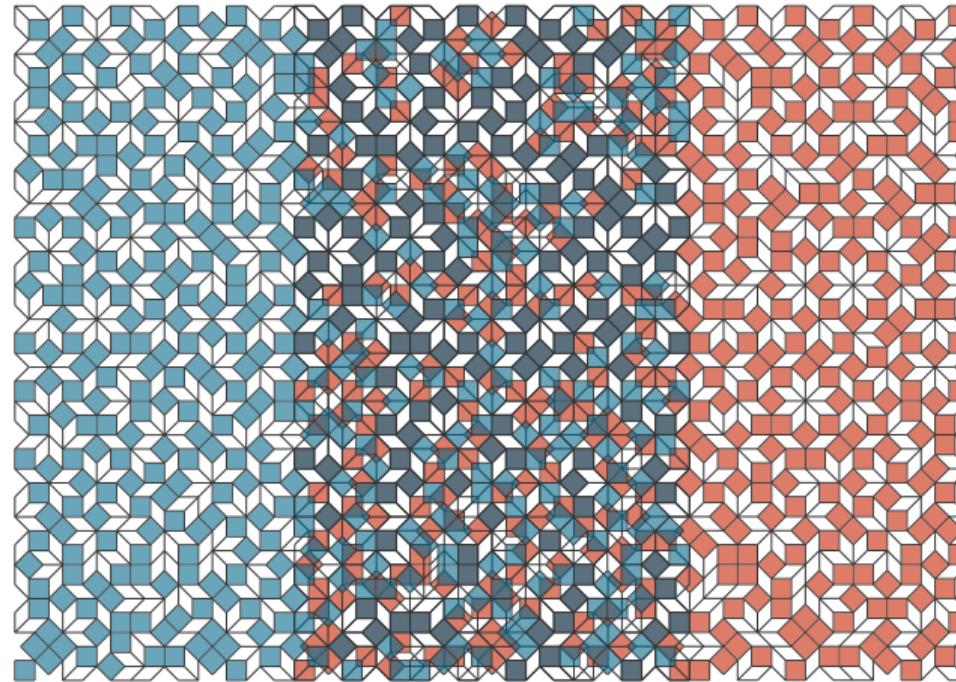


PERIODIC, QUASIPERIODIC AND RANDOM

Two copies of the tiling :

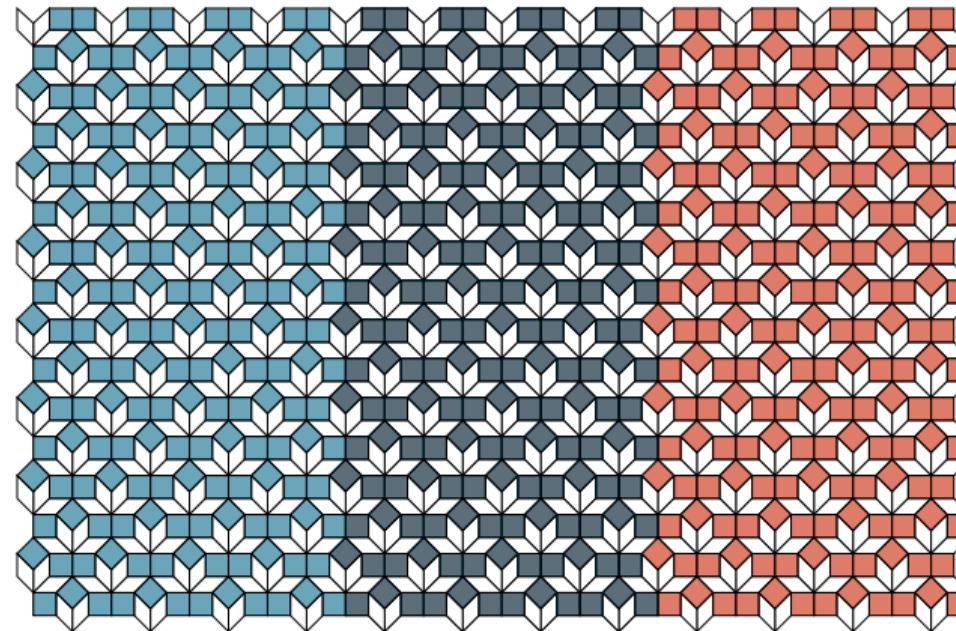


PERIODIC, QUASIPERIODIC AND RANDOM



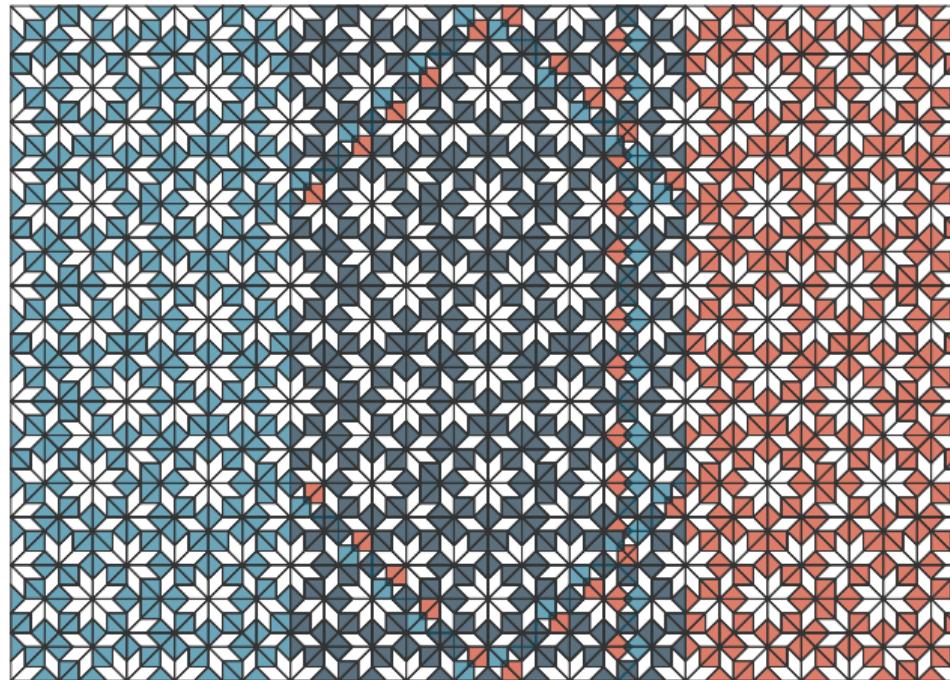
→ no overlap → no order

PERIODIC, QUASIPERIODIC AND RANDOM



## Perfect long range order : periodic

PERIODIC, QUASIPERIODIC AND RANDOM



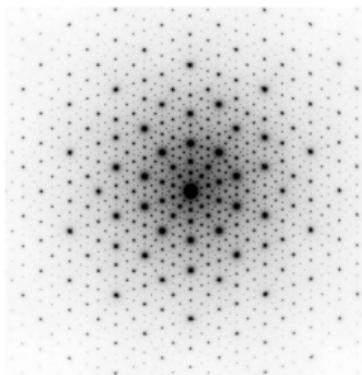
### Long range order : quasiperiodic

(see Chap. 2 of [Grimm, Baake 13])

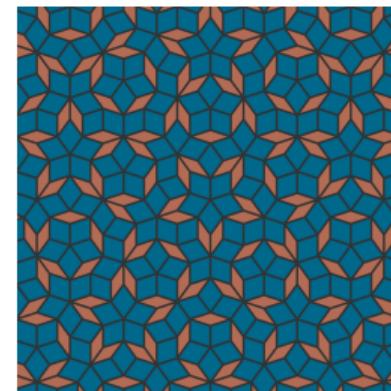
# QUASICRYSTALS

Quasicrystal → quasiperiodically arranged atoms :

- **aperiodicity**
- **long range order** (diffraction pattern exhibits sharp peaks).

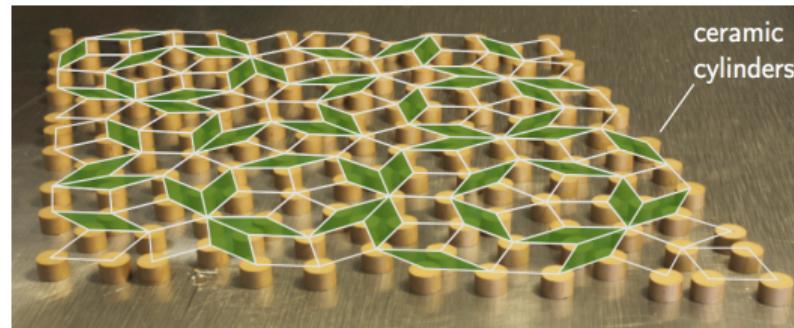


Diffraction pattern of a AlPdMn alloy  
(Conradin Beeli group)



A patch of the quasiperiodic Penrose tiling,  
used to model many quasicrystals.

## ARTIFICIAL QUASIPERIODIC STRUCTURES

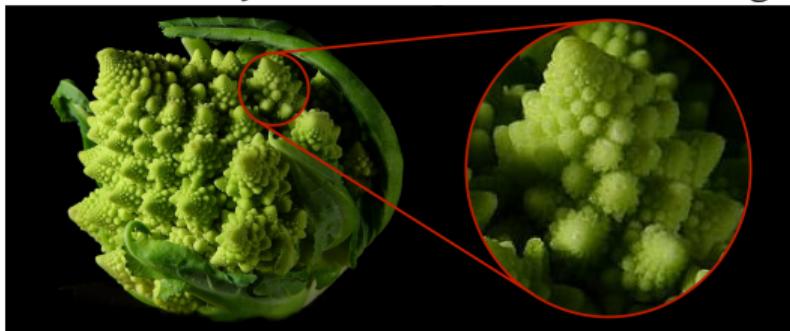


A network of dielectric resonators [Vignolo *et al.* 14]

- Plasmons in semiconductor stacks [Merlin *et al.* 85]
- Microwaves in perforated metallic films [Matsui *et al.* 07]
- Microwaves in dielectric resonator networks [Vignolo *et al.* 14]
- Light solitons [Freedman *et al.* 07]
- Cold atoms in laser potentials [Guidoni *et al.* 97]
- Polaritons in wire cavities [Tanese *et al.* 14]

# FRACTALS

Fractal : object invariant under rescaling



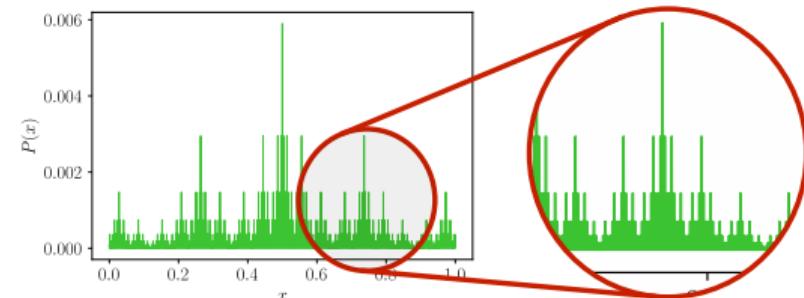
Romanesco broccoli (© Wikimedia commons)

Quasicrystals *not* fractal...

