An attempt to sketch out the landscape

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Multidimensional symbolic dynamics and lattice models of quasicrystals

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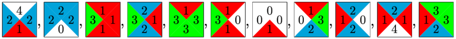


Motivations for this workshop

How and why many materials are ordered at low temperature?
(crystalline or quasicrystalline order)

Here the setting will be that of lattice ($= \mathbb{Z}^d$) systems (toy models).

Rich interplay between statistical mechanics, ergodic theory, (multidimensional) symbolic dynamics, and theoretical computer science.

Aperiodic Wang shifts (or tilings) play a prominent role when $d > 1$.

Pioneering work by Charles Radin and Jacek Miękisz.

Plan of the talk

- What can be a "quasi-crystal" in the context of lattice systems?
- Warming up by cooling down finite systems
- Gibbs states and equilibrium states on the lattice $\mathbb{Z}^d$
- Minimizing configurations, ground states and minimizing states
- What happens when temperature goes to 0?
- Can we reach a "quasi-crystal" at > 0 temperature?
- References (non-exhaustive list!)

Directly related talks

- Shmuel Friedland
- Guilhem Gamard
- Léo Gayral
- Juliano Gonschorowski
- Pascal Hubert
- Tamara Kucherenko
- Sébastien Labbé
- Jacek Miękisz
- Ronnie Pavlov
- Siamak Taati
- Philippe Thieullen
- Zizhu Wang

What can be a "quasi-crystal" in the context of lattice systems?

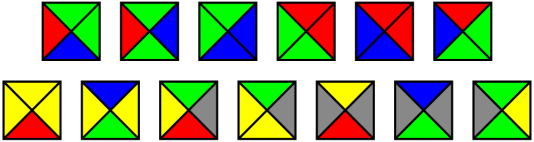
The game of statistical physics on the lattice $\mathbb{Z}^d$

Let $d \geq 1$ be an integer.

- We have a set S of different types of "particles". For instance, $S = \{-, +\}$ (Ising spins), or $S = \{0, 1\}$ (empty/occupied), etc.
- We place at each site of $\mathbb{Z}^d$ a "particle".
- A configuration is then an element of $S^{\mathbb{Z}^d}$.
- "Particles" interact through a potential which tells us what is the probability of having a given configuration in an arbitrary finite subset of $\mathbb{Z}^d$: this is called a Gibbs state or an equilibrium state.

A candidate for a "quasi-crystal" in $d = 2$

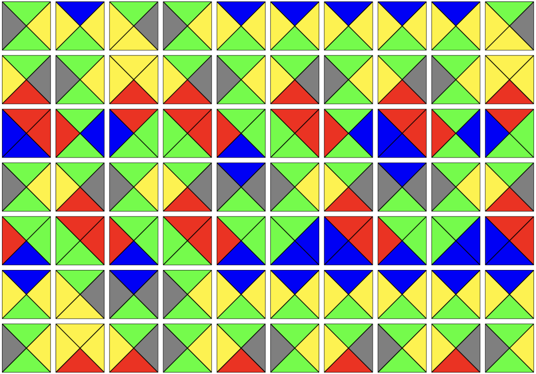
Now take $S = S_{KC}$ as the set of "tiles"



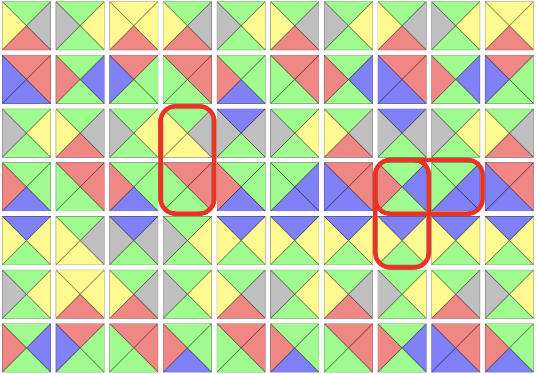
One can put a copy of one of these 1×1 squares centered at each $(i, j) \in \mathbb{Z}^2$ (without rotating them).

If two tiles are only allowed to touch along edges of the same colour, everywhere in $\mathbb{Z}^2$, then it can be proved that none of these tilings can be periodic (Kari-Culik).

This is an example of an aperiodic Wang shift, that is, an aperiodic subshift of finite type of $S_{KC}^{\mathbb{Z}^2}$.



A portion of a Kari-Culik tiling.



A portion of a Kari-Culik tiling with three “mistakes”.

