Analyticity for Classical Gasses via Recursion

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What is a classical gas/Gibbs point process?

For us, a *classical gas* (also known as *Gibbs point process*) is built from three ingredients:

1. A bounded set $S \subset \mathbb{R}^d$
2. A pair potential $\phi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$
3. An activity $\lambda \geq 0$.

For a finite set of points $\mathbf{X} = \{x_j\}_j$, define the *energy* $U(\mathbf{X}) = \sum_{i<j} \phi(x_i - x_j)$.

The *classical gas/Gibbs point process* $\mathbf{X} = \{x_j\}_j$ has density $\exp(-U(\mathbf{X}))$ against a Poisson point process of intensity λ in the set S.

For us, assume ϕ is *repulsive* so $\phi \geq 0$, and *tempered* so $\int_{\mathbb{R}^d} 1 - e^{-\phi(x)}\, dx < \infty$.

What does it behave like?

A Poisson point process of intensity λ wants to spread points in the set S at density λ with no interaction whatsoever (i.e. $\phi \equiv 0$ is a Poisson process).

When we introduce the potential ϕ, we pay a probabilistic penalty of $\exp(-\sum_{i<j} \phi(x_i - x_j))$ for a configuration $\mathbf{X} = \{x_j\}$.

Since we assumed $\phi \geq 0$, $\mathbf{X}$ "wants" to have a configuration with small energy $\sum_{i<j} \phi(x_i - x_j)$; this will mean it wants to have points further apart.

Another way to think about it: sample a Poisson point process $\mathbf{X}$ of intensity λ in S and accept it with probability $\exp(-\sum_{i<j} \phi(x_i - x_j))$.

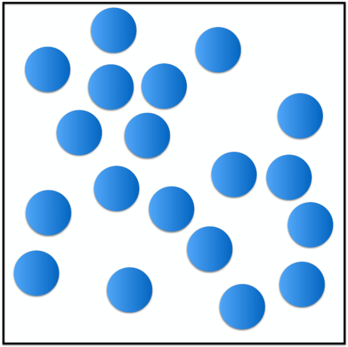
A special case: Hard spheres

Let $S \subset \mathbb{R}^d$ bounded, $\lambda > 0$, $r > 0$.

Define

$$\phi(x) = \begin{cases} +\infty & \text{if } |x| \leq 2r \\ 0 & \text{else} \end{cases} .$$

Think of the points as centers of spheres of radius r which are not allowed to overlap.



Some history

- A basic model of a gas.
- Studied by lots (e.g. Boltzmann, lots of others).
- Metropolis-Hastings algorithm was first used to sample the 2-dimensional hard sphere model.

Question

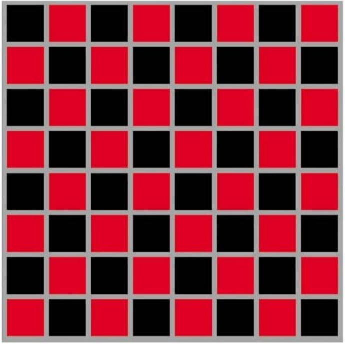
Does the hard-sphere model exhibit a phase transition for some dimension d?

Question

Is there any example of a Gibbs point process with pair potential that exhibits a phase transition?

Why has no one proved a phase transition?

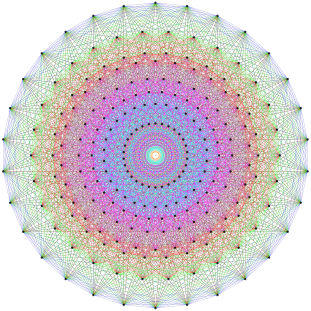
Compare to the hard-core model on $\mathbb{Z}^d$: the ground states are the odd and even states; there are only two of them.



For λ small, dependence on boundary condition decays exponentially; for λ large, either looks like a perturbation of all odd or all even.

Ground states for GPP/hard sphere?

