Exact results on electronic wavefunctions of 2D quasicrystals

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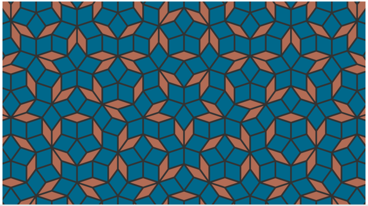
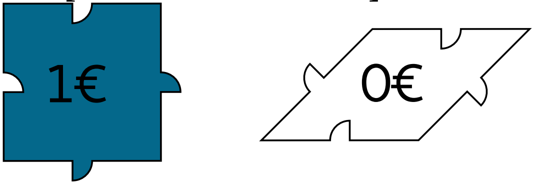
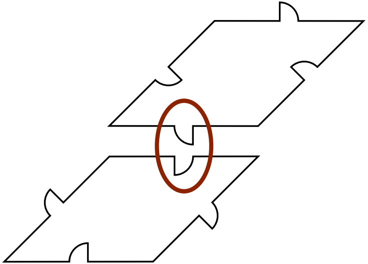


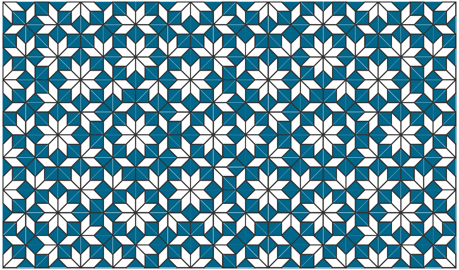
A QUASIPERIODIC PUZZLE [BÉDARIDE *ET AL.* 12]



Pay the squares, get the rhombuses for free!

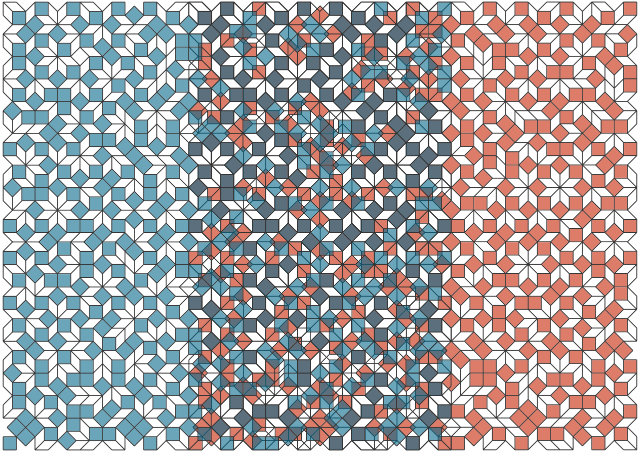


Forbidden configuration.



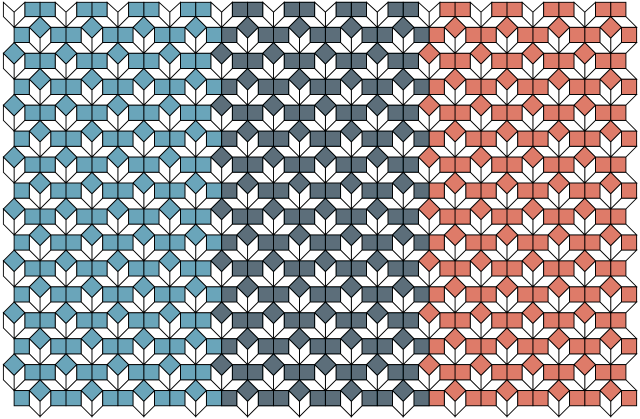
Patch of the Ammann-Beenker tiling.

