Gibbs measures and equilibrium states at low temperature

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Current Trends in Dynamical Systems and the Mathematical Legacy of Rufus Bowen

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Bowen's Lecture Notes (2682 citations): second, corrected edition (2017)

From Bowen's LN:

$$c_1 \leq \frac{\mu\{\underline{y} : y_i = x_i \ \forall\, i = 0, \ldots, m\}}{\exp\left(-Pm + \sum_{k=0}^{m-1} \phi(\sigma^k \underline{x})\right)} \leq c_2$$

for every $\underline{x} \in \Sigma_n$ *and* $m \geq 0$.

This measure μ is written μ_ϕ and called *Gibbs measure* of ϕ. Up to constants in $[c_1, c_2]$ the relative probabilities of the $x_0 \ldots x_m$'s are given by $\exp \sum_{k=0}^{m-1} \phi(\sigma^k \underline{x})$. For the physical system discussed above one takes $\phi = -\beta\phi^*$. In statistical mechanics Gibbs states are not *defined* by the above theorem. We have ignored many subtleties that come up in more complicated systems (*e.g.*, higher dimensional lattices), where the theorem will not hold. Our discussion was a gross one intended to motivate the theorem; we refer to Ruelle [9] or Lanford [6] for a refined outlook.

Motivation

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

This is a wide open program!

Perspective here: statistical mechanics of lattice systems (toy models)

Rich interplay between statistical mechanics, ergodic theory and (multidimensional) symbolic dynamics

Contents

Prelude: cooling down finite systems

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 $\nu(u) := \sum_{\omega\in\Omega} \nu(u) u(\omega)$.

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

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

Remarks:

- physically $\beta \geq 0$
- all configurations have a strictly positive probability wrt μ_β.

Zero temperature limit

The set of minimizing configurations for u:

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

As $\beta \to +\infty$

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

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

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

In particular

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

The variational principle

Theorem. Each Gibbs state μ_β satisfies

$$\sup_{\nu}\big(H(\nu) - \nu(\beta\boldsymbol{u})\big) = H(\mu_\beta) - \mu_\beta(\beta\boldsymbol{u}) = P(\beta),$$

where $P(\beta) := \log Z(\beta)$.

A state ν for which the 'sup' is attained is called an *equilibrium state* for $\beta\boldsymbol{u}$.

Thus Gibbs states are equilibrium states.

In fact μ_β is the only equilibrium state for $\beta\boldsymbol{u}$.

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

$$\mu_\infty(u) = \mathit{inf}_\nu\, \nu(u) = \min_\Omega u.$$

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

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

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

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 for u.

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

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

Also

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

Contents

GIBBS & EQUILIBRIUM STATES FOR INFINITE LATTICE SYSTEMS

Now the configuration space is

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

where S is a finite set of possible values of a configuration at a given site $\boldsymbol{i} \in \mathbb{Z}^d$, *e.g.*, $S = \{0, 1\}$.

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* $\left(T^{\boldsymbol{j}} : \boldsymbol{j} \in \mathbb{Z}^d\right)$:

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

(d-dimensional full shift.)

Interaction potentials, Hamiltonians & local energy functions

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

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

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

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

Local energy function ('potential', for dynamicists): $\phi : \Omega \to \mathbb{R}$

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

Example: the nearest-neighbor ($r = 1$) ferromagnetic Ising model

$S = \{-, +\}$ and

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

We have

$$\phi(\omega) = -\sum_{i=1}^{d} (\omega_{\mathbf{0}}\,\omega_{\mathbf{e}_i} + \omega_{\mathbf{0}}\,\omega_{-\mathbf{e}_i}).$$

Take Φ as above.

One can define (DLR equations), for each $\beta \in \mathbb{R}$, the *set* of Gibbs states (contains at least one shift-invariant Gibbs state).

An EQUILIBRIUM STATE for $\beta\phi$ is a **shift-invariant** measure μ such that

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

Theorem

The set of equilibrium states for $\beta\phi$ coincides with the set of *shift-invariant* Gibbs states for $\beta\Phi$.

Examples

- Take $d = 1$ and ϕ Hölder continuous, *i.e.*, $\exists C > 0$ and $\theta \in [0, 1)$ s.t.

$$\sup\{|\phi(\omega) - \phi(\omega')| : \omega_i = \omega'_i, |i| \leq n\} \leq C\,\theta^n, \forall n.$$

  Then, for each β, there is a unique Gibbs state μ_β for $\beta\phi$, which is also the unique equilibrium state (cf. Bowen's lect. notes). (Summability of 'sup ...' is enough.)

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- Back to the Ising model:
  - For $d = 1$, $\exists!$ Gibbs state for each β
  - For $d = 2$, there exists $\beta_c > 0$ such that $\exists!$ Gibbs state for each $\beta < \beta_c$, and the set of Gibbs states $\equiv [\mu_\beta^-, \mu_\beta^+]$ for each $\beta > \beta_c$, where μ_β^-, μ_β^+ are ergodic
  - For $d = 3$, for all β large enough, there exist non-shift invariant measures for $\beta\Phi$.

