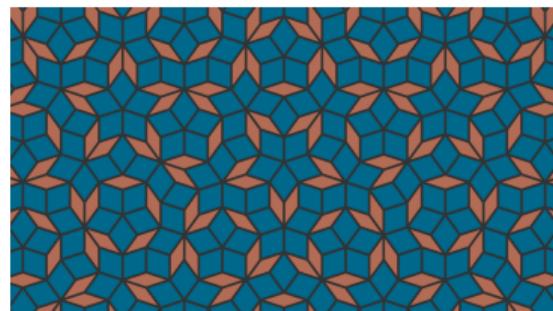


Electronic properties of quasicrystals

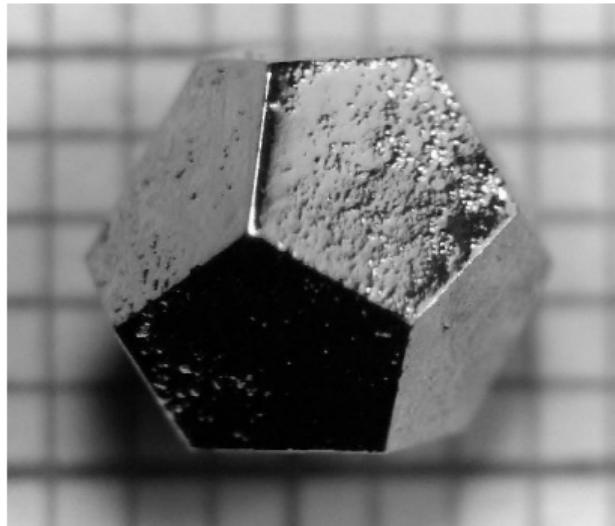
Single electron properties of tight-binding quasiperiodic models

Nicolas Macé

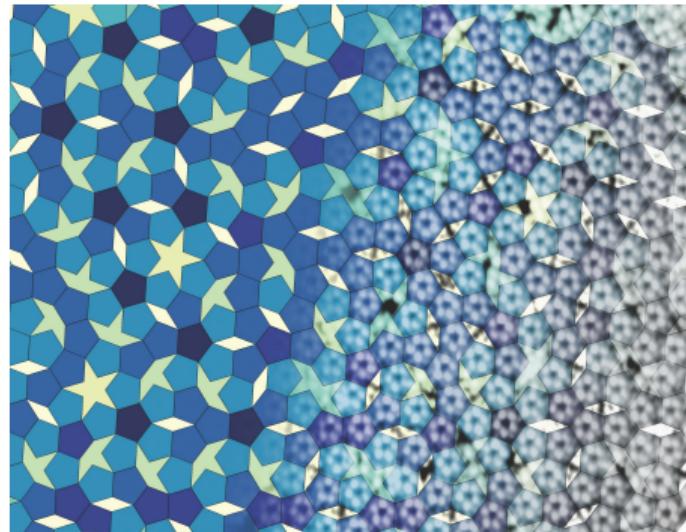
September 28, 2017



QUASICRYSTALS



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



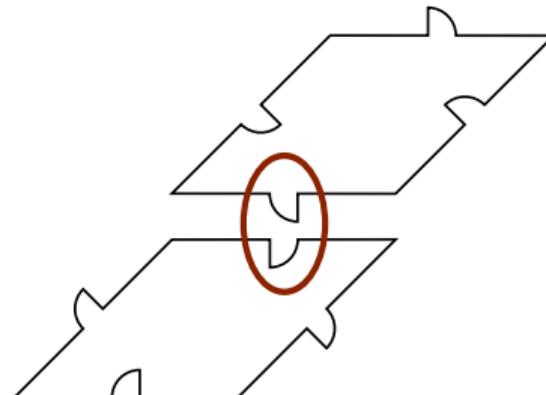
A 2D molecular quasicrystal
(doi:10.1038/nature12993)

- Fractal dimensions of wave functions and local spectral measures on the Fibonacci chain
Macé, Jagannathan, Piéchon, PRB 93 (20), 2016
 - Critical eigenstates and their properties in one-and two-dimensional quasicrystals
Macé, Jagannathan, Kalugin, Mosseri, Piéchon, PRB 96 (4), 2017

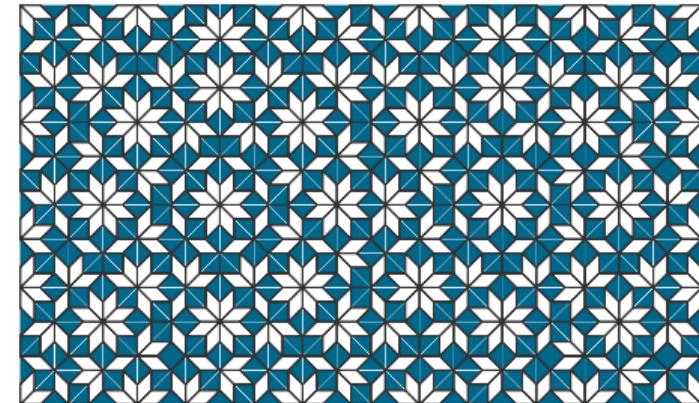
A QUASIPERIODIC PUZZLE [BÉDARIDE *ET AL.* 12]



Pay the squares, get the rhombuses for free!



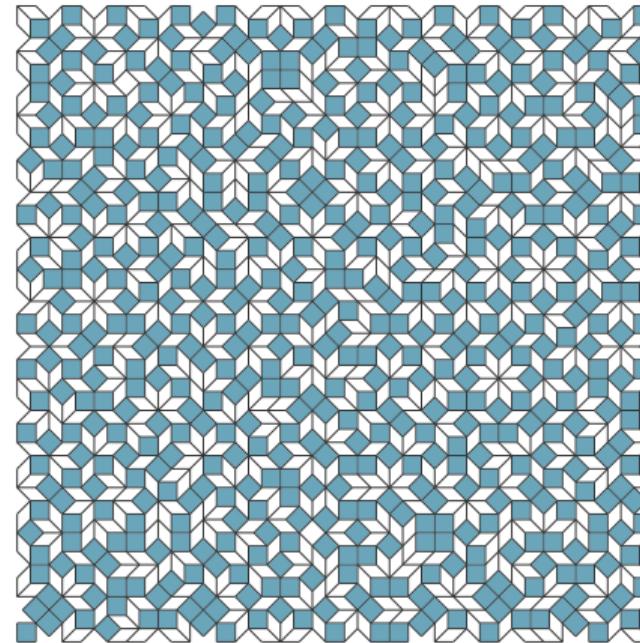
Forbidden configuration.



Patch of the Ammann-Beenker tiling.

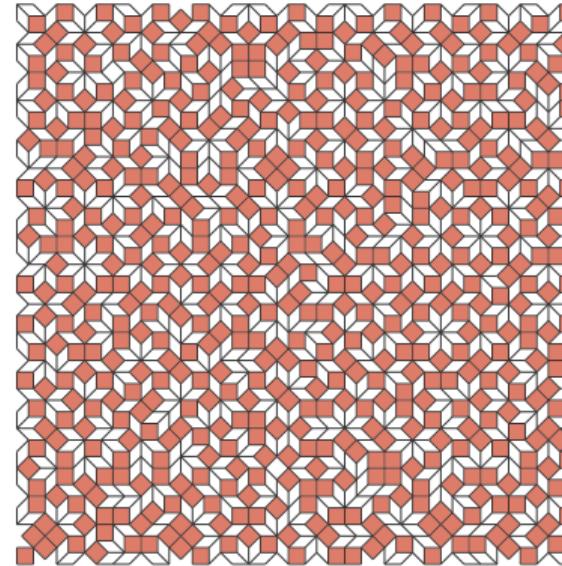
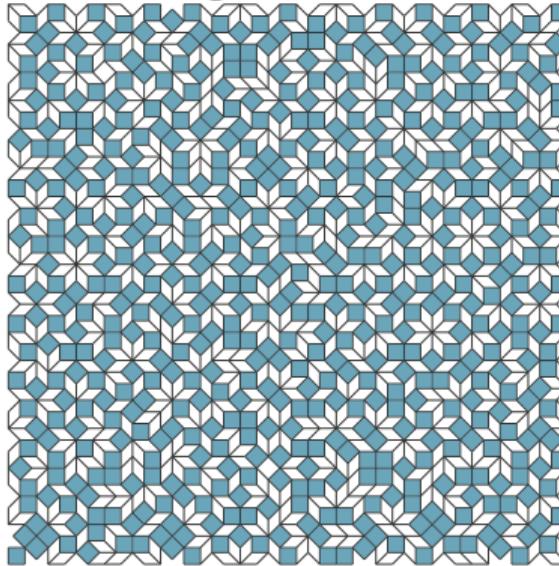
PERIODIC, QUASIPERIODIC AND RANDOM

A random tiling :

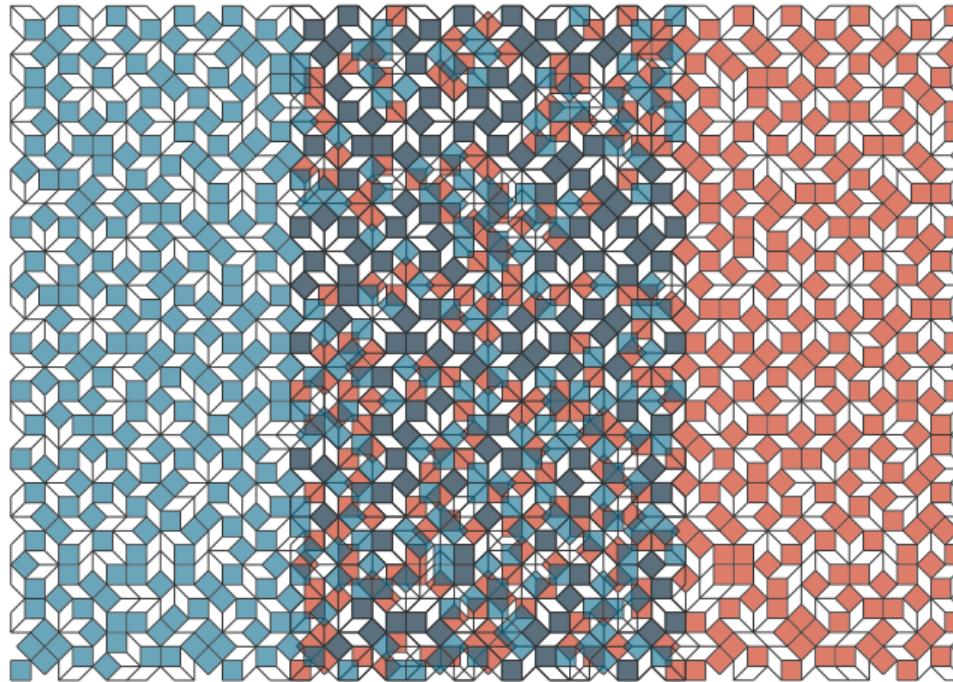


PERIODIC, QUASIPERIODIC AND RANDOM

Two copies of the tiling :