Periodic, quasiperiodic and random



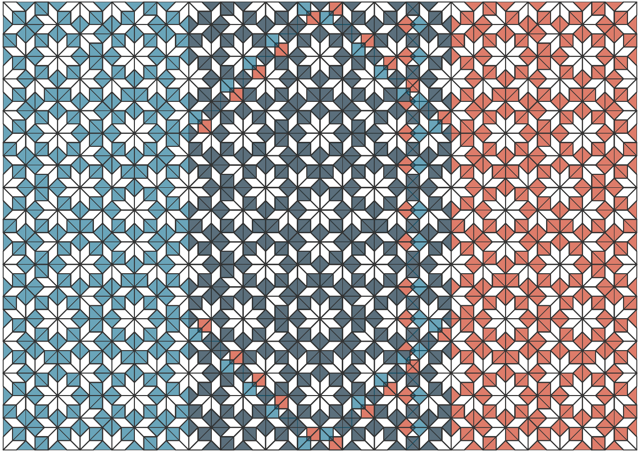
No long range order : random

Periodic, quasiperiodic and random



Perfect long range order : periodic

Periodic, quasiperiodic and random



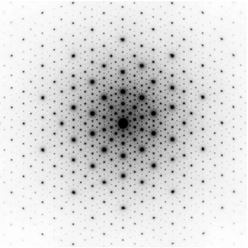
Long range order : quasiperiodic

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

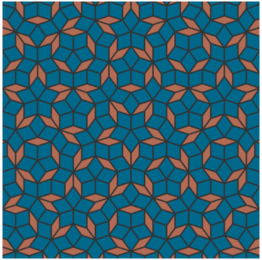
Quasicrystals

Quasicrystal → quasiperiodically arranged atoms :

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

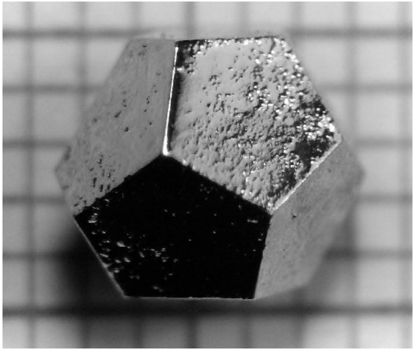


Diffraction pattern of a AlPdMn alloy
(Conradin Beeli group)

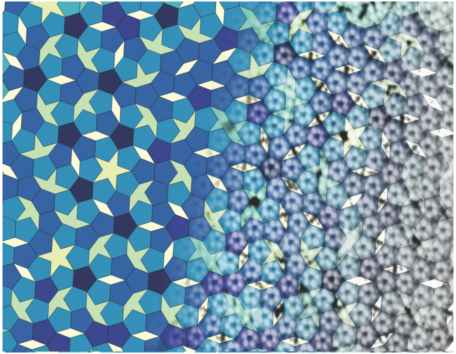


A patch of the quasiperiodic Penrose tiling,
used to model many quasicrystals.

Examples of quasicrystals



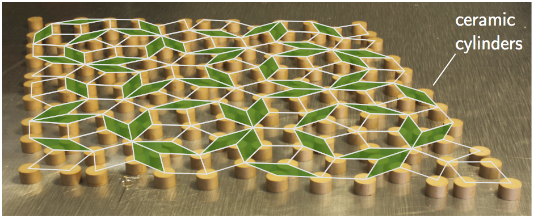
HoMgZn alloy in its icosahedral phase
(doi:10.1038/nmat1244)



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).

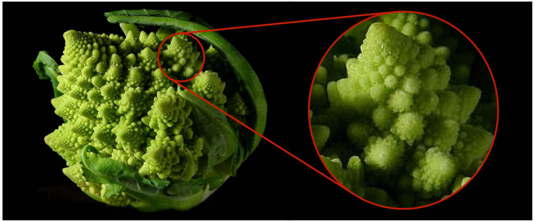
ENGINEERED QUASIPERIODIC STRUCTURES



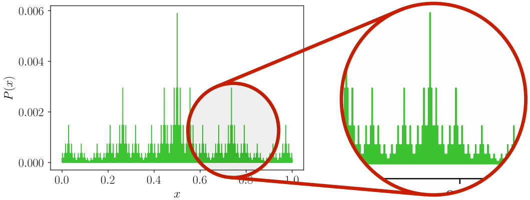
A network of dielectric resonators [Vignolo *et al.* 14]

