

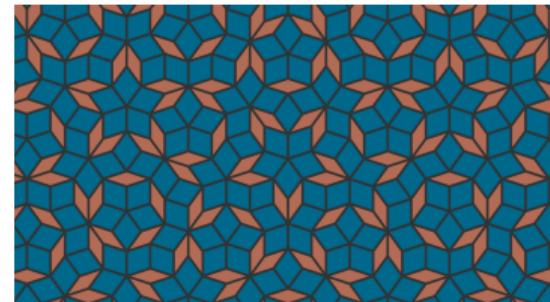
# Exact results on electronic wavefunctions of 2D quasicrystals

Nicolas Macé<sup>1</sup>, Anuradha Jagannathan<sup>1</sup>, Pavel Kalugin<sup>1</sup>, Rémy Mosseri<sup>2</sup>, Frédéric Piéchon<sup>1</sup>

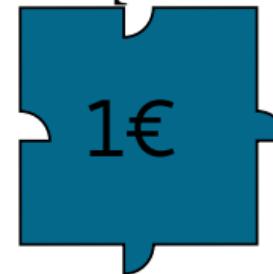
<sup>1</sup>Laboratoire de Physique des Solides, Université Paris-Saclay

<sup>2</sup>LPTMC, Université Pierre et Marie Curie

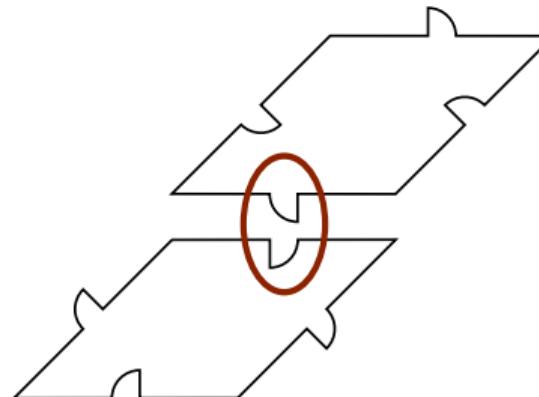
June 20, 2017



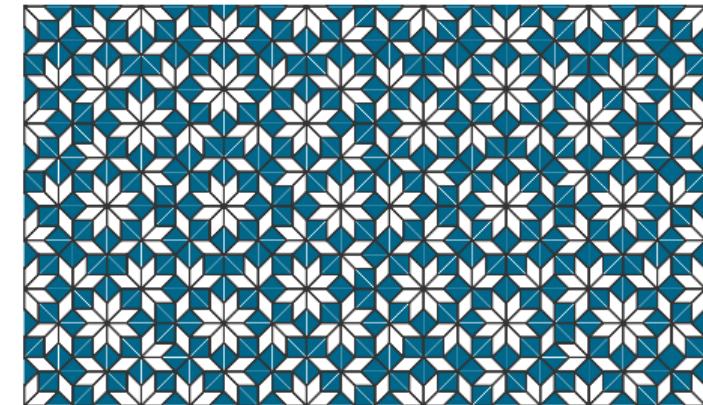
A QUASIPERIODIC PUZZLE [BÉDARIDE ET AL. 12]



Pay the squares, get the rhombuses for free!

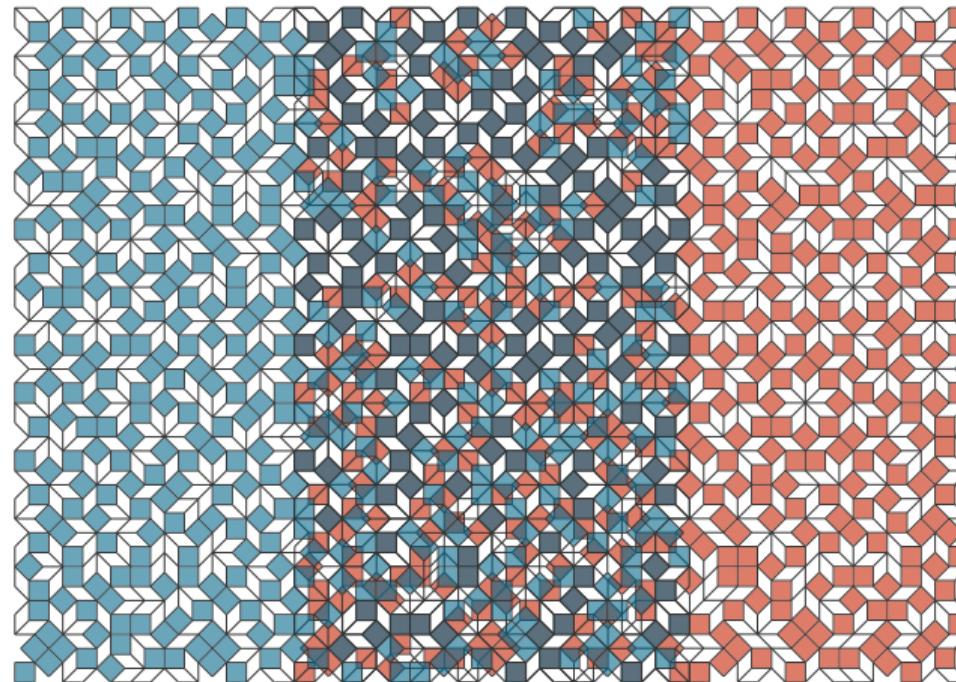


## Forbidden configuration



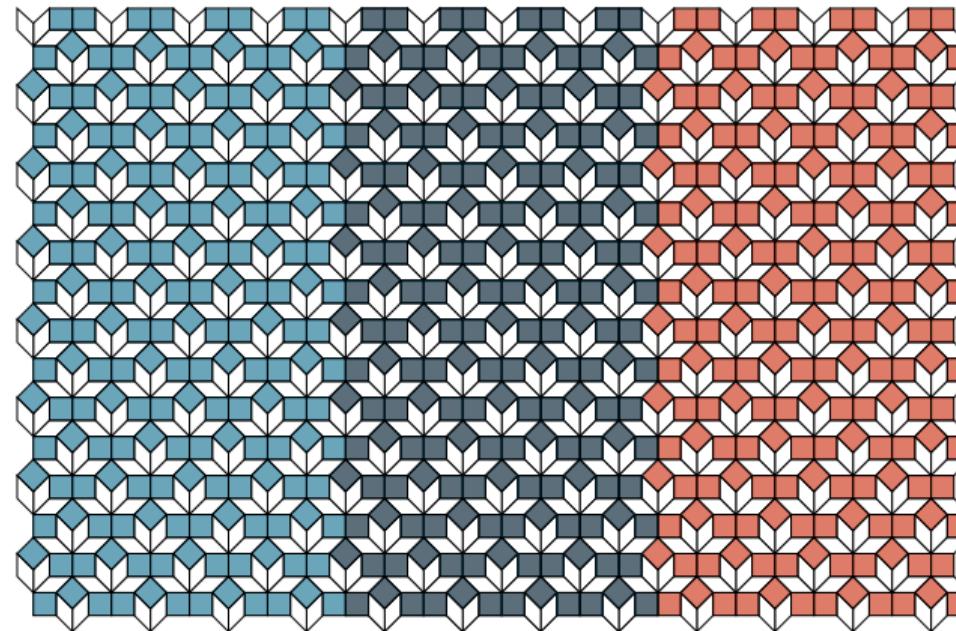
## Patch of the Ammann-Beenker tiling.

