Stable quasicrystal phases via cellular automata

Siamak Taati

Mathematical physics of non-periodic structures
Będlewo — July 2018

Statistical mechanics of (quasi)crystals

[see Radin, IJMPB, 1987]

Crystalisation problem

Why do most material take crystalline order at sufficiently low temperature?

- Find a reasonable model of a crystal!
- Explain the prevalence of crystals!

Inherently
a continuum problem

Quasicrystal problem

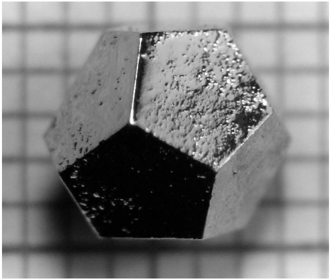
Explain the stability of quasicrystals at positive temperature!

- Find a reasonable (abstract) model of a quasicrystal!

Remains non-trivial
even on the lattice

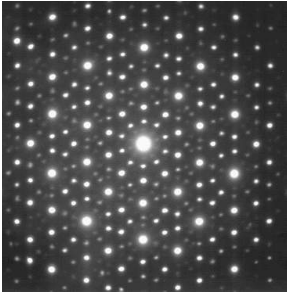
What are quasicrystals?

A Ho-Mg-Zn quasicrystal



from Wikipedia

Diffraction pattern



By Materialscientist [CC BY-SA 3.0]
via Wikimedia Commons

Five-fold rotational symmetry is inconsistent with translational symmetry!

Long-range orientational order but
no translational order

Quasicrystal problem (v1)

Problem

Construct a finite-range lattice-gas model
with a "quasicrystal phase" at positive temperature.

Question: What is a "quasicrystal phase"?

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Q1.1: What is "long-range order"?

[non-uniqueness of Gibbs measures]

Q1.2: What is "translational order"?

[existence of non-extremal ergodic Gibbs measures]

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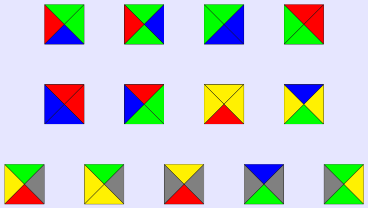
Answer 2: I don't know a perfect definition but ...
we may not need a perfect definition in order
to construct an example!

Q2.1: What are some desired properties?

Aperiodic Wang tiles

Wang tiles are combinatorial relatives of geometric tiles.

Example (Kari-Culik tiles)



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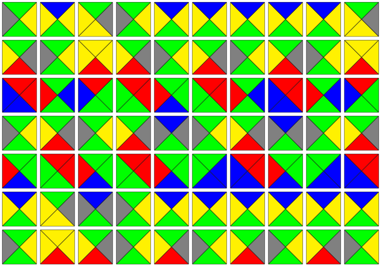


Adapted from C. Rocchini [CC BY-SA 3.0] via Wikimedia Commons

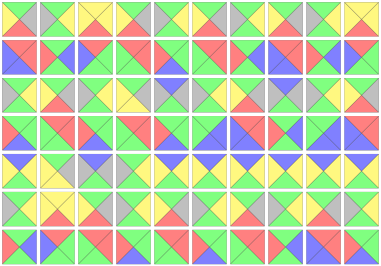
An aperiodic set of Wang tiles

- can tile the entire lattice, but [rotation not allowed]
- none of the valid tilings are periodic.

Quasicrystals at zero temperature

[Radin, JMP, 1985; PL, 1986]

Take your favorite aperiodic set of Wang tiles.
Assign interaction energy $+1$ to each tiling error.



- Every ground configuration is non-periodic.

  [Possibly with infinite lines of defect]

- The ground states are supported at ground configurations.

  [ground state $\equiv$ zero-temperature accumulation of Gibbs measures]

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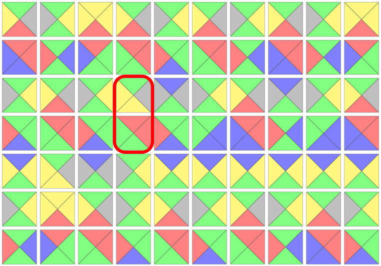

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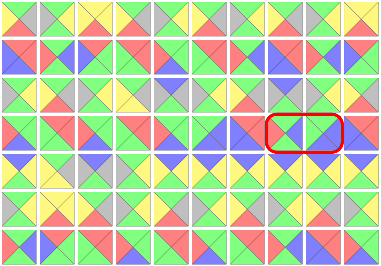