- 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 $\rightarrow$ discrete scale invariant objects.
- Discrete scale invariance $\rightarrow$ **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 :

$$\begin{aligned} F_0 &= 1 \\ F_1 &= 1 \\ F_2 &= F_1 + F_0 = 2 \\ F_3 &= F_2 + F_1 = 3 \\ F_4 &= F_3 + F_2 = 5 \\ F_5 &= F_4 + F_3 = 8 \\ &\vdots \end{aligned}$$

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

Fibonacci words

Letters instead of numbers, same rule :

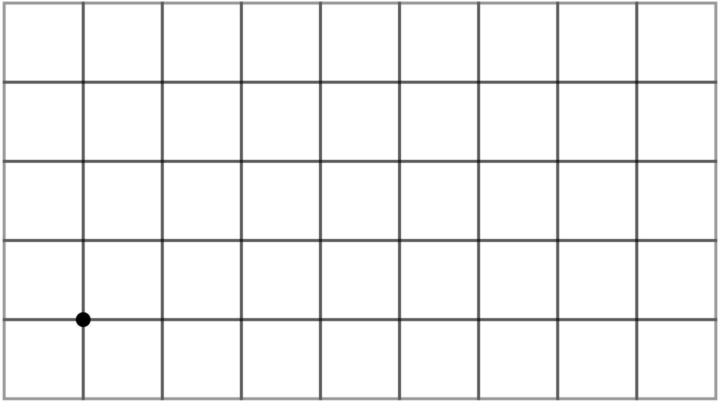
$$\begin{aligned} C_0 &= \mathrm{B} \\ C_1 &= \mathrm{A} \\ C_2 &= C_1 C_0 = \mathrm{AB} \\ C_3 &= C_2 C_1 = \mathrm{ABA} \\ C_4 &= C_3 C_2 = \mathrm{ABAAB} \\ C_5 &= C_4 C_3 = \mathrm{ABAABABA} \\ &\vdots \end{aligned}$$

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

Fibonacci word from above

(Infinite) Fibonacci word : ABAABABAABAAB...

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



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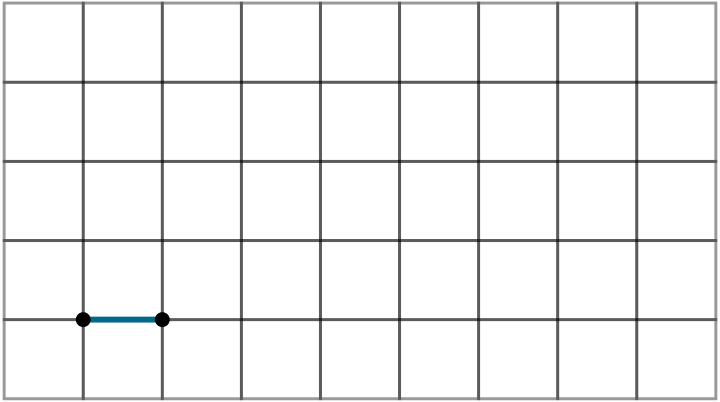

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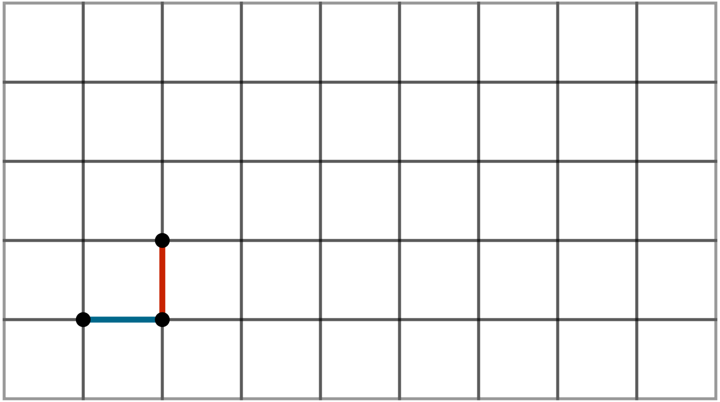