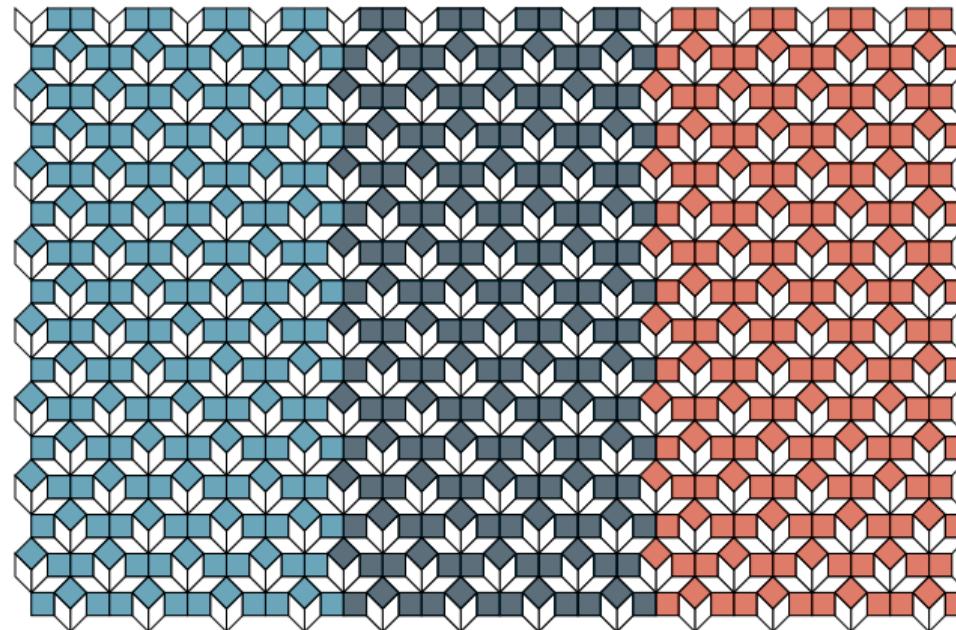


PERIODIC, QUASIPERIODIC AND RANDOM



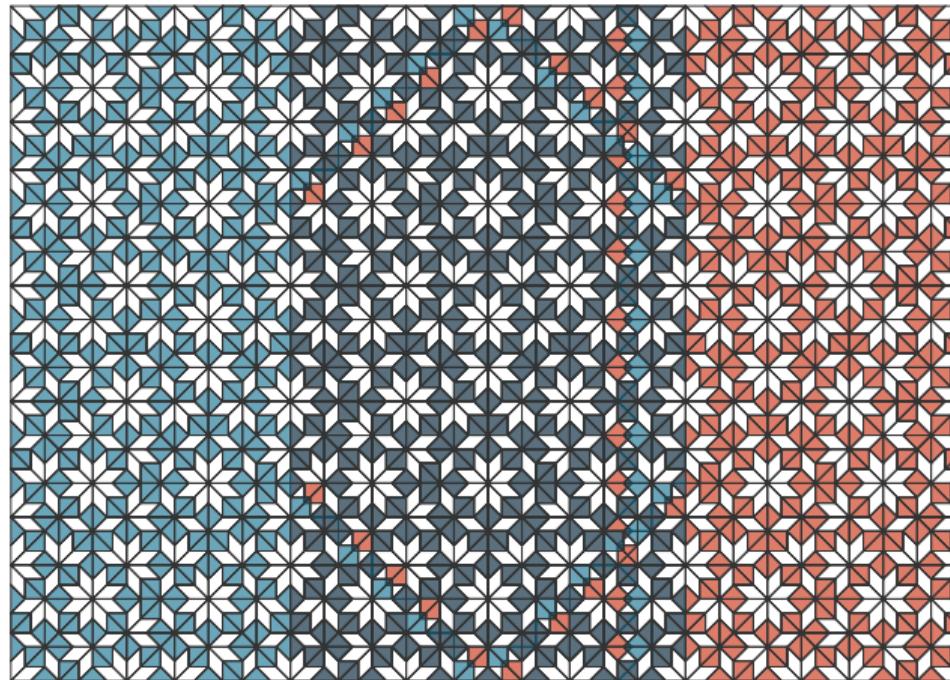
→ no overlap → no order

PERIODIC, QUASIPERIODIC AND RANDOM



Perfect long range order : periodic

PERIODIC, QUASIPERIODIC AND RANDOM



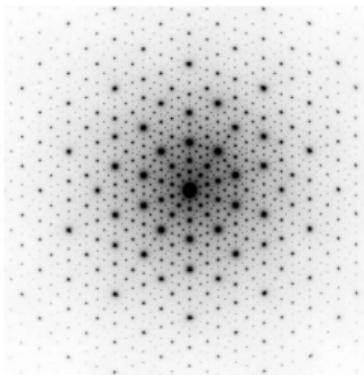
Long range order : quasiperiodic

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

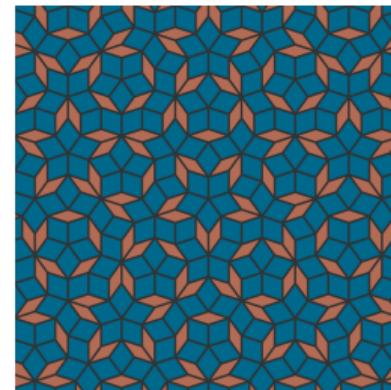
QUASICRYSTALS

Quasicrystal → quasiperiodically arranged atoms :

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

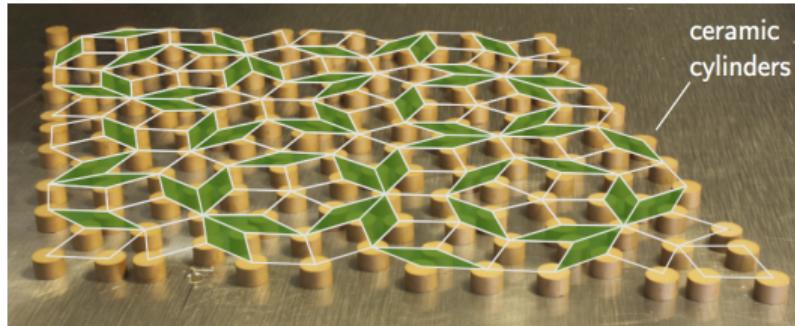


Diffraction pattern of a AlPdMn alloy
(Conradin Beeli group)



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

ENGINEERED QUASIPERIODIC STRUCTURES

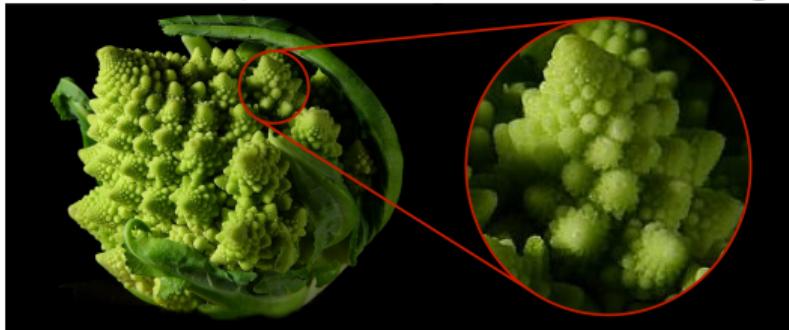


A network of dielectric resonators [Vignolo *et al.* 14]

- 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

Fractal : object invariant under rescaling



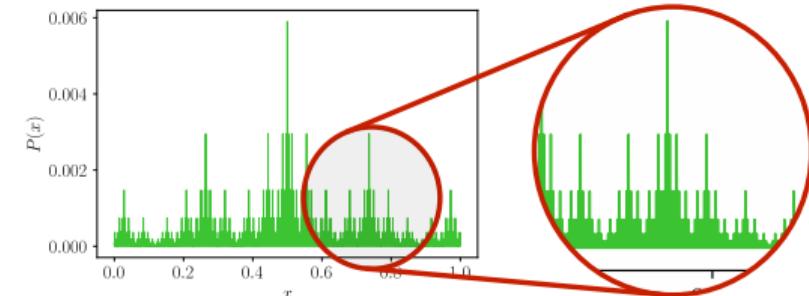
Romanesco broccoli (© Wikimedia commons)

