

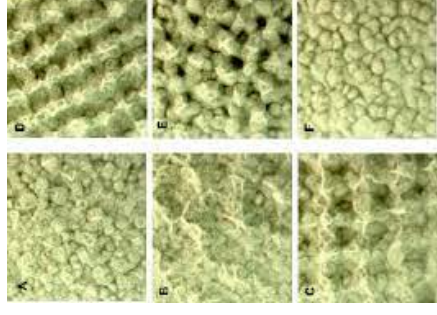
LECTURE 12

Widom-Rowlinson model with convex grains

In this lecture we focus on the Widom-Rowlinson model of interacting convex grains in \mathbb{R}^d , $d \geq 2$.

The extension from circular to convex grains turns out to be both interesting and challenging. It leads us into the world of granular media, where microscopic geometry has a profound effect on macroscopic behaviour.

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work in progress



§ STATICS: THREE EQUIVALENT FORMULATIONS

1. Let $\Lambda_n = [-n, n]^d$, and let

$$\tilde{\Gamma}_n = \{\tilde{\gamma} \subset \Lambda_n : N(\tilde{\gamma}) < \infty\}$$

be the set of **finite particle configurations** on Λ_n , where $N(\tilde{\gamma})$ denotes the **cardinality** of the set $\tilde{\gamma}$. Write $\tilde{\mathcal{C}}$ for the space of compact sets containing 0 endowed with the Hausdorff metric, which plays the role of a **shape space**. Observe that $\tilde{\mathcal{C}}$ is a locally compact Polish space, and write $\mathcal{B}(\tilde{\mathcal{C}})$ to denote its Borel σ -algebra.

Let $\Lambda_n \times \tilde{\mathcal{C}}$ denote the set of **particles** in Λ_n endowed with **random grains** drawn from $\tilde{\mathcal{C}}$, labelled

$$x = (\tilde{x}, K), \quad \tilde{x} \in \Lambda_n, K \in \tilde{\mathcal{C}},$$

and put

$$\Gamma_n = \{\gamma \subset \Lambda_n \times \tilde{\mathcal{C}} : N(\tilde{\gamma}) < \infty\}.$$

2. Let \mathbb{Q} be a **probability measure** on $\tilde{\mathcal{C}}$. Consider the space \mathcal{C} of non-empty compact subsets of $\Lambda_n \times \text{supp}(\mathbb{Q})$ endowed with the Hausdorff metric, which is also a locally compact Polish space.

3. Let λ_d be the Lebesgue measure on Λ_n . Given \mathbb{Q} and $z \in \mathbb{R}_+$, we write Π_n and Π_n^z to denote the **Poisson random measures** on the space of configurations Γ_n with intensity measures $\lambda_d \otimes \mathbb{Q}$ and $z\lambda_d \otimes \mathbb{Q}$, respectively. These satisfy

$$\Pi_n^z(\gamma) = z^{N(\gamma)} \Pi_n(\gamma), \quad \gamma \in \Gamma.$$

The **random cluster measure** $\mu_{n,z}^{\text{rc}}$ with **activity** z on Γ_n is defined as

$$\mu_{n,z}^{\text{rc}}(d\gamma) = \frac{1}{Z_n^{\text{rc}}} z^{N(\gamma)} 2^{k(\gamma)} \Pi_n(d\gamma),$$

where $k(\gamma)$ is the number of **connected components** of the random set $h(\gamma) = \cup_{(x,K) \in \gamma} (x + K)$, called the **halo** of γ , that do not intersect $\partial\Lambda_n$.