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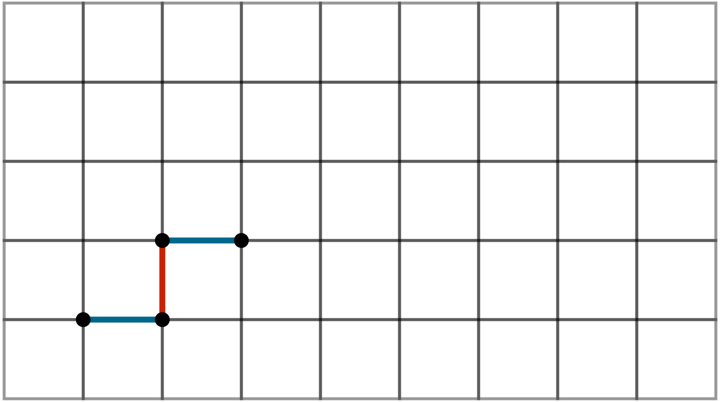

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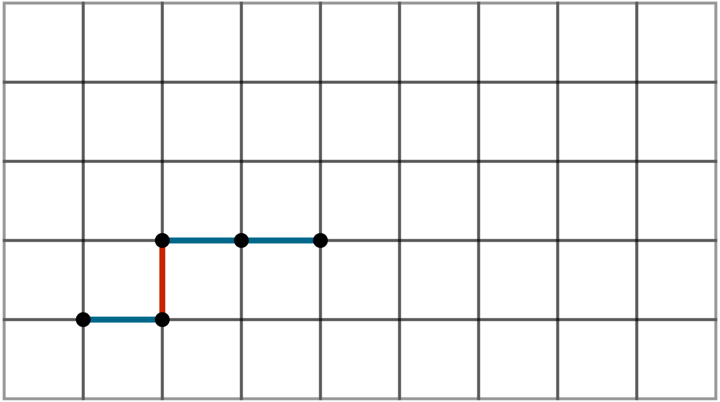

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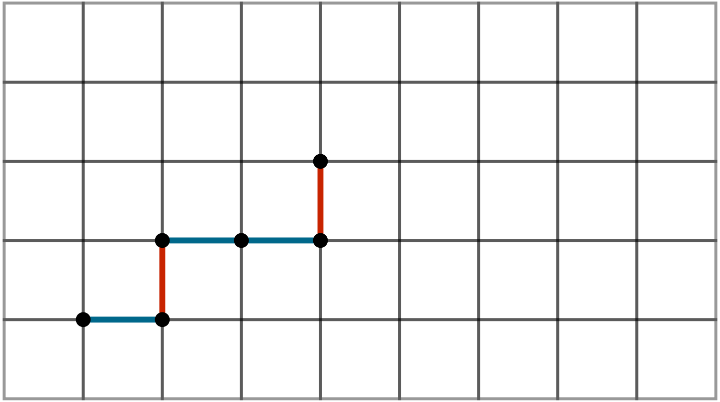

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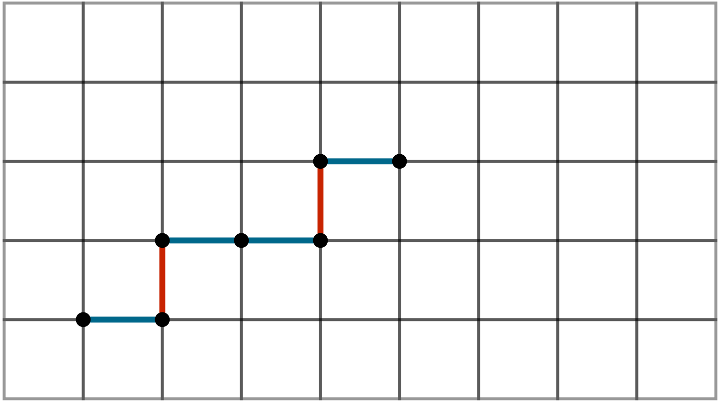

