Gibbsian germ-grain models

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1. Germ-grain models

2. Infinite volume Gibbsian germ-grain models

3. A percolation result

4. Parametric estimation for Quermass models
1 Germ-grain models
State space

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- $\mathcal{M}(\mathcal{E})$ the space of locally finite configurations in $\mathcal{E}$. We denote by $\gamma$ a configuration in $\mathcal{M}(\mathcal{E})$ and by $\tilde{\gamma}$ its associated germ-grain set

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- A Point Process $\Gamma$ is a random variable in $\mathcal{M}(\mathcal{E})$ and $\bar{\Gamma}$ is its associated germ-grain model.
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- A Point Process $\Gamma$ is a random variable in $\mathcal{M}(\mathcal{E})$ and $\tilde{\Gamma}$ is its associated germ grain model.
- First possible extension: The grains can be more complicated (convex sets, paths, etc)
- Second possible extension: The grains can be marked by a type (color). $\mathcal{E}$ becomes for example $\mathbb{R}^2 \times \mathbb{R}^+ \times \{1, \ldots, K\}$. 
Boolean model

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- On a bounded window $\Lambda : \pi^z_\Lambda$, $P^z_\Lambda$
Gibbsian modifications

On a finite window $\Lambda$.

$$P^{z,H} = \frac{1}{Z_\Lambda} e^{-H} P^z_{\Lambda}.$$ 

with $H$ an Hamiltonian which depends on $\tilde{\gamma}_\Lambda$ : a function from the space of finite union of balls to $\mathbb{R} \cup \{+\infty\}$ such that

$$0 < Z_\Lambda := \int e^{-H(\tilde{\gamma}_\Lambda)} P^z_{\Lambda}(d\gamma_\Lambda) < +\infty.$$
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with $H$ an Hamiltonian which depends on $\bar{\gamma}_{\Lambda}$: a function from the space of finite union of balls to $\mathbb{R} \cup \{+\infty\}$ such that

$$0 < Z_{\Lambda} := \int e^{-H(\bar{\gamma}_{\Lambda})} P^\gamma_{\Lambda}(d\gamma_{\Lambda}) < +\infty.$$ 

- $Z_{\Lambda} > 0 : H(\emptyset) = 0$. 
- $Z_{\Lambda} < +\infty :$ Stability

$$H(\bar{\gamma}_{\Lambda}) \geq -B\text{Card}(\gamma_{\Lambda}).$$
Examples of Hamiltonian

- **Quermass interaction** (Likos, Mecke and Wagner 95-Baddeley, Van Lieshout 99)

\[
H(\gamma) = \sum_{i=0}^{d} \theta_i W_i.
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with \(\theta_i\) in \(\mathbb{R}\) and \(W_i\) the ith Minkowski functional.
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- **Multi type Widom Rowlinson model** (Widom and Rowlinson 70)
  Inhibition model: non overlapping balls with different type.
Germ-grain models
Infinite volume Gibbsian germ-grain models
A percolation result
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Infinite volume Gibbsian germ-grain models
Why the infinite volume?

Motivations:

- Stationary model without boundary conditions
- Macroscopic quantities (mean value, percolation, conductivity, permeability)
- Phase transition via the non uniqueness of the Gibbs measures
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Issues:
- The infinite volume Hamiltonian is senseless
- Definition of local Hamiltonian
- Equilibrium equations via DLR equations
The Local Hamiltonian

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In some cases: a space \( \Omega^* \) of tempered configurations is needed.
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**Definition (Gibbs measures)**

An infinite volume germ-grain model $P$ is a Gibbs measure for the Hamiltonian $(H_{\Lambda})$ if $P(\Omega^*) = 1$ and if the law of $\gamma_{\Lambda}$ given $\gamma_{\Lambda^c}$ is absolutely continuous with respect to the Poisson law $\pi_{\Lambda}$ with the density

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\frac{1}{Z_{\Lambda}(\gamma_{\Lambda^c})} e^{-H_{\Lambda}(\tilde{\gamma})}
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Questions: Existence, uniqueness, non-uniqueness (phase transition).
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Some results

- **Widom Rowlinson exclusion model:**
  (Widom-Rowlinson 70, Chayes Kotecky 95) The law of radii $Q$ is concentrated on a singleton $R_0$: Existence and phase transition for large $z$ large enough.
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  $$\forall \theta > 0, \quad \int e^{\theta R^2} Q(dR) < +\infty.$$ 

- **Continuum random cluster model**: work in progress with my Phd Student, Pierre Houdebert. Existence and phase transition.
Stability of Quermass Model in $\mathbb{R}^2$

Is $e^{-H}$ intégrable under $\pi_\Lambda$?