4. $\mu_{n,z}^{rC}$ induces two probability measures μ_{n,z_r,z_b}^R and μ_{n,z_r,z_b}^B on the two-colour configuration space

$$\Gamma'_n = \{(\gamma^r, \gamma^b) : \gamma^r, \gamma^b \subset \Lambda_n \times \text{supp}(\mathbb{Q}), N(\gamma^r), N(\gamma^b) < \infty\}.$$

In fact, μ_{n,z_r,z_b}^R can be specified as

$$\begin{aligned} \mu_{n,z_r,z_b}^R(d\gamma^r, d\gamma^b) &= \frac{1}{Z_n^R} z_r^{N(\gamma^r)} z_b^{N(\gamma^b)} \chi(\gamma^r, \gamma^b) \\ &\quad \times \mathbb{1}_{h(\gamma^b) \cap \partial\Lambda_n = \emptyset} \Pi_n(d\gamma^r) \Pi_n(d\gamma^b), \end{aligned}$$

where χ is defined as

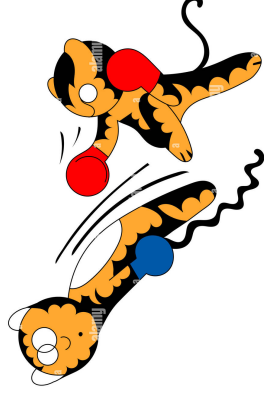
$$(*) \quad \chi(\gamma^r, \gamma^b) = \mathbb{1}_{h(\gamma^r) \cap h(\gamma^b) = \emptyset},$$

and similarly for μ_{n,z_r,z_b}^B . In words, μ_{n,z_r,z_b}^R and μ_{n,z_r,z_b}^B are obtained by independently assigning the colour red or blue to the connected components of the halo $h(\gamma)$ that are not intersecting $\partial\Lambda_n$, and assigning red or blue to all the connected components intersecting $\partial\Lambda_n$.

μ_{n, z_r, z_b}^R is the two-species Widom-Rowlinson measure on Λ_n with red boundary condition and with activities z_r and z_b . If $z_r = z_b = z$, then under the map $(\gamma^r, \gamma^b) \mapsto \gamma = \gamma^r \cup \gamma^b$ this measure is nothing but the random cluster measure, i.e.,

$$\mu_{n, z}^{\text{rc}}(d\gamma) = \int_{\mathbb{F}} \mathbb{1}_{\gamma = \gamma^r \cup \gamma^b} \mu_{n, z, z}^R(d\gamma^r, d\gamma^b).$$

5. The one-species Widom-Rowlinson measure is the γ^r marginal of the measure μ_{n, z_r, z_b}^R with $z_r = z$ and $z_b = \beta$. Its representation as a grand-canonical Gibbs measure is as follows.



LEMMA 12.1 Induced one-species measure

Consider the two-species Widom-Rowlinson measure $\mu_{n,z,\beta}^R$ on Γ'_n . Then the one-species Widom-Rowlinson measure, which is the marginal of $\mu_{n,z,\beta}^R$ on the red particles, is given by

$$\mu_{n,z,\beta}(\mathrm{d}\gamma) = \frac{1}{Z_n} e^{-\beta H(\gamma)} \Pi^z(\mathrm{d}\gamma),$$

where

$$H(\gamma) = \int_{\bar{\mathcal{C}}} |h(\gamma) \oplus (-K)| \mathbb{Q}(\mathrm{d}K)$$

plays the role of an effective Hamiltonian, where \oplus sums sets.

REMARK:

Suppose that $\mathbb{Q}(\cdot) = \delta_K(\cdot)$ for a compact subset K . Then

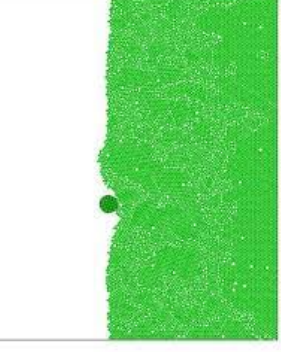
$$H(\gamma) = |\gamma \oplus K^*|,$$

where $K^* = K \oplus (-K)$ is the **symmetrisation** of the set K . Observe that K^* is always centrally symmetric.