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

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

Concatenate two words to get the next :

$$C_0 = B$$

$$C_1 = A$$

$$C_2 = C_1 C_0 = AB$$

$$C_3 = C_2 C_1 = ABA$$

$$C_4 = C_3 C_2 = ABAAB$$

⋮

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

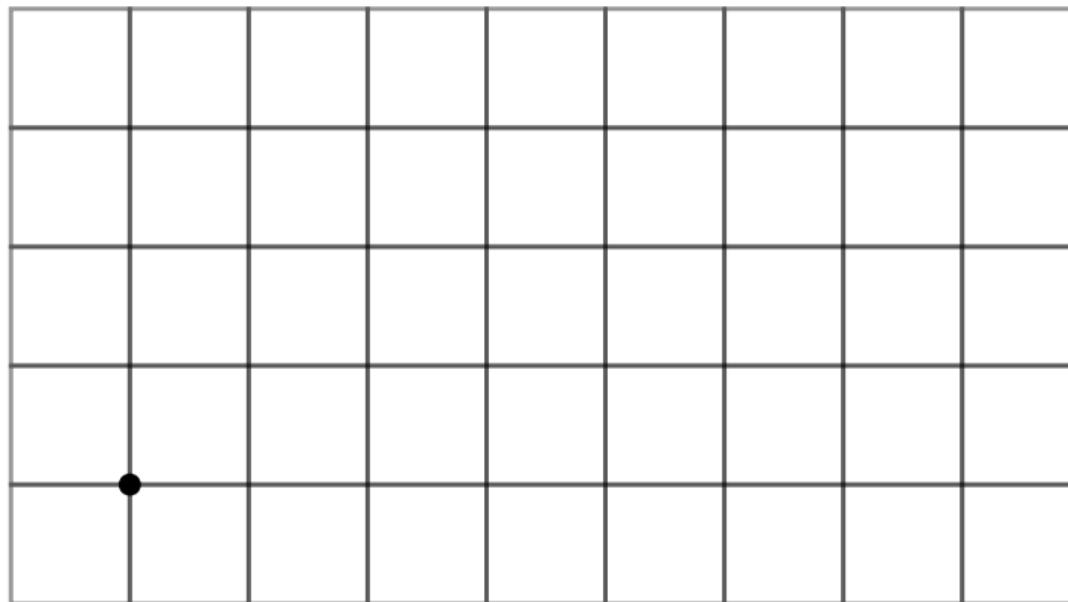
Properties of Fibonacci words

- 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 $\tau \simeq 1.61$ is the golden ratio.
- τ irrational \rightarrow infinite word **aperiodic**

FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

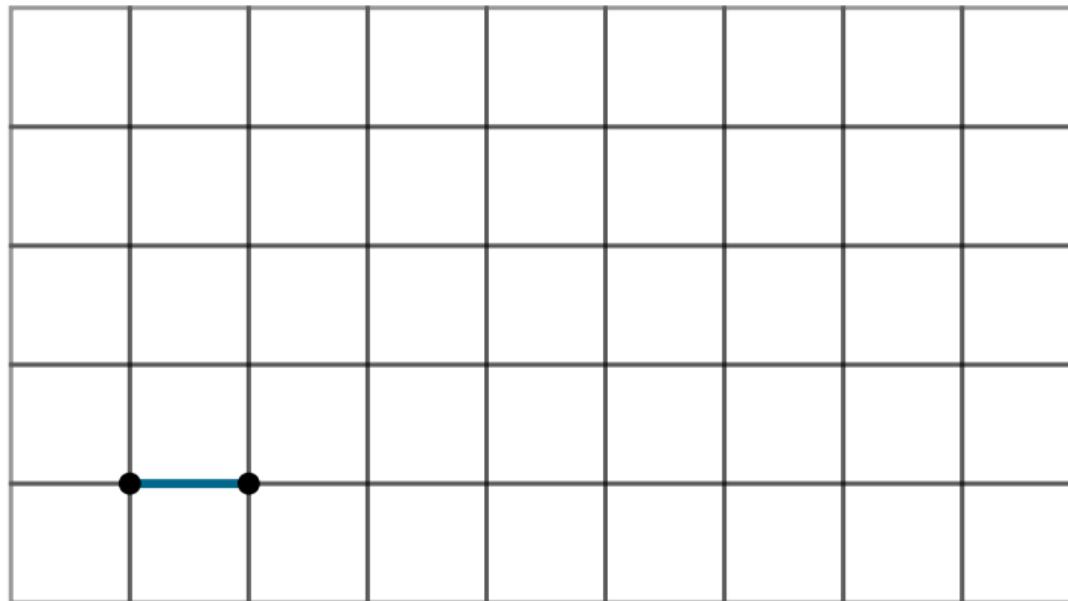
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

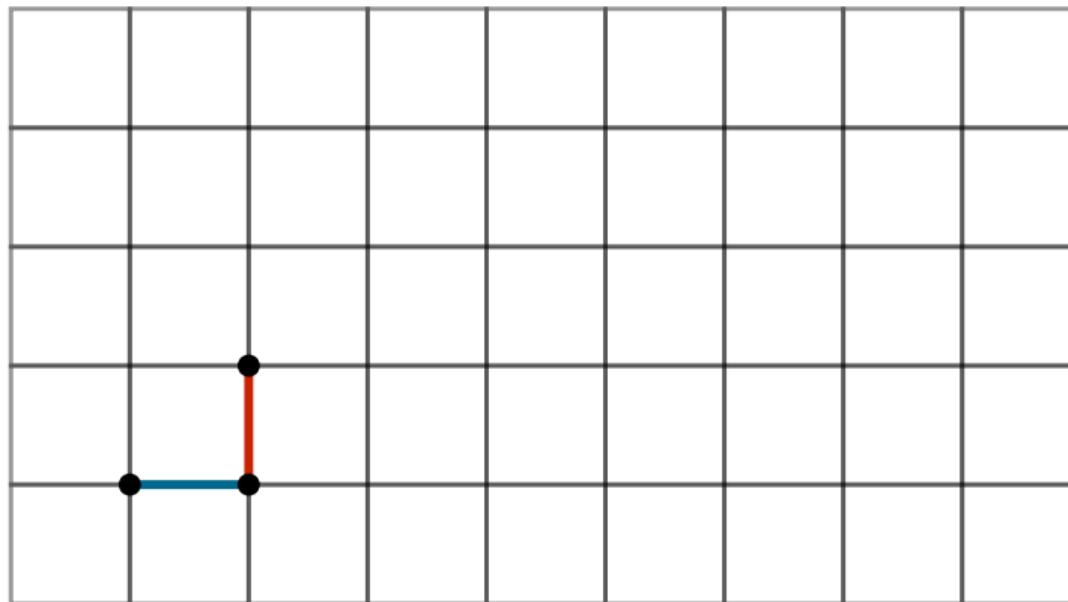
A \leftrightarrow horizontal step, **B** \leftrightarrow vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

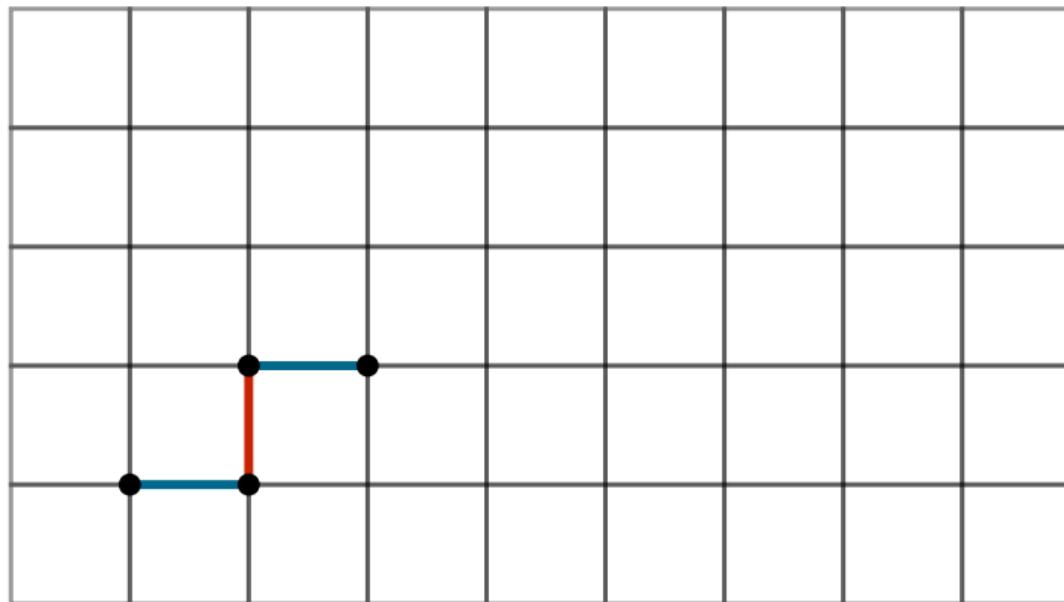
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

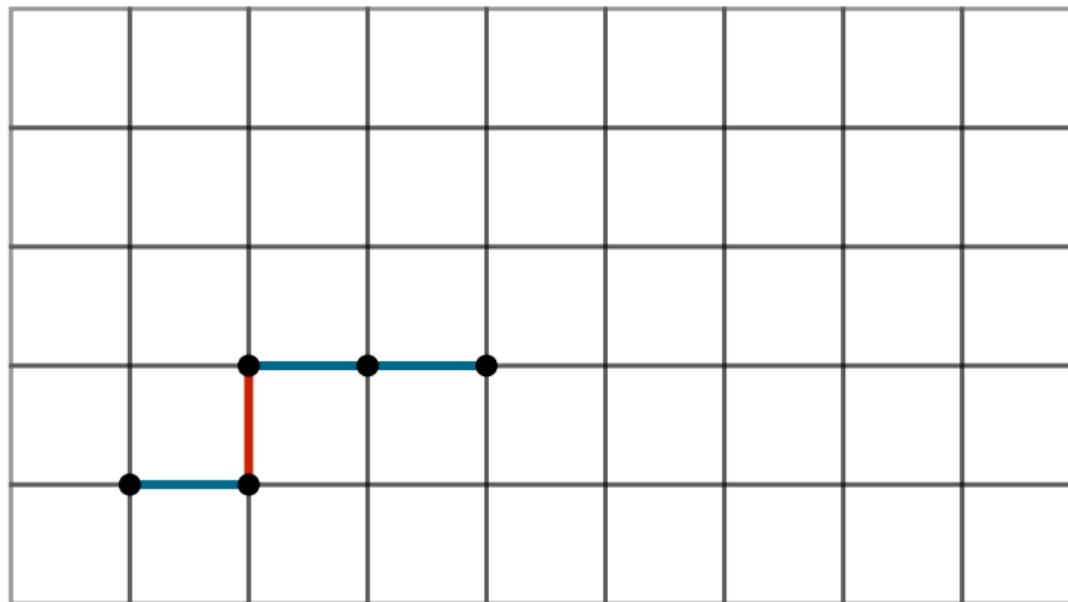
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