PERIODIC, QUASIPERIODIC AND RANDOM



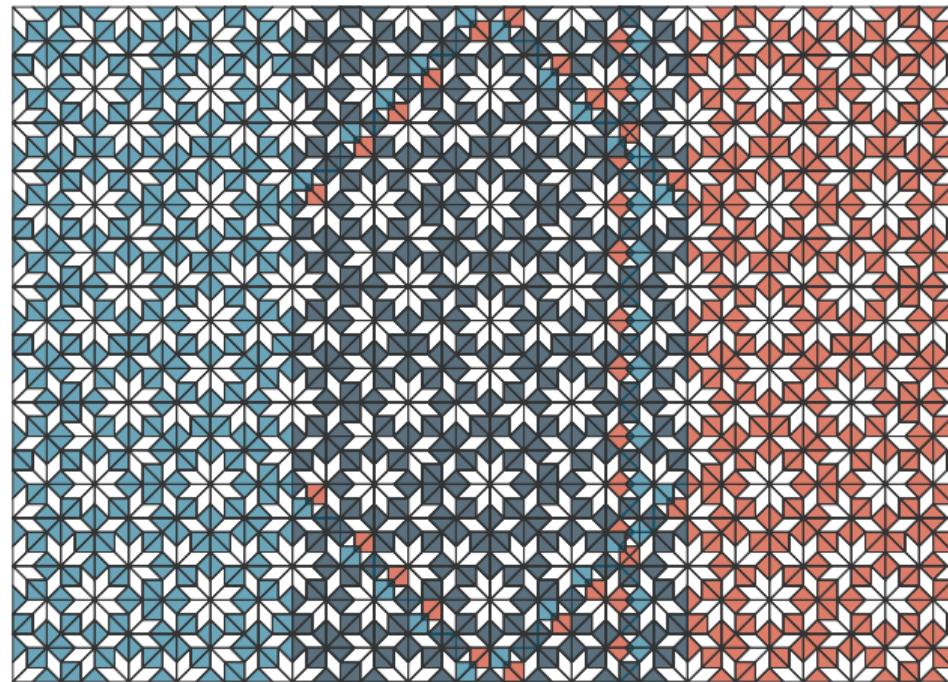
No long range order : random

PERIODIC, QUASIPERIODIC AND RANDOM



Perfect long range order : periodic

PERIODIC, QUASIPERIODIC AND RANDOM



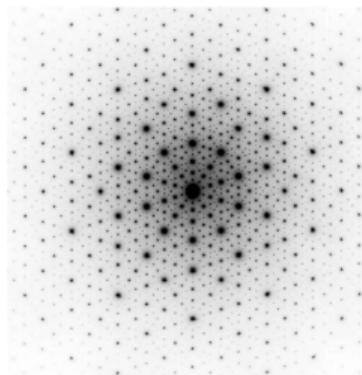
## Long range order : quasiperiodic

(Math : **Meyer sets**, see Chap. 2 of [Grimm, Baake 13])

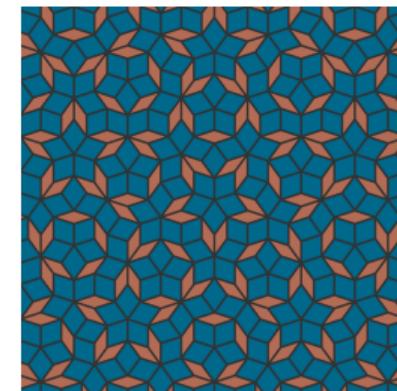
QUASICRYSTALS

Quasicrystal → quasiperiodically arranged atoms :

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

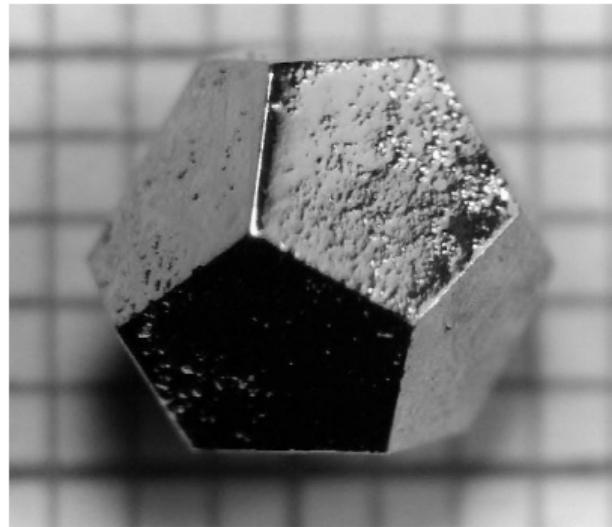


## Diffraction pattern of a AlPdMn alloy (Conradin Beeli group)



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

## EXAMPLES OF QUASICRYSTALS



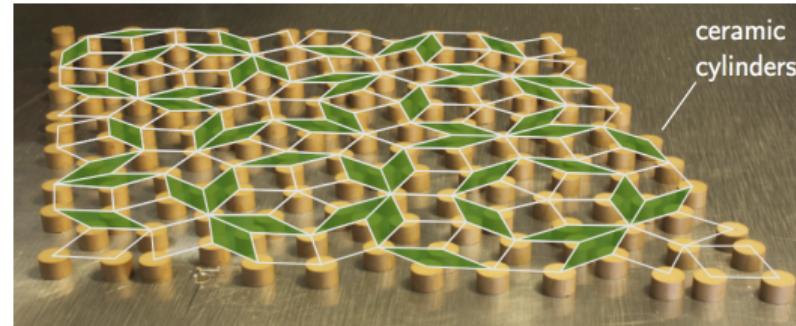
## HoMgZn alloy in its icosahedral phase (doi: 10.1038/nmat1244)



A 2D molecular quasicrystal  
(doi:10.1038/nature12993)

- many intermetallic alloys are quasiperiodic
  - a single natural example : Khatyrka meteorite hosts quasicrystals ([doi:10.1126/science.1170827](https://doi.org/10.1126/science.1170827)).