The **WRM** treated in **Lectures 9–11** corresponds to the choice $K = B_1(0)$. There, the activity z by choice included an additional factor $e^{-\beta V_0}$ with $V_0 = |B_1(0)|$, leading to the standard **grand-canonical** representation

$$\begin{aligned} \mu_{n, z e^{-\beta V_0}, \beta}(\mathrm{d}\gamma) \\ &= \frac{1}{Z_n} \sum_{N \in \mathbb{N}_0} \frac{z^N}{N!} e^{-\beta [H(x_1, \dots, x_N) - N V_0]} \mathrm{d}x_1, \dots, \mathrm{d}x_N. \end{aligned}$$

§ STATICS: PHASE TRANSITION



We need the following two assumptions.

ASSUMPTION I Finite connectivity

There exists a constant $c_d \in (0, \infty)$ such that, for $\lambda_d \times \mathbb{Q}$ a.e. $x = (\tilde{x}, K)$ and all $n \in \mathbb{N}$,

$$k(\gamma) - k(\gamma \cup x) \leq c_d \quad \forall \gamma \in \Gamma_n.$$

ASSUMPTION II Spherical interior

There exists a $t > 0$ such that $\mathbb{Q}\{K : B_0(t) \subset K\} > 0$.

Assumption I holds whenever $\mathbb{Q}\{K : B_0(t) \subset K\} = 1$ for some $t > 0$, and is much stronger than Assumption II.

The following lemma is the key behind the occurrence of a phase transition.

LEMMA 12.2 Stochastic domination

For $z \geq 0$ and $n \in \mathbb{N}$, let Π_n^z be the probability measure on the set of configurations Γ_n corresponding to the Poisson point process on Λ_n with intensity measure $z\lambda_d \times \mathbb{Q}$. Under Assumption I,

$$\Pi_n^{z2^{-cd}} \prec \mu_{n,z,z},$$

where \prec denotes stochastic domination.

THEOREM 12.3 Percolation transition in the Boolean model

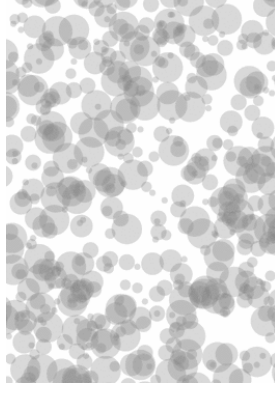
Under Assumption II, the Poisson Boolean model $h(\gamma)$ with general grains percolates for a.e. γ under $\Pi^z := \Pi_\infty^z$ for z large enough.

PROOF:

Couple with the **standard continuum percolation model** with grains $B_0(t)$. For the latter the same claim can be established via a Peierl's argument. Define

$$\underline{s}(K) = \sup\{\|B_t(0)\| : B_t(0) \subset K\}.$$

A standard sufficient condition is $\int \underline{s}(K) \mathbb{Q}(dK) > 0$, which is equivalent to **Assumption II**. \square



THEOREM 12.4 Phase transition in the two-species model

Under Assumptions I–II, symmetry breaking occurs in the two-species Widom-Rowlinson measure with red boundary condition $\mu_{n,z,z}^R$ for large z , i.e., for $z > z_t \in (0, \infty)$,

$$\liminf_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \left[\mu_{n,z,z}^R(N(\gamma^r)) - \mu_{n,z,z}^R(N(\gamma^b)) \right] > 0.$$

PROOF:

The proof relies on Lemma 12.2, Theorem 12.3 and (*), and uses similar arguments as in Chayes, Chayes, Kotecký 1995 for circular grains. The argument runs as follows.

Define

$k_n^r(\gamma)$ = number of red clusters in γ ,

$k_n^b(\gamma)$ = number of blue clusters in γ ,

$k_n(\gamma) = |\{\tilde{x} \in \tilde{\gamma} \cap \Lambda_n : \tilde{x} \in \text{infinite component of } h(\gamma)\}|$,

$k_{n,m}(\gamma) = |\{\tilde{x} \in \tilde{\gamma} \cap \Lambda_n : \tilde{x} \text{ intersects } \partial\Lambda_m\}|$.