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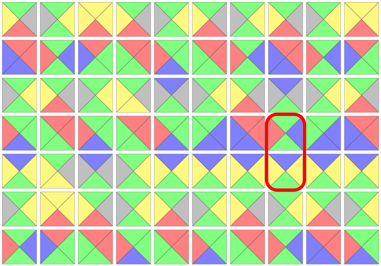

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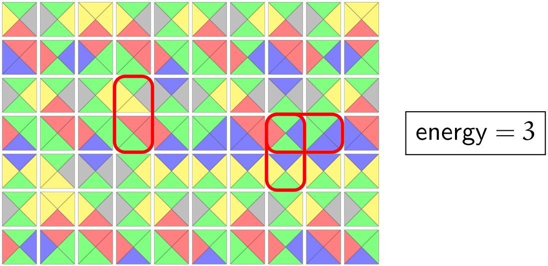

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Quasicrystal problem (v2)

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Construct an aperiodic tile set and a suitable finite-range interaction such that all (or some) non-periodic tilings are "stable at positive temperature".

Question: What does "stability at positive temperature" mean?

Answer: A ground configuration is stable if at any sufficiently low temperature, there is a Gibbs measure that is a "perturbation" of that configuration.

[Stability against thermal fluctuations]

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[Stability against thermal fluctuations]

- Q: What is a "perturbation"?
- A1: Close in weak topology [not sufficient]
- A2: Close in weak topology uniformly for all translations
- A3: Agree everywhere except on occasional finite (random) islands of fault. [Sea-island picture]

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Construct an aperiodic tile set and a suitable finite-range interaction such that all (or some) non-periodic tilings are "stable at positive temperature".

Our result

A four-dimensional finite-range lattice-gas model with 17 symbols (1 blank + 16 different types of particles) such that

- the non-blank symbols form an aperiodic tile set along two dimensions, and
- configurations that form valid tilings along two dimensions and are constant along the other two are strongly stable at positive temperature.

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Remarks

- The interaction window is included in a $2 \times 2 \times 2 \times 2$ box.
- Being periodic along two dimensions is not really a limitation.
  [Combine two independent copies, one rotated.]
- There are other "non-quasicrystalline" Gibbs measures.

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Corollary 1

At sufficiently low temperature, the model has non-periodic Gibbs measures supported on perturbations of a "cloned" tiling configuration. [sea-island picture]

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Corollary 2

At sufficiently low temperature, the model has a translation-invariant Gibbs measure with sea-island picture with respect to the orbit closure of a "cloned" tiling configuration.

Quasicrystal problem

Some related results

- van Enter, Miękisz and Zahradnik (1998):
  A three-dimensional model with infinite-range but exponentially decaying interactions that has a "quasi-crystal" ground configuration stable at positive temperature.
  [Thue-Morse sequence along one dimension, constant along the other two]
- Durand, Romashchenko and Shen (2012):
  A two-dimensional aperiodic set of Wang tiles that is stable against small Bernoulli noise. [How about thermal noise?]
- Gács (2001):
  A two-dimensional model with a continuum of distinct extremal Gibbs measures.
- Chazottes and Hochman (2010): [also van Enter and Ruszel, 2007]
  A three-dimensional finite-range model with no shift-invariant weakly stable ground state.

The construction

We simply put together three classic results about cellular automata (CA) and tilings.

The ingredients

I. Every d-dimensional CA can be simulated by a $(d+2)$-dimensional CA in a fashion that is robust against Bernoulli noise. [Gács and Reif (1988) based on Toom (1980)]

II. There are aperiodic tile sets that are deterministic in one direction. [Ammann (1980's), Kari (1992), ...]

III. The space-time diagrams of positive-rate probabilistic CA are Gibbs measures for an associated finite-range interaction. [Domany and Kinzel (1984), Goldstein, Kuik, Lebowitz and Maes (1989)]

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Cellular automata (CA)

CA are discrete-time dynamical systems on lattice configurations.

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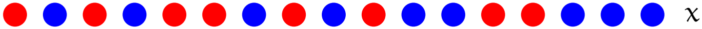

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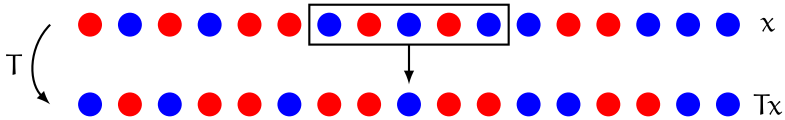

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Dynamics: The symbol at each site is updated according to a fixed local rule.

