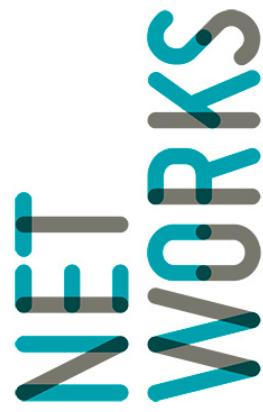


Metastability for the Widom-Rowlinson model with grains of general shape

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Inhomogeneous Random Systems,
Institut Curie & Institut Henri Poincaré, Paris, France,
24+25 January 2023.

CHALLENGE:

Questions about phase transitions, critical behaviour and metastability are **much more challenging** in the continuum than on lattices and graphs.



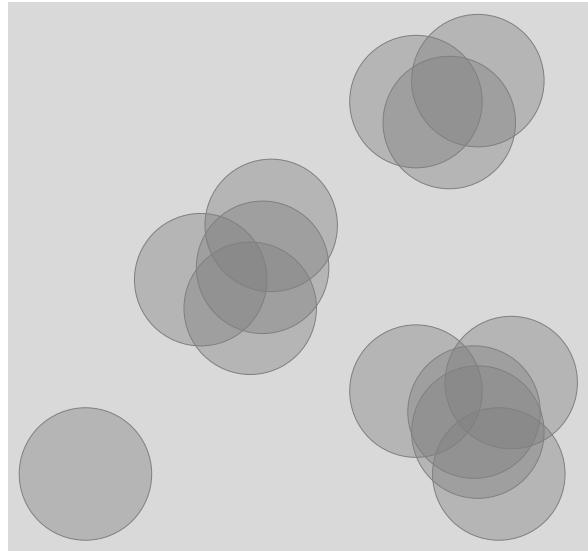
OUTLINE OF TALK:

- (1) Widom-Rowlinson model of interacting disks in \mathbb{R}^2 .
- (2) Extension to convex grains in \mathbb{R}^d , $d \geq 2$.

§ THE STATIC WIDOM-ROWLINSON MODEL

Let $\mathbb{T} \subset \mathbb{R}^2$ be a finite torus. The set of finite particle configurations in \mathbb{T} is

$$\Gamma = \{\gamma \subset \mathbb{T} : N(\gamma) \in \mathbb{N}_0\}, \quad N(\gamma) = \text{cardinality of } \gamma.$$



disks of radius 1 around γ

The grand-canonical Gibbs measure is

$$\mu(d\gamma) = \frac{1}{\Xi} z^{N(\gamma)} e^{-\beta H(\gamma)} \mathbb{Q}(d\gamma),$$

where

- \mathbb{Q} is the Poisson point process with intensity 1,
- $z \in (0, \infty)$ is the chemical activity,
- $\beta \in (0, \infty)$ is the inverse temperature,
- Ξ is the normalising partition function,

H is the interaction Hamiltonian given by

$$H(\gamma) = \left| \bigcup_{x \in \gamma} B(x) \right| - \sum_{x \in \gamma} |B(x)|,$$

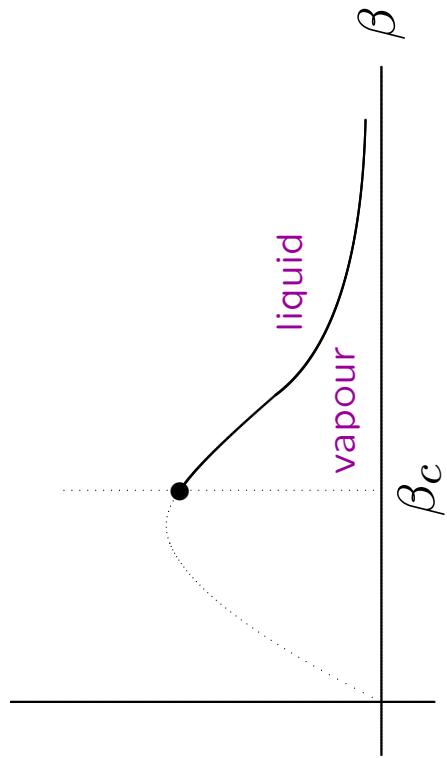
i.e., minus the total overlap of the disks of radius 1 around γ . This makes the interaction attractive.