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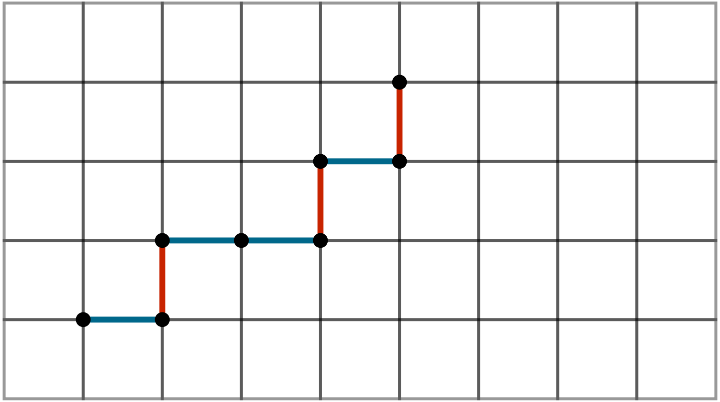

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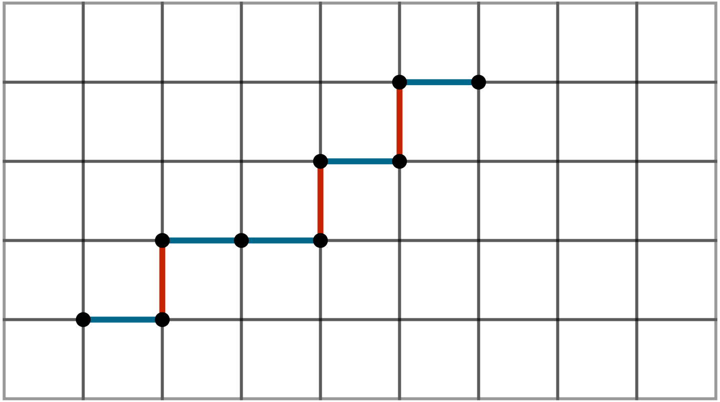

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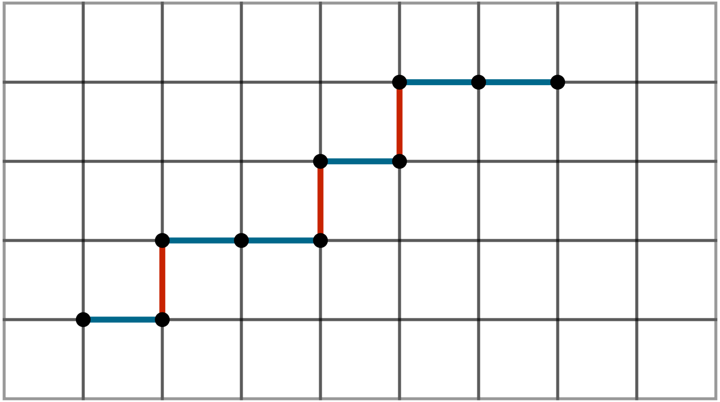

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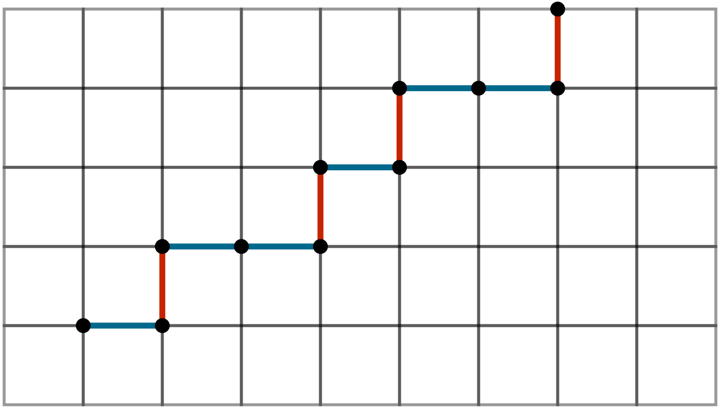