[Equivalently, T is continuous and commutes with translations.]

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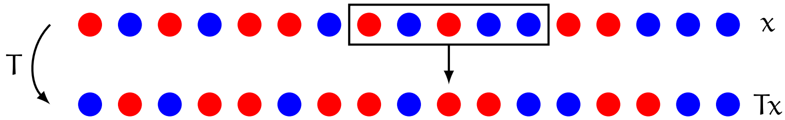

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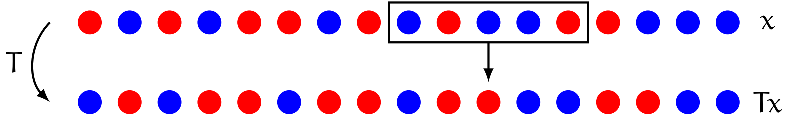

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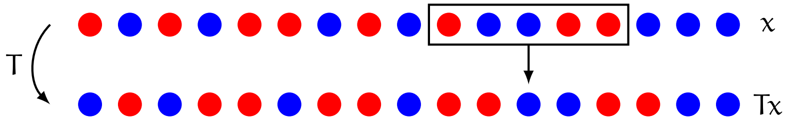

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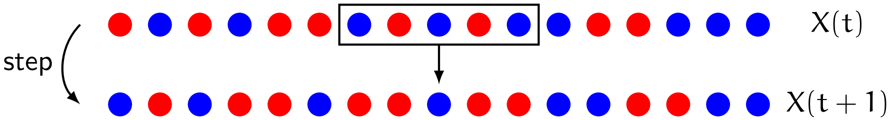

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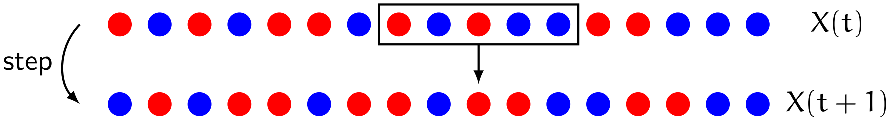

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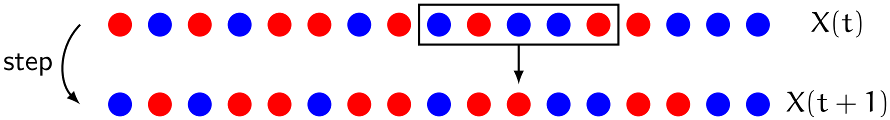

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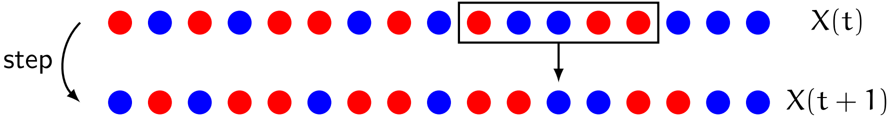

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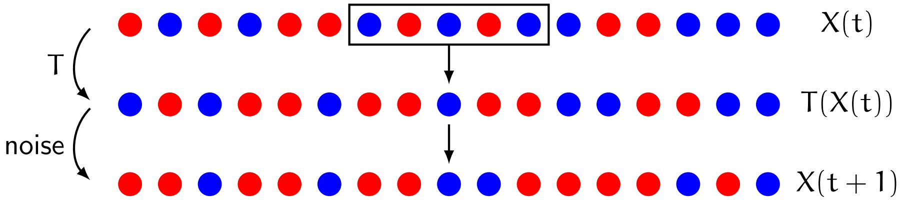
Noisy cellular automata (CA+noise)

A particular type of PCA.



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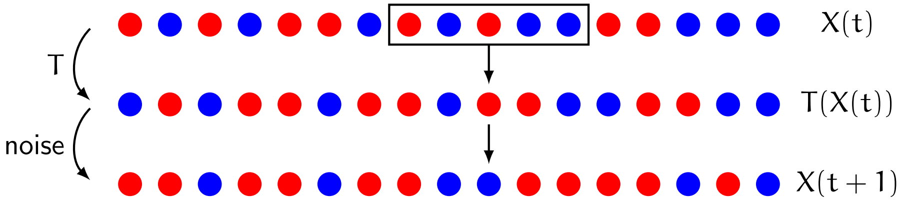