For $\beta > \beta_c$ a phase transition occurs at

$$z = z_c(\beta) = \beta e^{-\pi\beta}$$

in the thermodynamic limit, i.e., $\mathbb{T} \rightarrow \mathbb{R}^2$. No closed form expression is known for β_c .

$$z_c(\beta)$$

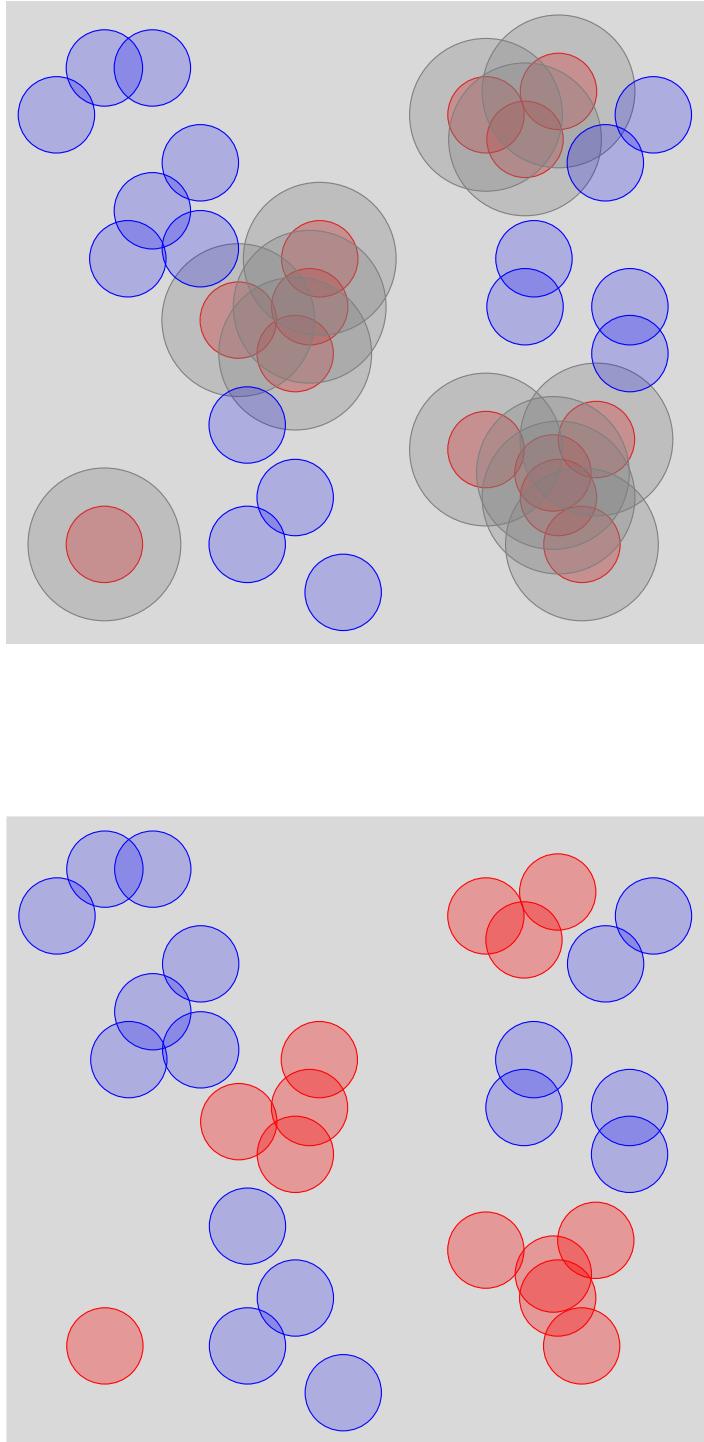


Ruelle 1971

Lebowitz, Gallavotti 1971

Chayes, Chayes, Koteky 1995

The one-species model can be seen as the projection of a two-species model with hard-core repulsion:

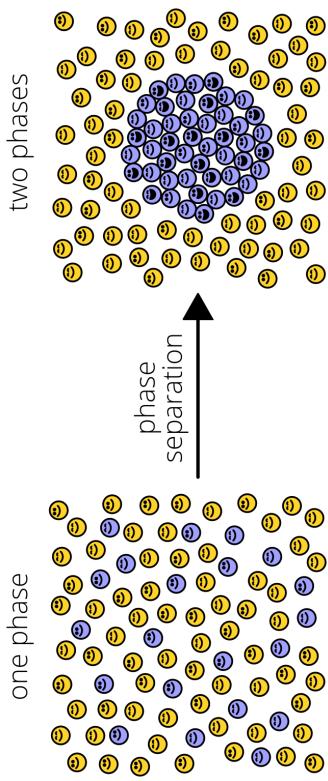


Disks of radius $\frac{1}{2}$ around γ^{red} and γ^{blue}
with chemical activities z^{red} and z^{blue} .

