Gibbsian germ-grain models

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1 Germ-grain models

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- 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 $\mathbb{R}^2 \times \mathbb{R}^+ \times \{1, \ldots, K\}$.

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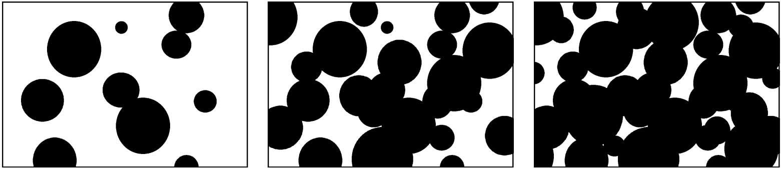
- On a bounded window Λ : π^z_Λ, P^z_Λ



Gibbsian modifications

On a finite window Λ.

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

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

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

$$H(\bar{\gamma}_\Lambda) \geq -B\mathrm{Card}(\gamma_\Lambda).$$

Examples of Hamiltonian

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

$$H(\bar{\gamma}) = \sum_{i=0}^{d} \theta_i W_i.$$

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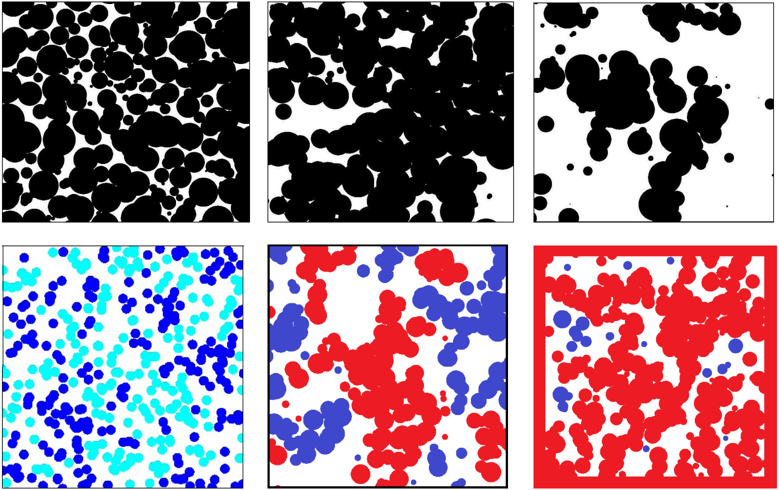
- **Multi type Widom Rowlinson model** (Widom and Rowlinson 70)
  Inhibition model : non overlapping balls with different type.



2. 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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Definition (Gibbs measures)

An infinite volume germ-grain model P is a Gibbs measure for the Hamiltonian (H_Λ) if $P(\Omega^*) = 1$ and if the law of γ_Λ given γ_{Λ^c} is absolutely continuous with respect to the Poisson law π_Λ^z with the density

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Questions : Existence, uniqueness, non-uniqueness (phase transition).

Some results

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- **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 π_Λ ?

Proposition (KVB99, MH08)

If

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

then

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

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

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 : $H(\gamma) \geq -K \ \mathrm{Card}(\gamma)$.

Tempered configurations for Quermass Model

$$\Omega_{K,K'} = \left\{ \gamma \text{ tq } \begin{array}{ll} -i) & \sup_{n\in\mathbb{N}^*} \frac{1}{\pi n^2} \sum_{(x,R)\in\gamma_{B(0,n)}} (1+R^2) \leq K \\ -ii) & \forall n \in \mathbb{N}^*, \quad \sup_{(x,R)\in\gamma_{B(0,n)}} R \leq \frac{1}{2} n + K' \end{array} \right\}.$$

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The cluster points in the construction of Gibbs measures by "entropy bounds" is tempered.

3 A percolation result

A Result

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Theorem (Coupier, Der.. 2012)

We assume that $Q([R_0, R_1]) = 1$ *with* ($R_0 > 0$ *and* $R_1 < \infty$), *then for any coefficients* $\theta_1, \theta_2, \theta_3$ *in* $\mathbb{R}$, *there exists* $z^* > 0$ *such that for any* $z > z^*$ *and any Quermass process* P *for parameters* z, $\theta_1, \theta_2, \theta_3$,

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Main issue : when $\theta_3 \neq 0$, it is impossible to obtain a stochastic minoration of P by Poisson processes

$$\text{For all } z' > 0, \qquad \pi_\Lambda^{z'} \not\preceq P_\Lambda.$$

The connection Lemma

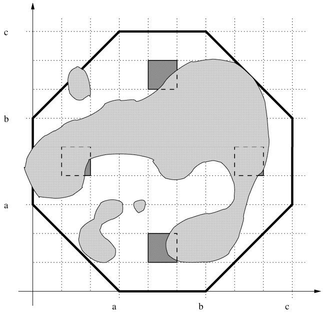
$\mathcal{D}$ = the diamond box

$\mathcal{D}$ 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 $\bar{\gamma}_{\mathcal{D}}$