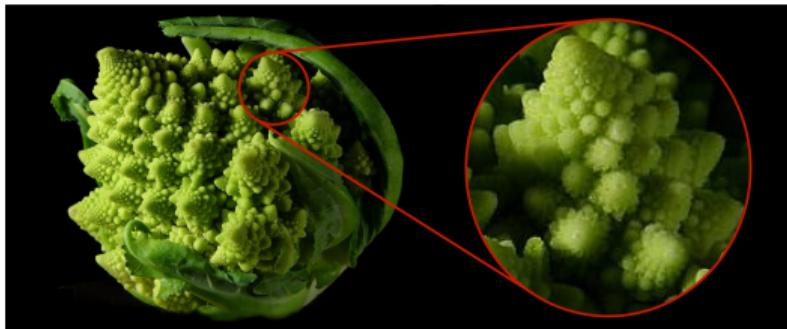
## ENGINEERED QUASIPERIODIC STRUCTURES



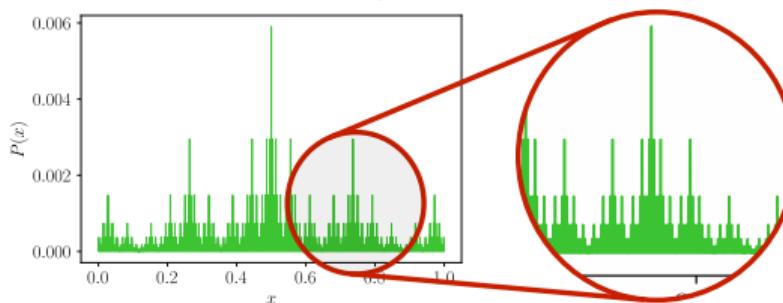
A network of dielectric resonators [Vignolo *et al.* 14]

- 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



Romanesco broccoli (© Wikimedia commons)



Electronic density along a quasiperiodic chain

- Broccoli & electronic density on a qp chain → discrete scale invariant objects.
- Discrete scale invariance → **fractal structure**.
- Fractals uncommon in general, but everywhere in the physics of quasicrystals!

Main matter

Link fractals and quasiperiodic geometry

# THE FIBONACCI CHAIN

## Fibonacci numbers

A simple rule for generating numbers :

$$F_0 = 1$$

$$F_1 = 1$$

$$F_2 = F_1 + F_0 = 2$$

$$F_3 = F_2 + F_1 = 3$$

$$F_4 = F_3 + F_2 = 5$$

$$F_5 = F_4 + F_3 = 8$$

⋮

$$F_{l+2} = F_{l+1} + F_l$$

## Fibonacci words

Letters instead of numbers, same rule :

$$C_0 = B$$

$$C_1 = A$$

$$C_2 = C_1 C_0 = AB$$

$$C_3 = C_2 C_1 = ABA$$

$$C_4 = C_3 C_2 = ABAAB$$

$$C_5 = C_4 C_3 = ABAABABA$$

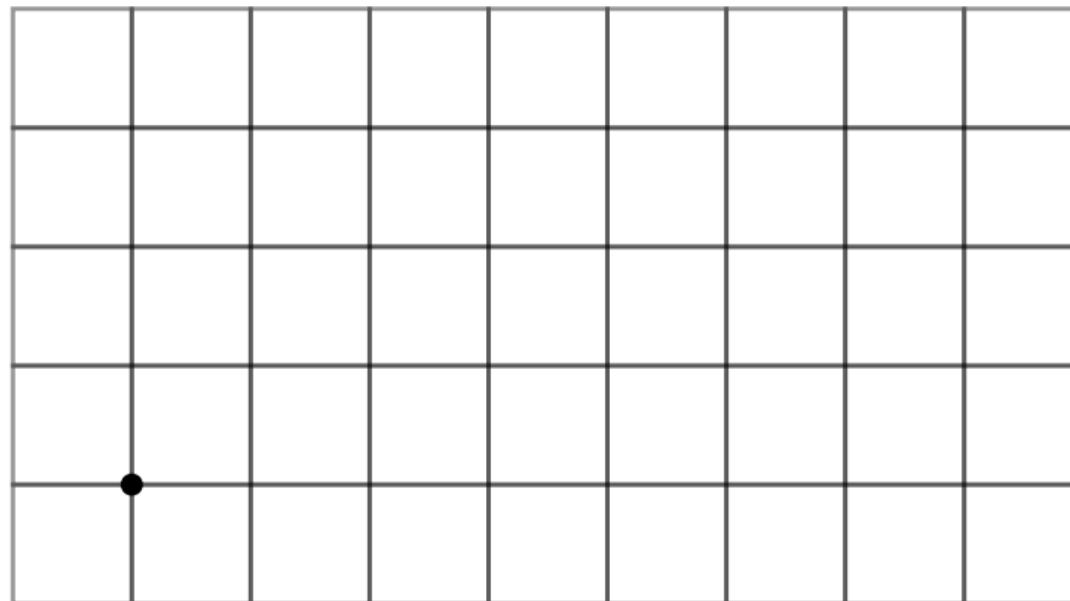
⋮

$$C_{l+2} = C_{l+1} C_l$$

## FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

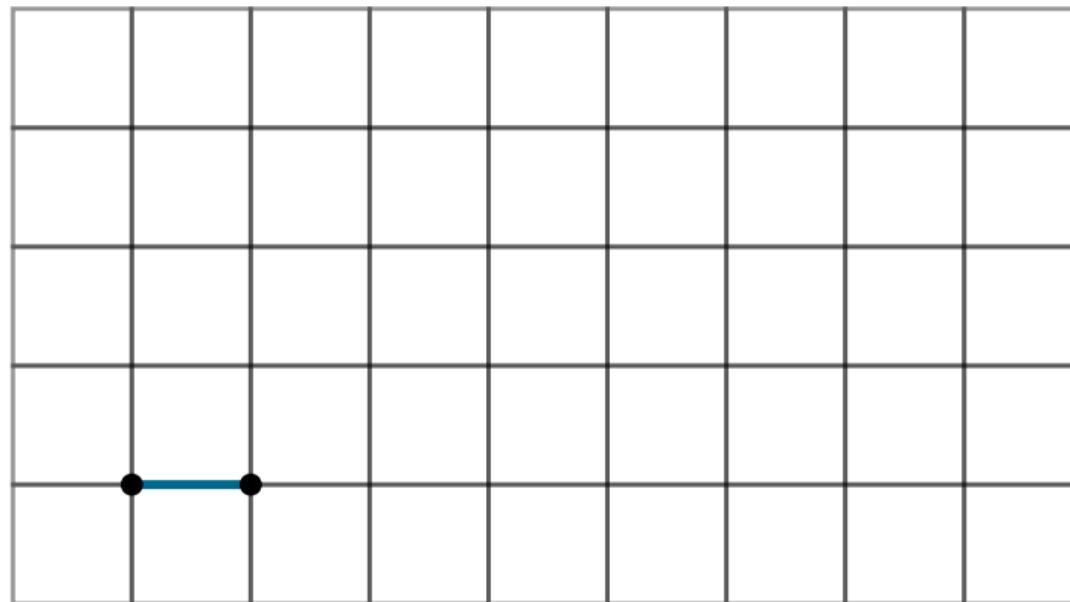
**A** ↔ horizontal step, **B** ↔ vertical step



