The Widom-Rowlinson model: from phase transition to metastability. Lecture 1

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"DFG SPP2265 Summer School on
Probability and geometry on configuration spaces"
Berlin, July 17-21, 2023

Plan of the mini-course

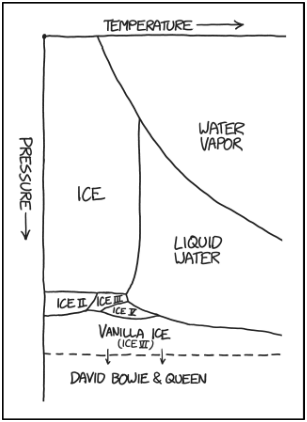
- Lecture 1:
  - Introduction and basic notions of equilibrium statistical mechanics
  - Widom-Rowlinson model: two equivalent formulations
  - Phase transition for the WR model
- Lecture 2:
  - Introduction to metastability and potential theory
  - Dynamic WR model
- Lecture 3:
  - Metastability for the WR model
  - Mesoscopic fluctuations of the critical droplet
  - Microscopic fluctuations and the parabolic interface model

Introduction and basic notions of equilibrium statistical mechanics

References:

- S. Friedli, Y. Velenik, Statistical Mechanics of Lattice Systems: A Concrete Mathematical Introduction Cambridge: Cambridge University Press, 2017.
- G. Gallavotti, Statistical Mechanics: A Short Treatise, Springer Verlag, Berlin, 1999.
- E. Presutti, Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics, Theoretical and Mathematical Physics, Springer, 2009.

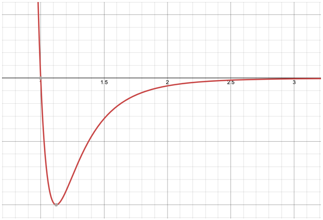
A central problem in equilibrium statistical mechanics is the derivation of phase diagrams of fluids.



From **xkcd.com**, Water Phase Diagram.
Vanilla Ice was produced in small quantities for years, but it wasn't until the 90s that experimenters collaborated to produce a sample that could survive at room temperature for several months.

"Phase diagrams are the beginning of wisdom-not the end of it"
Sir William Hume-Rothery

Fluids: identical point particles with no internal structure - electronically neutral atoms or molecules.
The inter-particles force is usually described by Lennard-Jones potential, that models soft repulsive and attractive interactions.



$$V_{\mathsf{LJ}}(r) = a\, r^{-12} - b\, r^{-6}$$

Conjecture: The phase diagram of a systems of particles interacting via a L-J potential agrees with the figure in previous slide.

• Existence of phase transitions is an experimentally well established fact.

• A complete rigorous derivation of phase diagrams or even the existence of phase transitions is still an open problem in statistical mechanics!

Introduction: phase transitions

Phase transitions may be much more complex, but we restrict to phase transitions of the first order with order parameter the density.
In Physics this means the following:

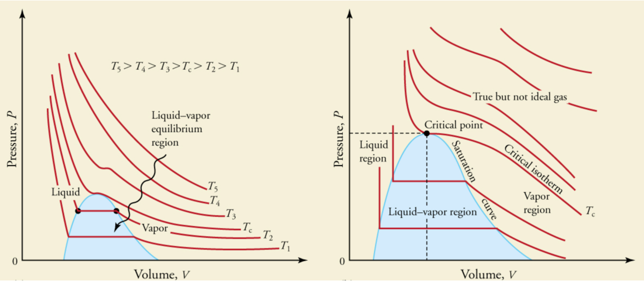
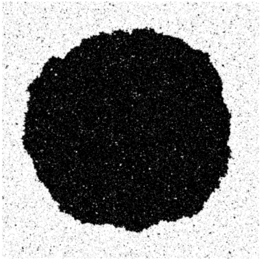


Figure from 13.5: Phase Changes by OpenStax is shared under a CC BY 4.0 license

Introduction: phase transitions

There is a forbidden interval of densities, say (ρ_-, ρ_+), so that if we put a mass $\rho|\Lambda|$ of fluid in the region Λ, with $\rho \in (\rho_-, \rho_+)$, then the fluid separates into a part with density ρ_- and another one with density ρ_+. It does not exist an equilibrium state with homogeneous density ρ.