Interaction potential : assign “energy” $+1$ to each “mistake”.
Thus, Kari-Culik tilings minimize energy, by construction.

The formalism of Gibbs states/equilibrium states allows to interpret "mistakes" as "thermal fluctuations" , using a "temperature" parameter.

Now, we can ask questions like :

Is the "Kari-Culik quasi-crystal" stable against thermal fluctuations ?

Warming up by cooling down finite systems

Setting

Let Ω be a **finite set** (space of ‘configurations’) :

- ‘state’ $\equiv$ probability vector $\nu = (\nu(\omega) : \omega \in \Omega)$
- Entropy of ν : $H(\nu) = -\sum_{\omega\in\Omega} \nu(\omega) \log \nu(\omega)$.
- Energy function $u : \Omega \to \mathbb{R}$ (assumed to take at least two distinct values).
  In state ν‘ the system has energy $\nu(u) := \sum_{\omega\in\Omega} \nu(\omega) u(\omega)$.

Remark. The set of states is a (finite-dimensional) simplex.

Gibbs states

For $\beta \in \mathbb{R}$ (*inverse temperature*) the Gibbs state μ_β is defined by

$$\mu_\beta(\omega) := \frac{e^{-\beta u(\omega)}}{Z(\beta)}$$

where

$$Z(\beta) = \sum_{\omega \in \Omega} e^{-\beta u(\omega)} \quad \text{(normalization).}$$

Remarks :

- Physically $\beta \geq 0$ (inverse temperature).
- All configurations have a strictly positive probability wrt μ_β.

Zero temperature limit

The set of *minimizing configurations* for u :

$$\Omega_{\min} = \{\omega : u(\omega) = \min_{\Omega} u\}.$$

As $\beta \to +\infty$

$$\mu_\beta(\omega) \to \mu_\infty(\omega) := \frac{\mathbb{1}_{\{\omega \in \Omega_{\min}\}}}{\text{card}(\Omega_{\min})} \quad (\textbf{zero-temperature limit}),$$

that is, equidistribution on $\Omega_{\min}$.

The support of μ_β becomes $\Omega_{\min} \subsetneq \Omega$, but when $\beta \to +\infty$.
(For all finite β, supp$(\mu_\beta) = \Omega$.)

Finally

$$H(\mu_\infty) = \log \text{Card}(\Omega_{\min}) \quad (= 0 \text{ if and only if } \text{Card}(\Omega_{\min}) = 1).$$

The variational principle

By definition, a state maximizing $\nu \mapsto H(\nu) - \nu(\beta u)$ is an *equilibrium state* of βu.

Theorem

The Gibbs state μ_β is the equilibrium state, that is,

$$\max_\nu \big(H(\nu) - \nu(\beta u) \big) = H(\mu_\beta) - \mu_\beta(\beta u) = P(\beta)$$

where the max is attained only at μ_β, and where $P(\beta) := \log Z(\beta)$ is the "pressure" of βu.

(Recall that $\nu(u) = \int u \, \mathrm{d}\nu = \sum_{\omega \in \Omega} u(\omega)\nu(\omega)$.)

Minimizing states (ground states)

By the variational principle : for all $\beta > 0$ and for any state ν

$$\frac{H(\nu)}{\beta} - \nu(u) \leq \frac{H(\mu_\beta)}{\beta} - \mu_\beta(u)$$

thus, taking $\beta \to +\infty$,

$$\mu_\infty(u) \leq \nu(u)$$

so

$$\mu_\infty(u) = min_\nu \, \nu(u) = \min_\Omega u.$$

A state ν for which the *min* is attained is called a **minimizing state** of u.

The zero-temperature limit μ_∞ is a minimizing state :

$$\mu_\infty(u) = \sum_{\omega \in \Omega} u(\omega)\mu_\infty(\omega) = \sum_{\omega \in \Omega_{\min}} \frac{1}{\mathrm{Card}(\Omega_{\min})} u(\omega) = \min_{\Omega} u.$$

Write $\Omega_{\min} = \{\omega^{(1)}, \ldots, \omega^{(k)}\}$ where $k := \mathrm{Card}(\Omega_{\min})$.

Then, any convex combination of the $\delta_{\omega^{(i)}}$ is a minimizing state of u.

