Continuum percolation for Gibbsian point processes with attractive interactions

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Context

Setting: Classical statistical mechanics, particles with short-range, attractive pair potential, Gibbsian point processes.

Classical questions:

1. phase transitions (non-analyticity of thermodynamic potentials, non-uniqueness of Gibbs measures)? for continuum models, open (but: special models...).
2. percolation transitions? Some results available Mürmann '75, Zessin '08, Pechersky, Yambartsev '09, Aristoff '12, Stucki '13.

Caution: in general, percolation transition and phase transitions are two different things.

This talk: percolation thresholds at low temperature for attractive interactions. *At low temperature, percolation is induced by particle attraction and not by high density: percolation threshold small compared to that of the ideal gas (Poisson point process).*

Proofs: combine known results with cluster expansions and large deviations results J., König, Metzger '11, J '12, equivalence of ensembles Georgii, Zessin '93, Georgii '94.

Overview

Model ingredients

- $\beta > 0$ inverse temperature
- $\mu \in \mathbb{R}$ chemical potential
- $z = \exp(\beta\mu)$ activity
  (intensity parameter of a reference Poisson point process)
- $v(r)$ pair potential: $v : [0, \infty) \to \mathbb{R} \cup \{\infty\}$
  (with or without hard core , superstable, compact support, attractive)
- total energy of a configuration $\{x_1, \dots, x_N\} \subset \mathbb{R}^d$:

$$U(\{x_1, \dots, x_N\}) := \sum_{i<j} v(|x_i - x_j|)$$

- $\mathcal{G}(\beta, \mu) =$ infinite volume Gibbs measures

We will be interested in $\beta \to \infty$, $\mu < 0$ fixed, $z = \exp(\beta\mu) \to 0$.
Waring: Because of interaction, it is possible that $z = \exp(\beta, \mu) \to 0$ but density $\rho(\beta, \mu)$ ($=$ expected number of particles per unit volume) bounded away from zero.

Infinite volume Gibbs measure

- Locally finite point configurations in $\mathbb{R}^d$:

$$\Omega = \{\omega \subset \mathbb{R}^d \mid \forall r > 0 : \ \#(\omega \cap \overline{B(0,r)}) < \infty\}.$$

- σ-algebra generated by the counting variables $N_B(\omega) := \#(\omega \cap B)$, $B \subset \mathbb{R}^d$ Borel sets.
- $\mathbf{k} \in \mathbb{Z}^d$, unit cube $C(\mathbf{k}) := [k_1 + 1) \times \cdots \times [k_d + 1)$.
- Probability measure P on $(\Omega, \mathcal{F})$ is *tempered* if

$$\sup_{\ell \in \mathbb{N}} \frac{1}{\ell^d} \sum_{\mathbf{k} \in \mathbb{Z}^d \cap [-\ell, \ell]^d} \Big(N_{C(\mathbf{k})}(\omega) \Big)^2 < \infty \quad P\text{-a.s.}$$

- $\Lambda = [-L, L]^d$, $\zeta \subset \Omega$. Finite volume Gibbs measure with boundary conditions ζ: a.c. wrt. Poisson point process of intensity 1, Radon-Nikodým derivative proportional to

$$z^{N_\Lambda(\omega)} \exp\Big(-\beta \Big[U(\omega \cap \Lambda) + W(\omega \cap \Lambda, \zeta \cap \Lambda^{\mathrm{c}} \Big] \Big)$$

  $W(\omega, \zeta)$: sum of pair interactions $v(x - y)$ $x \in \omega$, $y \in \zeta$.
- $P \in \mathcal{G}(\beta, \mu)$ iff (a) tempered, (b) for every Λ, conditional probability given configuration ζ outside the box is finite volume Gibbs measure with boundary condition ζ.