Back to freezing

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- Is it possible to have a 'freezing phase transition' (at *non-zero temperature, i.e., finite* β)?
- Does the regularity of the local energy function ϕ matter?
- Does the dimension d of the lattice matter?

The minimizing subshift

Fix Φ. Define

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

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

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

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

- $\Omega_{\min}(\Phi)$ is a subshift ($\equiv$ closed, shift-invariant subset), which we call the 'minimizing subshift' for Φ

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- One has

$$\mu \text{ shift-inv., } \operatorname{supp}(\mu) \subseteq \Omega_{\min}(\Phi) \iff \mu \text{ is a minimizing state for } \phi.$$

A general result on zero temperature

(Let Φ be a shift-invariant, absolutely summable interaction potential, and ϕ the corresponding local energy function.)

Folklore Theorem

For each β, let μ_β be any equilibrium state for $\beta\phi$. Then any accumulation point of $(\mu_\beta)_{\beta>0}$ (weak topology)

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

Basic observations about the existence of the zero-temperature limit

From the last two theorems, it follows at once that $\lim_{\beta\to+\infty}\mu_\beta$ exists

- if $\Omega_{\min}(\Phi)$ is a uniquely ergodic subshift
- or, if $\Omega_{\min}(\Phi)$ has a unique measure of maximal entropy.

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Zero-temperature limit: a positive result

We work with $\Omega = S^{\mathbb{N}}$.

Let $\phi : \Omega \to \mathbb{R}$ such that there exists $r \in \mathbb{N}$ such that

$$\phi(\omega) = \phi(\omega') \quad \text{whenever } \omega_i = \omega'_i,\, i = 0, \ldots, r.$$

Loosely, this means that $\phi(\omega) = \phi(\omega_0, \omega_1, \ldots, \omega_r)$.

For each β, the unique Gibbs/equilibrium state μ_β is nothing but the probability distribution of a certain stationary Markov chain with memory r and state space S.

Theorem (Brémont, 2003/ Leplaideur, 2005/ C., Gambaudo, Ugalde, 2011)

Let ϕ be such that there exists $r \in \mathbb{N}$ such that $\phi(\omega) = \phi(\omega_0, \omega_1, \ldots, \omega_r)$. Then

- the limit $\lim_{\beta\to\infty} \mu_\beta$ 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 $\lim_{\beta\to\infty} \mu_\beta$ over the ergodic minimizing states for ϕ (some coefficients may be equal to 0).

Remark. Generically, $\lim_{\beta\to\infty} \mu_\beta$ is equidistributed on a periodic orbit.

Zero-temperature limit: a negative result

Let $\Omega' \subset \Omega = \{0,1\}^{\mathbb{Z}}$ be any subshift, and ϕ the Lipschitz local energy function

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

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

By construction, the minimizing subshift for ϕ is Ω'.

We know (see Bowen) that, for each β, there is a unique Gibbs state μ_β which is also the unique equilibrium state for $\beta\phi$.

We can have 'chaotic temperature dependence':

Theorem (C., Hochman, 2010)

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

See also a paper by Coronel and Rivera-Letelier (2015).

A generic result

Take $\Omega = S^{\mathbb{N}}$.

Theorem (Contreras, 2016)

For an open and dense set of Lipschitz functions on Ω, the zero-temperature limit exists and is supported on a single periodic orbit.

Back to our original motivation

So far: we got, as $\beta \to \infty$, periodic order, sometimes 'chaotic order', or 'chaotic temperature dependence'.

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A (nontrivial) minimal uniquely ergodic subshift can be taken as a model of quasi-crystal:

- minimality $\equiv$ any pattern (word) appears again within a bounded distance
- unique ergodicity $\equiv$ the frequency of a pattern in a configuration ω converges uniformly wrt ω.

One can also ask for zero (topological) entropy.

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One can construct ϕ with a prescribed minimal uniquely ergodic subshift as a minimizing subshift, *e.g.*, the Thue-Morse substitution subshift. We know that $\lim_{\beta\to\infty} \mu_\beta = \mu_{TM}$.

An example of freezing phase transition

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

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

Then $\mathbb{K} := \overline{\bigcup_n T^n(\omega^{(0)})}$ is a subshift of $\{0,1\}^{\mathbb{N}}$ (the Thue-Morse subshift).
It has no periodic points and zero topological entropy.
It is uniquely ergodic. Denote by μ_{TM} its unique shift-invariant measure.