Using (*), monotonicity of $k_{n,m}(\gamma)$ in m for every fixed n , and Lemma 12.2, we find that

$$\begin{aligned} & \mu_{n,z}^R(N(\gamma^r)) - \mu_{n,z,z}^R(N(\gamma^b)) \\ &= \mu_{n,z}^{\text{rc}}(k_n^r(\gamma)) - \mu_{n,z}^{\text{rc}}(k_n^b(\gamma)) \\ &= \mu_{n,z}^{\text{rc}}(k_{n,n}(\gamma)) \geq \mu_{n,z}^{\text{rc}}(k_n(\gamma)) \geq \prod_n^z 2^{-c_d}(k_n(\gamma)). \end{aligned}$$

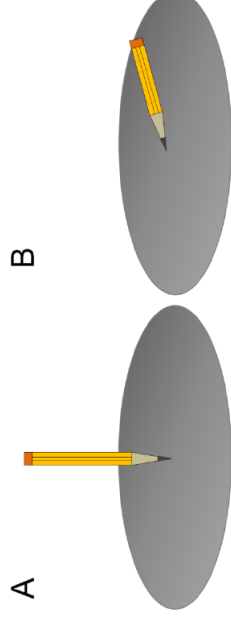
From [Theorem 12.3](#) and the ergodic theorem, we have that, for z large enough,

$$\liminf_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \prod_n^{z2^{-cd}} (k_n(\gamma)) > 0.$$

Hence we obtain [symmetry breaking](#) for z large enough, i.e.,

$$\begin{aligned} & \liminf_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} [\mu_{n,z,z}^R(N(\gamma^r)) - \mu_{n,z,z}^R(N(\gamma^b))] \\ &= \liminf_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} [\mu_{n,z}^{rc}(k_n^r(\gamma)) - \mu_{n,z}^{rc}(k_n^b(\gamma))] > 0, \end{aligned}$$

which settles the claim. \square



We can now characterise symmetry breaking in terms of percolation in the random-cluster model.

COROLLARY 12.5 Symmetry breaking

Under Assumptions I–II,

$$\lim_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \mu_{n,z}^{\text{rc}}(k_n(\gamma)) = \rho_\infty(z) \quad \text{exists,}$$

and symmetry breaking occurs if and only if $\rho_\infty(z) > 0$. The latter holds for z large enough.

PROOF:

The proof is an adaptation of the arguments in Chayes, Chayes, Kotecký 1995. The existence of the limit may be verified via ergodic-theoretic arguments. \square

§ STATICS: LARGE DEVIATIONS

Below we state a large deviation principle for the one-species Widom-Rowlinson measure μ_β on the torus \mathbb{T} in the low-temperature limit, and provide examples for which the rate function can be computed explicitly.

► LDP for the one-species model

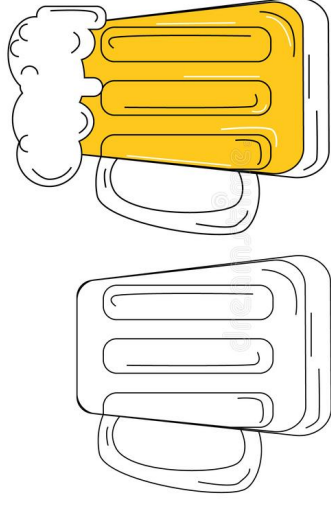
Set $z_b = \beta$ and $z_r = \kappa\beta$ for $\kappa \in (1, \infty)$ fixed. Then the induced one-species Widom-Rowlinson measure is given by

$$\mu_\beta(d\gamma) := \frac{1}{Z} e^{-\beta H(\gamma)} \Gamma^{\kappa\beta}(d\gamma).$$

REMARK: Reparametrisation

The two-colour model exhibits a phase transition for $z_r = z_b = \beta$ when $\beta > \beta_c$ for some $\beta_c \in (0, \infty)$.