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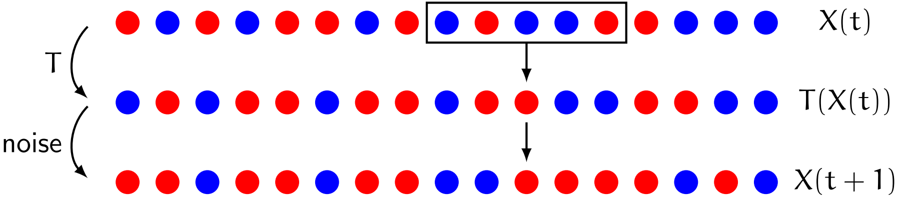

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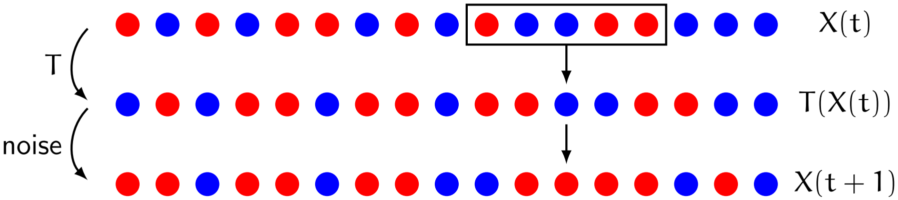

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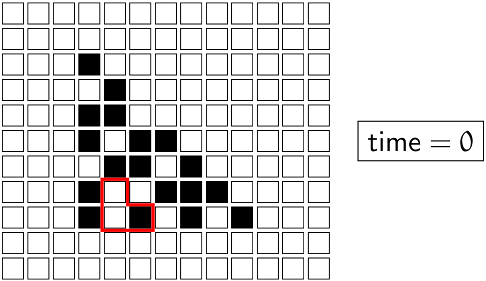
Toom's NEC CA

Two-dimensional deterministic CA with asymmetric majority rule.



Symbol set: {□, ■}

Local rule: North-East-Center majority

[$(Tx)_{i,j} \triangleq \text{majority}(x_{i,j},\, x_{i+1,j},\, x_{i,j+1})$]

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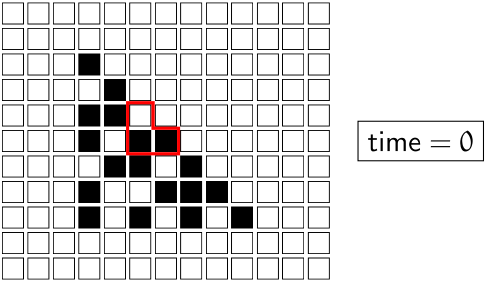

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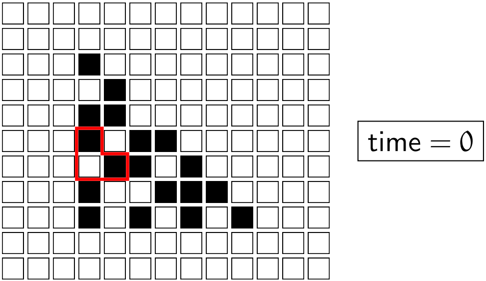

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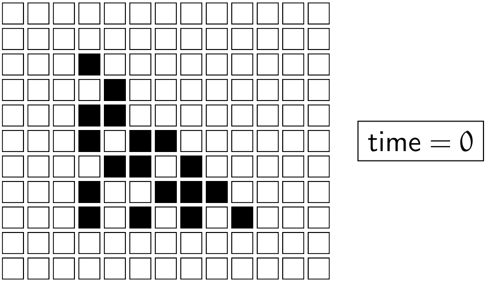

Cleaning finite islands

A finite island of black in a sea of white is quickly cleaned and vice versa! [A triangle of faults shrink.]

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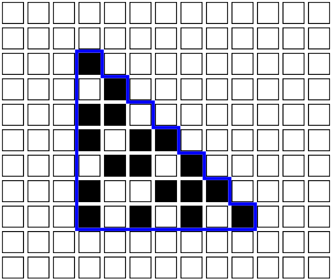

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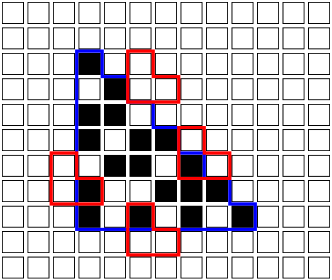

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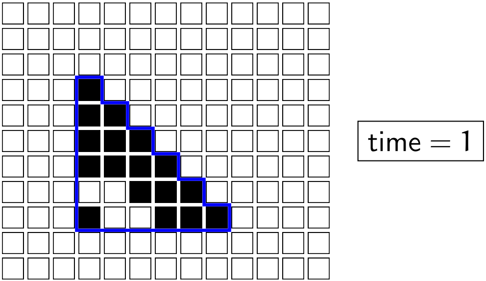