Proposition (KVB99, MH08)

If
\[ \int_{\mathbb{R}^+} e^{-\theta_1 \pi R^2 - 2\theta_2 R} Q(dr) < +\infty, \]

then
\[ \int e^{-H(\gamma)} \pi_\Lambda(d\gamma) < \infty. \]

Proof:
For one ball:
\[ \int e^{-\theta_1 A(B(x,R)) - \theta_2 L(B(x,R))} Q(dR) \]

Lemme (KVB99)

Let $n$ ($n \geq 3$) balls be in the plane. Then the number of holes is lower than $2n - 5$.

$H$ is stable: $H(\gamma) \geq -K \text{ Card}(\gamma)$. 
Tempered configurations for Quermass Model

\[ \Omega_{K,K'} = \left\{ \gamma \ \text{tq} \begin{array}{ll}
-i) & \sup_{n \in \mathbb{N}^*} \frac{1}{\pi n^2} \sum_{(x,R) \in \gamma_{B(0,n)}} (1 + R^2) \leq K \\
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\[ \Omega^* = \bigcup_{K \geq 2, K' \geq 2} M_{K,K'}(\mathcal{E}). \]
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is well defined for tempered configurations. The cluster points in the construction of Gibbs measures by "entropy bounds" is tempered.
3 A percolation result
A Result

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P(\bar{\gamma} \text{ percolates}) = 1,
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Remark: There exists Quermass process \( P \) such that \( 0 < P(\bar{\gamma} \text{ percolates}) < 1 \).

Main issue: when \( \theta_3 \neq 0 \), it is impossible to obtain a stochastic minoration of \( P \) by Poisson processes for all \( z' > 0 \), \( \pi_{z'} \Lambda \succeq P \Lambda \).
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For all $z' > 0$, $$\pi_{z'} \not\leq P_\Lambda.$$
The connection Lemma

$$D = \text{the diamond box}$$

$$D$$ is open for $$\bar{\gamma}$$ if

a) $$\bar{\gamma} \cap B_N \neq \emptyset$$

b) the same for $$B_E, B_W, B_S$$

c) $$B_N, B_E, B_W, B_S$$ are connected via $$\bar{\gamma}_D$$
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**Lemma (Connection Lemma)**

*There exists* \( C > 0 \) (depending on \( \theta_1, \theta_2 \) and \( \theta_3 \)) such that for any \( z > 0 \) and any Quermass process \( P \)

\[
\inf_{\gamma_{\Lambda^c}} P(D \text{ is open} \mid \gamma_{\Lambda^c}) \geq 1 - \frac{C}{z},
\]
Classical Bernoulli domination

Let \((V, E)\) be an undirected graph with uniformly bounded degrees and \(\xi\) a random variable in \(\{0, 1\}^V\)

Lemme (Liggett et al. 97)

Let \(p \in [0, 1]\). Assume that for all \(x \in V\),

\[
P(\xi_x = 1 \mid \xi_y : \{x, y\} \notin E) \geq p \quad \text{a.s.}
\]

Then the law of \(\{\xi_x, x \in V\}\) dominates stochastically a product \(\bigotimes_{x \in V} B_x\) of Bernoulli laws with parameter \(f(p)\), with \(\lim_{p \to 1} f(p) = 1\).
Representation of the multi-type Quermass model on $\Lambda$

For $K = 2$:
A one-type Quermass model $P_\Lambda$ on $\Lambda$ with density $2^{N_{cc}(\gamma)}$:

$$Q_\Lambda(d\gamma) = \frac{1}{Z_\Lambda} 2^{N_{cc}(\gamma)} P_\Lambda(d\gamma).$$

Example with $\theta_1 = -0.2$, $\theta_2 = 0.3$ and $\theta_3 = 0$:
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In colouring independently the connected components, we obtain a 2-type Quermass model on $\Lambda$ for the same parameters.
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2-type Quermass Process in \( \Lambda \) with red boundary condition.
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- When $\Lambda$ goes to $\mathbb{R}^2$, the 2-type Quermass process in $\Lambda$ with red boundary condition goes to a 2-type Quermass process in $\mathbb{R}^2$ with the red particle density bigger than the blue particle density (if percolation occurs).
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- Conversely for the 2-type Quermass process in $\Lambda$ with blue boundary condition.

