Flip dynamics on canonical cut and project tilings

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Outline

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The problem with local rules

Reminder: local rules can enforce (some) aperiodic structures.

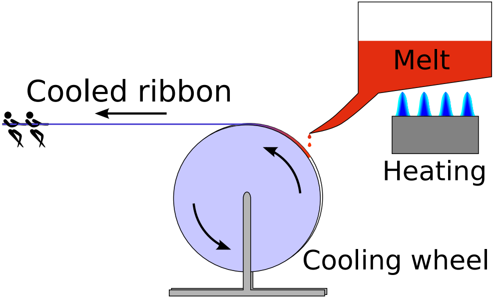
Proposition

Any local rules which allow only aperiodic tilings also allow finite patterns (called deceptions*) that appear in none of these tilings.*

The existence of a solution does not tell how to solve the puzzle!

Back to real quasicrystals

Real quasicrystals are *quenched* from high T:



Stability is governed by the minimization of the free energy F:

$$F = E - TS.$$

Random tilings of maximal entropy

Entropy of a tiling T of a region R:

$$S = \frac{\log(\#\ \text{rearrangements of}\ T)}{\#\ \text{tiles in}\ T} = \frac{\log(\#\ \text{tilings of}\ R)}{\#\ \text{tiles to tile}\ R}.$$

Two main issues:

1. Which region R does maximize the entropy?
2. How does a "typical" tiling T of R look like?

Underlying question: is there some "random order"?

The $2 \to 1$ case

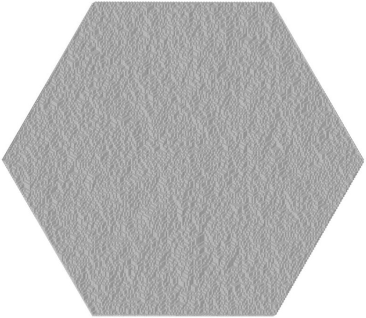
Both issues are solved for tilings of the line by two type of tiles:

1. For a and b tiles of each type, the tiling has entropy $\binom{a+b}{a}$. This is maximal for $a = b$.
2. The *fluctuations* of a tiling by n tiles are in $\Theta(\sqrt{n})$. A typical tiling thus looks like a line...

The 3 → 2 case (dimer tilings)

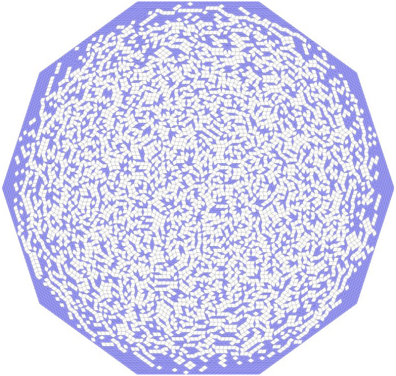
Much harder, but powerful results exist:

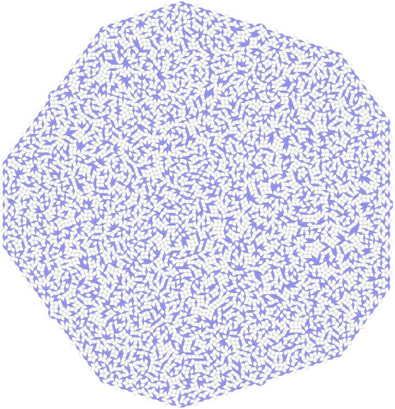
- Kasteleyn matrix (1967)
- Lindström–Gessel-Viennot lemma (1989)
- Cohn-Kenyon-Propp variational principle (2001)



Beyond the $3 \to 2$ case

Only simulations. . .





The problems with random tilings

At least two problems with random tilings:

1. Is it really easier to solve the puzzle?
2. Quenching has been dropped in favour of *slow cooling*. Why?

We shall here focus on the second problem. It is worth first asking:

How the previous pictures have been drawn?

Outline

Philosophy

Goal: draw an object at random in a (typically large) set.
The distribution is prescribed (*e.g.*, uniform).

This is easy if one can *index* all the elements, as the Rubik's cube:
Scrambling $\Leftrightarrow$ draw a number between 1 and $8! \times 3^7 \times 12! \times 2^{10}$.

This may be harder in other cases (Ising model, Tilings model...)
Moreover, one could prefer a sampling which is physically realist instead of algorithmically efficient.

A common solution: Markov chain methods.