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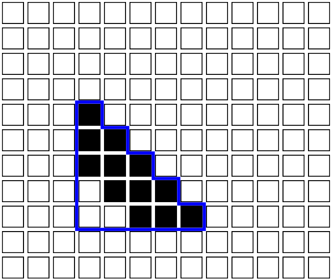

time = 2

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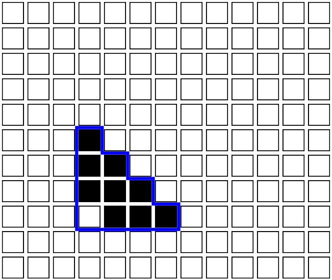

time $= 3$

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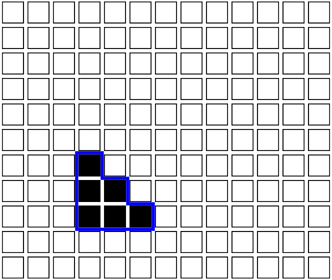

time $= 4$

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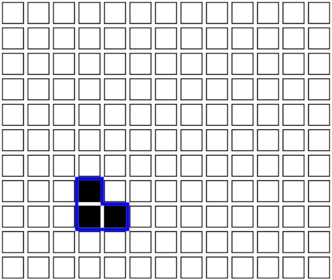

time = 5

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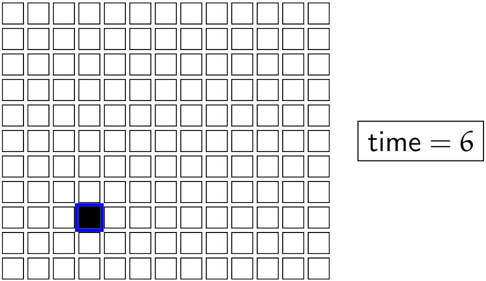

Cleaning finite islands

A finite island of black in a sea of white is quickly cleaned and vice versa! [A triangle of faults shrink.]

I. Robust simulation of CA

Toom's NEC CA

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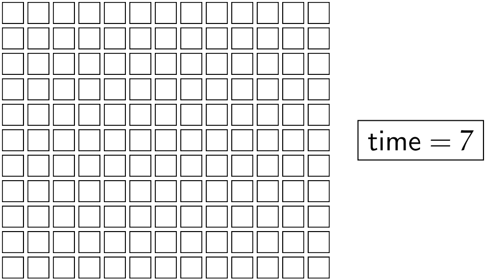

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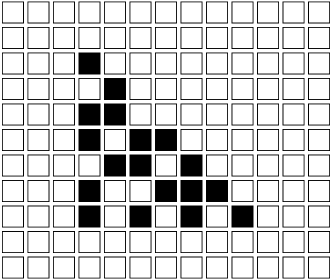


Theorem (Toom, 1980)

The trajectories of all-□ and all-■ are stable against small Bernoulli noise. *[The corresponding PCA has two distinct invariant measures.]*

I. Robust simulation of CA

Stacking simulation

[Gács and Reif (1988)]

Noise-resistant simulation of a d-dimensional CA with a $(d+2)$-dimensional CA.

To simulate a CA T,

- Replicate each symbol into a two-dimensional plane.

  [add two more dimensions]

- At each time step:
  1. Apply Toom's majority rule on each replicated plane.

     [Error correction!]

  2. Apply T on each d-dimensional space orthogonal to the replicated planes.

Theorem (Toom, 1980; Gács and Reif, 1988)

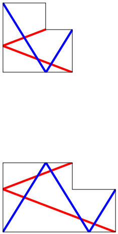
Every trajectory of the simulating CA corresponding to an initial configuration that is constant on each replicated plane is stable against independent noise.

II. Deterministic aperiodic Wang tiles

Ammann's golden tiles

[Ammann (1980's)]

Ammann's tile set A2 are geometric tiles with decorations.



- Rotations and reflections are allowed.
- The line decorations of adjacent tiles must match.