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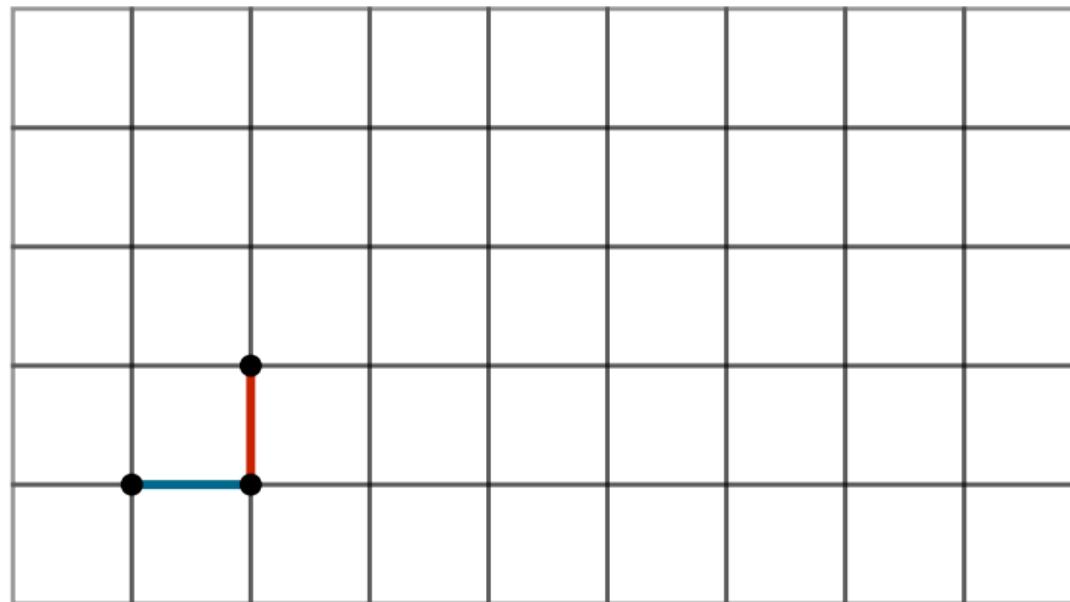
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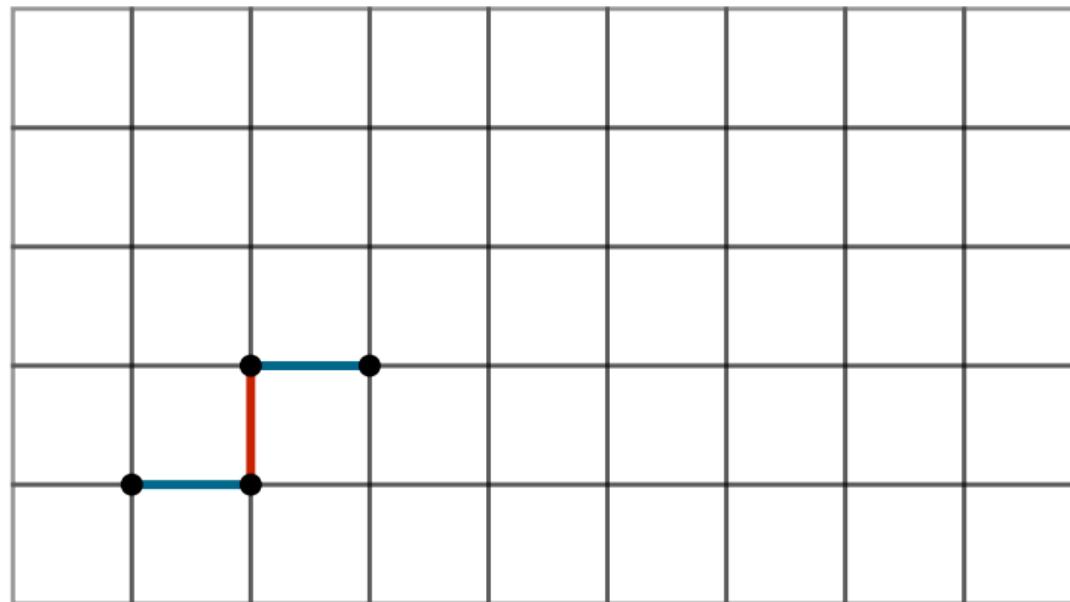
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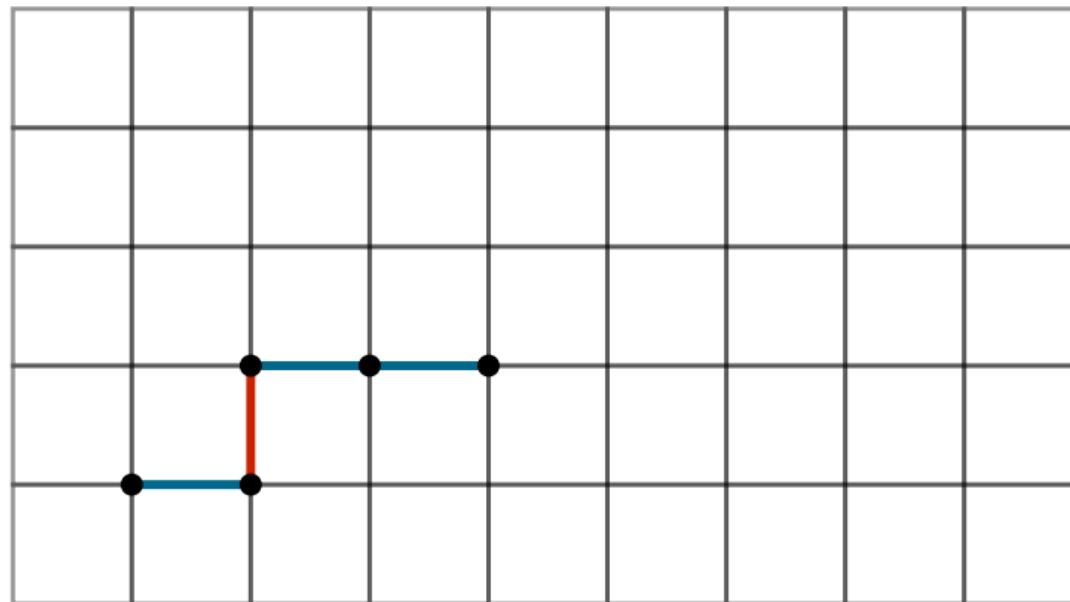