For hard-sphere: the ground states are *optimal sphere packings* and there are continuous symmetries. The only dimensions in which we know these are $1, 2$, 3 (Hales' 98), 8 (Viazovka '17) and 24 (Cohn-Kumar-Miller-Radchenko-Viazovska '17).



So large λ is hard.

So what can be done?

For $\lambda > 0$ and a set $S \subset \mathbb{R}^d$, define the partition function by

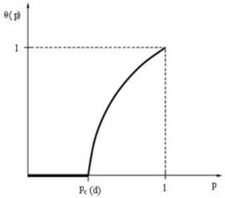
$$Z_S(\lambda) = \sum_{k \geq 0} \frac{\lambda^k}{k!} \int_{S^k} \exp\left(- \sum_{i<j} \phi(x_i - x_j) \right) \, d\mathbf{x} \,.$$

Think $\mathbb{P}(\mathbf{X}) \approx \frac{1}{Z_S(\lambda)} \frac{\lambda^k}{k!} e^{-U(\mathbf{X})} d\mathbf{X}$.

Define the *pressure* $p(\lambda) = \lim_{S \uparrow \mathbb{R}^d} \frac{1}{|S|} \log Z_S(\lambda)$.

Metatheorem (Yang-Lee, '52)

Phase transitions are points $\lambda > 0$ at which p is not analytic.



What has been done?

Define

$$C_\phi = \int_{\mathbb{R}^d} (1 - \exp(-\phi(x)))\, dx\,.$$

Theorem (Groenveld ('62), Penrose ('63), Ruelle ('63))

For a classical gas with pair potential ϕ, the pressure p is analytic for $\lambda \in [0, 1/(eC_\phi))$. In particular, there is no phase transition for $\lambda \in [0, 1/(eC_\phi))$.

For hard spheres $C_\phi = 2^d \cdot (\text{volume of ball})$.

Penrose and Ruelle show a bound for a more general class of potentials called *stable* potentials.

How do these proofs go?

Two (related) approaches:

(1) Show convergence of the *cluster expansion* for $\log Z_S(\lambda)$. An absolutely convergent series then implies analyticity.

(2) Show *uniqueness* via *Kirkwood-Salsburg* equations: Need $\mathrm{Id} - \lambda T$ to be invertible in a certain Banach space where T is some operator.

Both methods show analyticity of $\log Z_S(\lambda)$ for *complex* λ with $|\lambda| \leq 1/(eC_\phi)$.

(Check out Ruelle's classic text/Bible *Statistical Mechanics: Rigorous Results*)

Limits to these approaches

Note that $\log Z_S(\lambda)$ being analytic means $Z_S(\lambda)$ is zero-free.

These approaches show zero-freeness of $Z_S(\lambda)$ in a disk around the origin.

Phase transitions are about analyticity for *positive* λ, so singularities of $\log Z_S(\lambda)$ (uniformly) far from the positive real axis shouldn't correspond to a phase transition.

Fact (Groenveld ('62), Penrose ('63))

The closest singularity of $\log Z_S(\lambda)$ *to the origin is on the negative real axis, and the cluster expansion does not converge for* $|\lambda| = 1/C_\phi$.

Recall they showed analyticity/convergence for $|\lambda| \leq 1/(eC_\phi)$.

Some other approaches

For hard spheres, Hofer-Temmel ('19) and Dereudre ('19): uniqueness for $\lambda \in [0, 1/C_\phi + o_d(1))$. A probabilistic proof using *disagreement percolation*.

Also for hard spheres, Helmuth, Perkins, Petti ('20) showed uniqueness for $\lambda \in [0, 2/C_\phi)$ via a path coupling approach. Established an equivalence of correlation decay (specifically *strong spacial mixing*) and fast mixing of block dynamics.

In a little-noticed work, Meeron ('70) showed uniqueness for repulsive classical gasses for $\lambda \in [0, 1/C_\phi)$. Related to Kirkwood-Salsburg approach.