Assumptions on the pair potential

1. With or without hard core:

$$\exists r_{\mathrm{hc}} \geq 0 : \quad v(r) = \infty \text{ in } (0, r_{\mathrm{hc}}), \quad v(r) < \infty \text{ in } (r_{\mathrm{hc}}, \infty).$$

2. Compact support (range r_1), attractive "tail":

$$\exists 0 < r_0 < r_1 : \quad v(r) < 0 \text{ in } (r_0, r_1), \quad v(r) = 0 \text{ in } (r_1, \infty).$$

3. Superstable (e.g.: hard core $r_{\mathrm{hc}} > 0$).
   Needed for existence of infinite volume Gibbs measures.
4. Integrable in $\{v < \infty\}$: Allows us to apply a cluster expansion bound by Brydges, Federbush '78.
5. N-particle minimizers of U have interparticle distance bounded away from zero, uniformly in N (e.g. hard core $r_{\mathrm{hc}} > 0$), and
6. ... and diameter bounded by $CN^{1/d}$.
   Proven (and much more) in dimension two for some potential classes Radin '81, Theil '06. In general, difficult!

5. and 6. needed to apply earlier large deviations results J, König, Metzger '11.

Percolation. Cluster densities

Fix $R > 0$. Think $R \approx$ potential range r_1. Draw line between points $x, y \in \omega$ if $|x - y| \leq R$. Configuration splits into R-connected components $=$ clusters.
Let $P \in \mathcal{G}(\beta, \mu)$ (tempered!). Percolation occurs if

$$P\Big(\omega \text{ has infinite connected component }\Big) > 0.$$

Cluster of x: $\mathcal{C}_\omega(x)$ $=$ connected component of x.
Density $\rho(P)$: P shift-invariant, P° Palm measure,

$$\rho(P) = P^\circ(\Omega) = N_{[0,1]^d}(\omega).$$

Cluster densities $\rho_k(P)$: P shift-invariant, $k \in \mathbb{N}$,

$$\rho_k(P) = \frac{1}{k} P^\circ(\#\mathcal{C}_\omega(x) = k) = \int_\Omega \sum_{x \in [0,1]^d} \mathbf{1}(\#\mathcal{C}_\omega(x) = k) P(\mathrm{d}\omega).$$

Always have

$$\boxed{\sum_{k=1}^\infty k \rho_k(P) \leq \rho(P).}$$

Percolation iff inequality is strict.

Activity thresholds: definitions and conjecture

Percolation thresholds: Consider the conditions

$$\forall \mu > \mu_+ \ \forall P \in \mathcal{G}(\beta,\mu) \ P(\text{there is an infinite } R\text{-cluster}) = 1 \qquad (*)$$
$$\forall \mu < \mu_- \ \forall P \in \mathcal{G}(\beta,\mu) \ P(\text{there is an infinite } R\text{-cluster}) = 0. \qquad (**)$$

Set

$$\mu_+(\beta,R) := \inf\{\mu_+ \in \mathbb{R} \mid \mu_+ \text{ satisfies } (*)\},$$
$$\mu_-(\beta,R) := \sup\{\mu_- \in \mathbb{R} \mid \mu_- \text{ satisfies } (**)\}.$$

Percolation with probability 1 above $\mu_+(\beta,R)$, percolation probability vanishes below $\mu_-(\beta,R)$.

Ground state energies:

$$E_N := \inf\{U(\omega) \mid \#\omega = N\}, \quad e_\infty := \lim_{N\to\infty} \frac{E_N}{N} < 0.$$

Conjecture: for every $R >$ potential range,

$$\boxed{\lim_{\beta\to\infty} \mu_-(\beta,R) = \lim_{\beta\to\infty} \mu_+(\beta,R) = e_\infty}$$

and $\mu_-(\beta,R) = \mu_-(\beta,R)$ for large β. Activity threshold $z_\pm = \exp(\beta\mu_\pm) \to 0$.