The hard-core repulsion in the two-species model implies that the centers of the disks of one species must stay outside the halo of radius 1 around the centers of the disks of the other species.

When we integrate out over one species, we precisely get the Widom-Rowlinson interaction for the other species.

The crossover in the one-species model from vapour to liquid corresponds to a phase separation of species in the two-species model.



§ THE DYNAMIC WIDOM-ROWLINSON MODEL

The particle configuration evolves as a **continuous-time Markov process** $(\gamma_t)_{t \geq 0}$ with state space Γ and generator

$$(\mathcal{L}f)(\gamma) = \int_{\mathbb{T}} dx b(x, \gamma) [f(\gamma \cup x) - f(\gamma)] + \sum_{x \in \gamma} d(x, \gamma) [f(\gamma \setminus x) - f(\gamma)],$$

i.e., particles are **born at rate b** and **die at rate d** , given by a **heat bath dynamics**

$$\begin{aligned} b(x, \gamma) &= z e^{-\beta[H(\gamma \cup x) - H(\gamma)]}, & x \notin \gamma, \\ d(x, \gamma) &= 1, & x \in \gamma. \end{aligned}$$

The grand-canonical Gibbs measure is the unique reversible equilibrium of this stochastic dynamics.

particles do not move!

KEY QUESTION:



Let \square and \blacksquare denote the set of configurations where \mathbb{T} is **empty**, respectively, **full**.

- Start with \mathbb{T} empty, i.e., $\gamma_0 = \square$.
[preparation in vapour state]
- Choose $z = \kappa z_c(\beta)$, $\kappa \in (1, \infty)$.
[reservoir is super-saturated vapour]
- Wait for the first time τ_\blacksquare when the system fills \mathbb{T} .
[condensation to liquid state]

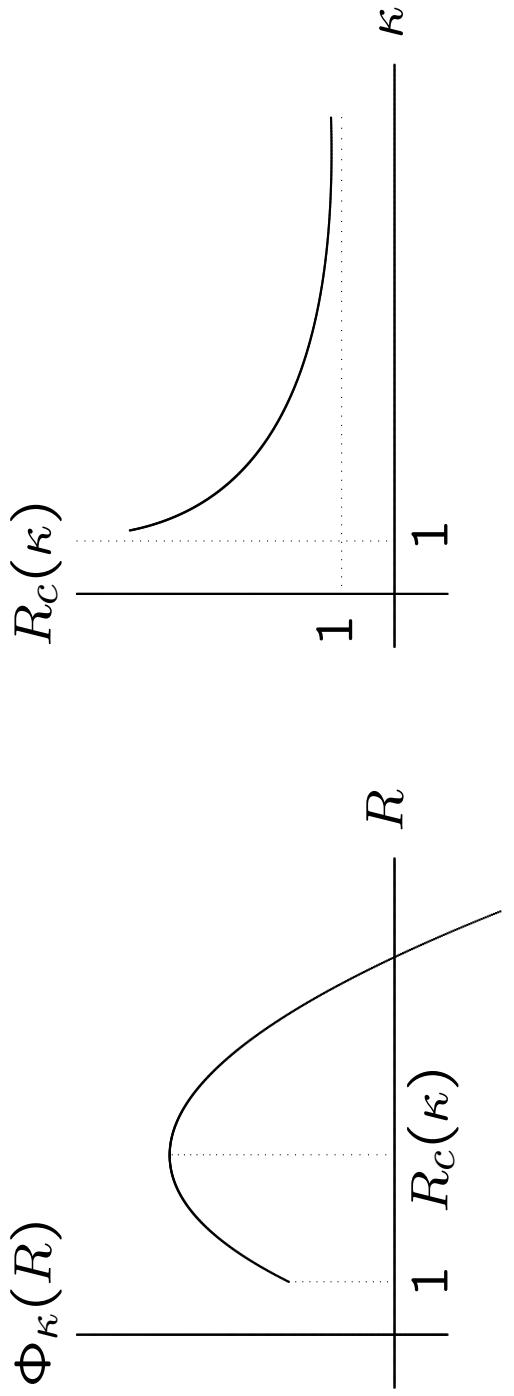
What can be said about the law of τ_\blacksquare in the limit as $\beta \rightarrow \infty$ for fixed \mathbb{T} and κ ?