Markov chain

A Markov chain (X_t) is a memoryless random process:

$$\mathbb{P}(X_{t+1} = x \mid X_1 = x_1, \dots, X_t = x_t) = \mathbb{P}(X_{t+1} = x \mid X_t = x_t).$$

Here: finite state space Ω. Description by a transition matrix P.

Acts on the distributions over Ω. *Stationary distribution*: $\pi = P\pi$.

A Markov chain is said to be

- *irreducible* if the state space is strongly connected;
- *aperiodic* if the gcd of the cycles through any state is 1;
- *Ergodic* if it is both irreducible and aperiodic.

Convergence

Total variation between two distributions over a space Ω:

$$||\mu - \nu|| := \max_{A \subset \Omega} |\mu(A) - \nu(A)| = \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|.$$

This allows to measure the distance to stationarity:

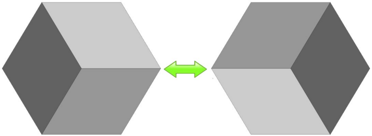
$$d(t) := \max_{x \in \Omega} ||P^t(x, \cdot) - \pi||.$$

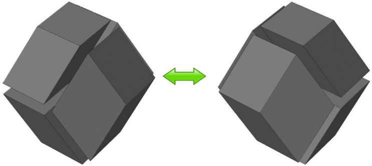
Theorem (Exponential convergence)

For any ergodic Markov chain, there is $\alpha < 1$ s.t. $d(t) \leq Cst \times \alpha^t$.

Flips and tiling spaces

Whenever a vertex of a $n \to d$ tiling belongs to exactly $d + 1$ tiles, translating each of them by the vector shared by the d other ones yields a new tiling. This elementary operation is called a *flip*.





The *tiling space* associated with a region R is the graph

- whose vertices are the tilings of R;
- whose edges connect tilings which differ by a flip.

We want to sample by performing a random walk on this graph.

Ergodicity

Orient the flips and define the random walk which at each step

1. pick uniformly at random a vertex x;
2. choose a flip direction (coin tossing);
3. try to perform the flip around x.

This is an aperiodic Markov chain (self-loops). Is it irreducible?

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Theorem (Kenyon, 1993)

The $n \to 2$ tilings of a simply connected region are flip-connected.

Theorem (Desoutter-Destainville, 2005)

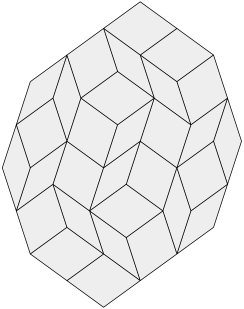
The $n \to d$ tilings of a simply connected region are flip-connected for $d \geq n-2$, but not always for $n-3 \geq d \geq 3$ (cycle obstruction).

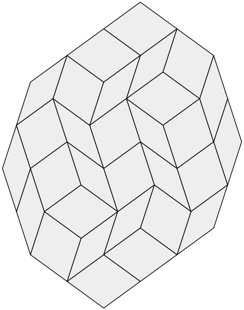
Beyond ergodicity

A path of flips is *direct* if no two flips involve exactly the same tiles.

Theorem (Bodini-Fernique-Rao-Rémila, 2011)

The $n \to 2$ tilings of a simply connected region are connected by direct paths of flips for $n \leq 4$, but not always for $n \geq 5$.





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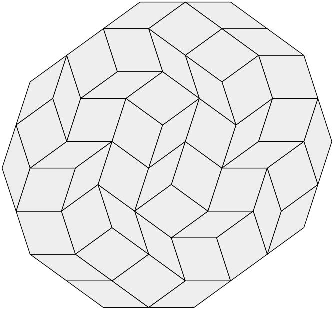

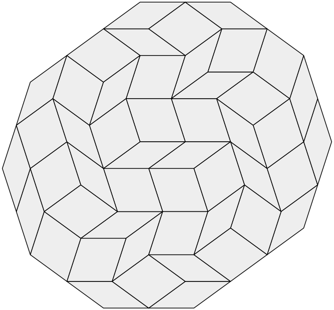

Eternity is really long, especially near the end

“The convergence is exponential, hence fast”. . . as in Chernobyl!

It is often important to be more precise:

- How many moves to scramble your Rubik’s cube?
- How many steps to shuffle a deck of cards?
- How many flips to have a typical tiling?

The point is: how does the exponent depend on the space size?

Outline

Definition

Mixing time: $\tau_{\text{mix}} := \min\{t \mid d(t) \leq 1/4\}$. Arbitrary threshold?

Theorem (Half-life)

A Markov chain is two times closer to stationarity after τ_{mix} steps.