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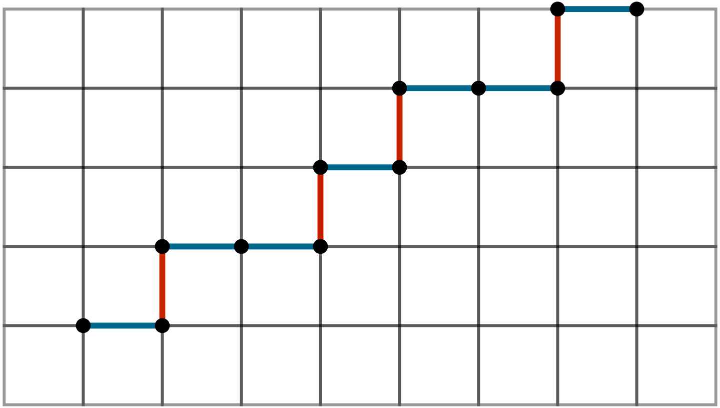

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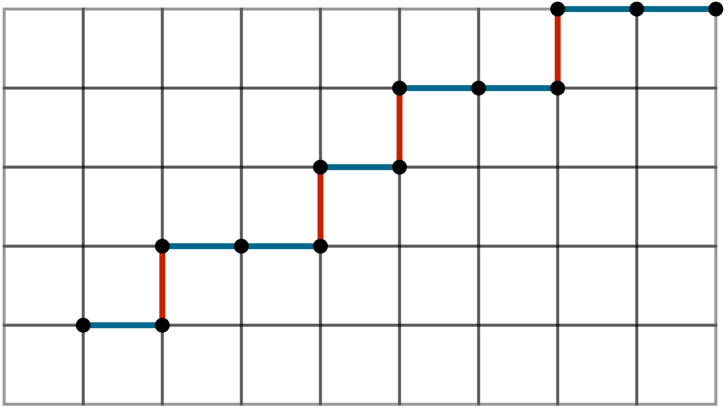
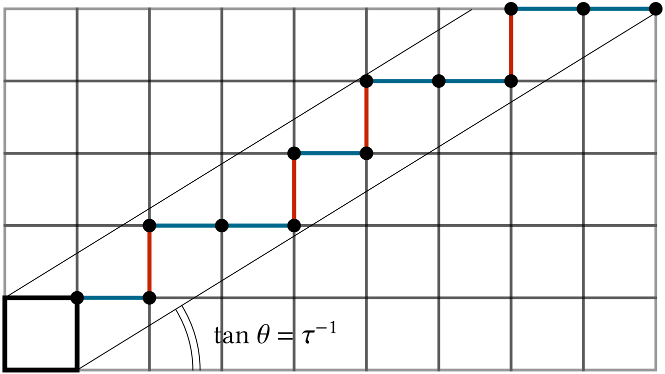


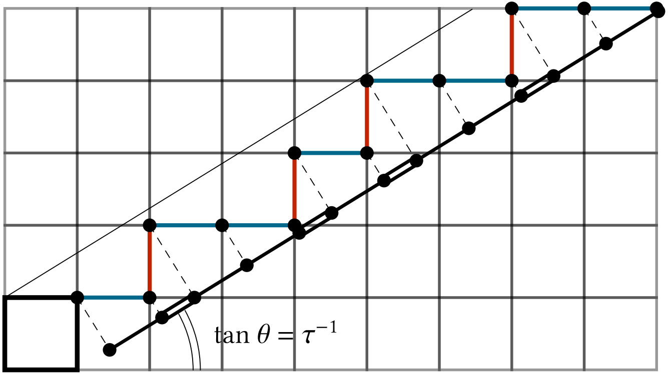
Quasiperiodicity of the Fibonacci word



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

$\rightarrow$ similar environments everywhere
$\rightarrow$ quasiperiodicity [Duneau, Katz 85]

Cut-and-project



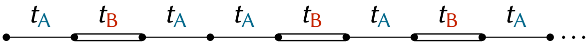
C&P $\rightarrow$ quasiperiodic (or periodic) tiling !