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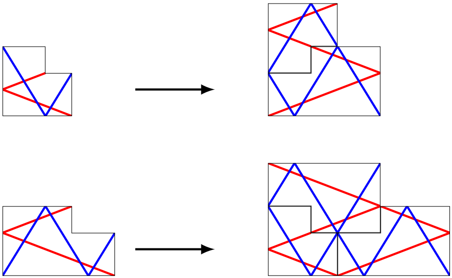

- The two tiles can be combined to simulate larger copies of themselves, with equivalent matching conditions.
  $\Longrightarrow$ existence of "self-similar" tilings

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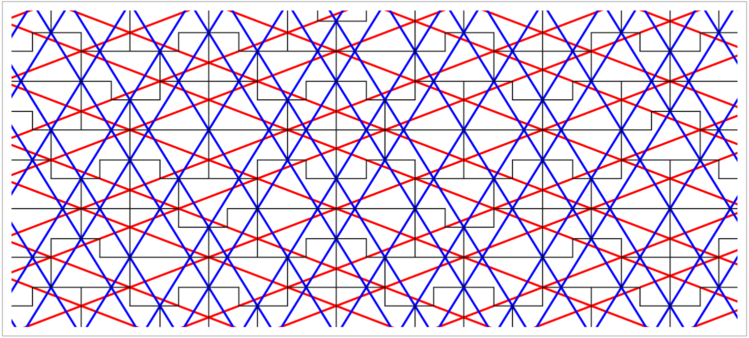

- Moreover, every valid tiling can be decomposed into such super-tiles in a unique fashion.

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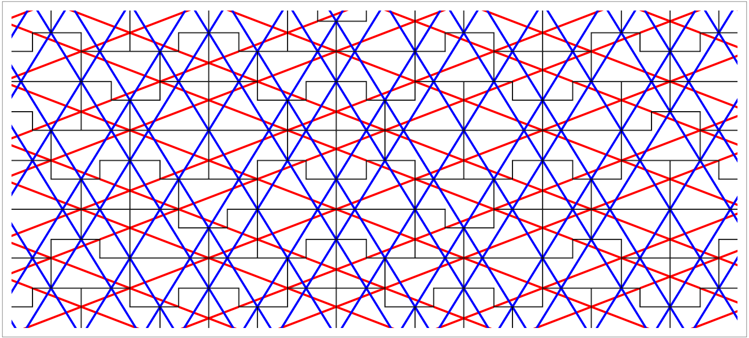


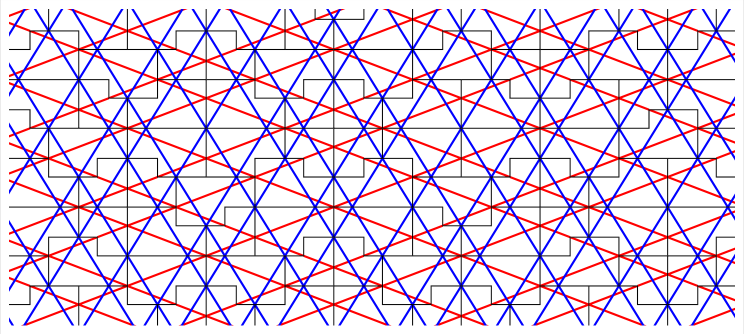
Theorem (Ammann, Grünbaum, Shephard, 1992)

Ammann's tile set is aperiodic.

II. Deterministic aperiodic Wang tiles

Ammann's golden tiles

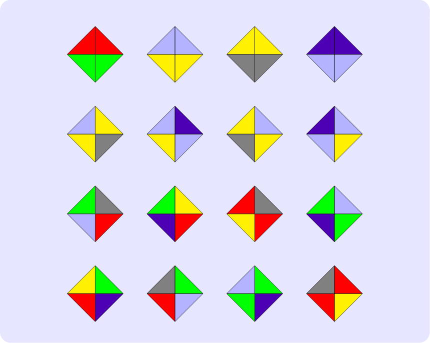
[Ammann (1980's)]



- The blue lines form a lattice!
  Furthermore, there are only 16 different blue parallelograms.
  These parallelogram can be symmetrized to obtain Wang tiles.

II. Deterministic aperiodic Wang tiles

Ammann's Wang tiles



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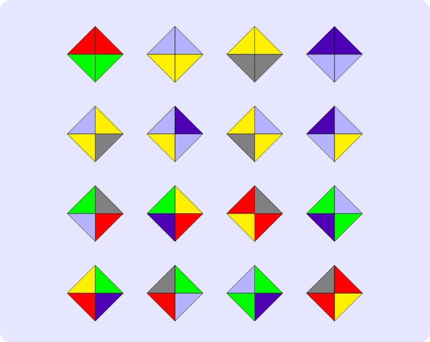


Determinism property

The two colors on the top determine the tile uniquely!

[So do the two on the bottom.]

