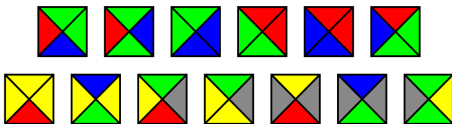


THERMODYNAMIC FORMALISM, SYMBOLIC DYNAMICS, AND MODELS OF QUASICRYSTALS

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INTRODUCTION

Mathematically open problem (even in the non-quantum setting) :

HOW AND WHY DO MANY MATERIALS ORDER
AT “SUFFICIENTLY LOW TEMPERATURE” ? (“PHASE TRANSITION”)
(CRYSTALLINE ORDER, SOMETIMES QUASI-CRYSTALLINE)

Very few results to date!

Toy models : lattice models (\mathbb{Z}^d).

Goal of this talk : A brief overview of this field of research...
... while minimizing the technical aspects. 😊.

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

THERMODYNAMIC FORMALISM : **A (VERY BRIEF) OVERVIEW**

INGREDIENTS :

- Ω : **finite set** (space of “configurations”).
- “state” : probability vector $\nu = (\nu(\omega) : \omega \in \Omega)$.
- **Entropy** of ν : $H(\nu) = - \sum_{\omega \in \Omega} \nu(\omega) \log \nu(\omega) (\in [0, \log \text{Card}(\Omega)])$.
- **Energy function** $u : \Omega \rightarrow \mathbb{R}$ (supposed to take at least two distinct values).
In state ν , the energy of the system is $\nu(u) := \sum_{\omega \in \Omega} \nu(\omega) u(\omega)$.

GIBBS STATES

For $\beta \geq 0$ ($\beta = 1/T$, T = “temperature”), the Gibbs state μ_β for the energy function u is

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

where

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

Remarks :

- When $\beta = 0$, $\mu_\beta(\omega) = 1/\text{card}(\Omega)$ (equidistribution, maximal entropy)
- All configurations have a > 0 μ_β -probability.
- What happens when $\beta \rightarrow +\infty$ (that is, when temperature goes to 0)?

THE VARIATIONAL PRINCIPLE AND EQUILIBRIUM STATES

Definition.

A state that minimizes $\nu \mapsto \nu(\beta u) - H(\nu)$ is an *equilibrium state* for βu .

PROPOSITION

For a state ν , one has

$$\nu(\beta u) - H(\nu) \geq -\log Z(\beta)$$

with equality if and only if $\nu = \mu_\beta$.

Remark : $P(\beta) := -\log Z(\beta)$ is the “free energy” for βu .

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

PROOF

Fix a state ν .

Apply Jensen's inequality to the convex function $\theta(x) = x \log x$, and since $\mu_\beta(\omega) := e^{-\beta u(\omega)} / Z(\beta)$:

$$\begin{aligned} \nu(\beta u) - H(\nu) + \log Z(\beta) &= \sum_{\omega \in \Omega} \nu(\omega) \log \frac{\nu(\omega)}{\mu_\beta(\omega)} \\ &= \sum_{\omega \in \Omega} \mu_\beta(\omega) \theta\left(\frac{\nu(\omega)}{\mu_\beta(\omega)}\right) \\ &\geq \theta\left(\sum_{\omega \in \Omega} \mu_\beta(\omega) \frac{\nu(\omega)}{\mu_\beta(\omega)}\right) \\ &= \theta(1) = 0. \end{aligned}$$

θ is strictly convex, hence equality holds if and only if $\omega \mapsto \frac{\nu(\omega)}{\mu_\beta(\omega)}$ is constant.



MINIMIZING CONFIGURATIONS, GROUND STATES AND ZERO-TEMPERATURE LIMIT ($\beta \rightarrow +\infty$)

The set of *minimizing configurations* for u :

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

$\beta \rightarrow +\infty$:

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

i.e., equidistribution on Ω_{\min} .

Hence the **support** of μ_{β} becomes $\Omega_{\min} \subsetneq \Omega$ in the limit $\beta \rightarrow +\infty$.
(For every **finite** β , $\text{support}(\mu_{\beta}) = \Omega$.)