Observe that μ_∞ is the evenly weighted centroid of the $\delta_{\omega^{(i)}}$'s :

$$\mu_\infty = \frac{1}{\mathrm{Card}(\Omega_{\min})} \sum_{i=1}^{k} \delta_{\omega^{(i)}}.$$

Also

$$H(\mu_\infty) = \log \mathrm{Card}(\Omega_{\min}) = \max\{H(\nu) : \nu \text{ minimizing state of } u\}.$$

Gibbs & equilibrium states for infinite lattice systems on the lattice $\mathbb{Z}^d$ (in a nutshell)

Setting

Now the configuration space is

$$\Omega = S^{\mathbb{Z}^d}$$

where S is a finite set.

So $\omega = (\omega_{\boldsymbol{i}})_{\boldsymbol{i} \in \mathbb{Z}^d}$, with $\omega_{\boldsymbol{i}} \in S$.

Dynamics : $\mathbb{Z}^d$ acts on Ω by the *shift* $T = \left(T^{\boldsymbol{j}} : \boldsymbol{j} \in \mathbb{Z}^d\right)$:

$$\left(T^{\boldsymbol{j}}\omega\right)_{\boldsymbol{i}} = \omega_{\boldsymbol{i}+\boldsymbol{j}}.$$

So (Ω, T) is the d-dimensional full shift.

Interaction potentials, Hamiltonians & local energy functions

Interaction potential $\Phi = (\Phi_\Lambda)_{\Lambda \Subset \mathbb{Z}^d}$:

- $\Phi_\Lambda : \Omega \to \mathbb{R}$ is continuous for each $\Lambda \Subset \mathbb{Z}^d$.
- $\Phi_\Lambda = \Phi_{\Lambda + \boldsymbol{j}} \circ T^{\boldsymbol{j}}$ for all $\boldsymbol{j} \in \mathbb{Z}^d$, $\Lambda \Subset \mathbb{Z}^d$ (shift-invariance).
- $\sum_{\Lambda \ni \mathbf{0}} \|\Phi_\Lambda\|_\infty < \infty$ ("absolute summability").

Fundamental subclass : finite-range interaction potentials
(*i.e.*, $\exists r \in \mathbb{N}$ s.t. $\Phi_\Lambda \equiv 0$ whenever $\mathrm{diam}(\Lambda) > r$)

Hamiltonian ("Energy") : $U_\Lambda^\Phi(\omega) = \sum_{\Delta \cap \Lambda \neq \emptyset} \Phi_\Delta(\omega)$.

Local energy function $\phi : \Omega \to \mathbb{R}$:

$$\phi(\omega) = \sum_{\Lambda \ni \mathbf{0}} \frac{\Phi_\Lambda(\omega)}{\mathrm{Card}(\Lambda)} \quad \text{(continuous)}\,.$$

(called "potential" by dynamicists)

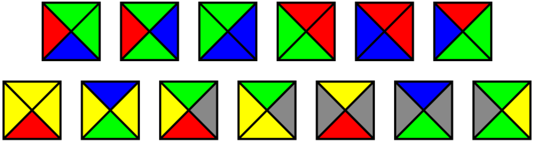
Dynamical systems ($d = 1$) :
An Axiom A diffeomorphism can be "coded" by a subshift of finite type and ϕ is a Hölder/Lipschitz continuous function.

Statistical physics ($d \geq 1$) : (ferromagnetic) Ising model
$S = \{-, +\}$ and

$$\Phi_\Lambda(\omega) = \begin{cases} -\omega_{\boldsymbol{i}}\,\omega_{\boldsymbol{j}} & \text{if} \quad \Lambda = \{\boldsymbol{i}, \boldsymbol{j}\} \quad \text{s.t.} \quad |\boldsymbol{i} - \boldsymbol{j}|_1 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

When $d = 1$, this is just a Markov chain.
When $d = 2$ it becomes much more interesting !

Statistical physics ($d = 2$) :

S : 

The 13 prototiles (= tileset) of Kari-Culik Wang shift

HAMILTONIAN U^{Φ}_{Λ} :

Given $\Lambda \Subset \mathbb{Z}^2$ (a $N \times N$ square, say), the energy of each configuration in Λ is equal to the number of links such that the colours of the facing edges are different.
So, the energy of the exactly matched configurations is zero, otherwise it is > 0.

Remark. About Kari-Culik Wang shift, see see the talk of G. Gamard.

Gibbs states & equilibrium states

I will not define directly Gibbs states in this talk.

For each $\beta \in \mathbb{R}$, the *set* of Gibbs states of $\beta\Phi$ contains at least one shift-invariant Gibbs state.