Results

Theorem (M.-Perkins, '20)

For a classical gas with (repulsive, tempered) pair potential ϕ, the pressure p is analytic for $\lambda \in [0, e/C_\phi)$ where

$$C_\phi = \int_{\mathbb{R}^d} (1 - \exp(-\phi(x)))\, dx\,.$$

There is no phase transition for $\lambda \in [0, e/C_\phi)$.

Compare to "Tree threshold" $\lambda_\Delta \sim \frac{e}{\Delta}$ for hardcore model of max degree Δ. Think "$\Delta \approx C_\phi$."

The idea is to work in a small neighborhood of the positive real axis.

Strategy

Take inspiration from work on hard core model and other discrete systems (e.g. Weitz).

Define some important statistics in terms of partition functions that act as continuous version of occupation probabilities.

Prove some recursion for these statistics: write these statistics for a given parameter in terms of those statistics for other parameters.

Use this recursion to prove analyticity "inductively."

Ideas: Setting things up

Allow λ to be a function $\boldsymbol{\lambda} : S \to \mathbb{C}$. This only makes physical sense if $\boldsymbol{\lambda} \geq 0$, but we can still make sense of $Z_S(\boldsymbol{\lambda})$ for complex $\boldsymbol{\lambda}$:

$$Z_S(\boldsymbol{\lambda}) = \sum_{k \geq 0} \frac{1}{k!} \int_{S^k} \exp\left(-\sum_{i<j} \phi(x_i - x_j) \right) \prod_{i=1}^{k} \boldsymbol{\lambda}(x_i)\, d\mathbf{x}\,.$$

If $Z_S(\boldsymbol{\lambda}) \neq 0$, define the *density* as

$$\rho_{\boldsymbol{\lambda}}(v) = \boldsymbol{\lambda}(v) \frac{Z_S(\boldsymbol{\lambda} e^{-\phi(v-\cdot)})}{Z_S(\boldsymbol{\lambda})}\,.$$

Think of $\boldsymbol{\lambda} e^{-\phi(v-\cdot)}$ as the activity we get when we add a point at v.

If $\boldsymbol{\lambda} \geq 0$, then $\rho_{\boldsymbol{\lambda}}(v)$ has a natural interpretation: the expected number of points of the process in a set U is $\int_U \rho_{\boldsymbol{\lambda}}(u)\, du$. This means that probability there is a point in a small set dV centered at v is $\approx \rho_{\boldsymbol{\lambda}}(v) dV$.

Ideas: A recursion

Lemma

We have

$$\rho_{\boldsymbol{\lambda}}(v) = \boldsymbol{\lambda}(v) \exp\left(- \int_{\mathbb{R}^d} \rho_{\boldsymbol{\lambda}_{v\to w}}(w)(1 - e^{-\phi(v-w)})\, dw \right)$$

where

$$\boldsymbol{\lambda}_{v\to w}(x) = \begin{cases} \boldsymbol{\lambda}(x) e^{-\phi(v-x)} & \text{if } |x-v| \le |w-v| \\ \boldsymbol{\lambda}(x) & \text{if } |x-v| > |w-v| \end{cases}$$

provided all densities $\rho_{v\to w}$ make sense.

To understand $\boldsymbol{\lambda}_{v\to w}$: points closer to v than w "see" a point at v but others don't.

Moral of the story: write $\rho_{\boldsymbol{\lambda}}$ in terms of densities with activities of the form $\boldsymbol{\lambda}_{v\to w} = \boldsymbol{\alpha} \cdot \boldsymbol{\lambda}$ where $\boldsymbol{\alpha} \in [0,1]$; think $\boldsymbol{\lambda}_{v\to w} \preceq \boldsymbol{\lambda}$.

(Think of this as a version of the recurrence that gives Weitz' tree.)