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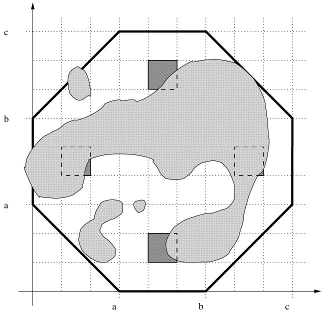


Lemma (Connection Lemma)

There exists $C > 0$ (depending on θ_1, θ_2 and θ_3) such that for any $z > 0$ and any Quermass process P

$$\inf_{\gamma_{\Lambda^c}} P(\mathcal{D} \textit{ is open } | \gamma_{\Lambda^c}) \geq 1 - \frac{C}{z}.$$

Classical Bernoulli domination

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

Lemme (Liggett et al. 97)

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

$$P\left(\xi_x = 1 \,|\, \xi_y : \{x,y\} \notin E\right) \geq p \quad a.s.$$

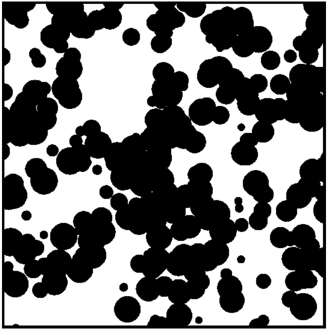
Then the law of $\{\xi_x, x \in V\}$ dominates stochastically a product $\otimes_{x \in \mathcal{V}} B_x$ of Bernoulli laws with parameter $f(p)$, with $\lim_{p \to 1} f(p) = 1$.

Representation of the multi-type Quermass model on Λ

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

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

Example with $\theta_1 = -0.2$, $\theta_2 = 0.3$ and $\theta_3 = 0$:



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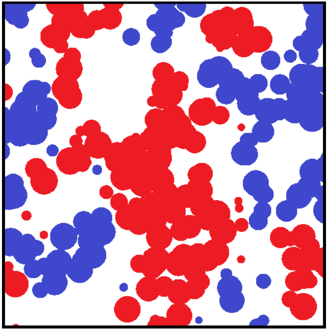
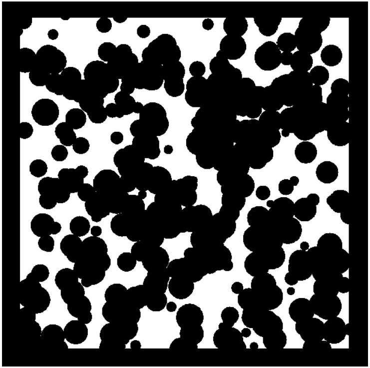


In colouring independently the connected components, we obtain a 2-type Quermass model on Λ for the same parameters.

The phase transition proof

Let $\frac{1}{Z_\Lambda} 2^{N_{cc}} P^z_\Lambda(.|\gamma_{\Lambda^c})$ be a modified one-type Quermass process with a full boundary condition



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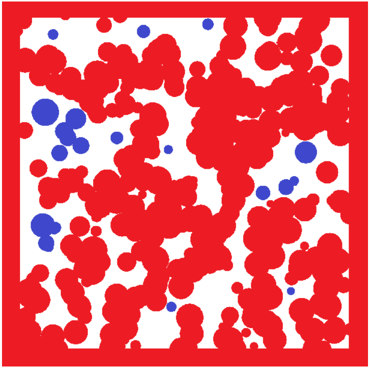

2-type Quermass Process in Λ
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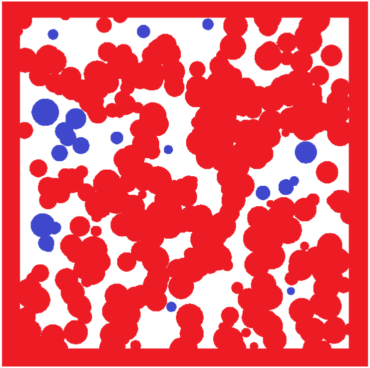

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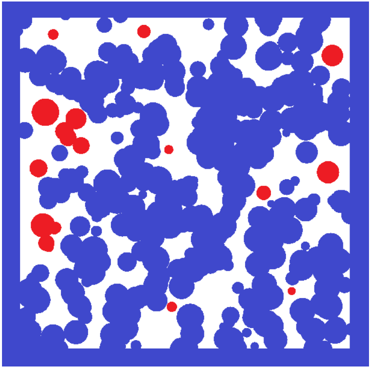

2-type Quermass Process in Λ with blue boundary condition

The phase transition proof

- When Λ goes to $\mathbb{R}^2$, the 2-type Quermass process in Λ 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 Λ with blue boundary condition.
- We build two different 2-type Quermass processes in $\mathbb{R}^2$.