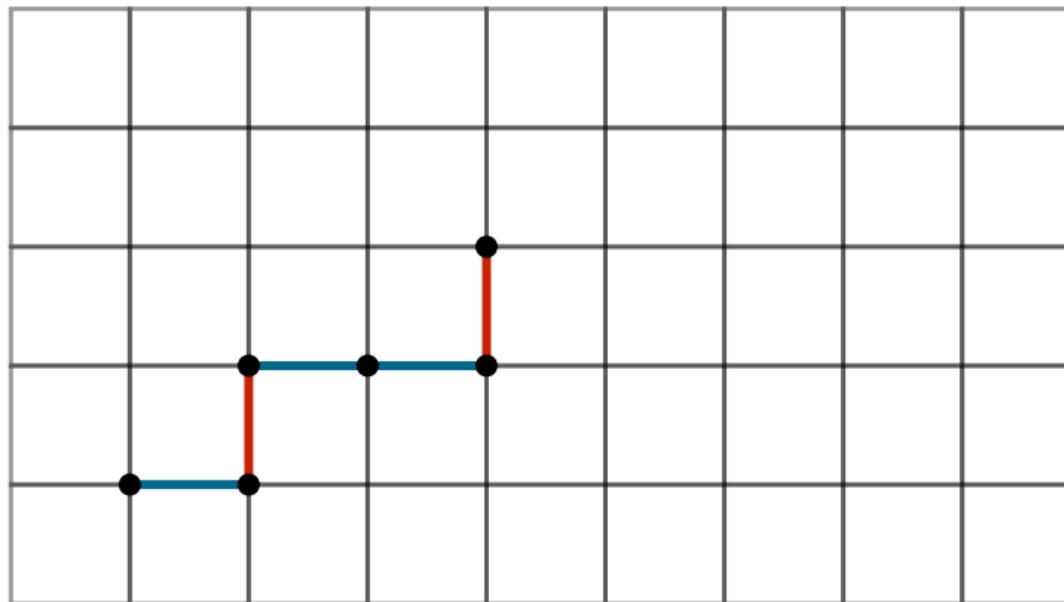
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

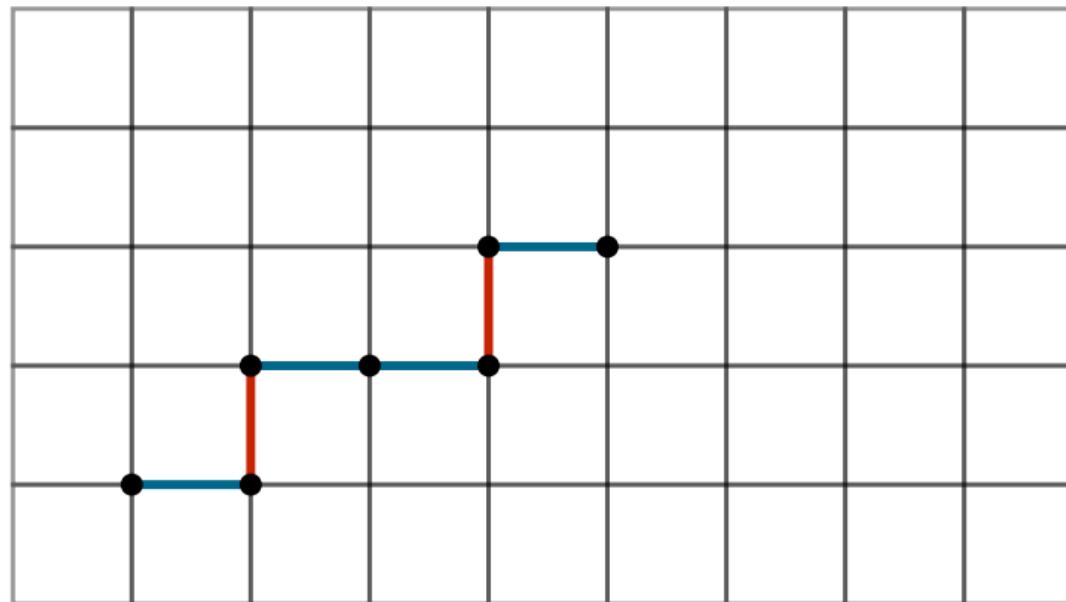
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

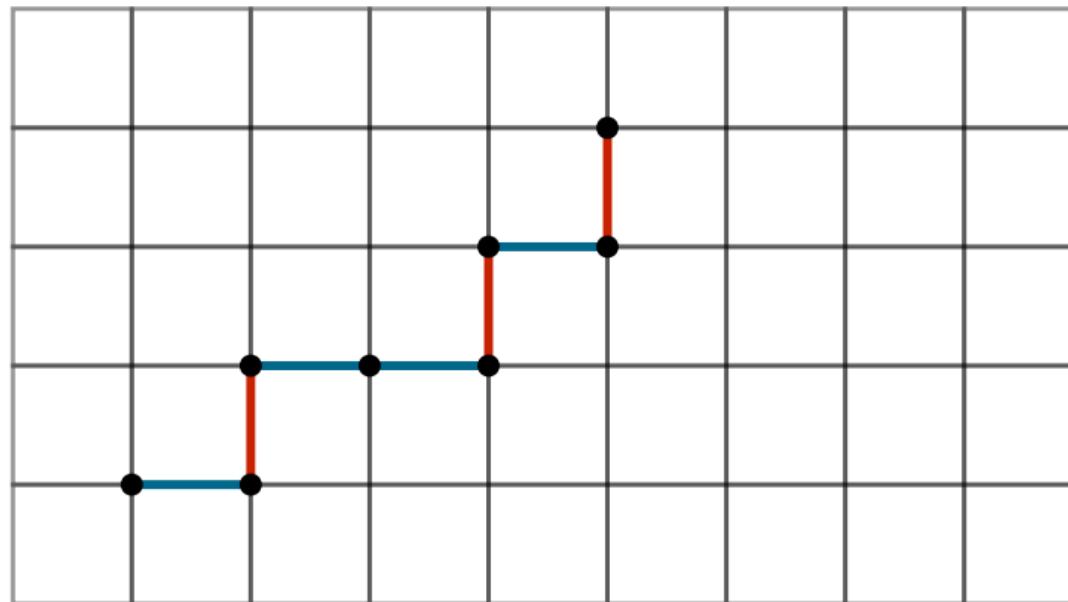
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

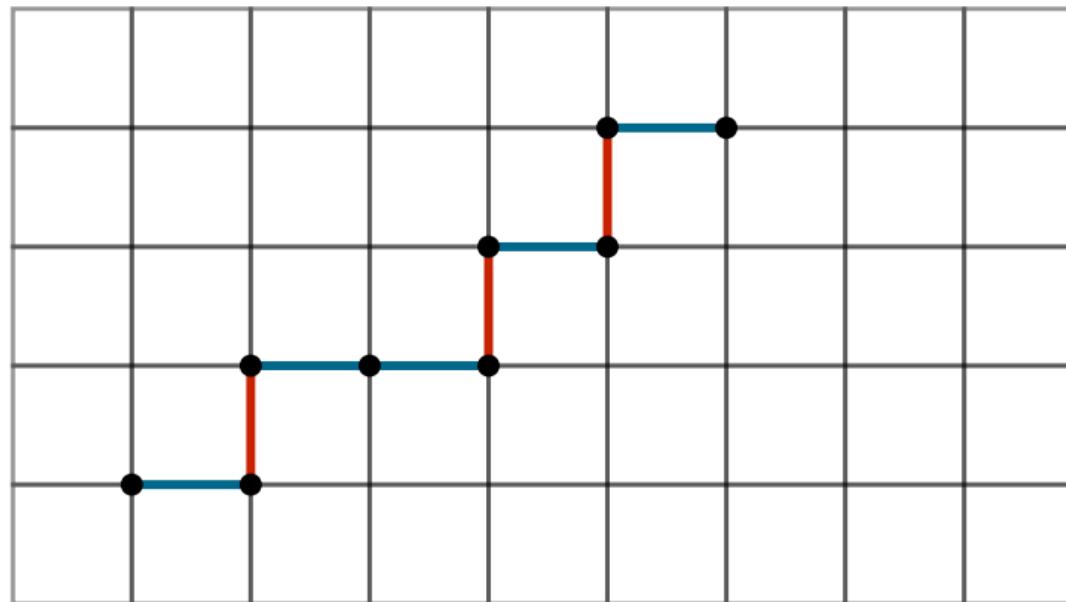
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

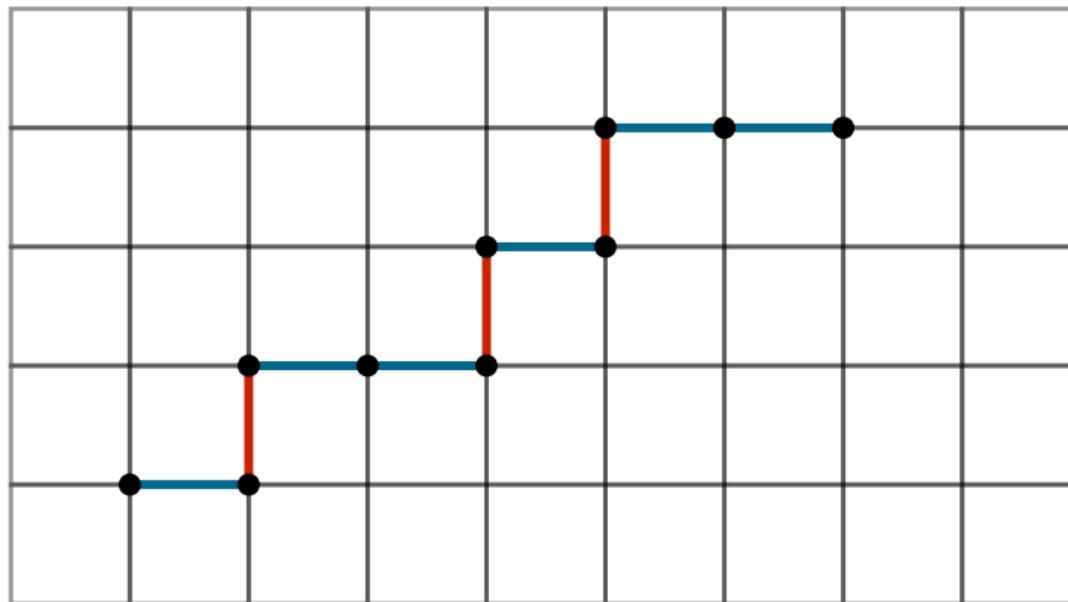
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