...but electrons on quasicrystals → fractal behavior

Goal :

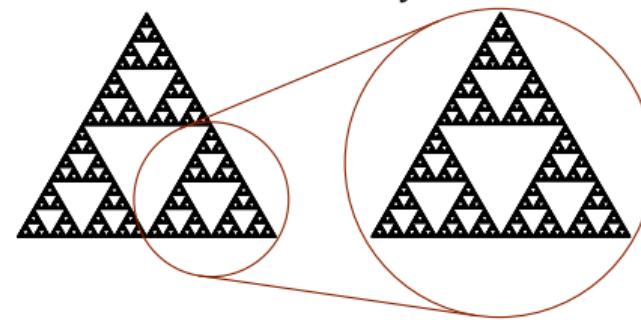
**Link the fractal behavior of the electrons to quasiperiodicity**



Electronic density along a quasiperiodic chain

## FRACTAL DIMENSIONS

- $M(L) \propto L^d$  for a non-fractal  $d$ -dimensional object...What happens for a fractal one?



A Sierpiński triangle

$$M(L) \sim L^{d_0}, \text{ with } d_0 = \log 3 / \log 2$$

- $d_0$  is the Hausdorff fractal dimension
- $1 < d_0 \simeq 1.58 < 2$ , signature of a fractal object
- Probe fractality of the  $q^{\text{th}}$  moment of a distribution  $\rightarrow$  generalized fractal dimensions  $d_q$ .

# CONTENT

- 1** Introduction
- 2** A 1D quasicrystal : the Fibonacci chain
- 3** Renormalization group on the Fibonacci chain
- 4** A 2D quasicrystal

# CONSTRUCTING THE FIBONACCI CHAIN

## Fibonacci words

Substitution rule :

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

Generate a sequence of words  $C_l$

$$C_{l+1} = S(C_l)$$

$$C_0 = B$$

$$C_1 = S(C_0) = S(B) = A$$

$$C_2 = S(C_1) = S(A) = AB$$

$$C_3 = S(C_2) = S(A)S(B) = ABA$$

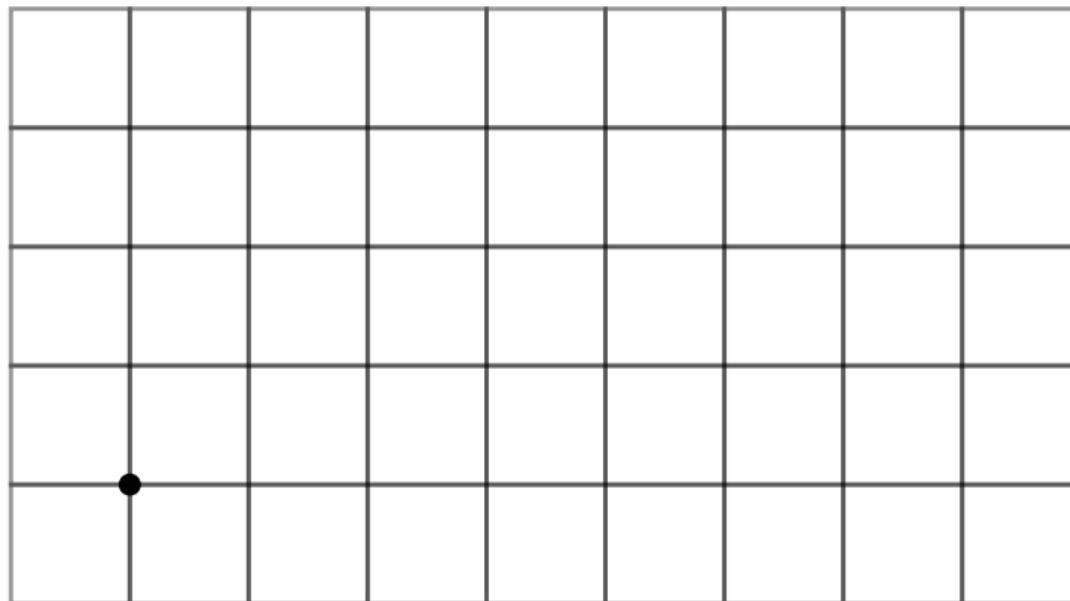
$$\dots C_6 = ABAABABAABAAAB$$

## Properties of Fibonacci words

- Number of letters follows the Fibonacci sequence :  
 $\#A$  in  $C_{1,2,3,4,\dots} = 1, 1, 2, 3, 5, \dots$
- $\#A/\#B \underset{l \rightarrow \infty}{\sim} \tau$ , where  
 $\tau = \frac{1+\sqrt{5}}{2} \simeq 1.61$  is the golden ratio.
- $\tau$  irrational  $\rightarrow$  infinite word **aperiodic**

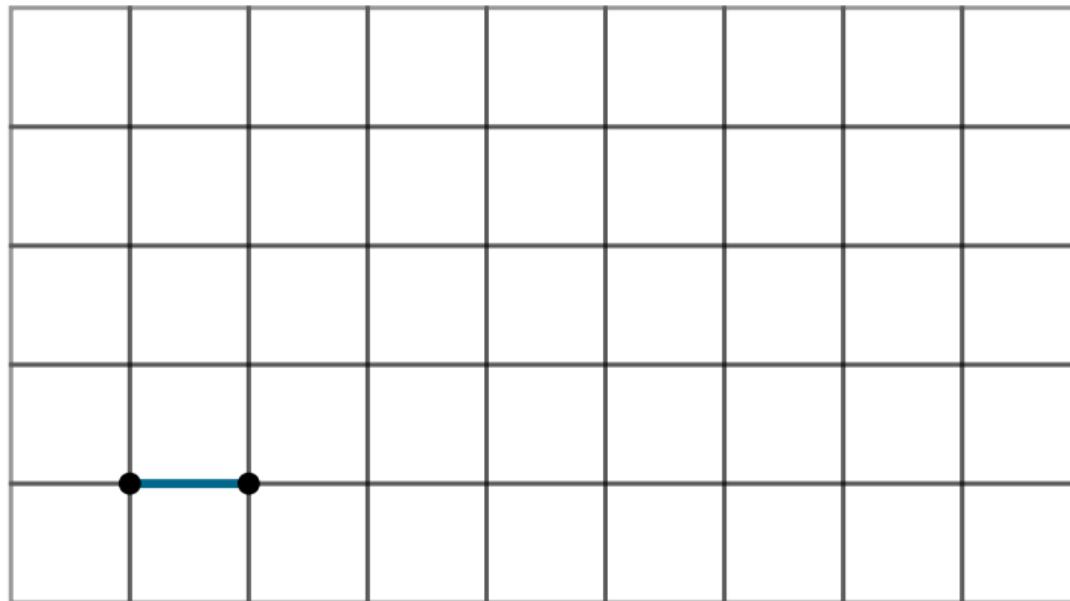
# FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABAA...  
 $A \leftrightarrow$  horizontal step,  $B \leftrightarrow$  vertical step