4 Parametric estimation for Quermass models

MLE and MPLE procedures

-P a Quermass Model for $\Theta^* = (z^*, \theta_1^*, \theta_2^*, \theta_3^*)$.
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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 :

$$E_P\Big(\sum_{X\in\gamma} f(X,\gamma\backslash X)\Big) = E_P\Big(\int f(X,\gamma)e^{-h^{\Theta^*}(X,\gamma)} z^*\lambda\otimes Q(dX)\Big),$$

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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 $\sum_{X\in\gamma_\Lambda} f_0\big(X,\gamma\backslash X\big) \approx \mathcal{L}(\bar{\gamma}_\Lambda))$.

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We have to choose f such that the empirical sum are computable.

-Examples of such functions f :

- $f_0(X,\gamma)=\mathcal{L}(\partial B(X)\cap\bar{\gamma}^c)$.
  In this situation $\sum_{X\in\gamma_\Lambda} f_0\big(X,\gamma\backslash X\big)\approx\mathcal{L}(\bar{\gamma}_\Lambda))$.
- $f_\alpha(X,\gamma)=\mathcal{L}(\partial B(x,R+\alpha)\cap(\bar{\gamma})^c_\alpha)$.
  In this situation $\sum_{X\in\gamma_\Lambda} f_\alpha\big(X,\gamma\backslash X\big)\approx\mathcal{L}((\bar{\gamma}_\Lambda)_\alpha)$.

Takacs-Fiksel procedure.

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  In this situation $\sum_{X\in\gamma_\Lambda} f_\alpha\big(X,\gamma\backslash X\big) \approx \mathcal{L}((\bar{\gamma}_\Lambda)_\alpha)$.
- $f_{iso}(X,\gamma) = \mathbb{1}_{B(X)\cap\bar{\gamma}=\emptyset}$.
  In this situation $\sum_{X\in\gamma_\Lambda} f_{iso}\big(X,\gamma\backslash X\big)$ is equal to the number of isolated balls in $\bar{\gamma}_\Lambda$.

Takacs-Fiksel procedure

For any function f we define

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

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TFE :

$$\hat{\Theta} := argmin_\Theta\Big(\Delta^2_{f_1,\Lambda} + \Delta^2_{f_2,\Lambda} + \Delta^2_{f_3,\Lambda} + \Delta^2_{f_4,\Lambda}\Big).$$

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By the GNZ equation :

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

and by ergodicity

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

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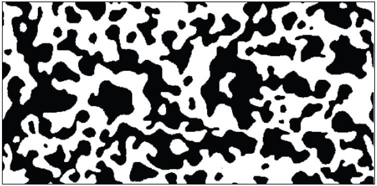
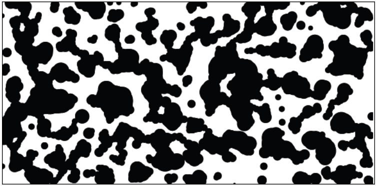
- Application for the Quermass model : Der., Helisova and Lavancier 2013.

Heather Dataset

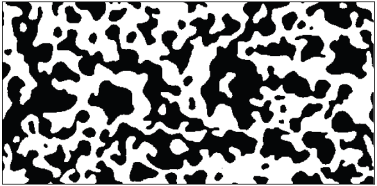


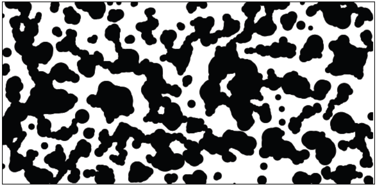
Heather : Real data



Approximation by balls

Heather Dataset



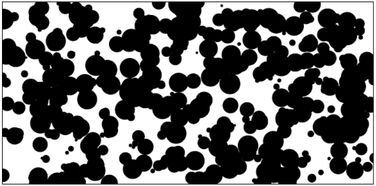


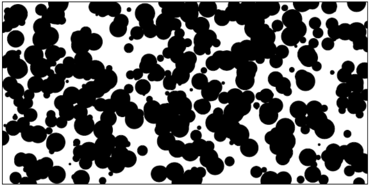
Heather : Real data

Approximation by balls

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

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





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