Results I: percolation thresholds, grand-canonical

Theorem

- *Let $R \geq r_1$ (potential range). Then*

$$e_\infty \leq \liminf_{\beta\to\infty} \mu_-(\beta; R).$$

In addition, for every $\mu < e_\infty$ and sufficiently large β, there is a unique (β,μ)-Gibbs measure P; it is shift-invariant, has no infinite cluster (P-almost surely), and satisfies

$$k\rho_k(P) \leq ke^k |B(0,R)|^{k-1} \exp\big(-\beta k(e_\infty - \mu)\big).$$

- *Suppose that v is continuous in (r_0, r_1). Let $0 > -m > \inf_{(r_0,r_1)} v(r)$, $\tilde{r}_m$ such that $v(\tilde{r}_m) \leq -m$, and $R_m \geq \sqrt{(d+3)}\tilde{r}_m$. Then*

$$\limsup_{\beta\to\infty} \mu_+(\beta; R_m) \leq -m$$

Note: $-m > \inf_{r\in(r_0,r_1)} v(r) > e_\infty$. Bounds consistent with conjecture.

Density thresholds: definitions and conjecture

Gibbs measures at given density:

$$\mathcal{G}_\theta(\beta,\rho) := \Big\{\{P \in \bigcup_{\mu\in\mathbb{R}} \mathcal{G}(\beta,\mu) \,\Big|\, \text{shift-invariant},\ \rho(P)=\rho\Big\}$$

Density thresholds: definition analogous to $\mu_\pm(\beta,R)$.

- percolation probability equal to 1 above $\rho_+(\beta,R)$
- percolation probability vanishes below $\rho_-(\beta,R)$.

Energetic quantity:

$$\nu^* := \inf_{N\in\mathbb{N}} (E_N - Ne_\infty) > 0.$$

Conjecture: for $R > r_1$ and large β,

$$\rho_-(\beta,R) = \exp\Big(-\beta\nu^*(1+o(1))\Big) \to 0,$$

$$\rho_+(\beta,R) \text{ bounded away from } 0.$$

Conjectured formula for $\rho_-(\beta,R)$ motivated by work J, König, Metzger '11, in agreement with Clausius-Clapeyron equation (thermodynamics). For $\rho_- < \rho < \rho_+$, expect non-ergodic Gibbs measures with percolation probability in $(0,1)$. Phase coexistence region.

Results II

Set $\rho(\beta,\mu) := \inf\{\rho(P) \mid P \in \mathcal{G}(\beta,\mu),\ \text{shift-invariant}\}$ and $\rho_m := \liminf_{\beta\to\infty} \rho(\beta, -m)$.

Theorem

- *Let $R \geq r_1$. Then*

$$-\nu^* \leq \liminf_{\beta\to\infty} \beta^{-1} \log \rho_-(\beta; R).$$

In addition, for every fixed $\nu > \nu^*$, sufficiently large β, $\rho = \exp(-\beta\nu)$, there is a unique measure P in $\mathcal{G}_\theta(\beta,\rho)$. It has no infinite cluster, P-almost surely, and satisfies

$$k\rho_k(P) \leq C\rho \exp(-\beta c k)$$

for suitable $C, c > 0$ and all $k \in \mathbb{N}$ (uniform in $\rho \leq \exp(-\beta(\nu^* + \varepsilon))$.)

- *Suppose that v is continuous in (r_0, r_1). Let $\inf_{(r_0,r_1)} v(r) < -m < 0$ and $R_m > \max(\sqrt{d+3}\,\tilde{r}_m, r_1)$. Then*

$$\limsup_{\beta\to\infty} \rho_+(\beta; R_m) \leq \rho_m.$$

A partial result for $\rho \geq \exp(-\beta\nu^*)$

Previous theorem: tells us that if $\rho \ll \exp(-\beta\nu^*)$, then no percolation.

Expect: if $\rho \gg \exp(-\beta\nu^*)$ and $d \geq 2$, then strictly positive percolation probability.