To make sure that the **pure gas state** (= torus filled with blue particles) is the **metastable state**, we choose $z_r = \kappa\beta$, $\kappa \in (1, \infty)$, which implies that the **pure liquid state** (= torus filled with red particles) is the **stable state** in the low-temperature limit.



Recall the definition of $\mathbb{T} \times \text{supp}(\mathbb{Q})$ and \mathcal{C} . We can extend the notion of **halo** to all sets in \mathcal{C} by putting

$$h: \mathcal{C} \rightarrow \tilde{\mathcal{C}}, \quad F \mapsto \cup_{(x,K) \in F} (x + K).$$

Assumption III Continuity of the halo

Let $\text{supp}(\mathbb{Q}) \subset \mathcal{K}_0$ be the collection of all convex sets with the origin in their **interior**. The halo function restricted to $\mathbb{T} \times \text{supp}(\mathbb{Q})$ is continuous.

Assumption III trivially holds when $\text{supp}(\mathbb{Q})$ is a singleton. Similar to the above definition of halo for general sets, we define the **volume** of the halo for general sets as

$$H(F) = \int_{\tilde{\mathcal{C}}} |h(F) \oplus (-K)| \mathbb{Q}(dK) = \mathbb{E}[|h(F) \oplus (-K_1)|],$$

where K_1 is a convex set with distribution \mathbb{Q} . Note that, under Assumption III, $F \mapsto H(F)$ is continuous.

The following large deviation principle for the configuration plays a crucial role in what follows.

THEOREM 12.6 LDP for the configuration

Under Assumption III, the family of probability measures $\{\mu_\beta(\cdot)\}_{\beta \geq 1}$ satisfies the LDP with rate β and with good rate function I_{WR} given by

$$I_{\text{WR}}(F) = J_{\text{WR}}(F) - \min_{\mathcal{C}} J_{\text{WR}}, \quad F \in \mathcal{C},$$

with

$$J_{\text{WR}}(F) = H(F) - \kappa(\lambda_d \otimes \mathbb{Q})(F)$$

and

$$\min_{\mathcal{C}} J_{\text{WR}} = (1 - \kappa)|\mathbb{T}|.$$

PROOF:

Clearly, $\Pi^{\kappa\beta}$ satisfies the LDP with good rate function

$$\mathbb{P}(\Pi^{\kappa\beta} \subset \tilde{F} \times \mathcal{A}) = e^{-\kappa\beta|\mathbb{T}|} e^{-\kappa\beta|\tilde{F}|\mathbb{Q}(\mathcal{A})}.$$

Consequently, the rate function is given by

$$I_{\text{PP}}(F) = \kappa|\mathbb{T}| - \kappa(\lambda_d \otimes \mathbb{Q})(F).$$

By Assumption III, $\gamma \mapsto h(\gamma)$ is continuous because $\gamma \mapsto H(\gamma)$ and $h(\gamma) \mapsto H(\gamma)$ are continuous.

Using exponential tilting, we obtain the LDP for μ_β with good rate function I_{WR} . Using the expression for I_{PP} , we can write I_{WR} as

$$I_{\text{WR}}(F) = J_{\text{WR}}(F) - \inf_{F' \in \mathcal{C}} J_{\text{WR}}(F').$$

The proof is completed by showing that the infimum equals $(1 - \kappa)|\mathbb{T}|$. \square

From Theorem 12.6 we can deduce LDPs for the shape and the volume of the halo via the contraction principle.

Define $S = h(\mathcal{C}) = \{S \subset \mathbb{T} : S = h(F) \text{ for some } F \in \mathcal{C}\}$.