§ THEOREMS

F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti,
work in progress

For $R \in [1, \infty)$ and $\kappa \in (1, \infty)$, let

$$\Phi_\kappa(R) = \pi R^2 - \kappa \pi (R-1)^2, \quad R_c(\kappa) = \frac{\kappa}{\kappa-1}.$$



THEOREM 1 [Arrhenius formula]

For every $\kappa \in (1, \infty)$,

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = \exp \left[\beta \Phi(\kappa) - \beta^{1/3} \Psi(\kappa)(1 + o(1)) \right], \quad \beta \rightarrow \infty,$$

where

$$\Phi(\kappa) = \Phi_{\kappa}(R_c(\kappa)) = \frac{\pi \kappa}{\kappa - 1},$$

$$\Psi(\kappa) = \Psi_{\kappa}(R_c(\kappa)) = s_* \frac{\kappa^{2/3}}{\kappa - 1},$$

where $s_* \in \mathbb{R}$ is a constant that comes from an effective
microscopic model with hard-core constraints.



For $\delta > 0$, let

$$\mathcal{C}_\delta(\kappa) = \left\{ \gamma \in \Gamma : \exists x \in \mathbb{T} \text{ such that } \right.$$

$$B_{R_c(\kappa)-\delta}(x) \subset \text{halo}(\gamma) \subset B_{R_c(\kappa)+\delta}(x) \Big\}.$$

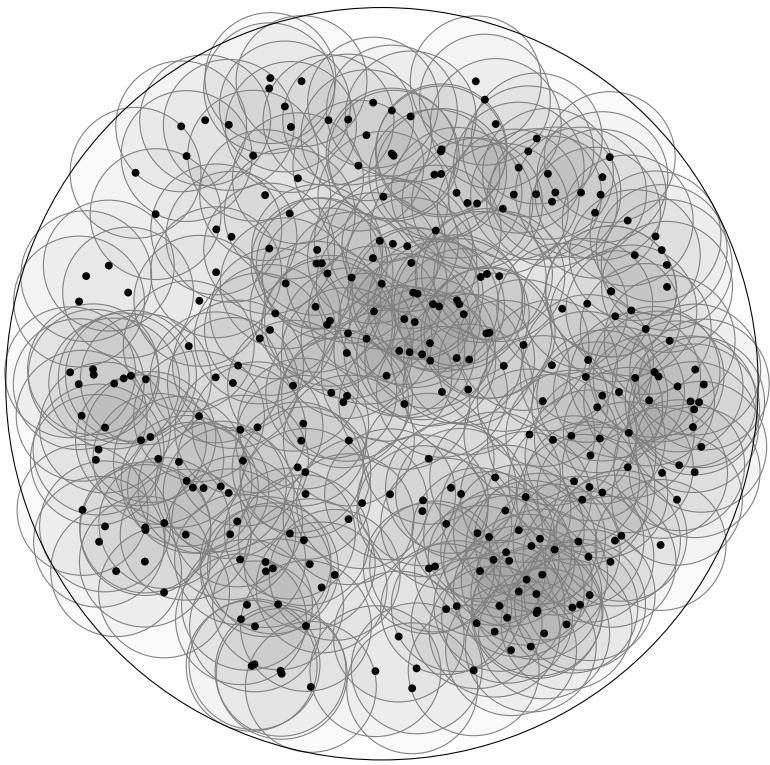
THEOREM 2 [Critical droplet]

For every $\kappa \in (1, \infty)$,

$$\lim_{\beta \rightarrow \infty} \mathbb{P}_\square \left(\tau_{\mathcal{C}_\delta(\beta)}(\kappa) < \tau_\blacksquare \mid \tau_\square > \tau_\blacksquare \right) = 1$$

when

$$\lim_{\beta \rightarrow \infty} \delta(\beta) = 0, \quad \lim_{\beta \rightarrow \infty} \beta^{2/3} \delta(\beta) = \infty.$$



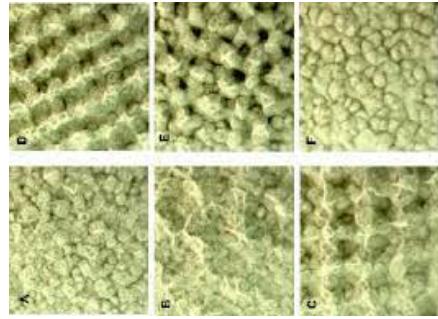
Critical droplet has radius $R_c(\kappa)$ and is filled with 1-disks:
 $\asymp \beta$ disks in the interior, $\asymp \beta^{1/3}$ disks on the boundary

Stillinger, Weeks 1995
capillary waves

§ GRAINS OF GENERAL SHAPE

We next 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.