In other words: $d(t) \leq 2^{-t/\tau_{\text{mix}}}$ (exponential convergence again).

Problem: bound the mixing time as a function of the space size.

Eigenvalues and the spectral gap

Theorem (Perron-Frobenius, 1907-1912)

The largest eigenvalue of a non-negative irreducible matrix is unique and simple.

An ergodic Markov Chain has a non-negative irreductible matrix.
Let $\lambda_1, \ldots, \lambda_n$ be its eigenvalues, ordered by decreasing moduli.
Since it is stochastic, $\lambda_1 = 1$, and by Perron-Frobenius, $|\lambda_2| < 1$.
Assume it diagonalizable (it can be adapted for Jordan forms).
By decomposing a vector $\vec{p}$ on an eigenbasis $(\vec{p}_1, \ldots, \vec{p}_n)$, one gets

$$|P^t \vec{p} - \vec{p}_1| = \left| \sum_{k \geq 2} \lambda_k^t \vec{p}_k \right| \leq |\lambda_2|^t \left| \sum_{k \geq 2} \vec{p}_k \right|.$$

This gives the exponent of the convergence... but what is $|\lambda_2|$?

Coupling

Alternative idea:

- a random walker is lost when he "forgot" its starting point;
- two random walkers are lost when they meet.

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Coupling: two random variables with equal marginal distributions.
Coupling time: $\tau_{\text{couple}} := \min\{t \mid X_t = Y_t\}$ (random variable).

Theorem

The mixing time is less than the expectation of any coupling time.

The random variables can be correlated: make a good choice!

Contraction

A typical way to bound the coupling time:

Proposition (Contraction)

Let (X_t, Y_t) *be a coupling and* $\varphi : \Omega \times \Omega \to \{0, \ldots, D\}$.
If there is $\beta < 1$ *such that*

$$\mathbb{E}(\varphi(X_{t+1}, Y_{t+1}) | (X_t, Y_t) = (x, y)) \leq \beta \varphi(x, y),$$

then

$$\tau_{mix} \leq \frac{\log(D)}{1 - \beta}.$$

The $2 \to 1$ case

Theorem (Wilson, 2004)

Let $h(v) := |v|_1 - |v|_2$ *and define*

$$\varphi(w, w') := \sum_{k=0}^{n} |h(w_1 \cdots w_k) - h(w'_1 \cdots w'_k)| \cos\left[\pi\left(\frac{k}{n} - \frac{1}{2}\right)\right].$$

Then, for x *and* y *such that* $h(x_1 \cdots x_k) \leq h(y_1 \cdots y_k)$ *for any* k*,*

$$\mathbb{E}(\varphi(X_{t+1}, Y_{t+1}) | (X_t, Y_t) = (x, y)) = (1 - \beta)\varphi(x, y),$$

with

$$\beta = \frac{1 - \cos(\pi/n)}{n - 1} \geq \frac{\pi^2}{2n^3}.$$

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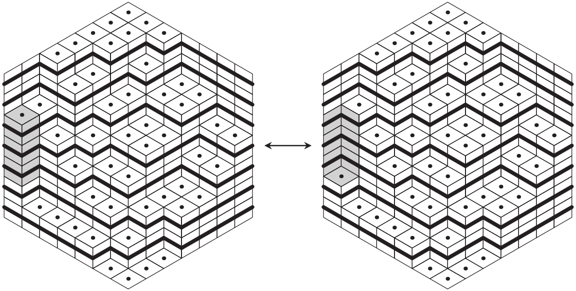
With $\varphi(w, w') \leq n$, this yields $\tau_{\text{mix}} \leq \frac{2}{\pi^2} n^3 \log(n)$. Actually tight.

The 3 → 2 case and beyond

One can rely on the 2 → 1 case up to a modification of the chain:



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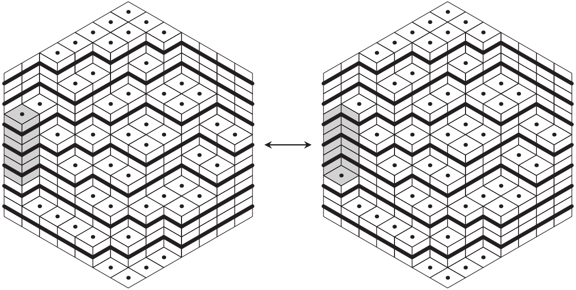