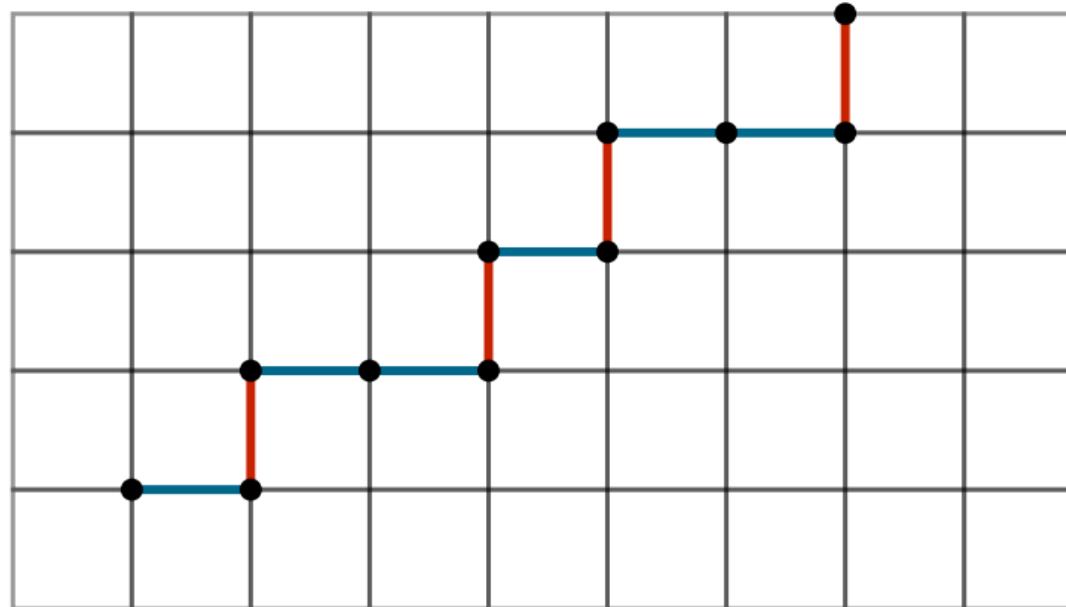
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

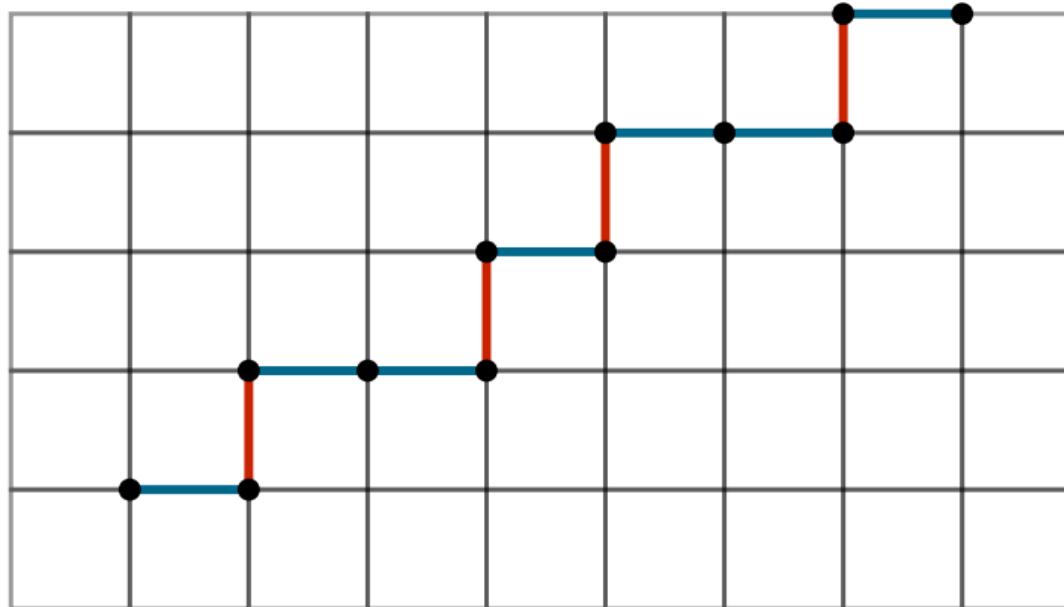
A ↔ horizontal step, **B** ↔ vertical step



FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

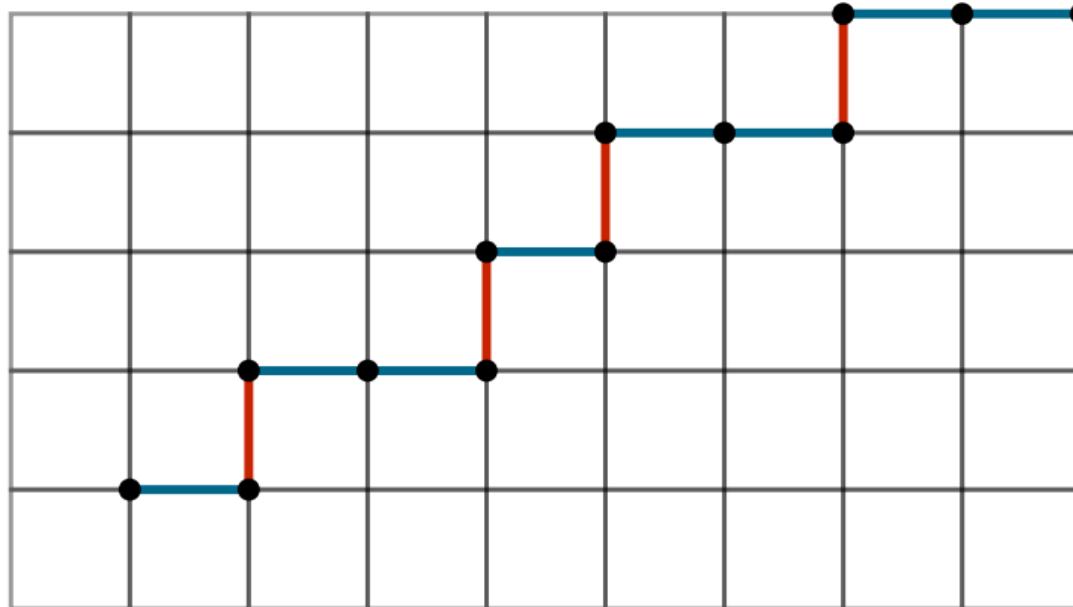
A ↔ horizontal step, **B** ↔ vertical step



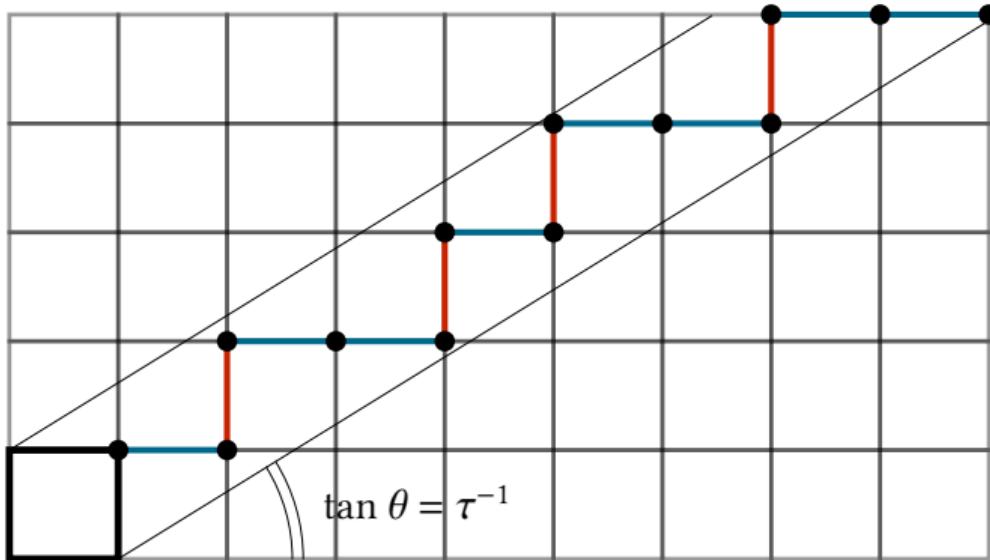
FIBONACCI WORD FROM ABOVE

(Infinite) Fibonacci word : ABAABABAABABAAB...

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



QUASIPERIODICITY OF THE FIBONACCI WORD



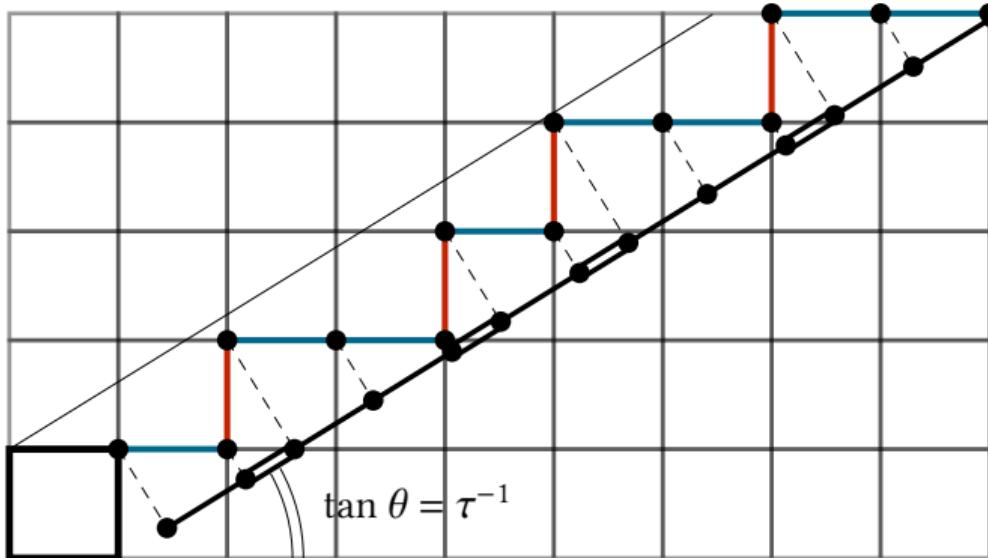
- average slope = inverse of the golden ratio ($\tau \simeq 1.6$)
 - bounded fluctuations

→ 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.