THEOREM 12.7 LDP for the halo shape

Under Assumption III, the family of probability measures $\{\mu_\beta(h(\gamma) \in \cdot)\}_{\beta \geq 1}$ satisfies the LDP with rate β and with good rate function I_h given by

$$I_h(S) = J_h(S) - (1 - \kappa)|\mathbb{T}|, \quad S \in \mathcal{S},$$

with

$$J_h(S) = \mathbb{E}[|S \oplus \tilde{K}_1|] - \kappa \sup_{F \in \mathcal{C} : h(F) = S} (\lambda_d \otimes \mathbb{Q})(F).$$

THEOREM 12.8 LDP for the halo volume

Under Assumption III, the family of probability measures $\{\mu_\beta(H(\gamma) \in \cdot)\}_{\beta \geq 1}$ satisfies the LDP with rate β and with good rate function I_H given by

$$I_H(a) = J_H(a) - \min_{[0, \infty)} J_H, \quad a \in [0, \infty),$$

with

$$J_H(a) = a - \kappa \sup_{F \in \mathcal{C}: H(F)=a} (\lambda_d \otimes \mathbb{Q})(F)$$

and

$$\min_{[0, \infty)} J_H = (1 - \kappa) |\mathbb{T}|.$$



§ EXAMPLES

- Fixed convex grains

If $K \in \mathcal{K}_0$ and $\mathbb{Q} = \delta_K$, then

$$J_H(a) := \Phi_\kappa(R_a, K), \quad a \in [0, \infty),$$

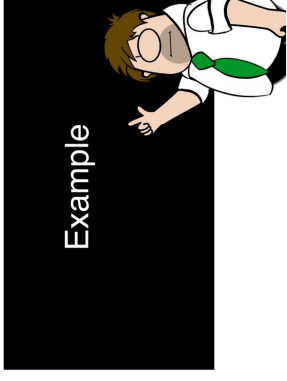
where $\Phi_\kappa(R, K) = R^d |K^*| - \kappa(R - 1)^d |K^*|$ with $K^* = K \oplus (-K)$, and R_a is chosen such that $a = R^d |K^*|$.

It is easy to show that $R \mapsto \Phi_\kappa(R, K)$ achieves its maximum at

$$R(\kappa) = \frac{\kappa^{1/(d-1)}}{\kappa^{1/(d-1)} - 1},$$

with the maximum given by

$$\Phi(\kappa, K) = \Phi_\kappa(R(\kappa), K) = |K^*| R(\kappa)^{d-1}.$$



Example

The latter is the volume free energy of the critical droplet. Note that it has a product form: the first term depends only on the volume of K^* and not on the shape, the second term depends only on κ and the dimension d .

► Uniform rotation of convex grain

The critical droplet is a ball.

► Partial rotation of a polygon

The critical droplet is a polygon, whose shape depends on the set of allowed rotations.

► Dilation of a convex grain

The critical droplet is the same as without dilation.

§ DYNAMICS: METASTABILITY

So far we only considered the static WRM. We now turn to the dynamic WRM, and focus on the average crossover time when the system starts with an empty torus and tries to condense to a full torus. Our goal is:

- To identify the leading order asymptotics:
volume free energy
- To speculate about the order of the correction term:
surface free energy

We are particularly interested in scaling properties as a function of β, κ .

THEOREM 12.9 Average crossover time for fixed grain shape

Let $\mathcal{Q} = \delta_K$ for some $K \in \mathcal{K}_0$. Then, for every $\kappa \in (1, \infty)$,

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = \exp[\beta \Phi(\kappa, K) + o(\beta)], \quad \beta \rightarrow \infty,$$

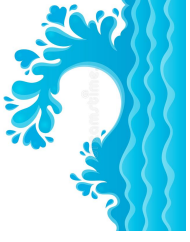
where

$$\Phi(\kappa, K) = |K^*|R(\kappa),$$

with $K^* = K \oplus (-K)$.