This yields $\tau_{\text{mix}} = \Theta(n^2 \log(n))$ for this modified chain.
One can derive $\tau_{\text{mix}} = O(n^4)$ for the original chain.
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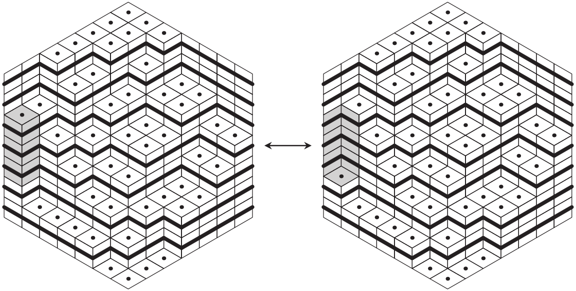

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One can derive $\tau_{\text{mix}} = O(n^4)$ for the original chain.
Simulations however suggest $\tau_{\text{mix}} = \Theta(n^2 \log(n))$.

Simulations actually suggest this bound for any $n \to 2$ tiling...

Coupling from the past

Assume that we simultaneously run the chain on all the states.
Assume that after some steps, all the states have coalesced.
Is the obtained state randomly drawn?

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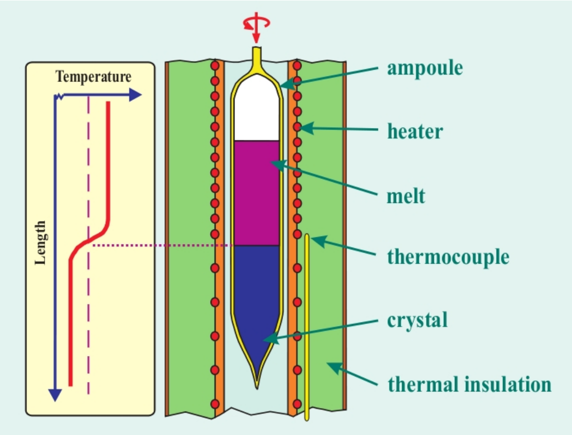
Sometimes, the coalescence of *some* chains, eventually modified, ensures the global coalescence (*sandwiching* or *bounding chains*).

Outline

Bridgeman-Stockbarger method



Minimization of $F = E - TS$: from max. entropy to min. energy.

Flip mechanism for atomic diffusion

Maximal entropy S (high T): modeled by random tilings.

Minimal energy E (low T): modeled by tilings with local rules, with the energy being the number of occuring forbidden patterns.

We model the transformation by flips:

- correspond to an observed mechanism of atomic diffusion.
- do not modify the entropy of a tiling but can lower its energy.

Random flips

Markov chain on the tilings of a given region:

1. choose uniformly at random a vertex;
2. choose a flip to be performed;
3. perform it, if possible, with probability $\min(1, \exp(-\Delta E/T))$.

Ergodicity is ensured at $T > 0$ for $n \to 1$ and $n \to 2$ tilings.
At fixed T, Boltzmann/Gibbs stationary distribution:

$$\pi(x) = \frac{1}{Z(T)} \exp(-E(x)/T).$$

At $T = \infty$: uniform distribution (random sampling).
At $T = 0$: Dirac distribution (error-correcting chain).

The $2 \to 1$ case at $T = 0$

Tiling space: words with as many a as b.
Energy: number of pairs of neighboor equal letters.
At $T = 0$, the flips $abab \to aabb$ and $baba \to bbaa$ are forbidden.
Any word is eventually corrected. How fast?

The $2 \to 1$ case at $T = 0$

Tiling space: words with as many *a* as *b*.
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At $T = 0$, the flips $abab \to aabb$ and $baba \to bbaa$ are forbidden.
Any word is eventually corrected. How fast?

$$\text{For} \quad \varphi(w) = \sum_{v \in \mathrm{DF}(w)} \sqrt{|v|} \quad \text{one shows} \quad \mathbb{E}(\Delta\varphi(w)|w)) \leq -\frac{1}{4n\sqrt{n}}.$$

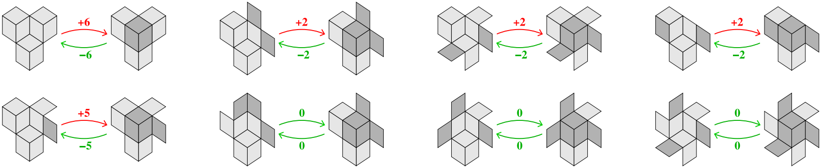
Theorem (Bodini-Fernique-Regnault, 2010)

The coupling time, hence the mixing time, is $O(n^3)$.