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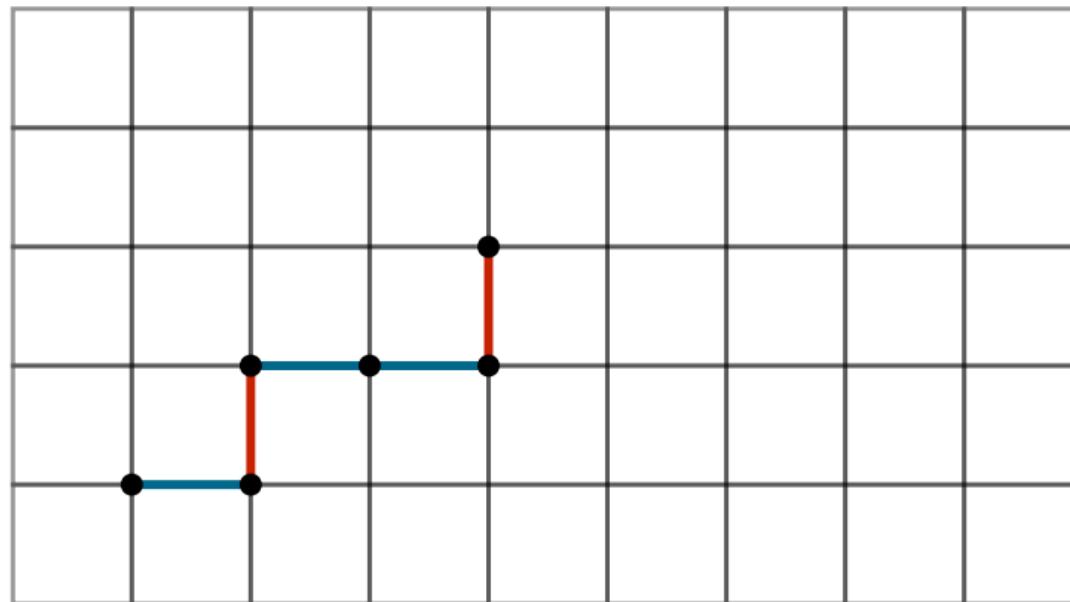
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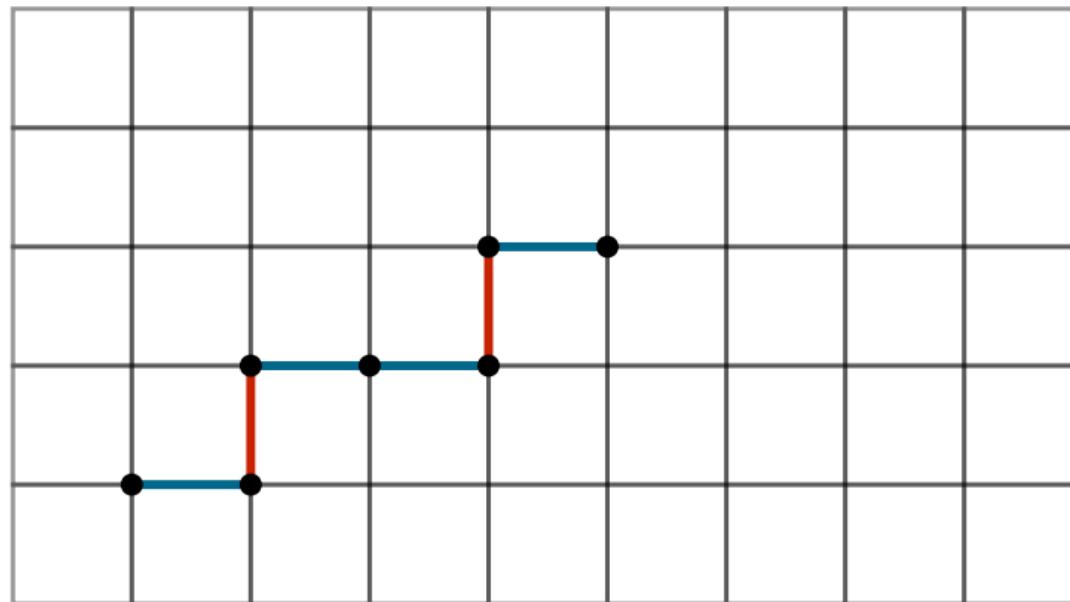
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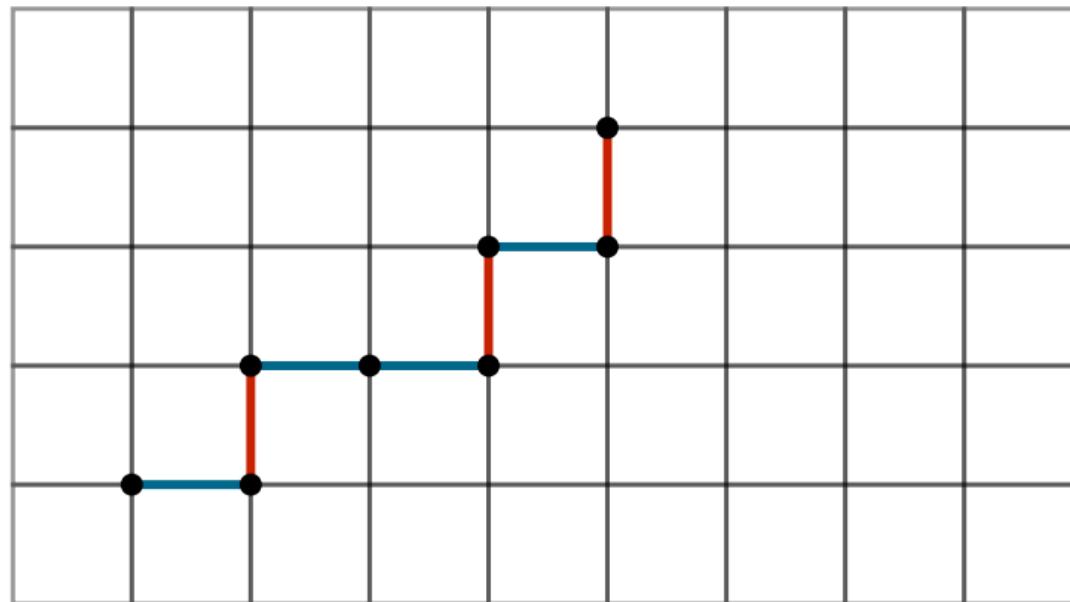
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