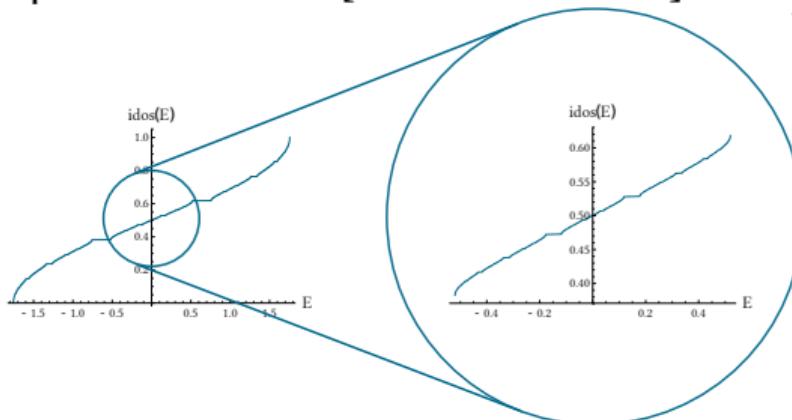
Schrödinger equation for the eigenstate of energy E :

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

FIBONACCI SPECTRUM AND EIGENSTATES

Numerical results

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



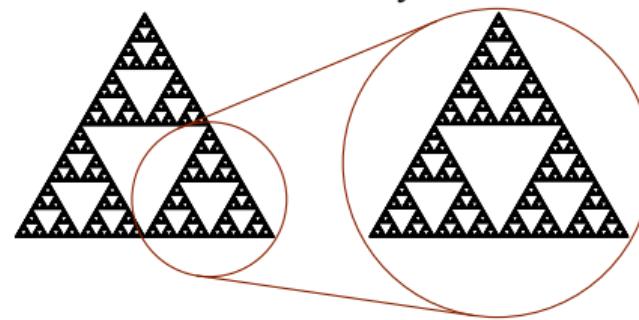
- Eigenstates : (almost all) fractal [Kohmoto *et al.* 83]

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]

FRACTAL DIMENSIONS

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

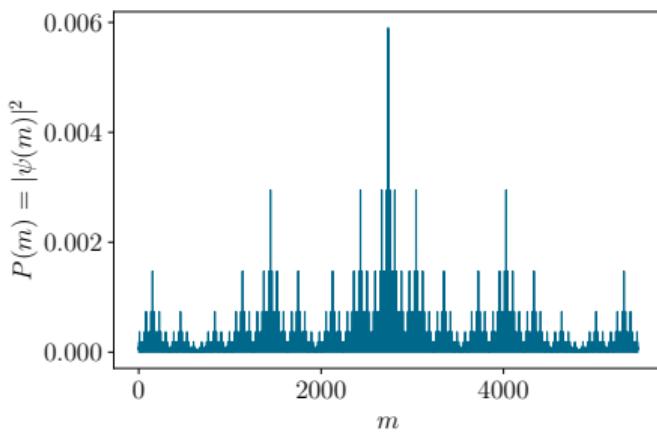


A Sierpiński triangle

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

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

THE BROCCOLI $E = 0$ STATE

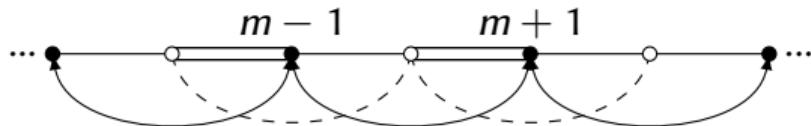


“Romanesco broccoli” fractal state at energy $E = 0$

- 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

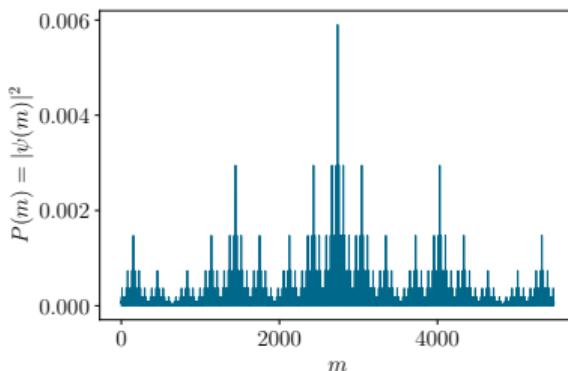
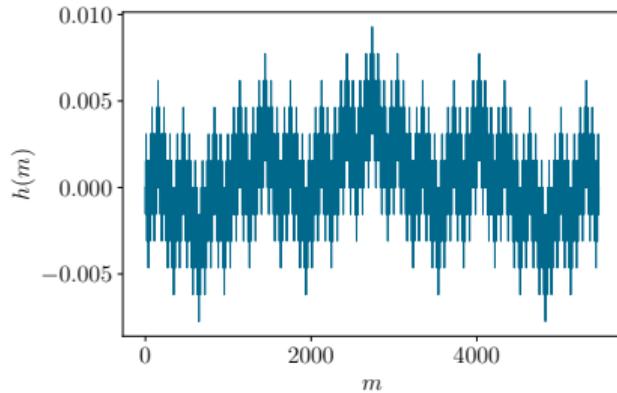
STRUCTURE OF THE BROCCOLI

- Effective chain



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

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

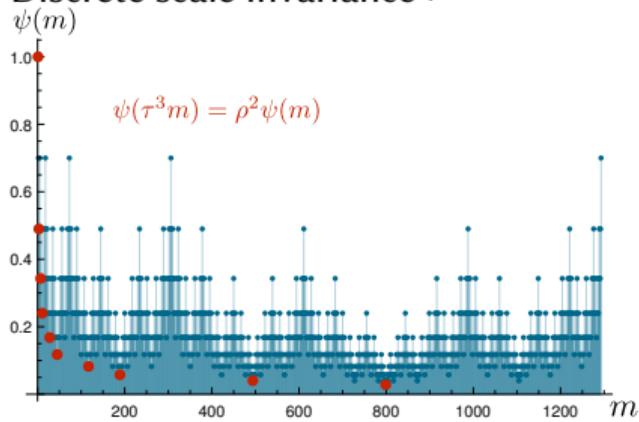


GEOMETRY AND EIGENSTATE PROPERTIES

- Arbitrary chain **AAABBABB...** (not necessarily Fibonacci)
- $E = 0$ state : $\psi(m) = (-1)^m \rho^{h(m)}$
- Geometry $\leftrightarrow h(m)$ function
- Periodic chain : **AAAAA...**
 - 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 $|\psi(m)| \sim m^{-\alpha}$
- **critical state** [Kohmoto *et al.* 87]

UNDERLYING SCALE INVARIANCE

Fibonacci chain *itself* scale invariant?

- Fibonacci words by concatenation :

$$C_2 = AB$$

$$C_3 = ABA$$

$$C_4 = C_3 C_2 = ABAAB$$

- Fibonacci words by **substitution** :

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

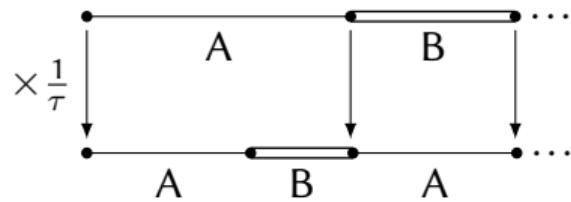
$$C_3 = ABA$$

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

- Infinite chain = fixed point of the substitution :

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

- Geometric substitution :



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

UNDERLYING SCALE INVARIANCE

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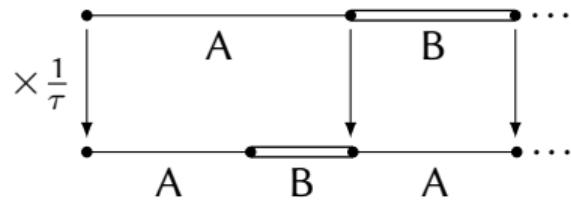
$$C_3 = ABA$$

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

- Infinite chain = fixed point of the substitution :

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

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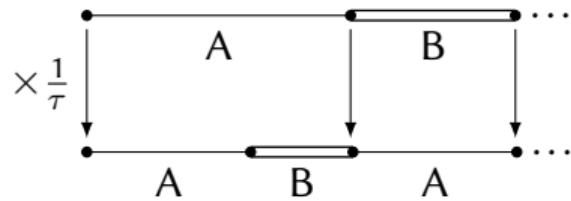
$$C_3 = ABA$$

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

- Infinite chain = fixed point of the substitution :

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

- Geometric substitution :



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UNDERLYING SCALE INVARIANCE

Fibonacci chain *itself* scale invariant?