PROOF:

The proof is based on the LDPs described in Theorems 12.7–12.8, which allow us to approximate the Dirichlet form for $\text{cap}(\square, \blacksquare)$, in combination with the tools from potential theory described in Lecture 2, rephrased in the continuum space setting. \square



§ SURFACE CORRECTIONS

What is written below is **conjectural**. Only for the case of spherical grains in two dimensions are rigorous proofs available, which are highly complex. See **Lectures 9–11**.

CONJECTURE 12.10

Let $Q = \delta_K$. For every $\kappa \in (1, \infty)$,

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = \exp\left[\beta \Phi(\kappa, K) - \beta^\alpha \Psi(\kappa, K) + o(\beta^\alpha)\right], \quad \beta \rightarrow \infty,$$

where $\alpha \in [0, 1)$ is a scaling exponent and

$$\Psi(\kappa, K) = \text{surface entropy of critical droplet.}$$

We next give heuristics for some special cases, leading to conjectures for the **scaling exponent** of the **surface free energy** of the critical droplet.

► Spherical grains

Let $K = B_1 \subset \mathbb{R}^d$. Suppose that a grain of unit radius sticks out of a sphere of radius R by a perpendicular distance $0 < s \ll 1$. Then the volume that sticks out is

$$V(s) \asymp s \left(\frac{R}{R-1} \right)^{(d-1)/2},$$

while the surface on the sphere that is covered by the grain is

$$S(s) \asymp \left(\frac{R}{R-1} \right)^{(d-1)/2}.$$

Because of the Boltzmann cost factor, the typical volume is $V(s) \asymp \beta^{-1}$. Consequently,

$$s \asymp \left(\beta^{-1} \left(\frac{R}{R-1} \right)^{-(d-1)/2} \right)^{2/(d+1)}.$$

Since the particles that stick out cover the entire surface of the sphere, the number of particles sticking out is

$$N(s) \asymp \frac{R^{d-1}}{S(s)} = \beta^{(d-1)/(d+1)} R \left(\frac{R}{R-1} \right)^{-(d-1)/(d+1)}.$$

Picking $R = R(\kappa)$, we find that the surface entropy is

$$\beta^{(d-1)/(d+1)} R(\kappa)^{d-1} \left(\frac{R(\kappa)}{R(\kappa)-1} \right)^{-(d-1)/(d+1)},$$

from which we conclude that

$$\alpha = \frac{d-1}{d+1}, \quad \Psi(\kappa, B_1) \asymp \frac{\kappa^{d/(d+1)}}{(\kappa^{1/(d-1)} - 1)^{d-1}}.$$

► Polygonal grains

Pick $K = P_1$ with P_1 a unit polygon in \mathbb{R}^d . We argue in the same way as for spherical grains. Suppose that a unit polygonal grain sticks out of a polygon of linear size R by a perpendicular distance $0 < s \ll 1$. Then

$$V(s) \asymp s, \quad S(s) \asymp 1,$$

which with $V(s) \asymp \beta^{-1}$ gives

$$N(s) \asymp R^{d-1}.$$

Hence

$$\alpha = 0, \quad \Psi(\kappa, P_1) \asymp R(\kappa)^{d-1}.$$

► Lebesgue grains

Both of the above cases can be subsumed into the more general case $K = K_p$ with

$$K_p = \{x \in \mathbb{R}^d : \|x\|_p \leq 1\},$$

where $\|\cdot\|_p$ denotes the l_p -norm with $p \in (1, \infty]$. Spherical grains correspond to $p = 2$ and polygonal grains to $p = \infty$.

We conjecture that the **scaling exponent** α equals

$$\alpha = \alpha_p = \frac{d-1}{d-1+p}.$$

§ CONCLUSION

The Arrhenius formula for the average condensation time involves both the volume free energy and the surface free energy of the critical droplet. Both depend on the shape of the grains.

There are many challenges in understanding the details of the Widom-Rowlinson model with grains of general shape. The world of granular media has lots to offer, not only in physics but also in mathematics.