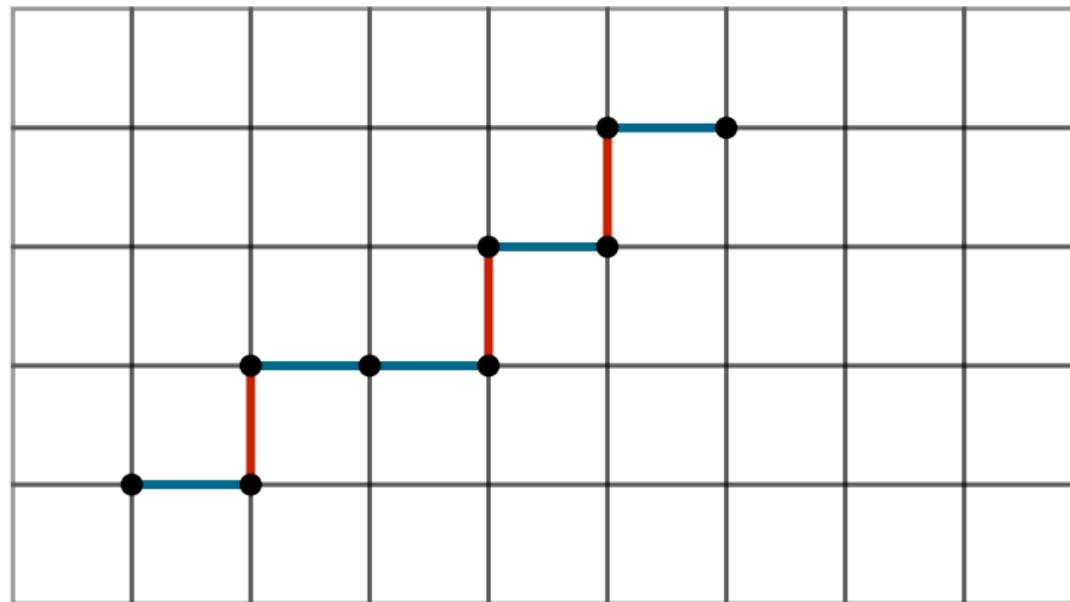
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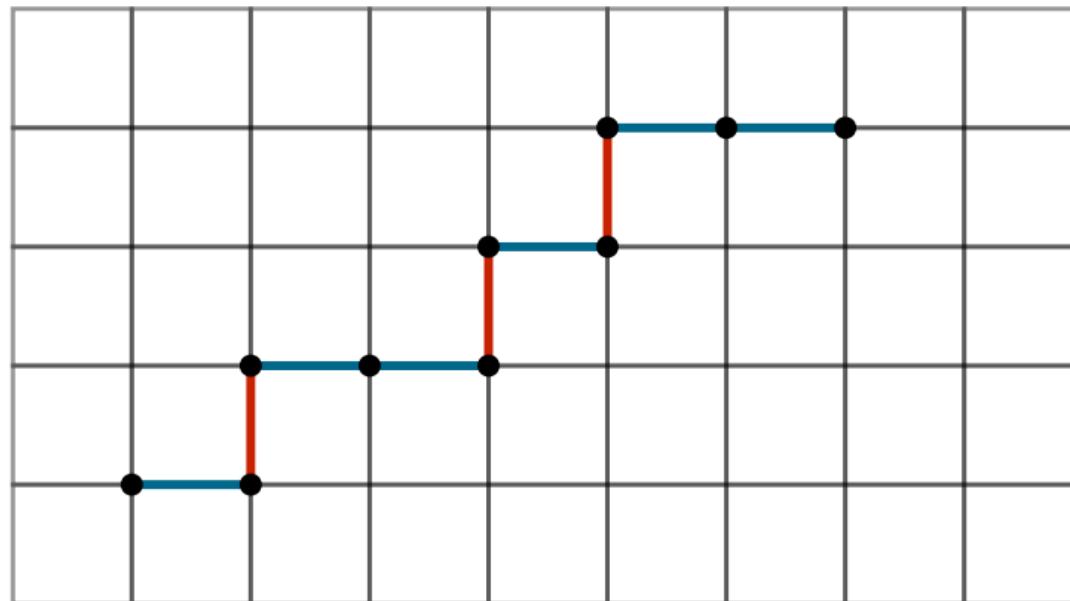
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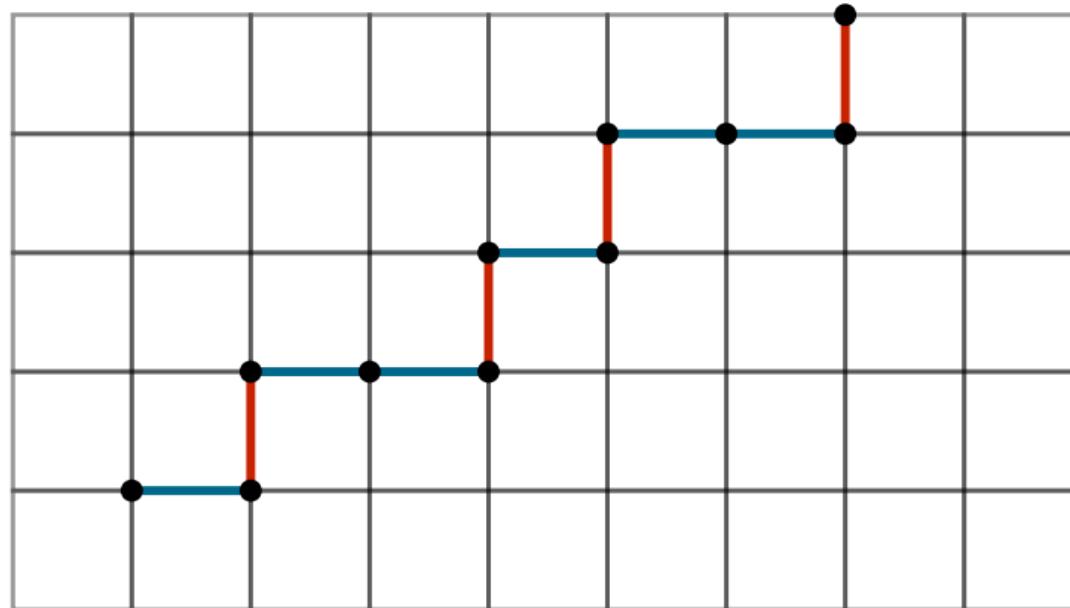
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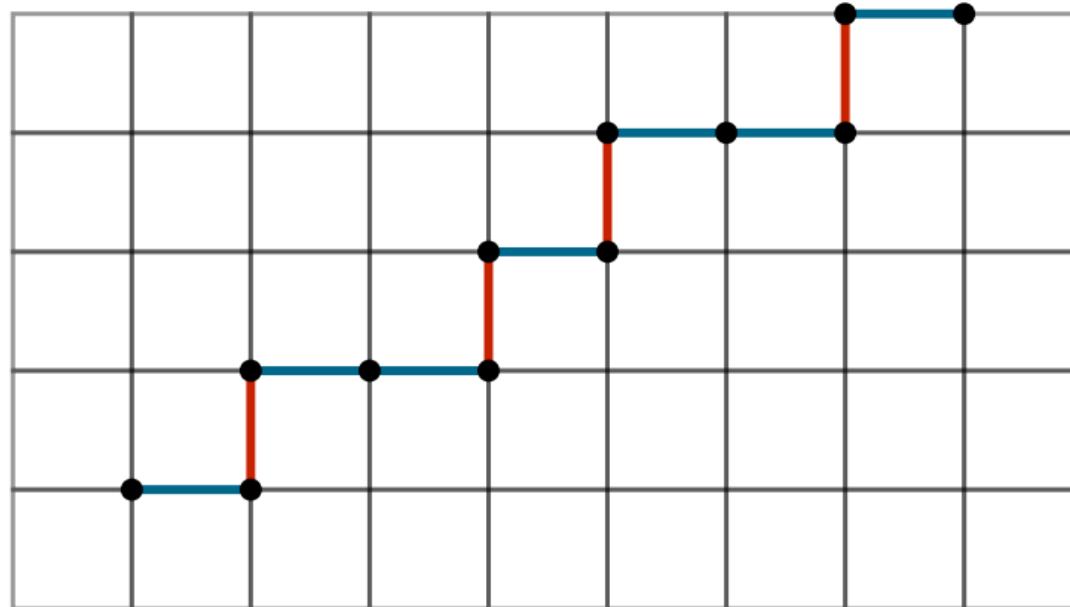