Finally

$$H(\mu_{\infty}) = \log \text{card}(\Omega_{\min}) \quad (= 0 \text{ iff } \text{card}(\Omega_{\min}) = 1).$$

A state ν is called a “ground state” for u if for every other state ν' , we have

$$\nu'(u) \geq \nu(u).$$

However, by the variational principle :
for every $\beta > 0$ and for every state ν ,

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

Hence, si $\beta \rightarrow +\infty$, on a

$$\nu(u) \geq \mu_\infty(u).$$

Therefore μ_∞ is a ground state (for u).

One can check that $\min_\nu \nu(u) = \min_\Omega u = \mu_\infty(u)$.

LATTICE MODELS ON \mathbb{Z}^d :

A (VERY) BRIEF OVERVIEW OF GIBBS STATES AND EQUILIBRIUM STATES

INGREDIENTS :

- A finite set S , for instance :

- $S = \{-, +\}$ (“spins”);
- $S = \{0, 1\}$ (“empty/occupied” site);
- $S = \left\{ \begin{array}{cccccc} \begin{array}{c} \color{red}\blacktriangle \color{green}\blacktriangle \\ \color{blue}\blacktriangle \color{red}\blacktriangle \end{array} & \begin{array}{c} \color{red}\blacktriangle \color{green}\blacktriangle \\ \color{blue}\blacktriangle \color{red}\blacktriangle \end{array} & \begin{array}{c} \color{green}\blacktriangle \color{blue}\blacktriangle \\ \color{red}\blacktriangle \color{green}\blacktriangle \end{array} & \begin{array}{c} \color{red}\blacktriangle \color{blue}\blacktriangle \\ \color{green}\blacktriangle \color{red}\blacktriangle \end{array} & \begin{array}{c} \color{blue}\blacktriangle \color{red}\blacktriangle \\ \color{green}\blacktriangle \color{blue}\blacktriangle \end{array} & \begin{array}{c} \color{red}\blacktriangle \color{green}\blacktriangle \\ \color{blue}\blacktriangle \color{red}\blacktriangle \end{array} \\ \begin{array}{c} \color{yellow}\blacktriangle \color{red}\blacktriangle \\ \color{green}\blacktriangle \color{yellow}\blacktriangle \end{array} & \begin{array}{c} \color{blue}\blacktriangle \color{yellow}\blacktriangle \\ \color{green}\blacktriangle \color{blue}\blacktriangle \end{array} & \begin{array}{c} \color{red}\blacktriangle \color{yellow}\blacktriangle \\ \color{green}\blacktriangle \color{red}\blacktriangle \end{array} & \begin{array}{c} \color{yellow}\blacktriangle \color{green}\blacktriangle \\ \color{red}\blacktriangle \color{yellow}\blacktriangle \end{array} & \begin{array}{c} \color{gray}\blacktriangle \color{red}\blacktriangle \\ \color{green}\blacktriangle \color{gray}\blacktriangle \end{array} & \begin{array}{c} \color{blue}\blacktriangle \color{gray}\blacktriangle \\ \color{green}\blacktriangle \color{blue}\blacktriangle \end{array} & \begin{array}{c} \color{red}\blacktriangle \color{gray}\blacktriangle \\ \color{green}\blacktriangle \color{red}\blacktriangle \end{array} \end{array} \right\}.$

- **Configurations** : $\omega = (\omega_i)_{i \in \mathbb{Z}^d}$, $\omega_i \in S$, i site of the lattice \mathbb{Z}^d ;
 $\omega \in \Omega = S^{\mathbb{Z}^d}$.
- **Shift** (translation) : $(T^j \omega)_i = \omega_{i+j}$, $i, j \in \mathbb{Z}^d$.
- Interaction between sites : $\Phi = (\Phi_\Lambda)_{\Lambda \in \mathbb{Z}^d}$ (**potential**).

TWO EXAMPLES OF POTENTIALS

Ising ferromagnetic model with nearest neighbor interaction :

$$S = \{-, +\}, \Phi_\Lambda(\omega) = \begin{cases} -\omega_i \omega_j, & \text{if } \Lambda = \{i, j\}, |i - j|_1 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

A more general model (“long range”) :

$$\Phi_\Lambda(\omega) = \begin{cases} -J(i - j) \omega_i \omega_j, & \text{if } \Lambda = \{i, j\}, \\ 0 & \text{otherwise} \end{cases}$$

where $J(0) = 0$ et $\sum_{i \in \mathbb{Z}^d} |J(i)| < \infty$, for instance $J(i - j) = \frac{1}{|i - j|_1^\alpha}$, $\alpha > d$.