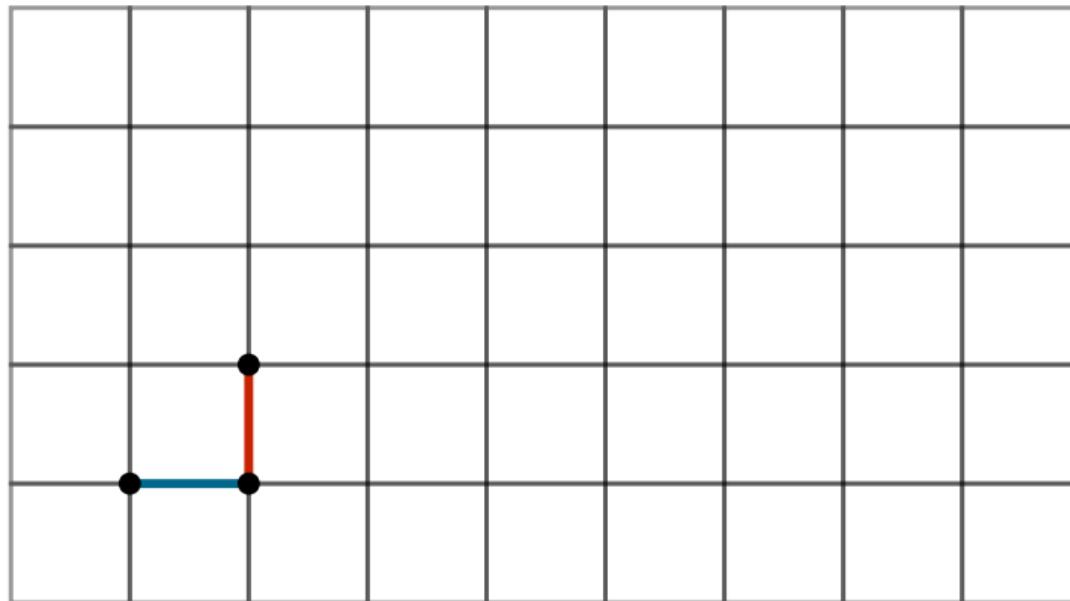
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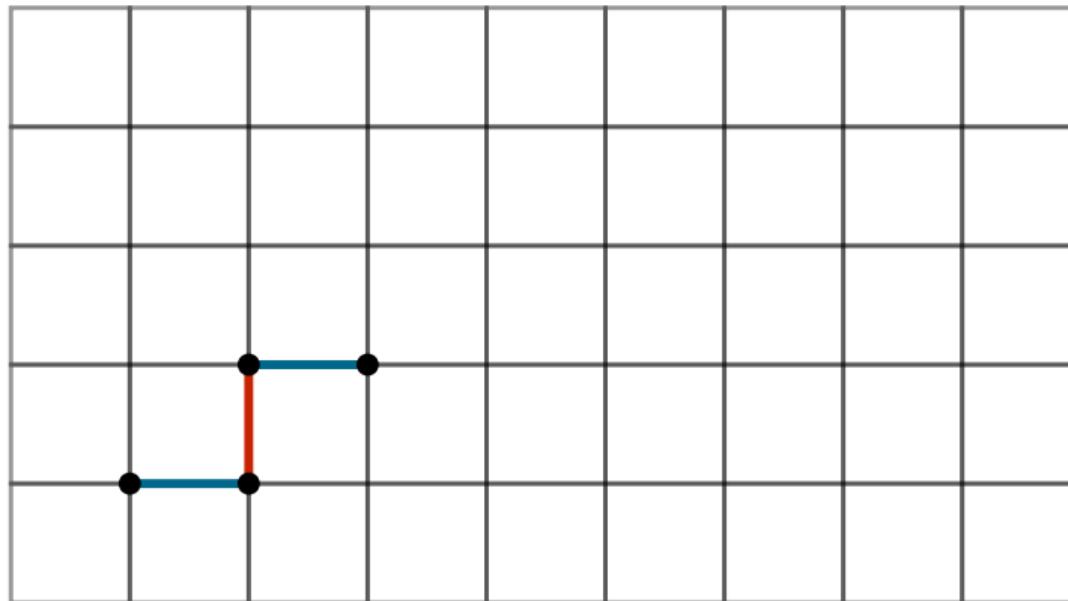
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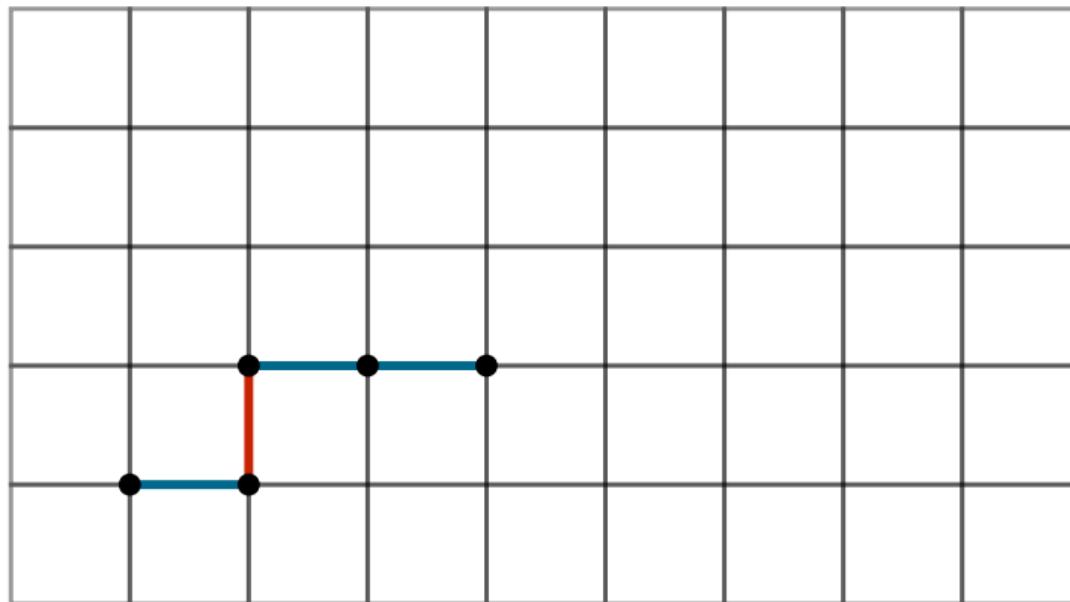
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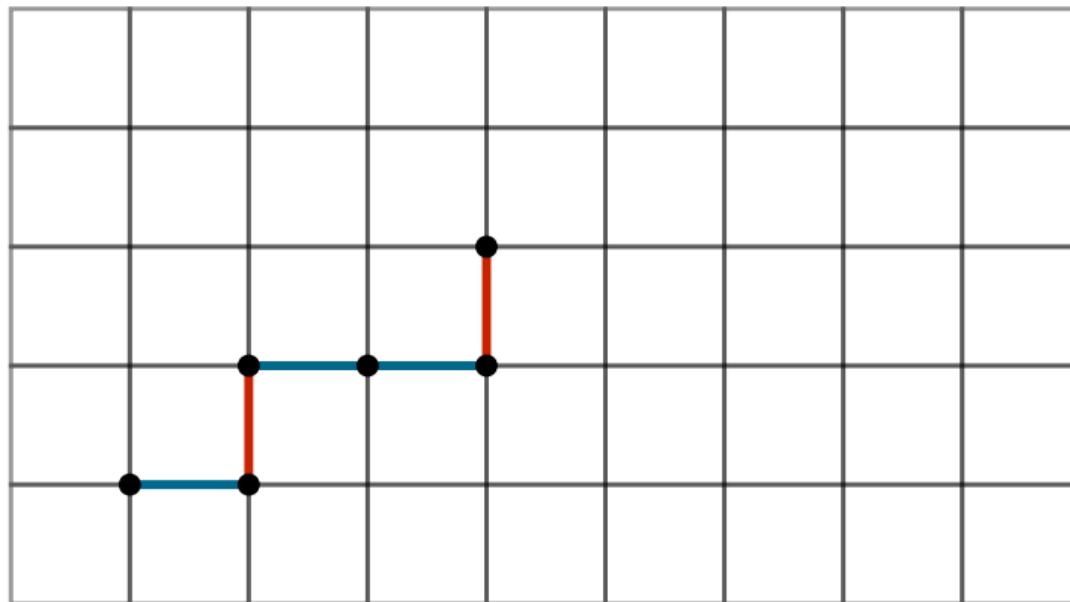
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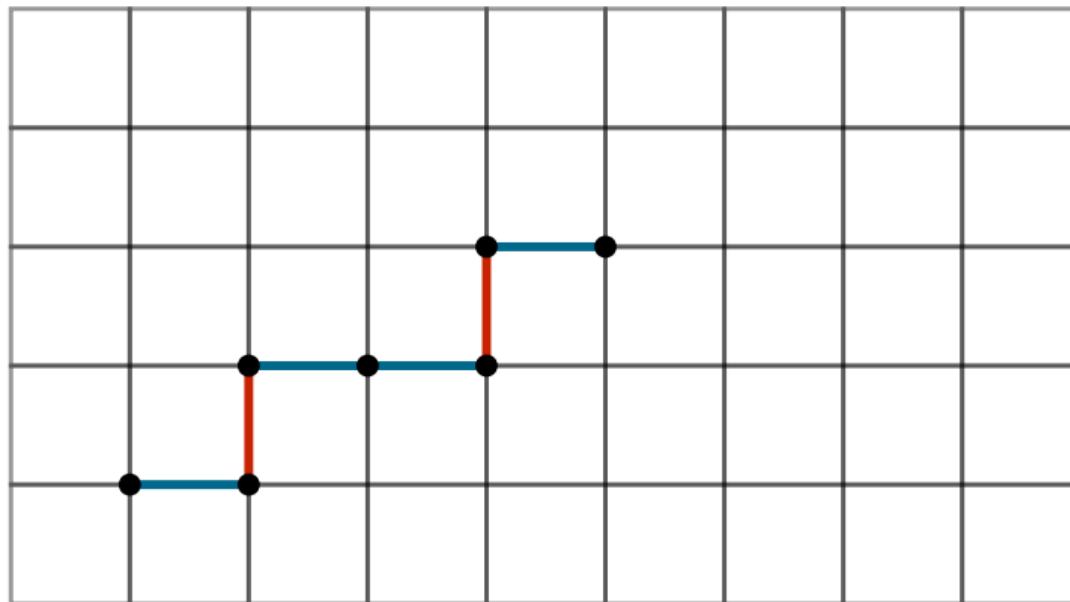
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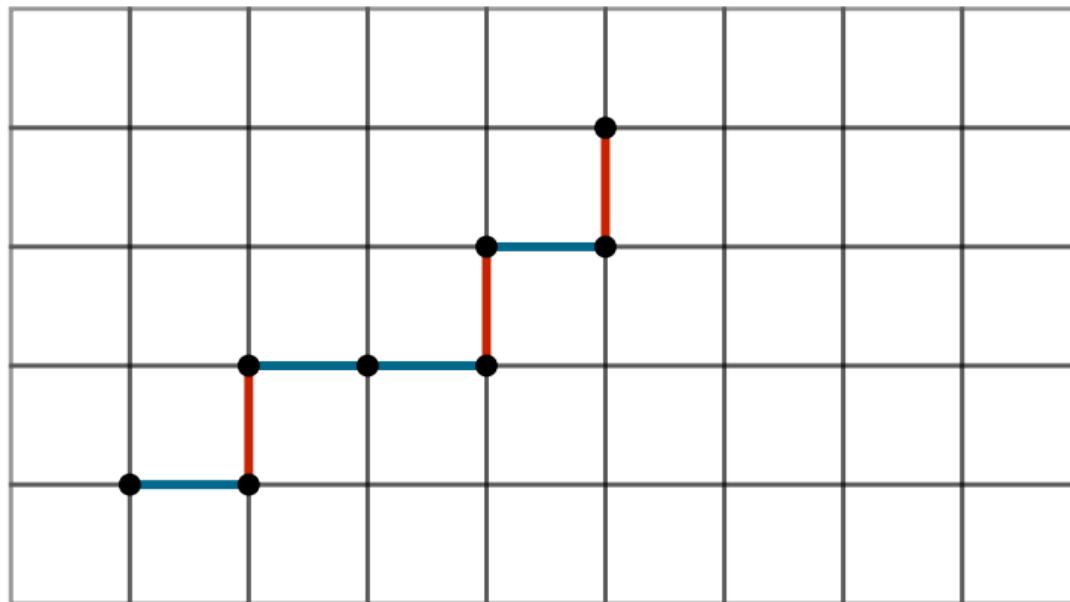