The simulation of the nearest-neighbor lattice gas was made by fixing the density
$\rho \in (\rho_-, \rho_+)$
with a boundary condition favouring the gas phase.
Phase separation occurs. In a typical configuration, a liquid droplet of density ρ_+ appears, immersed in a gas phase of density ρ_-.

Picture from "Statistical Mechanics of Lattice Systems", Sacha Friedli and Yvan Velenik.

Introduction: equilibrium statistical mechanics

- Thermodynamics is a phenomenological theory, developed during the 19th century with Carnot, Clausius, Kelvin, Joule, Gibbs... It is based on empirical principles and does not make any assumption regarding microscopic structures.
- A macroscopic state is described by thermodynamical laws in equilibrium. It is described by macroscopic quantities (e.g. energy, volume, pressure, number of particles, temperature,...).
- A microscopic state is described by classical mechanics. At a given instant, one has to specify the value of positions and momenta of each of the N particles $\rightarrow 6N$-dimensional phase space. Huge number of microscopic variables, $N \sim 10^{23}$!

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- A microscopic state is described by classical mechanics. At a given instant, one has to specify the value of positions and momenta of each of the N particles $\rightarrow 6N$-dimensional phase space. Huge number of microscopic variables, $N \sim 10^{23}$!
- The main object of statistical mechanics is the description of macroscopic systems starting from a microscopic description. $\rightarrow$ 19th century, with Maxwell, Boltzmann and Gibbs.

Idea: Probabilistic approach instead of deterministic! Define probability distributions ("ensembles") over the set of all microstates which are compatible with a certain observed macrostate.

Introduction: equilibrium statistical mechanics

- Averages of observables over long times (e.g. kinetic energy):

$$\frac{1}{T}\int_0^T \left(\sum_{i=1}^{N} \frac{1}{2}\dot{q}_i^2(s)\right) \mathrm{d}s, \qquad T \to \infty$$

- Ergodic hypothesis: "the time average of an observable equals its average on the surface of constant energy" (Boltzmann)
- N particles in box Λ. Energy/Hamiltonian:

$$H(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} \frac{1}{2}\dot{q}_i^2 + \sum_{1\le i<j\le N} V(q_i - q_j), \quad (\mathbf{q},\mathbf{p}) \in \Lambda^N \times (\mathbb{R}^3)^N$$

Introduction: equilibrium statistical mechanics

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- Let J_E be the domain of the variables $(\mathbf{p},\mathbf{q})$ where $E - \Delta E \le H(\mathbf{p},\mathbf{q}) \le E$ holds. Then

$$\lim_{T\to\infty} \frac{1}{T}\mathrm{d}s = \frac{\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}}{\int_{J_E} \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}}$$

Introduction: equilibrium statistical mechanics

Box $\Lambda \subset \mathbb{R}^3$. Call $\omega = (\mathbf{q}, \mathbf{p})$. Statistical ensembles.

- Microcanonical ensemble: Energy E and number of particles N fixed.

$$\nu^{\text{Mic}}_{E,N,\Lambda}(\omega) = 1/|\Omega(E,N,\Lambda)|, \qquad \text{if } \omega \in \Omega(E,N,\Lambda)$$

$$\Omega(E,N,\Lambda) = \{\omega \in \Lambda^N \times \mathbb{R}^{3N} | E - \Delta E \le H(\omega) \le E\}$$

- Canonical ensemble: $\beta = \frac{1}{kT}$ and number of particles N fixed.

$$Z(\beta, N, \Lambda) = \frac{1}{N!} \int_{\Lambda^N \times \mathbb{R}^{3N}} \mathrm{e}^{-\beta H(\omega)} \mathrm{d}\omega$$