Theorem (Bruin, Leplaideur, 2013)

Consider $\phi : \{0,1\}^{\mathbb{N}}$ s.t.

$$\phi(\omega) = \begin{cases} 0 & \text{if } \omega \in \mathbb{K} \\ \phi(\omega) = \frac{1}{n} + o\left(\frac{1}{n}\right) & \text{if } d(\omega, \mathbb{K}) = 2^{-n}. \end{cases}$$

Then, there exists $\beta_c \in (0, \infty)$ such that:

- for $\beta < \beta_c$, there is a unique Gibbs/equilibrium state μ_β and $\mathrm{supp}(\mu_\beta) = \{0,1\}^{\mathbb{N}}$
- for *all* $\beta > \beta_c$, the unique equilibrium state for $\beta\phi$ is μ_{TM}.

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Zero-temperature limit for $d \geq 3$: a negative result

Recall that given an interaction potential $\Phi = (\Phi_\Lambda)_{\Lambda \Subset \mathbb{Z}^d}$, there is an associated local energy function $\phi : \Omega \to \mathbb{R}$.

Here we take

$$\Omega = \{0, 1\}^{\mathbb{Z}^d}.$$

Theorem (C., Hochman, 2010)

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

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Open question: prove the same result for $d = 2$.

Modelling quasicrystals when $d \geq 2$

Quasicrystal $\equiv$ minimizing subshift which is minimal and uniquely ergodic (hence without periodic configurations), and with zero topological entropy.

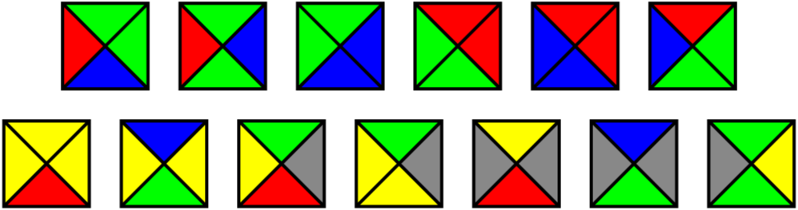
(Radin, Miękisz, van Enter, ...)

For $d = 1$, substitutions subshifts do the job (they are not subshifts of finite type).

What happens when $d \geq 2$?

A subshift of finite type without periodic configurations

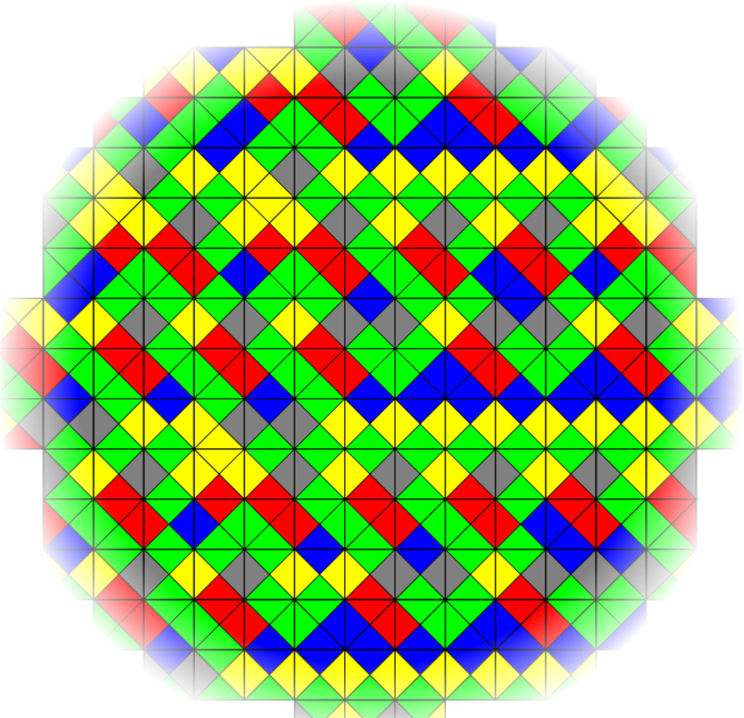
S :



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

Wang shift: $\mathcal{W} \subset S^{\mathbb{Z}^2}$ satisfying the (local) constraint:
'two tiles of are only allowed to touch along edges of the same colour'.

It is a subshift of finite type **without periodic configurations**.



Freezing phase transitions in dimension $d \geq 2$?

One can trivially define a nearest-neighbor interaction potential (range one) whose minimizing sushift is the previous Wang shift!

One can construct Wang shifts which are minimal and uniquely ergodic. They automatically have zero topological entropy.

Open question: find examples of freezing phase transitions to a minimal and uniquely ergodic Wang shift.

Warning: trichotomy & undecidability for Wang tilesets

There are three kinds of Wang tilesets:

1. those which cannot tile a n by n square for some n (so they can't tile the plane)
2. those which can tile a n by n square for some n with the same colors on the sides (periodic tiling)
3. those which can tile the plane but not periodically.

There is no algorithm to decide in which case a given tileset falls!

This has dramatic consequences on the structure of the set of finite-dimensional marginals of shift-invariant measures... but this is another story.