An equilibrium state of $\beta\phi$ is a **shift-invariant** measure μ such that

$$\sup\left\{h(\nu) - \nu(\beta\phi) : \nu \textbf{ shift-invariant}\right\} = h(\mu) - \mu(\beta\phi) = p(\beta\phi).$$

Remark : $p(\phi)$ is called the "pressure" of ϕ in ergodic theory.
See the talks of T. Kucherenko, P. Hubert ($d = 1$), and S. Friedland, R. Pavlov and T. Meyerovich ($d \geq 1$).

Theorem

For each β :
$\big\{$equilibrium states of $\beta\phi\big\} = \big\{$*shift-invariant* Gibbs states of $\beta\Phi\big\}$.

A bunch of questions

We want to do the same as for finite systems.

Given an interaction potential Φ :

1. What kind of set is the set of minimizing configurations ?
2.
   - Does the limit of $\mu_{\beta\phi}$ (in weak topology) always exist ? Answer : NO
   - If it does, is it equidistribution on the set of minimizing configurations ? Answer : NO
   - What about its entropy ?
3. Is it possible that the support of $\mu_{\beta\phi}$ become the set of minimizing configurations corresponding to a quasi-crystal, for all $\beta \geq \beta_c$, for some $\beta_c < +\infty$ (that is, $T_c = 1/\beta_c > 0$) ? ("freezing phase transition") Answer : YES when $d = 1$, WE DON'T KNOW when $d = 2$
4. Does the regularity of ϕ matter ? Answer : YES
5. Does the dimension d of the lattice matter ? Answer : YES

Minimizing configurations, ground states and minimizing states

The minimizing subshift

Define the subset of minimizing configurations

$$\Omega_{\min}(\Phi) = \left\{\omega \in \Omega : U_\Lambda^\Phi(\omega) \leq U_\Lambda^\Phi(\omega'_\Lambda \omega_{\mathbb{Z}^d\setminus\Lambda}),\ \forall \omega' \in \Omega,\ \forall \Lambda \Subset \mathbb{Z}^d\right\}.$$

Any measure whose support $\subseteq \Omega_{\min}(\Phi)$ is called a **ground state**.

In the above two examples :

- Ferromagnetic Ising model, $d = 2$:
  $\Omega_{\min}(\Phi) = \{$"all $+$ configuration", "all $-$ configuration"$\}$
- For the Kari-Culik interaction potential :
  $\Omega_{\min}(\Phi) \equiv$ Kari-Culik Wang shift.

A shift-invariant measure μ is said to be a **minimizing state** of ϕ if

$$\mu(\phi) \le \nu(\phi), \text{ for all shift-invariant measures } \nu.$$

Connecion between ground states and minimizing states :

Theorem (Schrader, 1970 ; Garibaldi-Thieullen, 2014)

- $\Omega_{\text{min}}(\Phi)$ is a subshift ($\equiv$ closed, shift-invariant subset), which we call the "minimizing subshift" of Φ.
- $\{\text{shift-invariant ground states of } \Phi\} = \{\text{minimizing states of } \phi\}$.

What happens when temperature goes to 0 (i.e., $\beta \to +\infty$)?

A general result

Folklore theorem

Let $(\beta_k)_{k\geq 1}$ be any sequence of inverse temperatures. For each β_k, pick up one of the equilibrium states of $\beta_k\phi$, call it μ_k.
Then, any accumulation point of $(\mu_k)_{k\geq 1}$ (in weak topology)

- is a minimizing state of ϕ,
- has maximal entropy among all the minimizing states of ϕ.

Corollary of the last two theorems :

$\lim_{\beta\to+\infty} \mu_\beta$ exists in at least two situations, namely

1. when $\Omega_{\min}(\Phi)$ is a uniquely ergodic subshift

   or

2. when $\Omega_{\min}(\Phi)$ has a unique measure of maximal entropy.

When $d = 1$, take for instance the Thue-Morse subshift (case 1), or the subshift of finite type on $S = \{0, 1\}$ with 11 forbidden (case 2).

What happens in general ?

- The cases $d = 1$ and $d \geq 2$ drastically differ.
- When $d = 1$, finite-range potentials behave differently from Lipschitz continuous potentials.

$d = 1$: THE FINITE-RANGE CASE

W.l.o.g., ϕ is of *finite range* if $\phi(\omega) = \phi(\omega')$,whenever $\omega_0 = \omega'_0, \omega_1 = \omega'_1$.
(Notice that $\mu_{\beta\phi}$ is the joint distribution of a stationary Markov chain.)