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$$C_3 = ABA$$

$$C_4 = C_3 C_2 = ABAAB$$

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

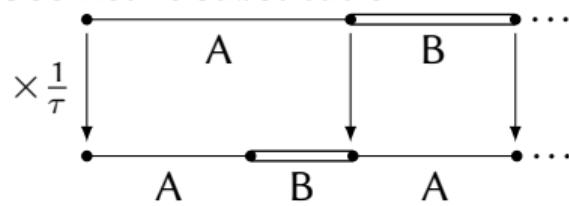
$$C_3 = ABA$$

$$C_4 = S(C_3) = ABAAB$$

- Infinite chain = fixed point of the substitution :

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

- Geometric substitution :



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

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

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

→ access to the distribution of heights

Height grows slowly :

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

Fractal dimensions of the $E = 0$ state :

$$d_q = \frac{q\omega(2\kappa) - \omega(2\kappa q)}{q - 1}, \text{ with } \kappa = |\log \rho|$$

$0 < d_q < 1 \rightarrow \text{fractal state}$

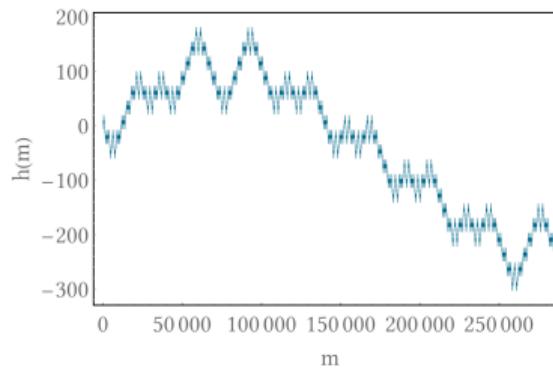
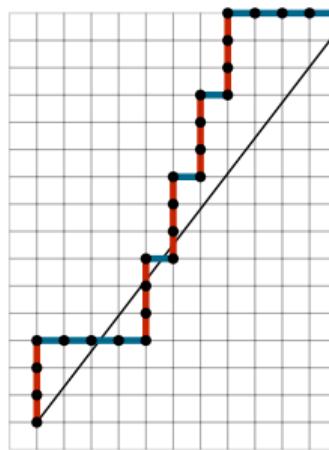
[Macé *et al.* 17]

BEYOND QUASIPERIODICITY

B3 chain :

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

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



Height : power-law growth [Dumont 89]

$$h(m) = C(m)m^\alpha$$

→ **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 :

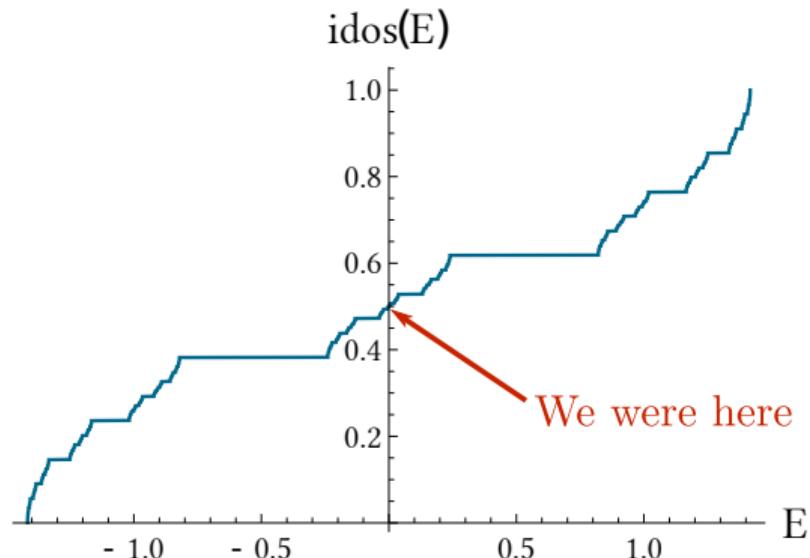
- Height field $h(m) \rightarrow \psi(m) = (-1)^m \rho^{h(m)}$

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...

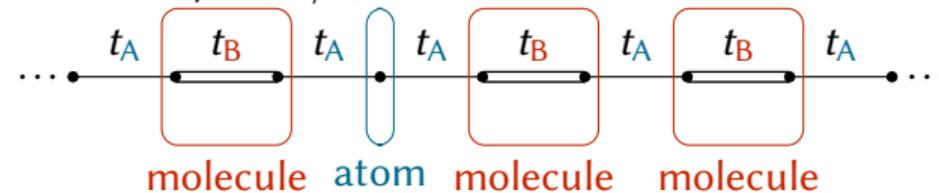


Integrated density of states (IDoS) of the Fibonacci chain

...what about the rest of the spectrum?

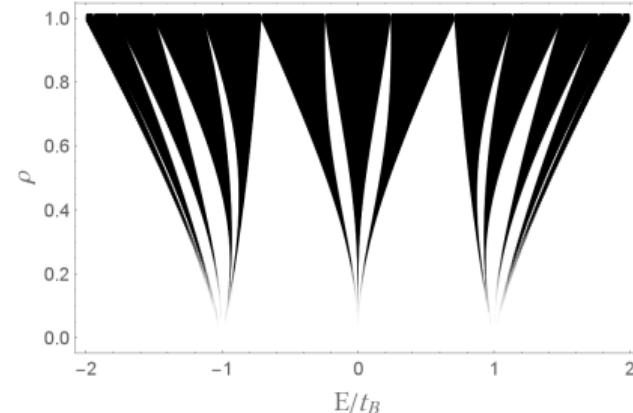
ATOMS AND MOLECULES

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



→ collection of decoupled atoms and diatomic molecules

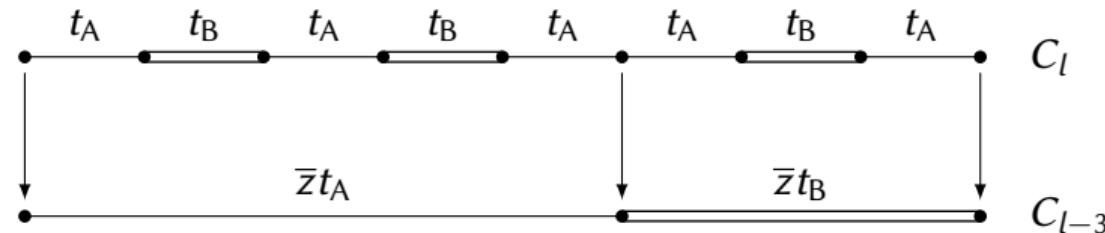
$\rho \neq 0, \rho \ll 1 \rightarrow$ lifted degeneracy, atomic and molecular energy clusters :



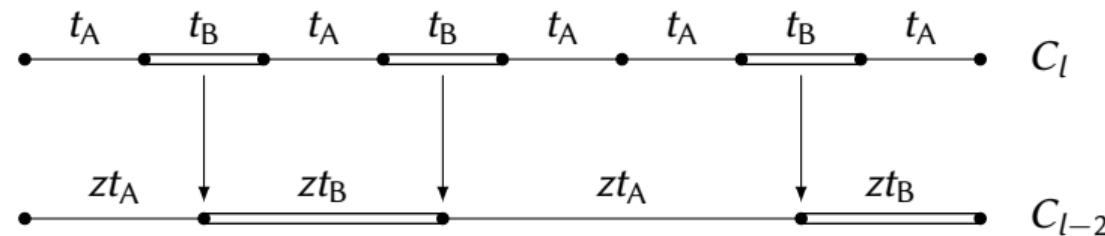
RENORMALIZATION

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)

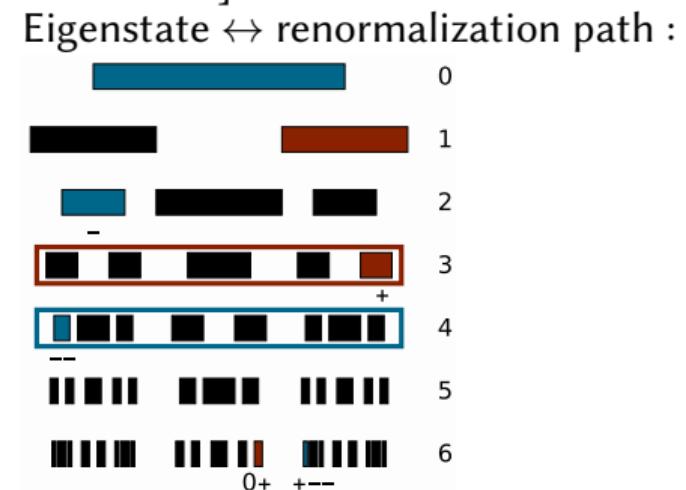
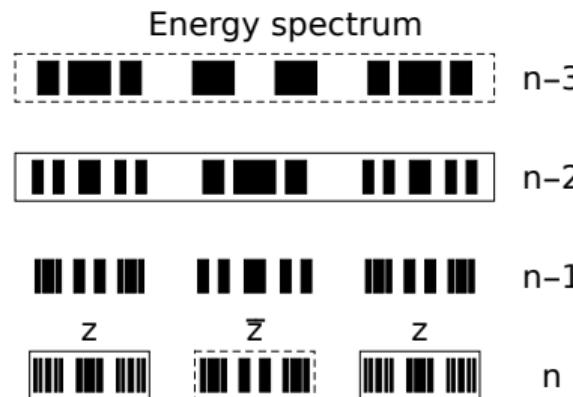


In the limit $\rho \ll 1$, $z = \rho/2$, $\bar{z} = \rho^2$

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]



FRACTALITY OF THE EIGENSTATES

RG → renormalization of the eigenstates [Macé *et al.* 16]

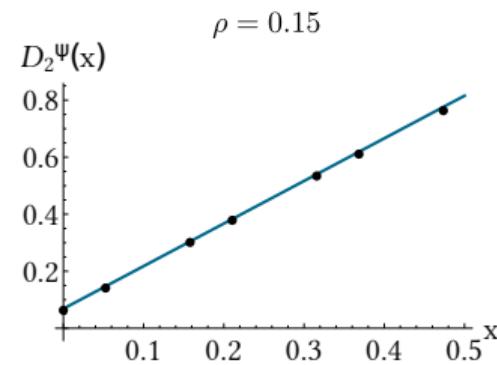
$$|\psi_m^{(l)}(E)|^2 = \bar{\lambda} |\psi_{m'}^{(l-3)}(E')|^2 \text{ if } E \text{ atomic level}$$

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

Fractal dimensions of the eigenstates :

$$d_q(x) = \frac{\log \left[\left(\frac{\lambda(\rho)^q}{\bar{\lambda}(\rho^q)} \right)^x \left(\frac{\bar{\lambda}(\rho)^q}{\bar{\lambda}(\rho^q)} \right)^{(1-2x)/2} \right]}{(q-1) \log \tau^{-1}}$$

x : fraction of molecular RG steps in a path
 $d_q(0)$: dimensions of the “broccoli state”