- We build two different 2-type Quermass processes in $\mathbb{R}^2$. 
Parametric estimation for Quermass models
MLE and MPLE procedures

- $P$ a Quermass Model for $\Theta^* = (z^*, \theta_1^*, \theta_2^*, \theta_3^*)$.
- $h^{\Theta^*}$ and $h^{\Theta}$ are the local energies for $\Theta^*$ and $\Theta$.
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This procedure does not work since, from the data, we don’t know where are the balls.
Takacs-Fiksel procedure.

This procedure is based on the GNZ equilibrium equation:

\[ E_P\left( \sum_{X \in \gamma} f(X, \gamma \setminus X) \right) = E_P\left( \int f(X, \gamma) e^{-h(\Theta^* (X, \gamma))} z^* \lambda \otimes Q(dX) \right), \]
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- Examples of such functions $f$:
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    In this situation $\sum_{X \in \gamma \Lambda} f_0(X, \gamma \setminus X) \approx \mathcal{L}(\bar{\gamma}_\Lambda)$.
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  - \( f_\alpha(X, \gamma) = \mathcal{L}(\partial B(x, R + \alpha) \cap (\bar{\gamma})^c_\alpha) \).
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- Examples of such functions \(f\):
  - \(f_0(X, \gamma) = \mathcal{L}(\partial B(X) \cap \bar{\gamma}^c)\).
    In this situation \(\sum_{X \in \gamma} f_0(X, \gamma \setminus X) \approx \mathcal{L}(\bar{\gamma}_\Lambda)\).
  - \(f_{\alpha}(X, \gamma) = \mathcal{L}(\partial B(x, R + \alpha) \cap (\bar{\gamma})^c_{\alpha})\).
    In this situation \(\sum_{X \in \gamma} f_{\alpha}(X, \gamma \setminus X) \approx \mathcal{L}((\bar{\gamma}_\Lambda)^{\alpha})\).
  - \(f_{iso}(X, \gamma) = \mathbb{1}_{B(X) \cap \bar{\gamma} = \emptyset}\).
    In this situation \(\sum_{X \in \gamma} f_{iso}(X, \gamma \setminus X)\) is equal to the number of isolated balls in \(\bar{\gamma}_\Lambda\).
Takacs-Fiksel procedure

For any function $f$ we define

$$\Delta_{f,\Lambda} := \sum_{X \in \gamma_\Lambda} f(X, \gamma \setminus X) - \int f(X, \gamma)e^{-h^{\Theta}(X, \gamma)} \lambda_\Lambda \otimes Q(dX).$$
Takacs-Fiksel procedure

For any function $f$ we define

$$\Delta_{f,\Lambda} := \sum_{X \in \gamma_\Lambda} f(X, \gamma \setminus X) - \int f(X, \gamma) e^{-h^\Theta(X, \gamma)} \lambda_\Lambda \otimes Q(dX).$$

**TFE** :

$$\hat{\Theta} := \arg\min_\Theta \left( \Delta_{f_1,\Lambda}^2 + \Delta_{f_2,\Lambda}^2 + \Delta_{f_3,\Lambda}^2 + \Delta_{f_4,\Lambda}^2 \right).$$
Takacs-Fiksel procedure

For any function $f$ we define

$$\Delta_{f,\Lambda} := \sum_{X \in \gamma \Lambda} f(X, \gamma \setminus X) - \int f(X, \gamma) e^{-h^\Theta(X, \gamma)} \lambda_\Lambda \otimes Q(dX).$$

TFE:

$$\hat{\Theta} := \arg\min_{\Theta} \left( \Delta^2_{f_1,\Lambda} + \Delta^2_{f_2,\Lambda} + \Delta^2_{f_3,\Lambda} + \Delta^2_{f_4,\Lambda} \right).$$

By the GNZ equation:

$$E_P(\Delta_{f_i,\Lambda}) = 0$$

and by ergodicity

$$\frac{1}{|\Lambda|} \Delta_{f_i,\Lambda} \xrightarrow{\Lambda \to \mathbb{R}^2} 0.$$
References

- The Takacs-Fiksel procedure is introduced in 1984-86 by Takacs and Fiksel.
- Application for the Quermass model: Der., Helisova and Lavancier 2013.
Heather Dataset

Heather : Real data

Approximation by balls
Heather Dataset

Heather : Real data 

Approximation by balls

TFE for Quermass model with $Q$ uniform in $[0, 0.5]$:

$z = 2.12$, $\theta_1 = 0$, $\theta_2 = 0.14$ and $\theta_3 = 0.22$. 


D. Der, Existence of Quermass processes for non locally stable interaction and non bounded convex grains, Adv. in Appl. probab. 41 664-681 (2009).

D. Der and F. Lavancier, Fitting all parameters of the Quermass model by the Takacs-Fiksel method, submitted.