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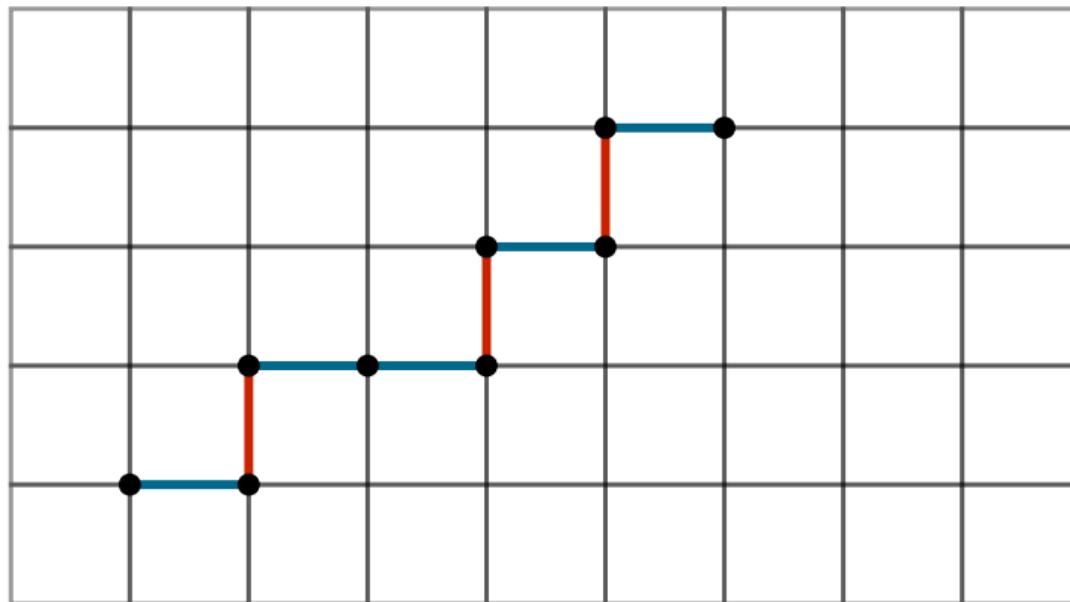
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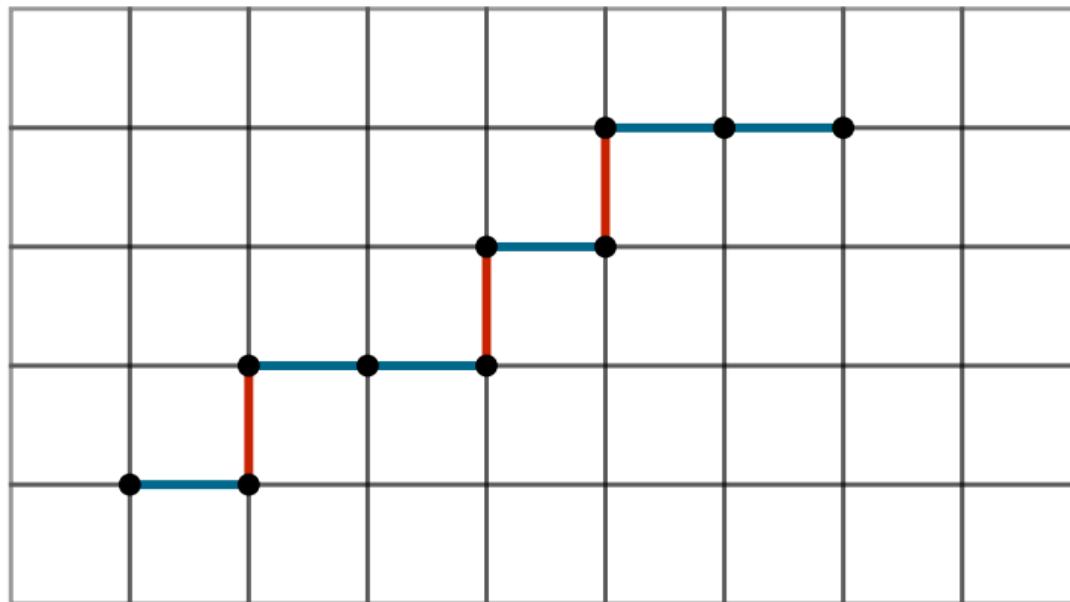
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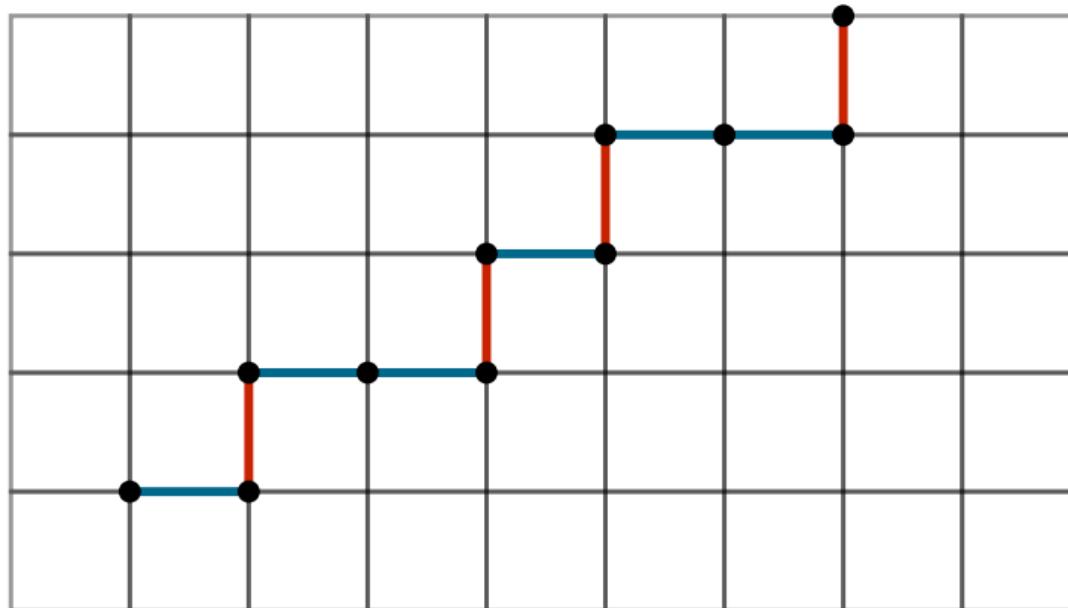
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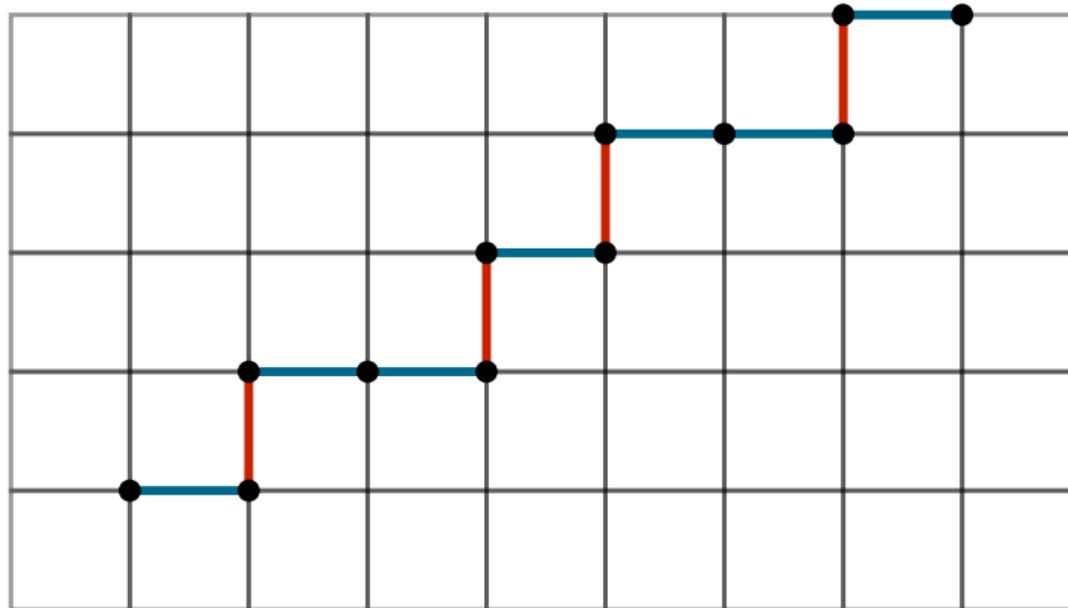
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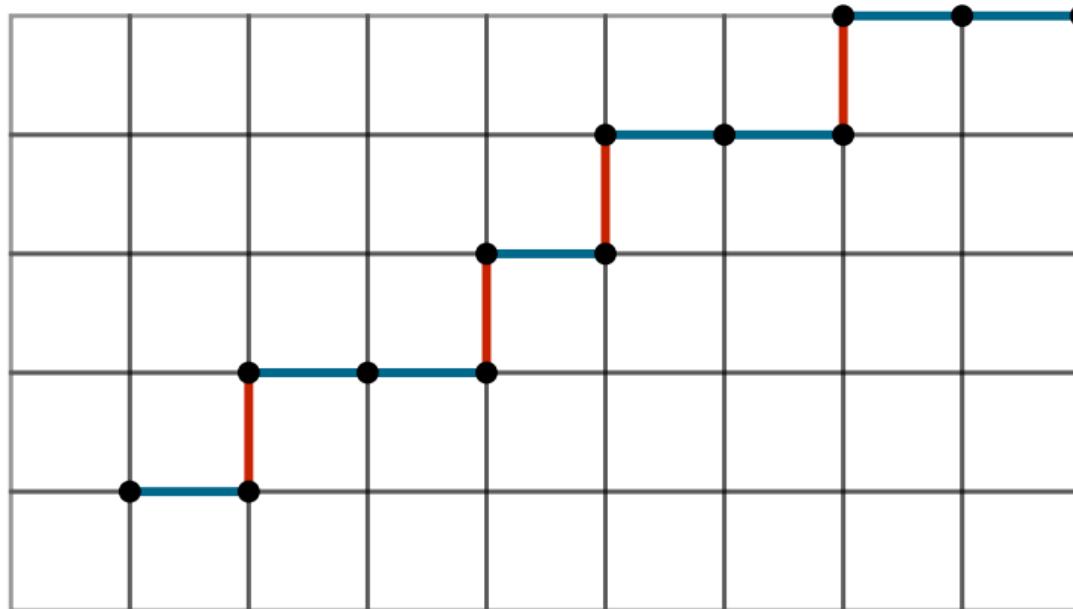
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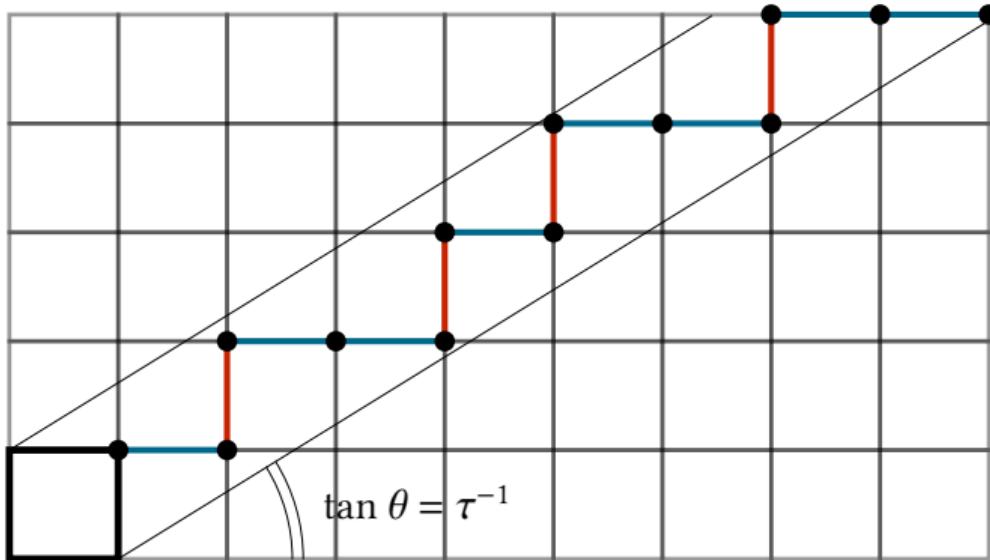