THEOREM (BRÉMONT [2003], LEPLAIDEUR [2005], JRC, GAMBAUDO, UGALDE [2011])

Let ϕ be of finite range. Then

- $\mu_\infty := \lim_{\beta\to\infty} \mu_\beta$ exists
- the minimizing subshift is a *subshift of finite type* (not necessarily transitive)
- there are finitely many ergodic minimizing states
- there is an "*algorithm*" to compute the barycentric decomposition of μ_∞ over the ergodic minimizing states (some coefficients may be equal to 0).

$d = 1$: THE LIPSCHITZ CONTINUOUS CASE

Let $\Omega' \subset \Omega = \{0,1\}^{\mathbb{Z}}$ be any subshift, and take

$$\phi(\omega) := d(\omega, \Omega')$$

where $d(\omega, \omega') = 2^{-\max\{k:\, \omega_i = \omega'_i,\, \forall |i| \leq k\}}$.

By construction, the minimizing states are supported on Ω'.

Fact : for each β, there is a unique equilibrium state for $\beta\phi$.

THEOREM (JRC, HOCHMAN [2010], CORONEL, RIVERA-LETELIER [2015]

One can construct subshifts $\Omega' \subset \{0,1\}^{\mathbb{Z}}$ such that the family $(\mu_\beta)_{\beta>0}$ does not converge, as $\beta \to \infty$.

Remark. Coronel and Rivera-Letelier prove a somewhat stronger result.

$d \geq 2$, finite-range potentials

Theorem (JRC, Hochman [2010])

Let $d \geq 3$. Then, there exist finite-range interaction potentials Φ such that for any family $(\mu_\beta)_{\beta>0}$ in which μ_β is an equilibrium state of $\beta\phi$, $\lim_{\beta\to\infty} \mu_{\beta\phi}$ does not exist.

Theorem (JRC, Shinoda [2021], Barbieri, Bissacot, Dalle Vedove, Thieullen [2022])

Let $d = 2$. Then, there exist finite-range interaction potentials Φ such that for any family $(\mu_\beta)_{\beta>0}$ in which μ_β is an equilibrium state of $\beta\phi$, $\lim_{\beta\to\infty} \mu_{\beta\phi}$ does not exist.

The previous theorems heavily rely on constructions (simulations by a Turing machine) of 1D (effective) subshifts by a 2D or 3D subshifts of finite type.

See the talks of Léo Gayral and Philippe Thieullen.

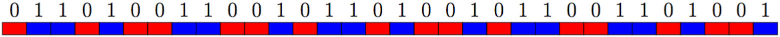
Can we reach a "quasi-crystal" at > 0 temperature?

$d = 1$, "weird" potentials

The Thue-Morse substitution $0 \mapsto 01$, $1 \mapsto 10$ has two fixed points

$$\omega^{(0)} = 01101001\ldots \quad \text{and} \quad \omega^{(1)} = 10010110\ldots$$

Thue-Morse subshift $\mathtt{TM} := \overline{\bigcup_n T^n(\omega^{(0)})}$. It has no periodic points, zero topological entropy, and uniquely ergodic.



A portion of a configuration.

Theorem (Bedaride, Cassaigne, Hubert, Leplaideur [2024])

Let $\phi(\omega) = \frac{1}{n}$ if $d(\omega, \mathtt{TM}) = 2^{-n}$. Then, there exists $\beta_c \in]0, \infty)$ such that :

- for $\beta < \beta_c$, there is a unique equilibrium state $\mu_{\beta\phi}$ with full support,
- for *all* $\beta \geq \beta_c$, the unique equilibrium state for $\beta\phi$ is μ_{TM}.

Other results in $d = 1$

- J. Buzzi, B. Kloeckner, R. Leplaideur (2023), see the list of references.
- See the talk of Tamara Kucherenko.

$d \geq 2$, FINITE-RANGE POTENTIALS

Phase transitions from a "disordered phase" to a "quasi-crystalline phase" :

Numerical evidences in $d = 2$: L. Leuzzi and G. Parisi (2000), D. Aristoff and C. Radin (2011), Z. Rotman, E. Eisenberg (2011).

A rigorous result :

For an example in $d = 4$, there is construction by S. Taati.
`https://siamak.isoperimetric.info/talks/Bedlewo2018.pdf`

There are many open problems!

A (non-exhaustive!) list of references

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- See several papers of J. Miękisz : `https://www.mimuw.edu.pl/~miekisz/quasicrystals.html`, some with A. van Enter.
- See several papers of Ch. Radin : `https://web.ma.utexas.edu/users/radin/tiling.html`.
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