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 :



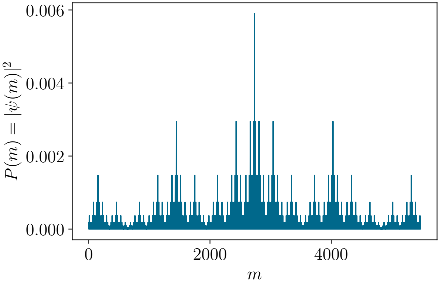
Hamiltonian :

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

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

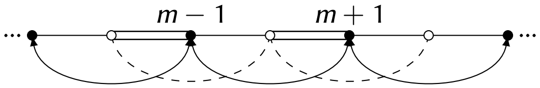


"Romanesco broccoli" fractal state at energy $E = 0$

- 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

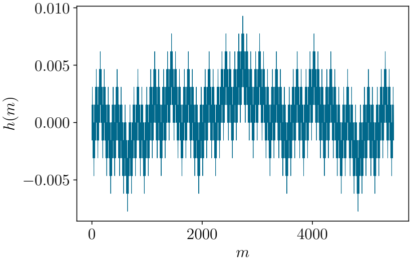
Structure of the broccoli

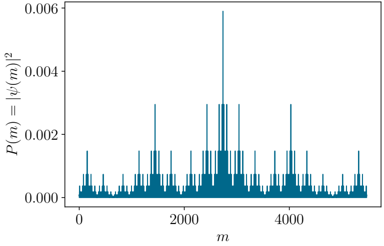
- Effective chain

$$\underbrace{AB}_{R}\ \underbrace{AA}_{U}\ \underbrace{BA}_{L}\ \underbrace{BA}_{L}\ \underbrace{AB}_{R}\ \underbrace{AA}_{U}\ \dots$$

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

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

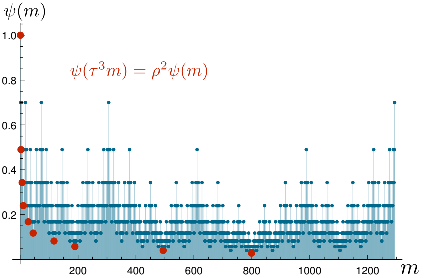




Geometry and eigenstate properties

- 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 : AAABBABB…
  - 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

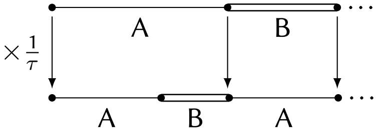
Fibonacci chain *itself* scale invariant ?

- Fibonacci words by concatenation :
  $C_2 = \mathsf{AB}$
  $C_3 = \mathsf{ABA}$
  $C_4 = C_3 C_2 = \mathsf{ABAAB}$
- Fibonacci words by **substitution** :

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

$C_3 = \mathsf{ABA}$
$C_4 = S(C_3) = \mathsf{S(A)\,S(B)\,S(A)}$

- Infinite chain = fixed point of the substitution :
  $S(\mathsf{ABAAB}\dots) = \mathsf{ABAAB}\dots$
- Geometric substitution :



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

UNDERLYING SCALE INVARIANCE

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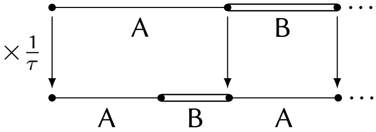

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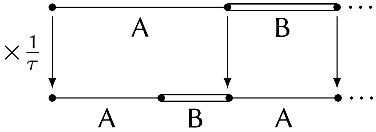

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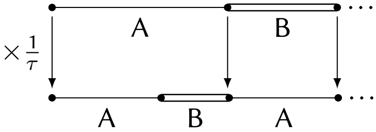

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Height distribution & multifractality

Partition function of the heights :

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

Scaling law behavior :

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

with

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

$\rightarrow$ access the distribution of heights !

Height diffuses slowly through the chain :

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

Fractal dimensions of the $E = 0$ state :

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

$0 < d_q < 1 \rightarrow$ fractal state indeed !

[Macé *et al.* 17]

Beyond quasiperiodicity

Conclusions