# FIBONACCI WORD FROM ABOVE

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## QUASIPERIODICITY OF THE FIBONACCI WORD

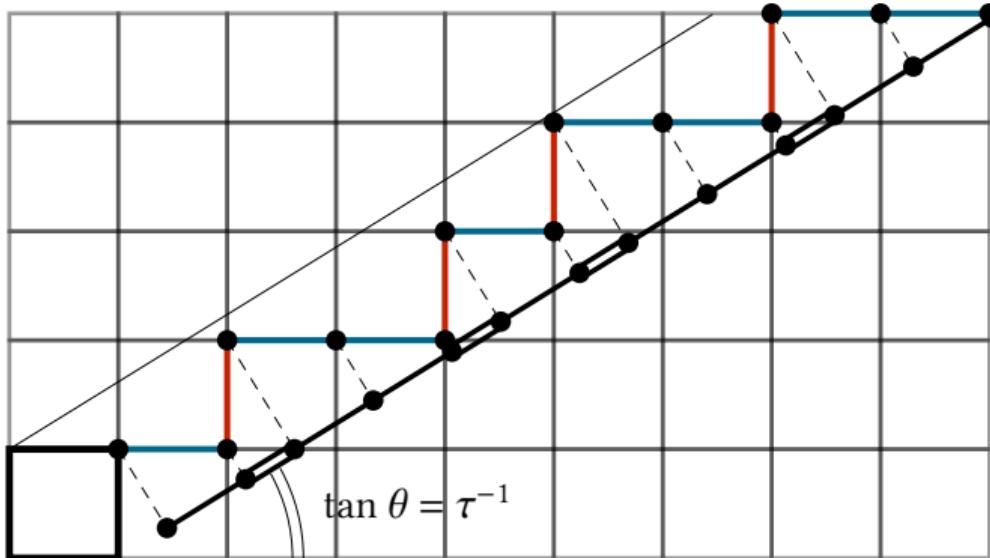


- average slope = inverse of the golden ratio ( $\tau \simeq 1.6$ )
  - bounded fluctuations

→ similar environments everywhere  
→ quasiperiodicity [Duneau, Katz 85]

# CUT-AND-PROJECT ILLUSTRATED IN THE 1D CASE

C&P : general method to construct quasiperiodic tilings

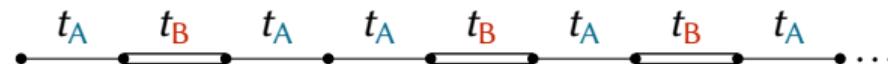


The cut-and-project algorithm :

- 1 choose a hypercubic lattice (here  $\mathbb{Z}^2$ )
- 2 choose a “physical plane”  $E_{\parallel}$  (here a slope)
- 3 select points by translating the unit hypercube along  $E_{\parallel}$
- 4 project them onto  $E_{\parallel}$ .

## FROM LETTERS TO ATOMS

- The Fibonacci word : ABAABABA...
- The Fibonacci (tight-binding) chain of atoms :



Pure-hopping Hamiltonian :

$$\hat{H} = - \sum_m t_m |m-1\rangle \langle m| + \text{H.c}$$

→  $\rho = t_A/t_B$  only free parameter.

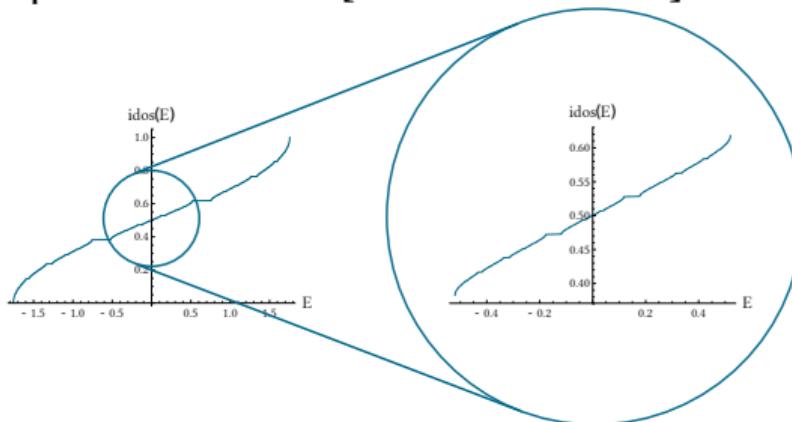
Schrödinger equation for the eigenstate of energy  $E$  :

$$E\psi(m) = -t_m\psi(m-1) - t_{m+1}\psi(m+1)$$

# FIBONACCI SPECTRUM AND EIGENSTATES

## Numerical results

- Spectrum : fractal [Kohmoto *et al.* 83]

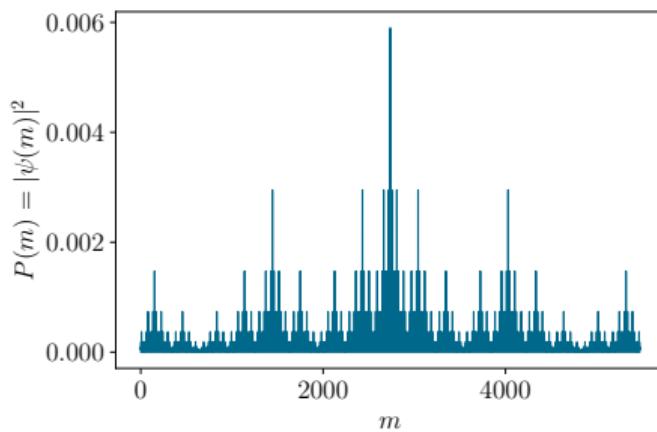


- Eigenstates : (almost all) fractal [Kohmoto *et al.* 83]

## Analytical results

- Gap labeling [Bellissard 86]
- Fractal dimensions of the spectrum
  - $\rho = t_A/t_B \ll 1$  : [Piéchon *et al.* 95]
  - $\rho \sim 1$  : [Rüdinger, Sire 96]
- Fractal dimensions of the eigenstates,  $\rho \ll 1$ 
  - leading order [Thiem, Schreiber 12]
  - next-to-leading order [Macé *et al.* 16]
- **exact description of the  $E = 0$  state [Kohmoto *et al.* 87], [Macé *et al.* 17]**

# THE BROCCOLI $E = 0$ STATE

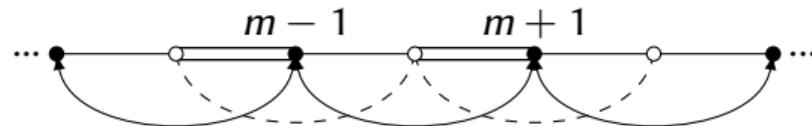


“Romanesco broccoli” fractal state at energy  $E = 0$

- State at 0 energy verifies

$$t_m \psi(m-1) + t_{m+1} \psi(m+1) = 0$$

- Fibonacci chain decouples into two chains :



- Work on groups of two letters :

- AB  $\leftrightarrow$  R
- BA  $\leftrightarrow$  L
- AA  $\leftrightarrow$  U
- BB : never occurs

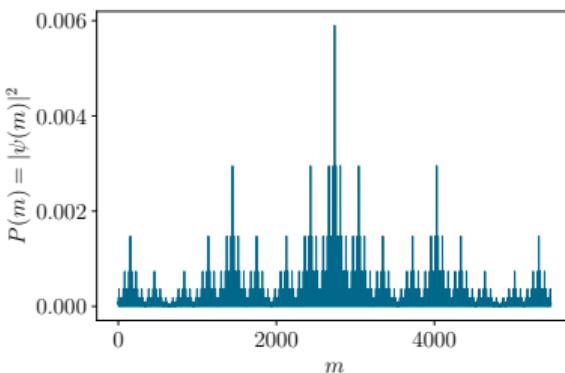
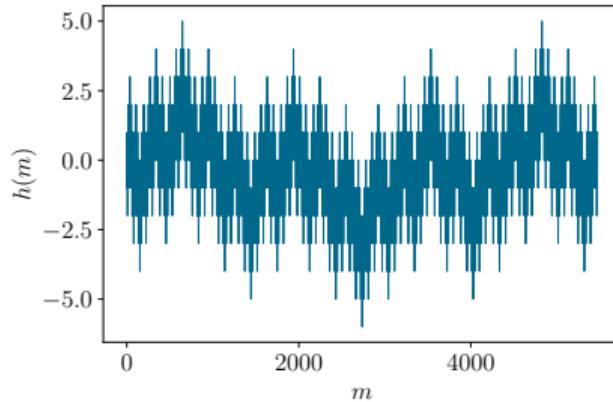
# STRUCTURE OF THE BROCCOLI

- Effective chain



- **Arrow function** :  $A(R) = +1$ ,  $A(L) = -1$ ,  $A(U) = 0$ .
- **Height function** :  $h(m) = \sum_{n \leq m} A_n$
- Let  $\rho = t_B/t_A$ .