II. Deterministic aperiodic Wang tiles

Determinism property

There are other aperiodic sets of Wang tiles with similar determinism property.

- Kari (1992): a variant of Robinson's aperiodic set.

  [The tiling problem remains undecidable (ibid.).]

- Kari and Papasoglu (1999): an aperiodic set that is deterministic in four directions.

  [Lukkarila (2009): The tiling problem remains undecidable.]

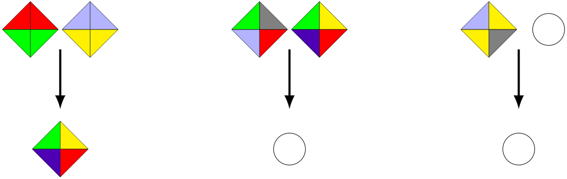
- Guillon and Zinoviadis (2016): an aperiodic set that is deterministic in all but two opposite (real) directions.

For us, any aperiodic set with determinism in one direction will do.

II. Deterministic aperiodic Wang tiles

CA from deterministic tiles

There is a natural way to construct a CA out of a deterministic tile set: [Kari (1992)]



if a matching tile exists.

if no matching tile exists.

blank leads to blank.

- Introduce a new blank symbol.
- By determinism, the matching tile (if it exists) is unique.
- Whenever no tile matches the color constraint, produce blank.

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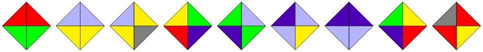

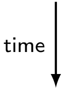

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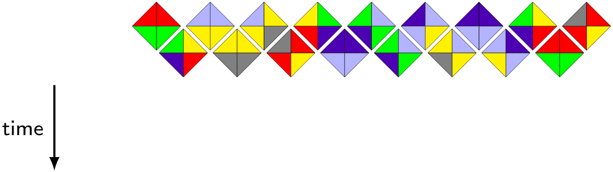

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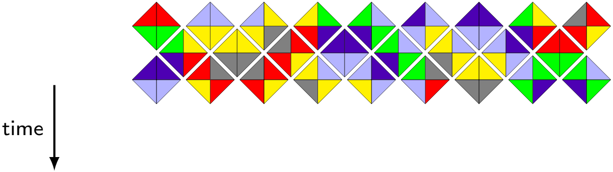

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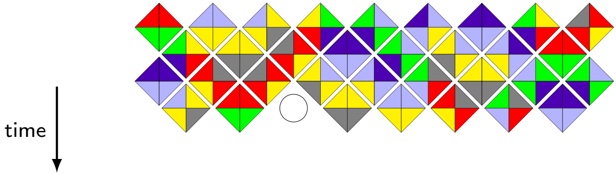

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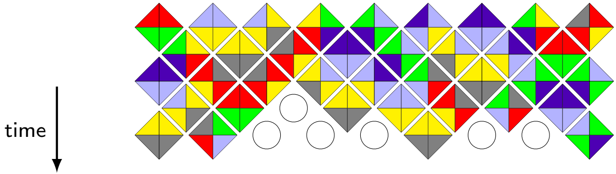

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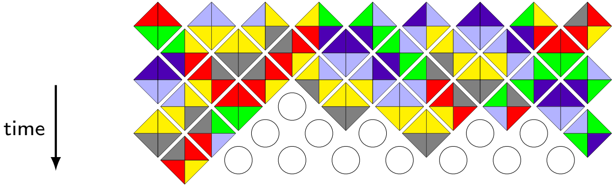

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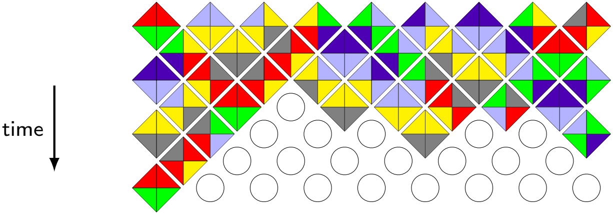

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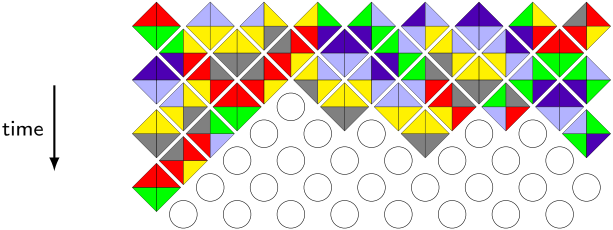