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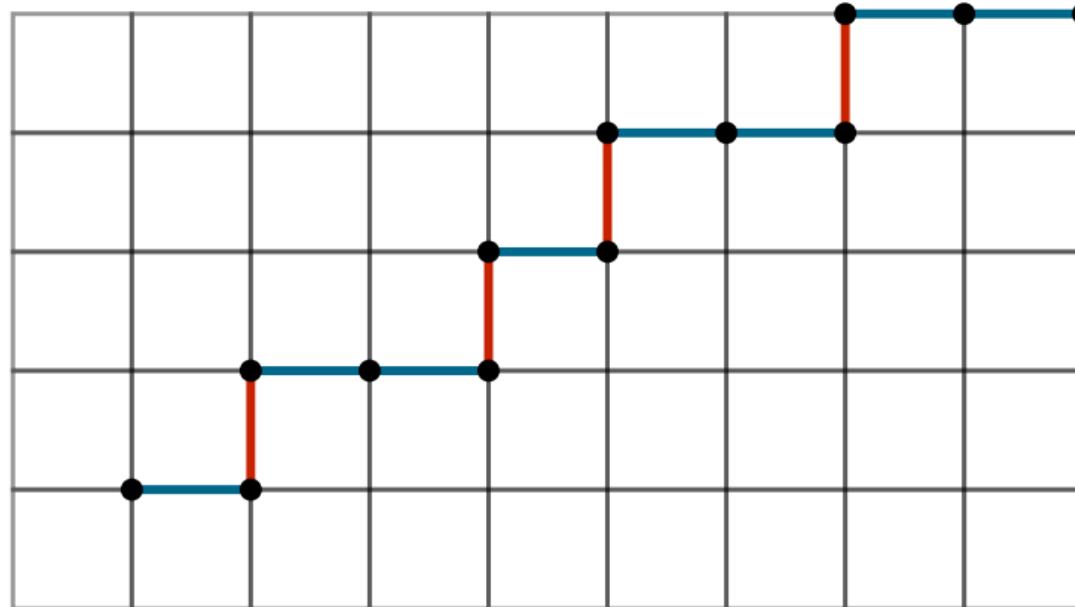
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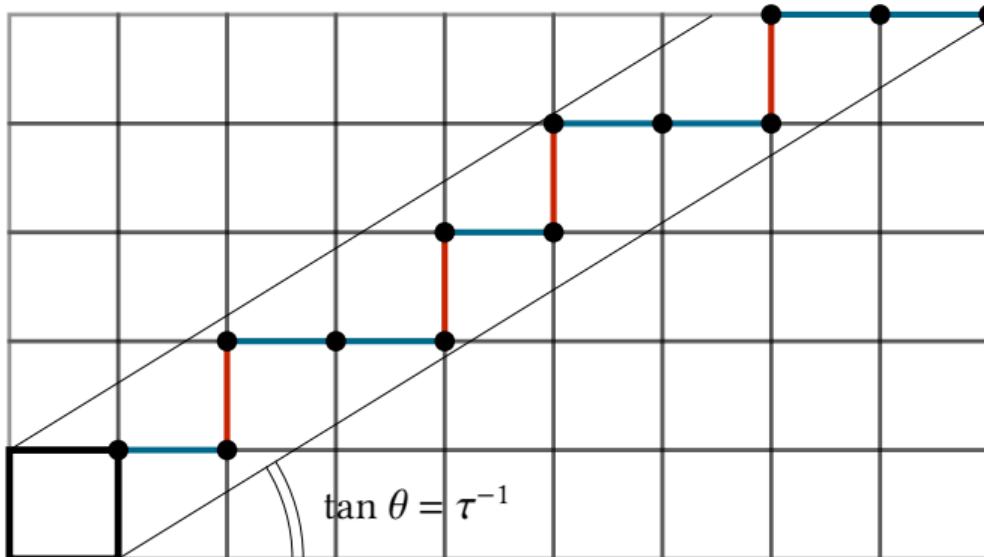
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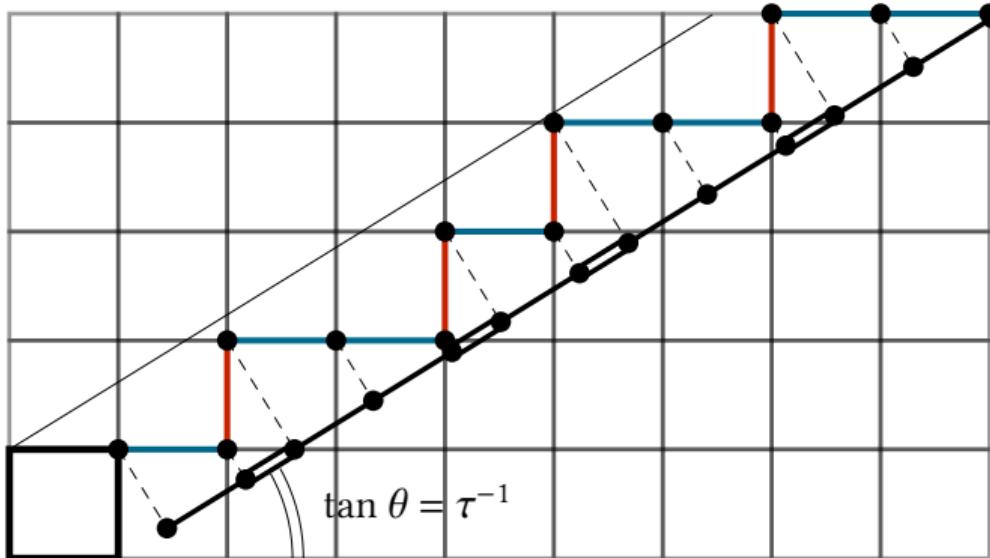