$$\psi(m) = (-1)^m \rho^{h(m)}$$

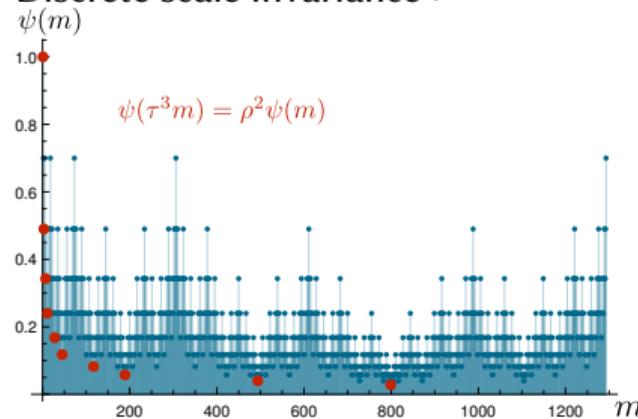


# GEOMETRY AND EIGENSTATE PROPERTIES

- Arbitrary chain **AAABBABB...** (not necessarily Fibonacci)
- $E = 0$  state :  $\psi(m) = (-1)^m \rho^{h(m)}$
- Geometry  $\leftrightarrow h(m)$  function
- Periodic chain : **AAAAAA...**
  - Arrows = 0  $\implies |\psi(m)| = \text{cst}$
  - **extended state**
- Disordered chain : **AAABBBABB...**
  - Random arrows  $\implies h(m) \underset{m \rightarrow \infty}{\sim} \sqrt{m}$   
 $\implies |\psi(m)| \sim e^{-\sqrt{m}/\xi}$
  - **localized state**

## ■ Quasiperiodic chain

- Discrete scale invariance :



- Local power-law behavior  $|\psi(m)| \sim m^{-\alpha}$
- Red points show such a local power-law,  
 $\alpha = 2|\log \rho|/(3\log \tau)$
- **critical state**

# HEIGHT DISTRIBUTION & MULTIFRACTALITY

Partition function of the heights :

$$Z_L(\beta) = \sum_{m \in \mathcal{R}(L)} e^{-\beta h(m)}$$

Substitution → scaling law behavior :

$$Z_L(\beta) \underset{L \rightarrow \infty}{\sim} L^{\omega(\beta)}$$

with

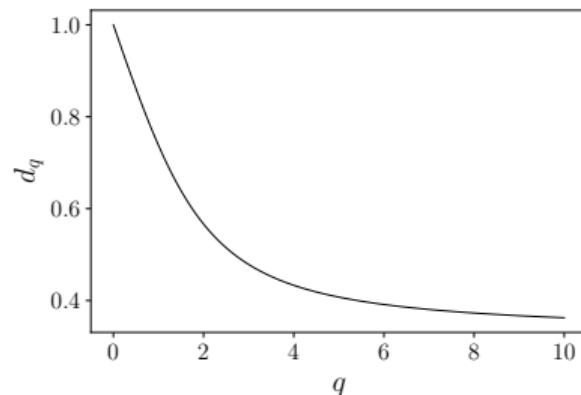
$$\omega(\beta) = \frac{\sinh^{-1}(1 + \cosh(\beta))}{\log(2 + \sqrt{5})}$$

→ access to the distribution of heights

Height grows slowly :

$$h_{\text{typ}}(L) \sim \sqrt{\log L}$$

Fractal dimensions of the  $E = 0$  state :



$0 < d_{q>0} < 1 \rightarrow \text{multifractal state}$

[Kohmoto *et al.* 87], [Macé *et al.* 17]

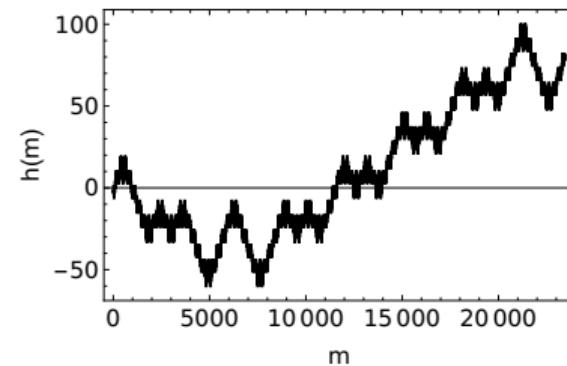
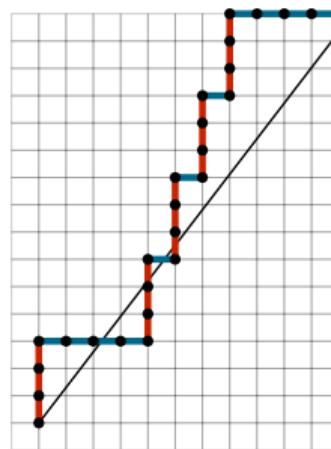
# BEYOND QUASIPERIODICITY

B3 chain :

$$S : \begin{cases} A \rightarrow ABBB \\ B \rightarrow A. \end{cases}$$

Unbounded fluctuations  
(non-Pisot inflation factor)

→ **not quasiperiodic**  
[Frank, Robinson 08]



Height : power-law growth [Dumont 89]

$$h(m) \sim m^\alpha$$

$$\alpha = \log 3 / \left( 3 \log \left( \frac{1 + \sqrt{13}}{2} \right) \right)$$

→ **non-fractal, localized state**

$$|\psi(m)| \underset{m \rightarrow \infty}{\sim} e^{-m^\alpha/\xi}$$

# CONCLUSIONS

$E = 0$  state of **two-letters** tight-binding chains :

- Height field  $h(m) \rightarrow \psi(m) = (-1)^m \rho^{h(m)}$

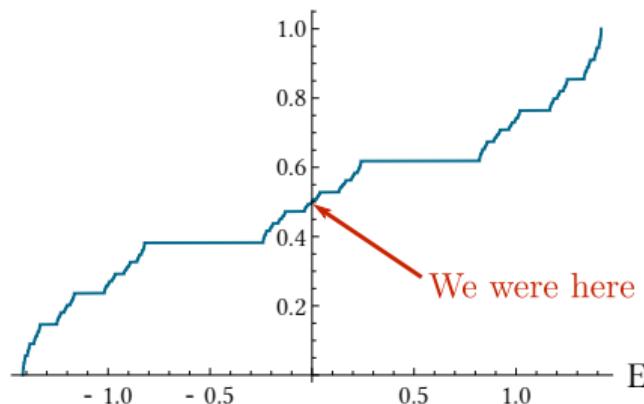
Effect of the (dis)order :

- **Periodic** → no height growth → **extended** state
- **Quasiperiodic** → slow height growth ( $h(L) \sim \sqrt{\log L}$ ) → critical, **fractal** state
- **Random/deterministic non-qp** → fast height growth ( $h(L) \sim L^\alpha$ ) → **localized** state

# RENORMALIZATION GROUP ON THE FIBONACCI CHAIN

Focused on the  $E = 0$  state...

idos( $E$ )



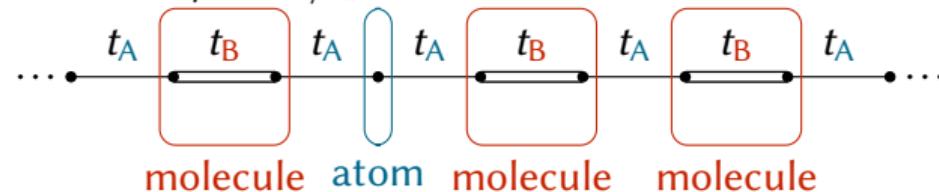
Integrated density of states (IDoS) of the Fibonacci chain  
...what about the rest of the spectrum?

## Analytical results

- Gap labeling [Bellissard 86]
- Fractal dimensions of the spectrum
  - $\rho = t_A/t_B \ll 1$  : [Piéchon *et al.* 95]
  - $\rho \sim 1$  : [Rüdinger, Sire 96]
- Fractal dimensions of the eigenstates,  
 $\rho \ll 1$ 
  - **leading order**  
[Thiem, Schreiber 12]
  - **higher order**  
[Macé *et al.* 16]
- exact description of the  $E = 0$  state  
[Kohmoto *et al.* 87], [Macé *et al.* 17]

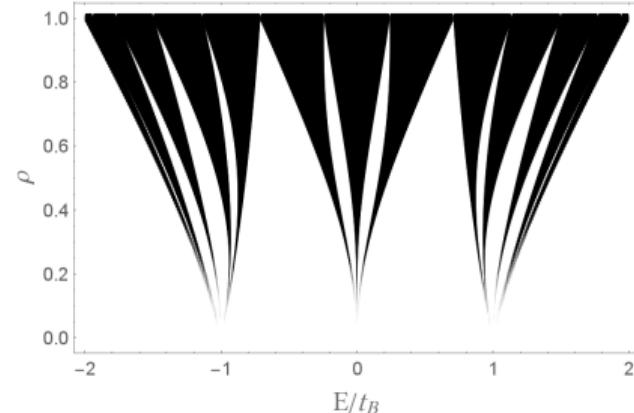
# ATOMS AND MOLECULES

Fibonacci chain in the limit  $\rho = t_A/t_B = 0$  :



→ collection of decoupled atoms and diatomic molecules

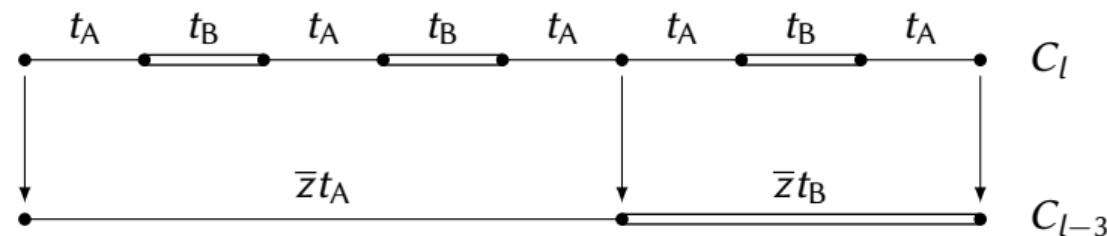
$\rho \neq 0, \rho \ll 1 \rightarrow$  lifted degeneracy, atomic and molecular energy clusters :



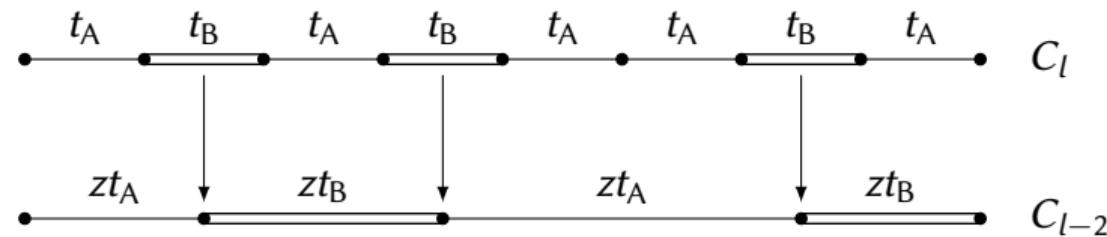
# RENORMALIZATION

Substitution rule :  $C_{l+1} = S(C_l)$   $\Rightarrow$  renormalization [Niu, Nori 86, Kalugin *et al.* 86]