Many more models : Potts, Blume-Capel, etc.

INTERLUDE : WHY CONSIDER INFINITE LATTICES ?

Because non-trivial phenomena of “phase transitions” can occur (while they are *impossible* for finite systems).

A possible type of phase transition : non-uniqueness of equilibrium states for certain temperature regimes (see, e.g., the Ising model).

We will see a different type of phase transition.

EQUILIBRIUM STATES

Given Φ and β , we seek the states (\equiv probability measures on Ω) that are shift-invariant and minimize

$$\nu \mapsto \nu(\beta\varphi) - \text{entropy}(\nu),$$

where $\varphi : \Omega \rightarrow \mathbb{R}$ is the “energy per site” (derived from Φ).

Comments :

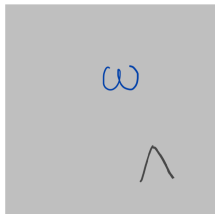
- $\varphi = \sum_{\Lambda \in \mathbb{Z}^d, 0 \in \mathbb{Z}^d} \Phi_\Lambda / \text{card}(\Lambda)$.
- $\text{entropy}(\nu)$: entropy “per unit volume” after taking the limit (“thermodynamic limit”).

GIBBS STATES

Gibbs state for Φ at temperature β^{-1} :
we want to construct measures on Ω
($=S^{\mathbb{Z}^d}$) such that

$$\text{Proba}(\omega \text{ in } \Lambda \mid \eta \text{ in } \Lambda^c) \\ \propto \exp(-\beta U_{\Lambda}^{\Phi}(\omega_{\Lambda} \eta_{\Lambda^c}))$$

(family of conditional probabilities)



for every $\Lambda \Subset \mathbb{Z}^2$ and for (almost) every “boundary condition” η .

SOME FACTS (THEOREMS)

Fix a potential Φ and an inverse temperature $\beta > 0$.

- There can exist *multiple Gibbs states*.
At least one must be shift-invariant, but not necessarily all.
- There can exist *multiple equilibrium states* (all of which are by *definition* shift-invariant).
Some of them may not be Gibbs states.
- For “absolutely summable” potentials $(^*)$:
 $\{ \text{shift-invariant Gibbs states} \} = \{ \text{equilibrium states} \}.$

(Recall : for a finite system, there is a unique Gibbs state, which is also the unique equilibrium state.)

$$(^*) : \sum_{\Lambda \in \mathbb{Z}^d, 0 \in \Lambda} \|\Phi_\Lambda\|_\infty < +\infty.$$

MODELS OF QUASICRYSTALS : APERIODIC TILINGS

AN EXAMPLE OF “QUASI-CRYSTAL” ($d = 2$): KARI-CULIK TILING

Take

$$S = \left\{ \begin{array}{cccccc} \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Yellow} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} \\ \hline \begin{array}{|c|} \hline \text{Yellow} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} \end{array} \right\} .$$

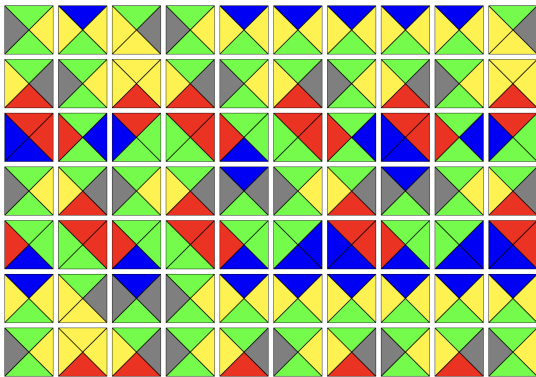
All possible configurations :

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

This gives the set $\left\{ \begin{array}{cccccc} \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Yellow} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} \\ \hline \begin{array}{|c|} \hline \text{Yellow} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} & \begin{array}{|c|} \hline \text{Green} \\ \hline \end{array} \end{array} \right\}^{\mathbb{Z}^2} .$

Now, let's select *only* the configurations satisfying the **constraint** :

the colors of the edges that touch must match.