Using the recurrence

Analyticity of $\log Z_S(\boldsymbol{\lambda}) \iff$ zero-freeness of $Z_S \iff$ uniform upper bound on $\rho_{\boldsymbol{\lambda}}(v)$.

Show *complex contraction*: for $\boldsymbol{\lambda}$ in a complex neighborhood of $[0, e(1-\varepsilon)/C_\phi]$ show that uniform upper bound on $\rho_{\boldsymbol{\lambda}_{v\to w}}$ implies the same bound upper bound on $\rho_{\boldsymbol{\lambda}}$.

In other words: say $\hat{\boldsymbol{\lambda}}$ is *good* if we have an upper bound on $\rho_{\hat{\boldsymbol{\lambda}}}$. Contraction says "If all $\boldsymbol{\lambda}_{v\to w}$ are good then $\boldsymbol{\lambda}$ is too."

The zero activity $\boldsymbol{\lambda} \equiv 0$ is good, and contraction let's us "induct" to show all $\boldsymbol{\lambda}$ in this neighborhood of $[0, e(1-\varepsilon)/C_\phi]$ are good.

(Inspired by Peters and Regts's work on zero-freeness of the hardcore model, and Weitz's work before them)

Where does the recursion come from?

Another recursion we prove and use is

$$\mathbb{P}(S \text{ has no points}) = \frac{1}{Z_S(\boldsymbol{\lambda})} = \exp\left(-\int_S \rho_{\hat{\boldsymbol{\lambda}}_x}(x)\,dx\right)$$

where

$$\hat{\boldsymbol{\lambda}}_x(y) = \begin{cases} 0 & \text{if } |y| \le |x| \\ \boldsymbol{\lambda}(y) & \text{if } |y| > |x| \end{cases}.$$

Heuristically:

$$\begin{aligned}
\mathbb{P}(S \text{ has no points}) &\approx \prod_x \mathbb{P}(S \text{ has no point at } x \,|\, S \text{ has no point } < x) \\
&\approx \prod_x (1 - \mathbb{P}(S \text{ has point at } x \,|\, S \text{ has no point } < x)) \\
&\approx \prod_x (1 - \rho_{\hat{\boldsymbol{\lambda}}_x}(x) dx) \\
&\approx \exp\left(-\int_S \rho_{\hat{\boldsymbol{\lambda}}_x}(x)\,dx\right)
\end{aligned}$$

Where does the recursion come from? (pt 2)

Want to show

$$\mathbb{P}(S \text{ has no points}) = \frac{1}{Z_S(\boldsymbol{\lambda})} = \exp\left(-\int_S \rho_{\hat{\boldsymbol{\lambda}}_x}(x)\,dx\right)$$

where $\hat{\boldsymbol{\lambda}}_x(y) = \boldsymbol{\lambda}(y)\mathbf{1}_{|y|>|x|}$.

Think: want "continuous version" of telescoping product. Take log to turn into telescoping sum.

Think: fundamental theorem of calculus is a continuous version of a telescoping sum.

Set $\boldsymbol{\lambda}_t(y) = \mathbf{1}_{|y|\geq t}\boldsymbol{\lambda}(y)$ and apply the fundamental theorem of calculus to $\int_0^\infty \frac{d}{dt}\log Z_S(\boldsymbol{\lambda}_t)\,dt = \log Z_S(\boldsymbol{\lambda}_\infty) - \log Z_S(\boldsymbol{\lambda}_0) = -\log Z_S(\boldsymbol{\lambda})$.

Open questions/future work

Question (Stable potentials)

Can these results be extended to stable potentials, i.e. those that are allowed to be negative at certain points?

The bound of analyticity for $\lambda \in [0, 1/(eC_\phi))$ of Penrose and Ruelle applies to stable potentials.

Question (Approximating)

Can the partition function $Z_S(\boldsymbol{\lambda})$ be approximated (perhaps using the recurrences for ρ?).

Thank you!