Open. **But**: preliminary result:

Theorem

Let $R \geq r_1$. There are $\beta_0, \rho_0, C > 0$ such that for all $\beta \geq \beta_0$, all $\rho \leq \rho_0$ and all $P \in \mathcal{G}_\theta(\beta, \rho)$, the following holds: if $\rho = \exp(-\beta\nu) > \exp(-\beta\nu^*)$, then

$$\forall K \in \mathbb{N}: \quad \sum_{k=1}^{K} k\rho_k(P) \leq \frac{C\rho\beta^{-1}\log\beta}{\nu^* - \nu}.$$

Thus at densities above $\exp(-\beta\nu^*)$, the fraction of particles in finite-size clusters is small.

$$\frac{1}{\rho(P)} P^\circ\Big(\#\mathcal{C}_\omega(x) \leq K\Big) = O(K\beta^{-1}\log\beta).$$

Something does happen around $\exp(-\beta\nu^*)$, though we don't know yet that it is a percolation transition.

Proof structure: activity thresholds

Percolation at high enough chemical potential:
Proven by Pechersky, Yambartsev '09 in $d = 2$. Their proof extends to $d \geq 3$ (noted independently by Stucki '13).

Basic idea: discretize space into cells = little cubes. Choose side-length ℓ so that $v(r) \leq -m + \delta$ in $(\ell - \varepsilon, \ell + \varepsilon)$ and $v(r) \leq 0$ for $r \geq \ell - \varepsilon$. Contour $\approx$ connected string of cubes. Show that "energy" penalty for large empty contours is large, then use standard contour arguments. "Energy": $U(\omega) - \mu \# \omega$.

Absence of percolation at low enough chemical potential:
Proven by Mürmann '75 for empty boundary conditions, Zessin '08 for general boundary conditions.

Our proof: extract temperature-dependence and exponential decay from Mürmann's proof. Use cluster expansion criterion for uniqueness of Gibbs measure at $\mu < e_\infty$.

Proof structure: density thresholds

Deduced from activity thresholds with the help of good control of $\rho(\beta, \mu)$.
Remember: increasing function, almost everywhere differentiable.

Absence of percolation at density $\rho \ll \exp(-\beta\nu^*)$:
Know (J 12):

$$\boxed{\forall \mu < e_\infty : \lim_{\beta\to\infty} \frac{1}{\beta} \log \rho(\beta, \mu) = -\inf_{k\in\mathbb{N}} (E_k - k\mu) < -\nu^*.}$$

If $\rho \ll \exp(-\beta\nu^*)$, then chemical potential $\mu < e_\infty$.
Theorem on density thresholds $\Rightarrow$ no ,percolation.

A.s. percolation at density $\rho \geq \rho_m > 0$:
Similar argument. For $\mu > -m$ have $\rho(\beta, \mu) \geq \rho(\beta, -m)$.
This is how $\rho_m = \liminf \rho(\beta, -m)$ enters.

Variational characterization of percolation

J, König, Metzger '11, J, König '12:
Start from finite volume, canonical ensemble. Look at vector of empirical cluster densities $(\rho_{k,\Lambda}(\omega))_{k\in\in\mathbb{N}}$. Random variable with values in $[0,\infty)^{\mathbb{N}}$. Satisfies large deviations principle with rate function $f(\beta,\rho,(\rho_k)_{k\in\mathbb{N}})$.

Proved bounds for large deviations rate function

$$f\left(\beta,\rho,(\rho_k)_{k\in\mathbb{N}}\right) \approx \sum_{k\in\mathbb{N}} \rho_k\left(E_k+\beta^{-1}\log\frac{\rho_k}{e}\right)+(\rho-\sum_{k\in\mathbb{N}} k\rho_k)e_\infty$$

and minimizers.

Connection with infinite volume Gibbs measures.

$$f\left(\beta,\rho,(\rho_k)_{k\in\mathbb{N}}\right)=\left\{U(P)-\beta^{-1}S(P)\mid P \text{ shift-invariant},\ \rho_k(P)=\rho_k,\ \rho(P)=\rho\right\}.$$

But minimizers are (shift-invariant) Gibbs measures...

Cluster densities $(\rho_k(P))_{k\in\mathbb{N}}$ minimize constrained free energy $f(\beta,\rho,(\rho_k)_{k\in\mathbb{N}})$.
Percolation iff $f(\beta,\rho,\cdot)$ has minimizer with $\sum_k k\rho_k<\rho$.