# QUASIPERIODICITY OF THE FIBONACCI WORD



- average slope = inverse of the golden ratio ( $\tau \simeq 1.6$ )
- bounded fluctuations
  - similar environments everywhere
  - quasiperiodicity [Duneau, Katz 85]

# CUT-AND-PROJECT



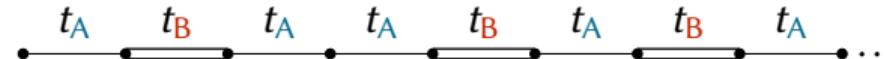
C&P → quasiperiodic (or periodic) tiling!

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 :



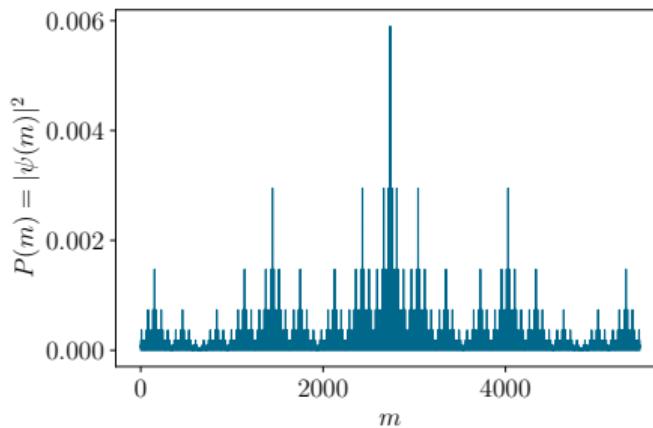
Hamiltonian :

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

Schrödinger equation for the eigenstate of energy  $E$  :

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

# THE BROCCOLI $E = 0$ STATE

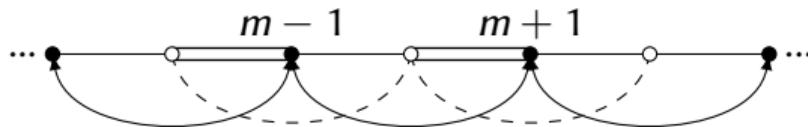


“Romanesco broccoli” fractal state at energy  $E = 0$

- 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

# STRUCTURE OF THE BROCCOLI

- Effective chain



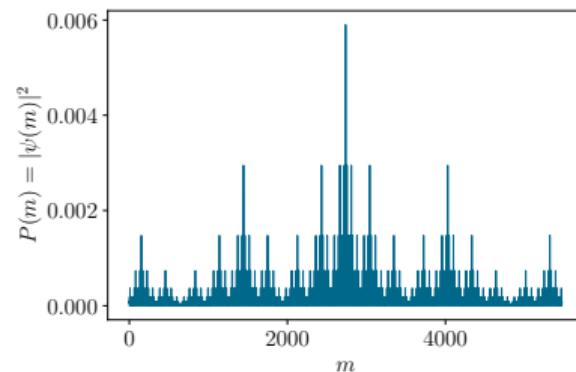
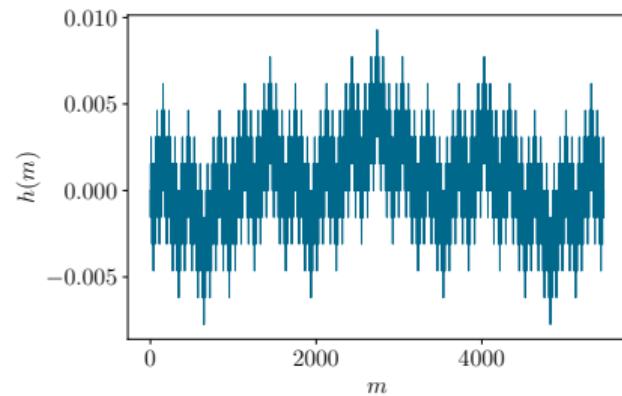
- **Arrow function** :  $A(R) = +1$ ,  $A(L) = -1$ ,

$$A(U) = 0.$$

- **Height function** :  $h(m) = \sum_{n \leq m} A_n$

- Let  $\rho = t_B/t_A$ .

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

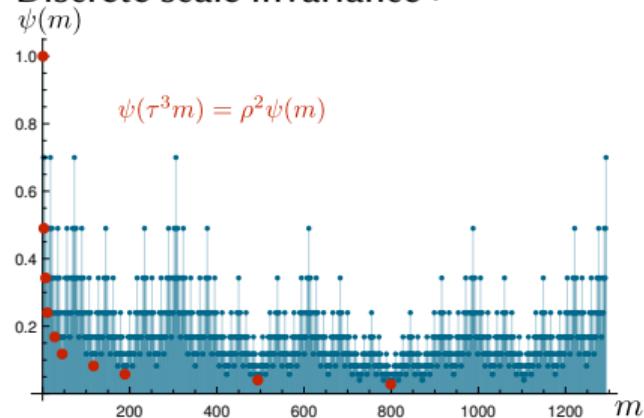


# GEOMETRY AND EIGENSTATE PROPERTIES

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

## Quasiperiodic chain

- Discrete scale invariance :



- Local power-law behavior  $|\psi(m)| \sim m^{-\alpha}$
- **critical state** [Kohmoto *et al.* 87]

## UNDERLYING SCALE INVARIANCE

Fibonacci chain *itself* scale invariant?

- ### ■ Fibonacci words by concatenation

$$C_2 = AB$$

$$C_3 = \text{ABA}$$

$$C_4 = C_3 C_2 = \text{ABAAB}$$

- ### ■ Fibonacci words by **substitution**

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

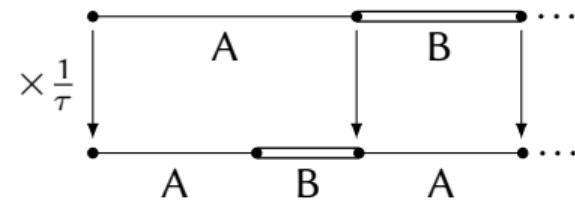
$$C_3 = \text{ABA}$$

$$C_4 = S(C_3) = S(A)S(B)S(A)$$

- Infinite chain = fixed point of the substitution :

$$S(ABAAB\dots) = ABAAB\dots$$

- ### ■ Geometric substitution :



- **Infinite chain scale invariant,**  
scaling factor  $1/\tau$ .

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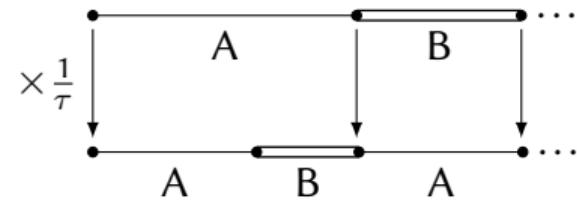
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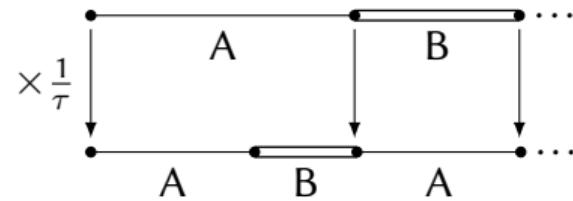
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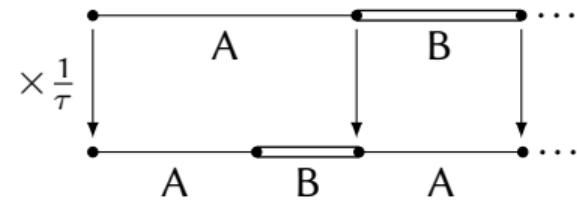
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- **Infinite chain scale invariant**, scaling factor  $1/\tau$ .

# HEIGHT DISTRIBUTION & MULTIFRACTALITY

# BEYOND QUASIPERIODICITY

# CONCLUSIONS