F. den Hollander, R. Kotecký, D. Yogeshwaran
work in progress

1. A configuration γ now consists of a collection of **centers** x and **shapes** K . For given γ define the set

$$h(\gamma) = \cup_{(x,K) \in \gamma} (x + K),$$

which is the **halo of γ** .

2. Let \mathcal{K} be the collection of all **compact convex sets** whose interior contains the origin. Let \mathbb{S} denote the probability distribution on \mathcal{K} according to which the shapes of the grains are drawn **independently**. Then

$$H(\gamma) = \int_{\mathcal{K}} |h(\gamma) \oplus (-K)| \mathbb{S}(dK)$$

is the **effective Hamiltonian**, where \oplus is the Minkowski sum for sets.

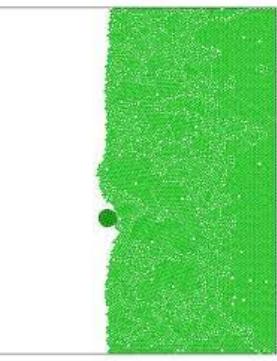
3. If $\mathbb{S}(\cdot) = \delta_K(\cdot)$ for a compact subset K , then

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

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

The standard **WRM** corresponds to the choice $K = B_1$,
the ball with radius 1 centered at the origin.

§ STATICS: PHASE TRANSITION



We need the following assumption.

ASSUMPTION: $\mathbb{S}(tB_1 \subset K) = 1$ for some $t > 0$.

Under this assumption it can be shown that the system has a phase transition between a liquid phase and a vapour phase for β large enough.

§ DYNAMICS: METASTABILITY

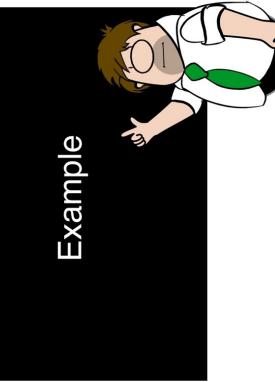
THEOREM 3

Subject to the assumption,

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = \exp \left[\beta \Phi(\kappa, K) (1 + o(1)) \right], \quad \beta \rightarrow \infty,$$

for a computable volume free energy $\Phi(\kappa, K)$.

§ EXAMPLES



► Fixed convex grain

If $K \in \mathcal{K}$ and $\mathbb{S} = \delta_K$, then the critical droplet **is** the set

$$R(\kappa)K$$

with

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

and the volume free energy **is**

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

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

- Uniform rotations of a convex grain
The critical droplet is $R(\kappa, K)B_1$, where $R(\kappa, K)$ scales with κ in the same way as for a fixed convex grain, and depends on the volume and surface K only.
- Random dilations of a convex grain
If $K = -K$, then the critical droplet is $R(\kappa, \mathcal{D})K$, where $R(\kappa, \mathcal{D})$ scales with κ in a way that depends on the first d moments of the probability distribution \mathcal{D} of the dilation.
- Random rotations of a polygon
The critical droplet is a polygon whose shape depends on the probability distribution of the rotations. For instance, if K is the unit square and the rotations are 0 and $\frac{\pi}{8}$, each with probability $\frac{1}{2}$, then the critical droplet is a multiple of a regular octagon.



§ 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.

CONJECTURE

Let $\mathbb{S} = \delta_K$. For every $\kappa \in (1, \infty)$,

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = \exp \left[\beta \Phi(\kappa, K) - \beta^{\alpha} \Psi(\kappa, K) (1 + o(1)) \right], \quad \beta \rightarrow \infty,$$

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

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

EXAMPLES BASED ON HEURISTICS:

- **Spherical grains:** $K = B_1 \subset \mathbb{R}^d$

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

- **Polygonal grains:** $K = P_1 \subset \mathbb{R}^d$

$$\alpha = 0, \quad \Psi(\kappa, P_1) = s_*(P_1) \frac{\kappa}{(\kappa^{1/(d-1)} - 1)^{d-1}}$$

§ 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.