- Atomic RG step (decimation of molecules)



- Molecular RG step (decimation of atoms)

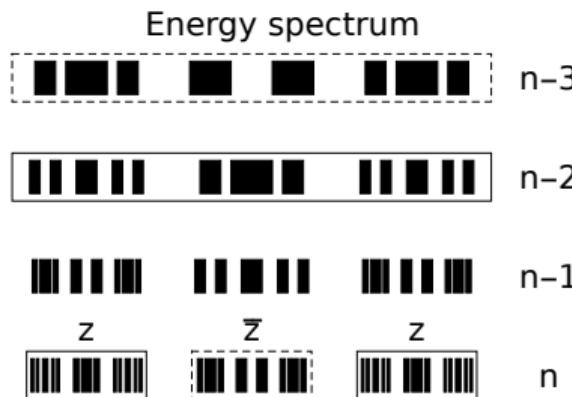


In the limit  $\rho \ll 1$ ,  $z = \rho/2$ ,  $\bar{z} = \rho^2$

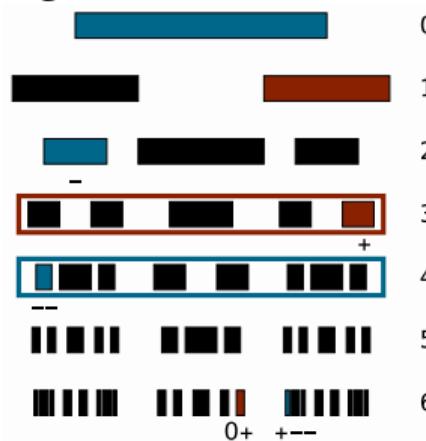
# RG CONSTRUCTION & RENORMALIZATION PATHS

$$H_l = \underbrace{(zH_{l-2} - t_s)}_{\text{bonding levels}} + \underbrace{(\bar{z}H_{l-3})}_{\text{atomic levels}} + \underbrace{(zH_{l-2} + t_s)}_{\text{antibonding levels}} + \mathcal{O}(\rho^4)$$

→ recursive construction of the spectrum [Piéchon *et al.* 95]



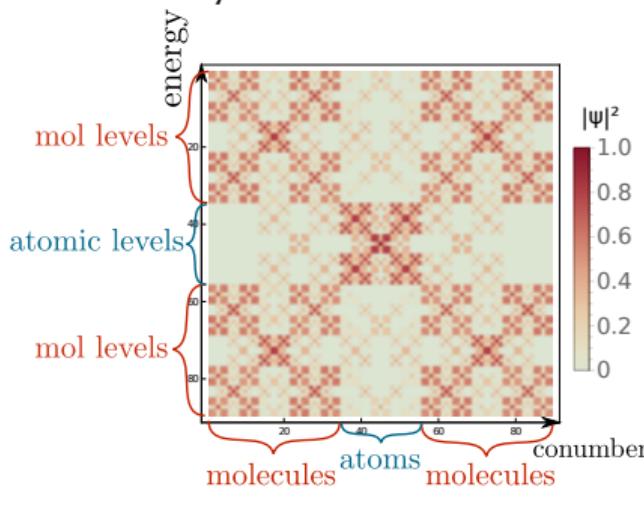
Eigenstate  $\leftrightarrow$  renormalization path :



# RG FOR THE EIGENSTATES

Reordering of the sites [Mosseri 88]

→ self-similarity :

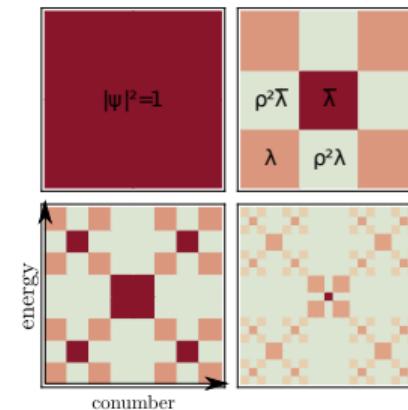


Renormalization factors :

**atomic** levels :

$$|\psi_m^{(l)}(E)|^2 = \bar{\lambda} |\psi_{m'}^{(l-3)}(E')|^2$$

RG reconstruction of the electronic density :



**molecular** levels :

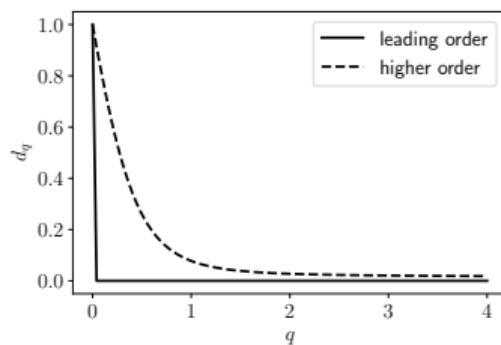
$$|\psi_m^{(l)}(E)|^2 = \lambda |\psi_{m'}^{(l-2)}(E')|^2$$

# FRACTALITY OF THE EIGENSTATES

Leading order [Thiem, Schreiber 12]

$$\bar{\lambda} = 1$$

$$\lambda = 1/2$$

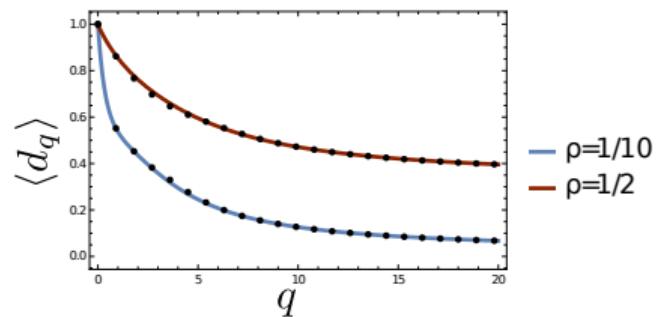


Fractal dimensions of the “broccoli state”,  $\rho = 0.1$   
→ higher order : captures multifractality

Higher order [Macé et al. 16]

$$\bar{\lambda} = \frac{1}{1+2\rho^2}$$

$$\lambda = \frac{1}{2+\rho^2}$$



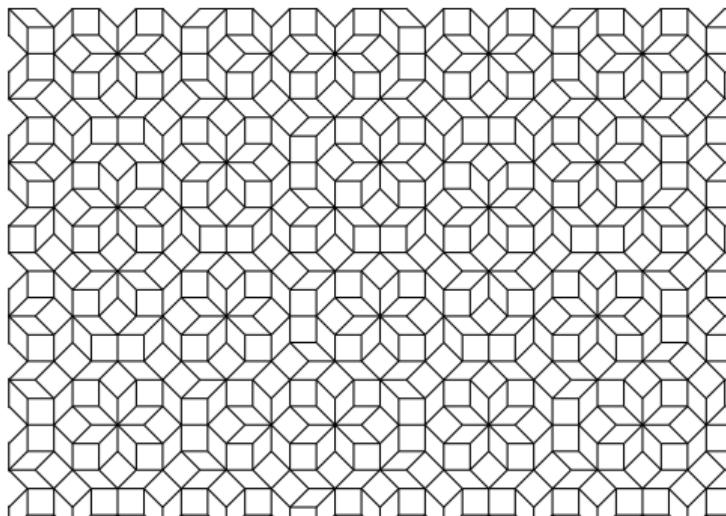
Fractal dimensions averaged over all states : numerics vs RG  
→ higher order accurate for large  $\rho$

# CONCLUSIONS

Focus on the Fibonacci tight-binding chain, in the limit  $\rho \ll 1$ .

- Substitution rule → **scale invariance** → renormalization group
- RG → eigenstates all **multifractal**
- Higher order in  $\rho$  : captures this multifractality

# GROUNDSTATE OF THE AMMANN-BEENKER TILING



A patch of the Ammann-Beenker tiling

**Fractal states described by **height** functions?**

$$\psi(m) = e^{\kappa h(m)}$$

- RG description [Sire, Bellissard 90]
- Fractal spectrum [Sire 94]
- **Exact eigenstates [Sutherland 87], [Grimm, Repetowicz 98]**
- **Exact groundstate [Kalugin, Katz 14], [Macé et al. 17]**

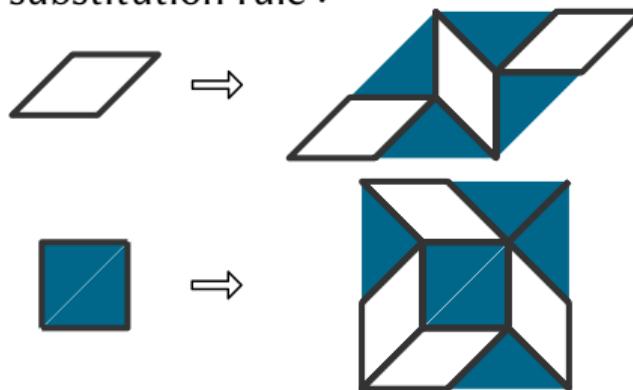
Pure hopping Hamiltonian :

$$\hat{H} = -t \sum_{\langle m,n \rangle} |m\rangle \langle n|$$

Quasiperiodicity encoded in adjacency

## LOOKING FOR ARROWS

Like 1D chains, Ammann-Beenker has a substitution rule :

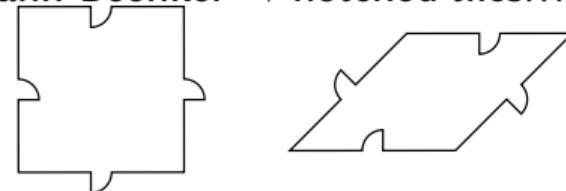


→ scale invariance.

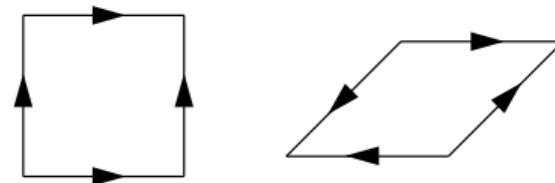
Height requires a field of arrows :

- invariant under substitution
- irrotational

Ammann-Beenker → notched tiles...