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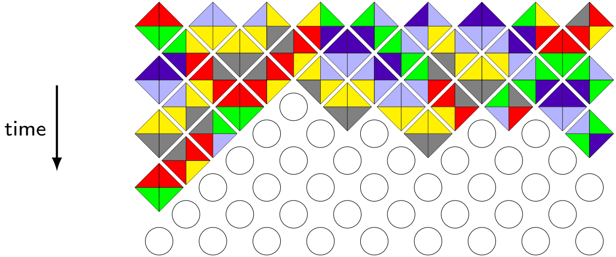

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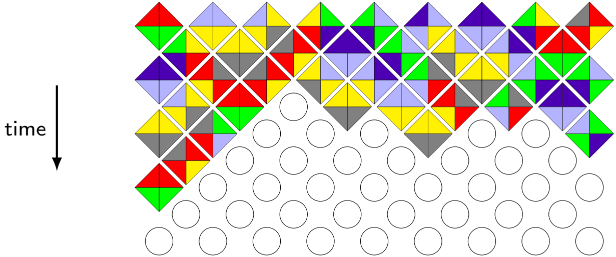
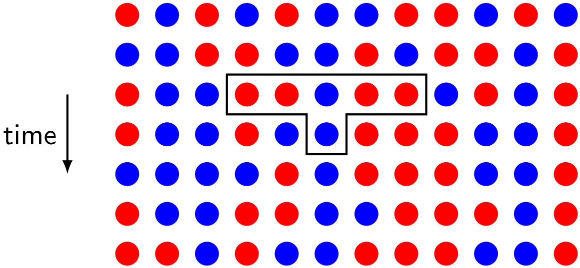


- The blank symbol spreads.
- The bi-infinite trajectories with no occurrence of the blank symbol are precisely the valid tilings.

III. Space-time diagram of PCA



Observation (Domany and Kinzel, 1984)

The distribution of any bi-infinite trajectory of any PCA is a Gibbs measure for an associated finite-range interaction.

[The zero-dimensional case is better known!]

The converse is also true for translation-invariant Gibbs measures.

[Goldstein, Kuik, Lebowitz and Maes (1989)]

The construction

We simply put together these three ingredients.

The ingredients

I. Every d-dimensional CA can be simulated by a $(d+2)$-dimensional CA in a fashion that is robust against Bernoulli noise. [Gács and Reif (1988) based on Toom (1980)]

II. There are aperiodic tile sets that are deterministic in one direction. [Ammann (1980's), Kari (1992), ...]

III. The space-time diagrams of positive-rate probabilistic CA are Gibbs measures for an associated finite-range interaction. [Domany and Kinzel (1984), Goldstein, Kuik, Lebowitz and Maes (1989)]

A quasicrystal at positive temperature

The construction

i) Take Ammann's aperiodic Wang tiles.

[...or any deterministic aperiodic set]

ii) Extend it to a 1d CA by introducing a blank symbol.

iii) Use Toom-Gács-Reif stacking to simulate this CA with a 3d CA that is resistant against noise.

iv) Add small symmetric noise to get a positive-rate PCA.

v) Consider the corresponding interaction in 4d.

Theorem

The 4d clone of every valid tiling with Ammann's tiles is a ground configuration that is strongly stable at positive temperature.

A quasicrystal at positive temperature

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Remarks

- Lowering the temperature corresponds to lowering the intensity of the noise. [$\tilde{\varepsilon}(\beta) = \frac{16(\varepsilon/16)^{\beta}}{(1-\varepsilon)^{\beta}+16(\varepsilon/16)^{\beta}}$]
- There are other Gibbs measures corresponding to immature tilings. [e.g., the all-blank configuration is also stable.]
- There might be other Gibbs measures that do not correspond to simulations of the 1d CA.

[I don't know all the invariant measures of Toom's CA + noise]

[Do all Gibbs measures correspond to space-time trajectories?]

Open problems

Q1: Is there a shift-invariant Gibbs measure with only non-periodic Gibbs measures in its extremal decomposition?

[Is Ammann's tile set α-aperiodic for some $\alpha > 0$?]

Q2: What is the advantage over independent Ising stacking?

[Here there is a simple order parameter ...]

Q3: Can we get rid of the non-quasicrystalline phases?

[Crystalization by decreasing the temperature]

Q4: Use Gács's (very sophisticated) construction (1986, 2001) to construct two-dimensional quasicrystals.

[Doesn't his model already contain quasicrystal phases?]

Q5: Show the (strong) stability of the aperiodic set of Durand, Romashchenko and Shen (2012) against thermal noise.

Q6: Is "low-temperature phase multiplicity" algorithmically (un)decidable?

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What to discuss next?