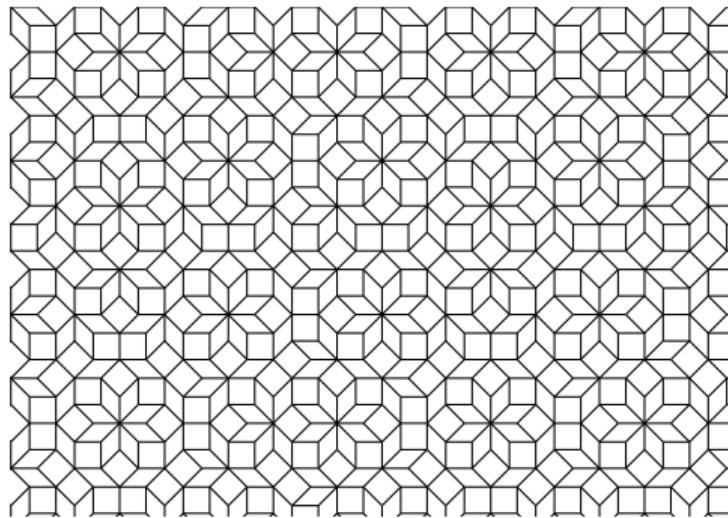
Fractal dimensions for $\rho = 0.15$: numerics vs RG predictions

CONCLUSIONS

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

- Substitution rule \rightarrow scale invariance \rightarrow renormalization group
- RG \rightarrow eigenstates all *fractal*
- Fractal dimensions depend only on x

GROUNDSTATE OF THE AMMANN-BEENKER TILING



A patch of the Ammann-Beenker tiling

Fractal states described by **height functions?**

Pure hopping Hamiltonian :

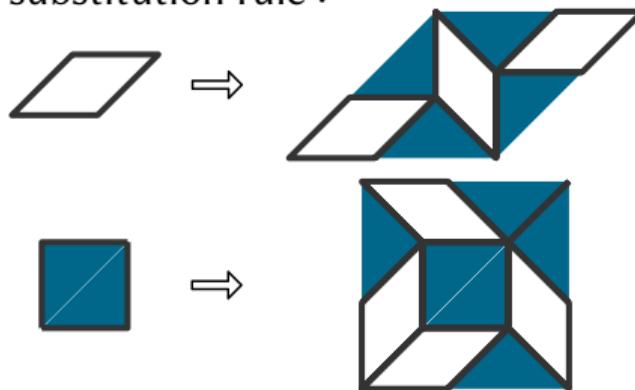
$$\hat{H} = -t \sum_{\langle m,n \rangle} |m\rangle \langle n|$$

Quasiperiodicity encoded in adjacency and on-site potentials

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

LOOKING FOR ARROWS

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

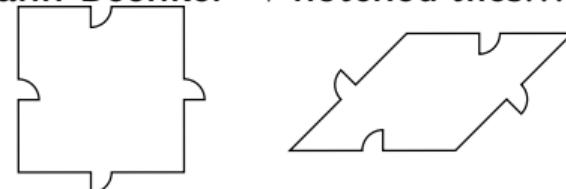


→ scale invariance.

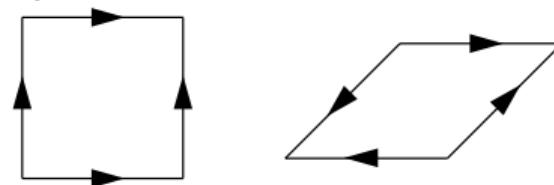
Height requires a field of arrows :

- invariant under substitution
- irrotational

Ammann-Beenker → notched tiles...



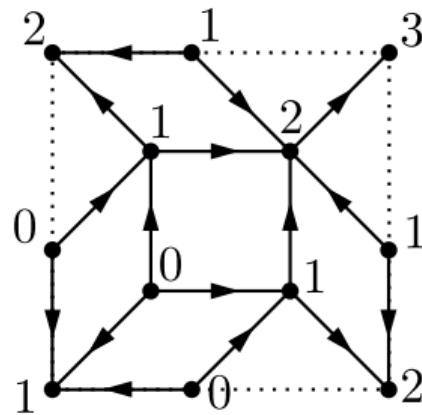
...exactly what we need!



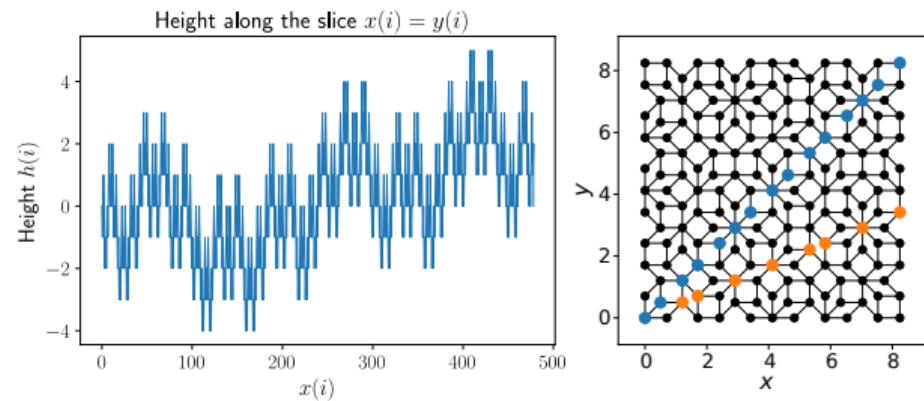
Height field :

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

PROPERTIES OF THE HEIGHT FIELD



The height field on a small patch of the tiling.



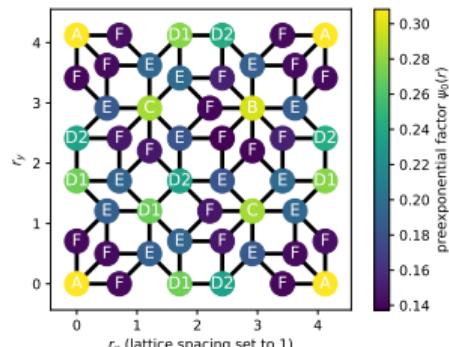
GROUNDSTATE

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

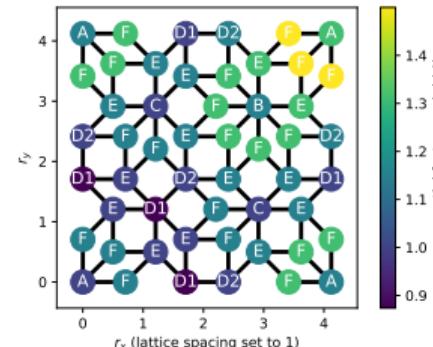
Conjecture [Kalugin, Katz 14] :

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

$C(m)$: local function :

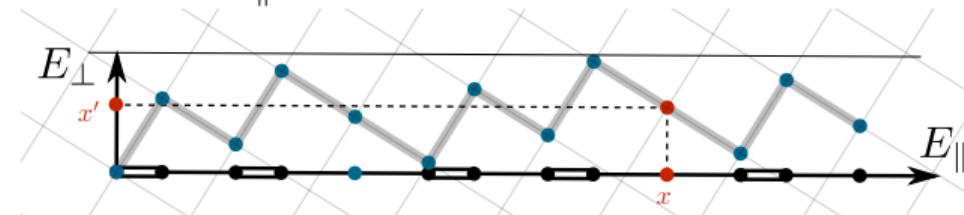


$e^{\kappa h(m)}$: non-local function :

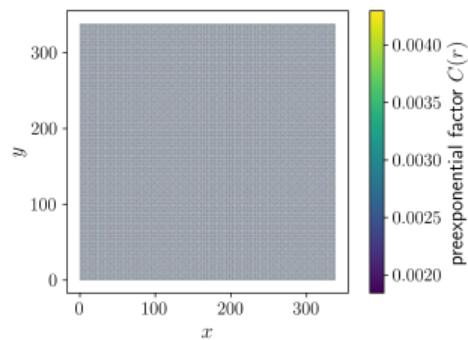


TESTING THE CONJECTURE

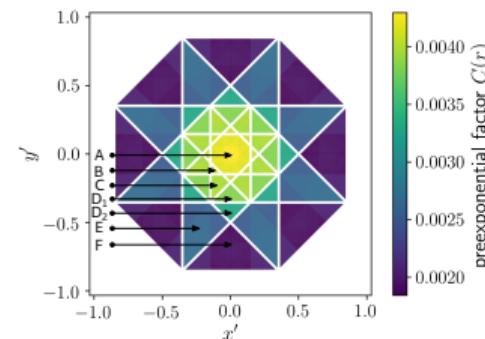
Cut-and-project \rightarrow physical (E_{\parallel}) and internal (E_{\perp}) space :



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

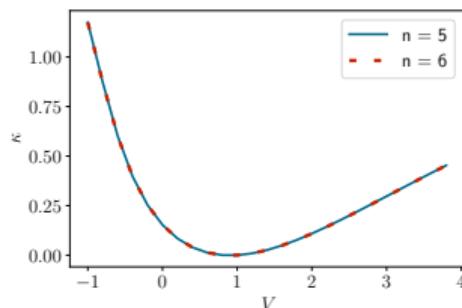
PERTURBING THE HAMILTONIAN

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] :

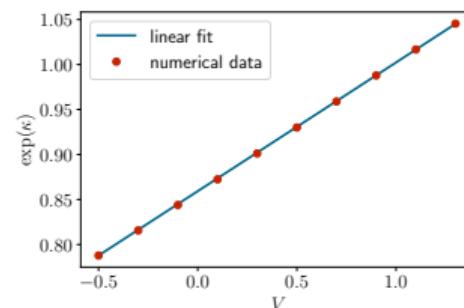
$$V_m = V z_m \\ \rightarrow \psi(m) = C(m) e^{\kappa h(m)}$$



Prefactor κ 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^κ 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
- 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
- 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 can be seen as a form of deterministic disorder. Although non-interacting eigenstates are not localized, many-body quasiperiodic systems seem to localize ...how ?