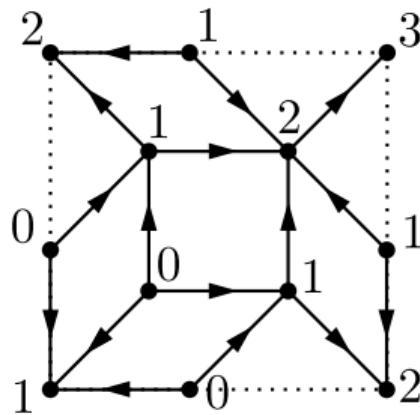
...exactly what we need!



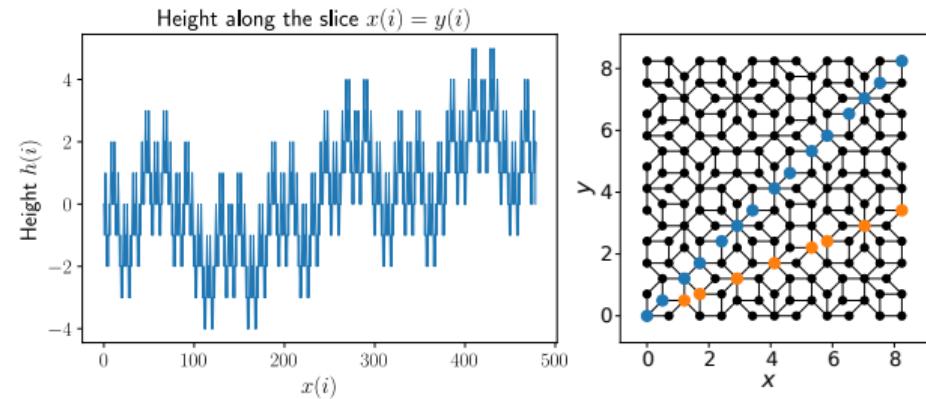
Height field :

$$h(m) = \sum_{0 \rightarrow m} \text{arrows}$$

# PROPERTIES OF THE HEIGHT FIELD



The height field on a small patch of the tiling.



Partition function :  $Z_L(\beta) \underset{L \rightarrow \infty}{\sim} L^{\omega(\beta)}$

→ slow growth :  $h_{\text{typ}}(L) \underset{L \rightarrow \infty}{\sim} \sqrt{\log L}$

→ states  $\psi(m) = e^{\kappa h(m)}$  fractal

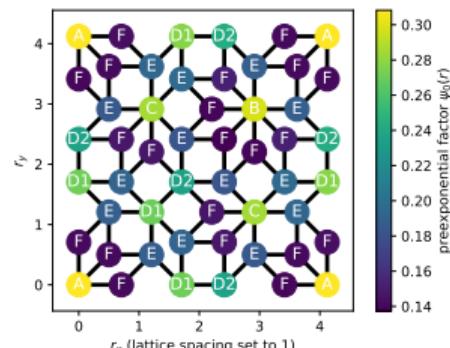
# GROUNDSTATE

$$\hat{H} = -t \sum_{\langle m,n \rangle} |m\rangle \langle n|$$

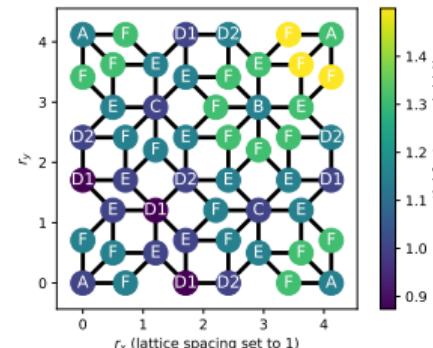
Conjecture [Kalugin, Katz 14] :

$$\psi_{\text{groundstate}}(m) = C(m) e^{\kappa h(m)}$$

$C(m)$  : local function :

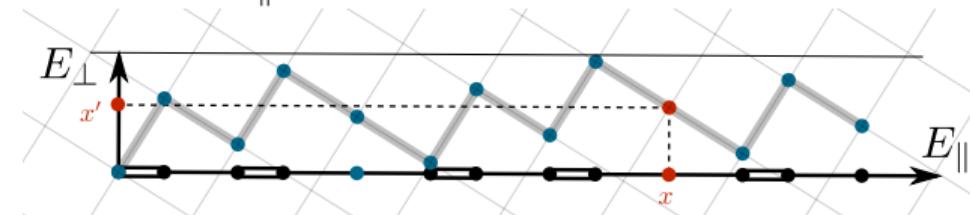


$e^{\kappa h(m)}$  : non-local function :

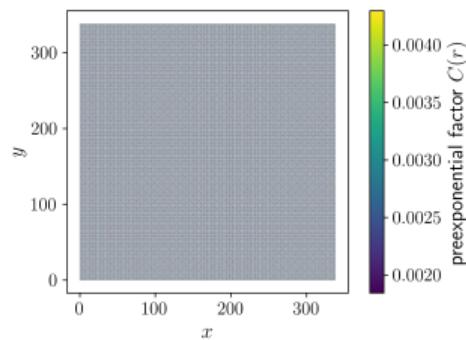


# TESTING THE CONJECTURE

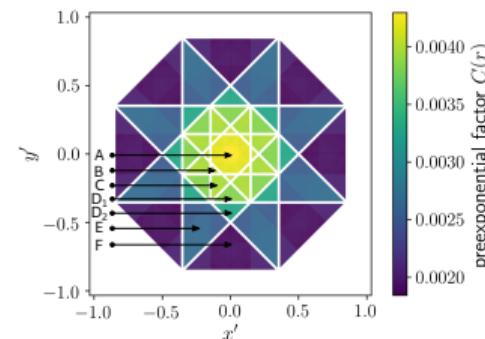
Cut-and-project  $\rightarrow$  physical ( $E_{\parallel}$ ) and internal ( $E_{\perp}$ ) space :



Internal space  $\rightarrow$  sites classified by local environment  $\rightarrow$  test the local nature of  $C$  :



$C$  part in physical space (finite system of  $\simeq 3 \times 10^5$  atoms)



The  $C$  part in internal space

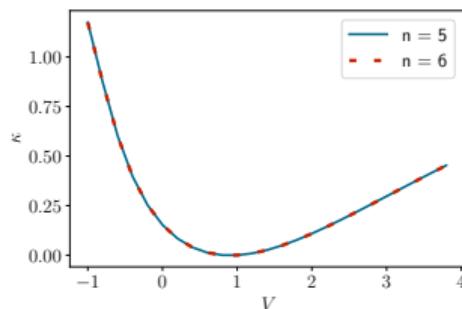
# PERTURBING THE HAMILTONIAN

Adding an on-site potential :

$$\hat{H} = -t \sum_{\langle m,n \rangle} |m\rangle \langle n| + \sum_m V_m |m\rangle \langle m|$$

Laplacian-like [Sire, Bellissard 90] :

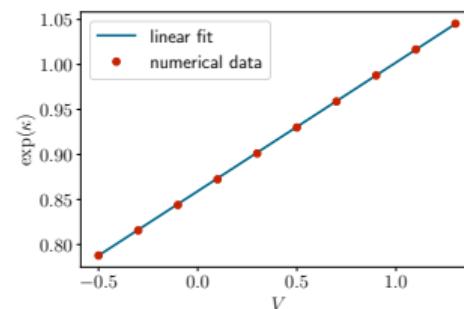
$$V_m = V z_m \\ \rightarrow \psi(m) = C(m) e^{\kappa h(m)}$$



Prefactor  $\kappa$  as a function of  $V$ .

An “arbitrary” potential :

$$V_m = V \text{ if } m \text{ has 3 neighbors, else } V_m = 0. \\ \rightarrow \psi(m) = C(m) e^{\kappa h(m)}$$



$e^\kappa$  as a function of  $V$ .

# CONCLUSIONS

Tight-binding models on a 2D quasiperiodic tiling

- Geometry (notches) → **height field**  $h(m)$  →  $\psi_{\text{groundstate}}(m) = C(m)e^{\kappa h(m)}$
  - Slow height growth ( $h(L) \sim \sqrt{\log L}$ ) → critical, **fractal** state
- Groundstate in 2D  $\leftrightarrow E = 0$  state in 1D
- Robust to symmetry-preserving on-site perturbations
  - Same conclusions for the 10-fold symmetric Penrose tiling.

# GENERAL CONCLUSION

Simple tight-binding models on 1D and 2D quasiperiodic tilings

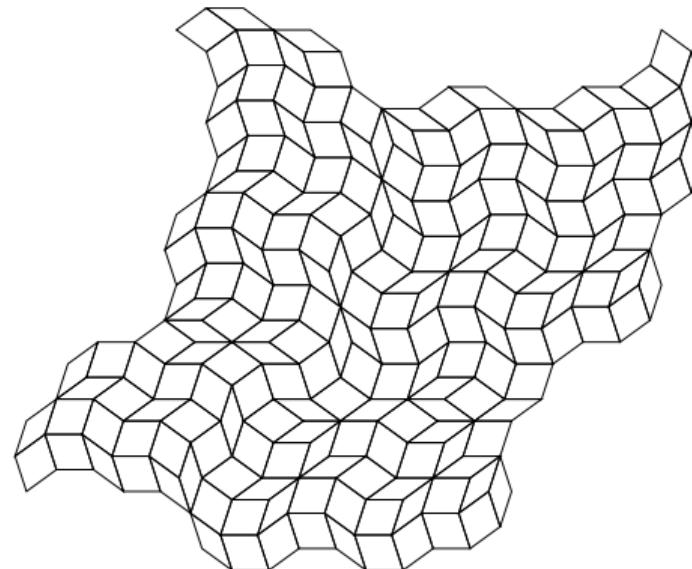
- Quasiperiodic structures : in between periodic and random, very close to periodic
- Critical, fractal eigenstates
- Consequence of quasiperiodic geometry

Perspectives

- Topology : the internal space degree of freedom can be used to probe topological properties, for the Fibonacci chain [Tanese *et al.* 14]. What about 2D quasicrystals?
- Interactions : quasiperiodicity  $\simeq$  deterministic disorder. Non-interacting eigenstates are not localized, yet many-body quasiperiodic systems seem to localize ...how?

## PERSPECTIVES : EXACT EIGENSTATES

Systematically study the exact eigenstates ( $E = 0$  state in 1D, groundstate in 2D) for different *classes* [Julien 10] of aperiodic structures.



The binary tiling : a non-Pisot 2D tiling [Godrèche, Lançon 92]

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