A portion of a Kari-Culik tiling.

(The spaces are only there to improve visualization.)

FACTS ABOUT KARI-CULIK TILINGS

- The set of all Kari-Culik tilings is a subset of $\left\{ \begin{array}{cccccccc} \color{red}\blacktriangle & \color{green}\blacktriangle & \color{blue}\blacktriangle & \color{red}\blacktriangle & \color{green}\blacktriangle & \color{blue}\blacktriangle & \color{red}\blacktriangle & \color{green}\blacktriangle \\ \color{yellow}\blacktriangle & \color{blue}\blacktriangle & \color{red}\blacktriangle & \color{yellow}\blacktriangle & \color{red}\blacktriangle & \color{yellow}\blacktriangle & \color{blue}\blacktriangle & \color{green}\blacktriangle \end{array} \right\}^{\mathbb{Z}^2}$, which is closed and invariant under the shift action.
- Using the Kari-Culik tiles and following the color-matching rules, *one can tile (entirely) the plane.*
- The set of Kari-Culik tilings is *uncountable* and contains *no periodic configurations.*

Remarks :

- There are other examples of aperiodic tilings, constructed using other methods (Ammann, Jeandel-Rao, Labbé, etc.), which are also Wang tilings (dominoes).
- All of this can be translated into the language of multidimensional subshifts of finite type (symbolic dynamics).

Let $d \geq 2$.

We can ask the following (very natural) question :

Given a set of tiles, can we decide whether or not it can tile the plane?

By “decide”, we mean “find an algorithm”.

Theorem (Berger, 1964) : This is, in general, undecidable.

(Idea of the proof : encode Turing machines into sets of tiles; this transforms the problem into the halting problem, which is undecidable.)

Remark. For $d = 1$, the problem is decidable.

THERMODYNAMIC FORMALISM

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APERIODIC TILINGS

APERIODIC TILINGS AS MINIMIZING CONFIGURATIONS

Let's return to our lattice models.

Take your favorite potential Φ .

In simple terms, the configurations whose energy can only increase when modified at a finite number of sites are the minimizing configurations for Φ .

The shift-invariant states supported by these fundamental configurations are the ground states for Φ .

Consider again the set of Kari-Culik tiles

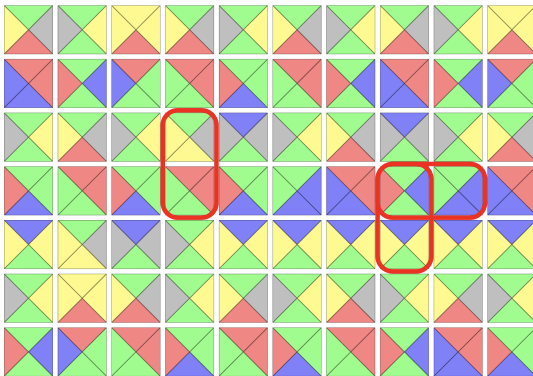
$$S = \left\{ \begin{array}{cccccc} \begin{array}{c} \text{red} \quad \text{green} \\ \text{blue} \quad \text{red} \end{array} & \begin{array}{c} \text{green} \quad \text{red} \\ \text{blue} \quad \text{green} \end{array} & \begin{array}{c} \text{green} \quad \text{blue} \\ \text{red} \quad \text{green} \end{array} & \begin{array}{c} \text{red} \quad \text{blue} \\ \text{green} \quad \text{red} \end{array} & \begin{array}{c} \text{blue} \quad \text{red} \\ \text{green} \quad \text{blue} \end{array} & \begin{array}{c} \text{red} \quad \text{green} \\ \text{blue} \quad \text{red} \end{array} \\ \begin{array}{c} \text{yellow} \quad \text{red} \\ \text{green} \quad \text{yellow} \end{array} & \begin{array}{c} \text{blue} \quad \text{yellow} \\ \text{red} \quad \text{blue} \end{array} & \begin{array}{c} \text{green} \quad \text{red} \\ \text{yellow} \quad \text{green} \end{array} & \begin{array}{c} \text{yellow} \quad \text{green} \\ \text{red} \quad \text{yellow} \end{array} & \begin{array}{c} \text{yellow} \quad \text{red} \\ \text{green} \quad \text{yellow} \end{array} & \begin{array}{c} \text{blue} \quad \text{yellow} \\ \text{red} \quad \text{blue} \end{array} & \begin{array}{c} \text{green} \quad \text{yellow} \\ \text{red} \quad \text{green} \end{array} \end{array} \right\}$$

and the corresponding Kari-Culik tilings.