It is conjectured to be $\Theta(n^3)$. At least, it is $\Omega(n^2)$ (diameter).

The $3 \to 2$ case at $T = 0$

Tiling space: patches with the boundary of a 6-fold planar tiling.
Energy: number of pairs of neighboor equal tiles.



Any tiling is eventually corrected. How fast?

Theorem (Fernique-Regnault, 2010)

The coupling time, hence the mixing time, is $O(n^2\sqrt{n})$ (for n tiles).

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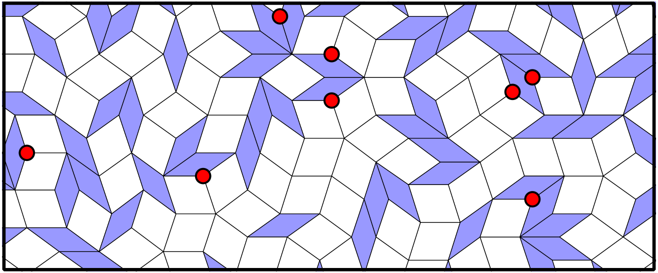
Beyond the $3 \to 2$ case at $T = 0$

Tiling space: patches with the boundary of, *e.g.*, a Penrose tiling.
Energy: number of forbidden patterns, *e.g.*, violated alternations.



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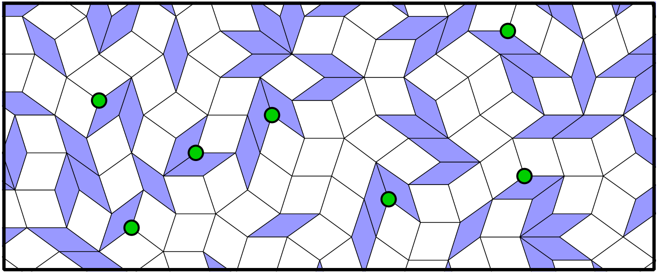

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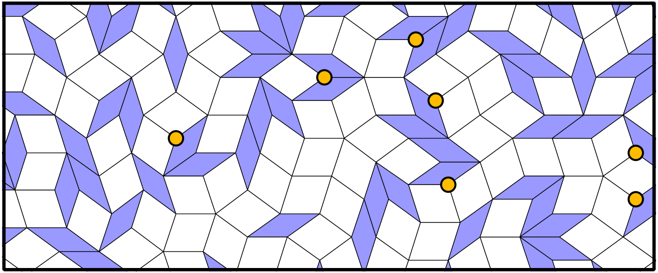

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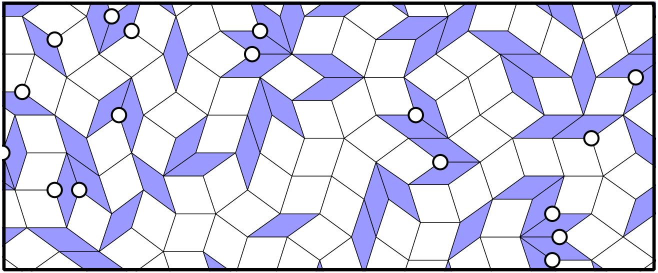

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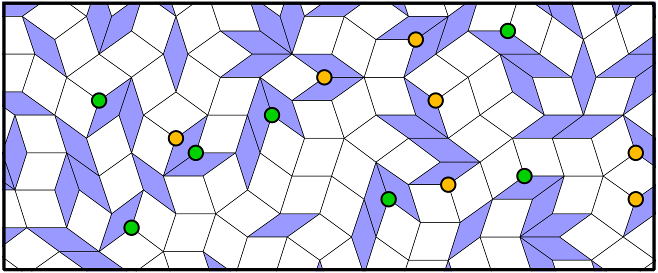

Simulations suggest a mixing time $\Theta(n^2)$...
...but it is still not proven that tilings are eventually corrected!

Cooling schedule

We considered Markov chains at two temperatures:

- $T = \infty$: random sampling;
- $T = 0$: error-correcting chain.

The chain at $T = 0$ aims to model the "quasicrystallization" but

- nothing really happens at $T = 0$ (frozen);
- flips allowed at $T > 0$ can fasten the correction (annealing).

Optimal cooling schedule?

Some open questions

- Do Penrose tilings have maximal entropy?
- Arctic circle phenomena beyond dimer tilings?
- Error-correcting "planarization" of $n \to d$ tilings?
- Mixing time of $n \to d$ tilings at $T = 0$? at any T?
- Phase transition (with T) in the mixing time?
- Optimal cooling schedule?