A *possible* potential : assign an “energy” of 0 when adjacent colors match, and +1 for each “error” (mismatch).

This is a nearest-neighbor potential.

Thus, the Kari-Culik tilings minimize the energy by construction, meaning they are minimizing configurations, all aperiodic and forming an uncountable set.



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

WHAT HAPPENS AT POSITIVE (FINITE) TEMPERATURE?

Having “quasicrystals” as minimizing configurations is thus easy and possible with nearest-neighbor potentials.

But this corresponds to the situation of zero temperature.

What happens if the temperature is > 0 ?

Thermal fluctuations can lead to “errors.”

Question : Can we maintain a “quasicrystal” at temperature > 0 (without any “errors”)?

FREEZING PHASE TRANSITION

Is it possible that the equilibrium states or Gibbs states “see” all possible configurations for every $\beta < \beta_c$ (“disordered phase”), but they only “see” the configurations of a given “quasicrystal” for every $\beta > \beta_c$?

By “seeing a given configuration” ω , we mean that, for every $\Lambda \in \mathbb{Z}^d$, the probability of the event “all configurations η such that $\eta|_{\Lambda} = \omega|_{\Lambda}$ ” is > 0 .

For the Kari-Culik example :

- we would see all possible configurations belonging to

$$S = \left\{ \begin{array}{cccccccc} \color{red}\blacktriangle & \color{green}\blacktriangle & \color{blue}\blacktriangle & \color{red}\blacktriangle & \color{green}\blacktriangle & \color{blue}\blacktriangle & \color{red}\blacktriangle & \color{green}\blacktriangle \\ \color{yellow}\blacktriangle & \color{green}\blacktriangle & \color{red}\blacktriangle & \color{yellow}\blacktriangle & \color{red}\blacktriangle & \color{green}\blacktriangle & \color{yellow}\blacktriangle & \color{green}\blacktriangle \end{array} \right\}^{\mathbb{Z}^2} \text{ for } \beta < \beta_c,$$

- we would only see configurations corresponding exactly to the Kari-Culik tilings for $\beta > \beta_c$.

Theorem (J.-R. C., Tamara Kucherenko, Anthony Quas, 2025)

- ◆ For every $d \geq 1$, and for every “crystal” or “quasi-crystal,” one can construct (explicitly) a potential with a freezing phase transition.
- ◆ This potential must have a “sufficiently” long range.
- ◆ A potential decaying in a “summable” manner cannot have a freezing phase transition.

Some comments :

- **The “true” theorem is actually much more precise!**
- The nearest-neighbor potential presented for the Kari-Culik example therefore cannot have a freezing phase transition.
- Below the critical temperature (i.e., when $\beta > \beta_c$), the equilibrium states coincide with the measures of maximal entropy for the given quasi-crystal. These states cannot be Gibbs states.

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SUPPLEMENTS

If you insist...

Minimizing configurations :

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

where $U_{\Lambda}^{\Phi} = \sum_{\Delta \cap \Lambda \neq \emptyset} \Phi_{\Delta}$ (“energy in the volume Λ ”).

By definition, a **minimizing state** μ for Φ (or φ) is a shift-invariant state such that

$$\nu(\varphi) \geq \mu(\varphi), \text{ for every shift-invariant state } \nu.$$

(Theorem : $\Omega_{\min}(\Phi)$ is a subshift of Ω ; every shift-invariant state with support $\subseteq \Omega_{\min}(\Phi)$ is a ground state, and every minimizing state has its support $\subseteq \Omega_{\min}(\Phi)$ [Garibaldi-Thieullen, 2015].)