- Grand canonical ensemble: $\beta = \frac{1}{kT}$ and chemical potential λ fixed

$$\Xi(\beta, \lambda, \Lambda) = \sum_{N \ge 0} \frac{\mathrm{e}^{\beta \lambda N}}{N!} \int_{\Lambda^N \times \mathbb{R}^{3N}} \mathrm{e}^{-\beta H(\omega)} \mathrm{d}\omega$$

Introduction: equilibrium statistical mechanics

- Thermodynamic limit: $N \sim 10^{23}$ very large $\Rightarrow$ approximate with limit $N, |\Lambda|, E \to \infty$ while $\beta, \lambda, u = \frac{E}{|\Lambda|}, \rho = \frac{N}{|\Lambda|}$ remain constant.

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- Orthodicity property: by taking the thermodynamic limit of the log of partition functions we obtain thermodynamic potentials.

  Example: Boltzmann-Entropy $S = k \log W$ (Wahrscheinlichkeit)

Wikipedia: Boltzmann's equation carved on his gravestone

- In the thermodynamic limit equivalence of ensembles.

Introduction: equilibrium statistical mechanics

The thermodynamic potentials

$$s(u,\rho) = \lim \frac{1}{|\Lambda|} \log |\Omega(E,N,\Lambda)|, \qquad \text{Entropy}$$

$$f(\beta,\rho) = -\lim \frac{1}{\beta|\Lambda|} \log Z(\beta,N,\Lambda), \qquad \text{Free energy}$$

$$p(\beta,\lambda) = \lim \frac{1}{\beta|\Lambda|} \log \Xi(\beta,\lambda,\Lambda), \qquad \text{Pressure}$$

- $f(\beta,\rho)$ is a convex function of ρ and $p(\beta,\lambda)$ a convex function of λ.
- They are one the Legendre transform of the other:

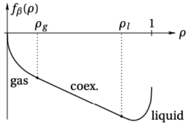
$$f(\beta,\rho) = \sup_{\lambda}\{\lambda\rho - p(\beta,\lambda)\}, \qquad p(\beta,\lambda) = \sup_{\rho}\{\lambda\rho - f(\beta,\rho)\}$$

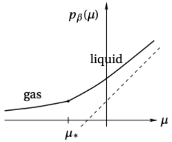
- The chemical potential is the change of energy when one adds one particle to the system

$$\lambda = \frac{\partial E}{\partial N}, \qquad \text{at fixed } S, |\Lambda|$$

Introduction: equilibrium statistical mechanics

- Phase transition: non convexity of $f(\beta, \rho)$ and non differentiability of $p(\beta, \lambda)$ for a certain range of the parameters (forbidden intervals).





Pictures from Friedli-Velenik, Section 4

- Other definition in terms of non-uniqueness of equilibrium measures.

  If there exist at least two distinct infinite-volume Gibbs measures, we say that there is a first-order phase transition. There are several "pure phases".

  When there is a unique Gibbs measure, the system lacks sensitivity to boundary conditions.

  $\Rightarrow$ Phase transition means sensitive dependence on boundary conditions.

Introduction: equilibrium statistical mechanics

State of the art:

- There is a great number of lattice models for which phase transitions are proven to take place, e.g. the Ising model on $\mathbb{Z}^d$ (Peierls '36, Onsager,...).
- Existence of phase transitions in models of fluids in the continuum: open.
- Simplified models for liquid-vapour phase transitions:
  - Hard rods in $d = 1$ with pairwise potential (attractive) decaying as $|r|^{-2+\alpha}, \alpha \in [0, 1)$, proof by Johansson '96;
  - Widom - Rowlinson model in $d \geq 2$, proof by Ruelle '71;
  - LMP model: four body potential (repulsive) + pair potential (attractive) in $d \geq 2$, proof by Lebowitz, Mazel and Presutti '99.

Widom-Rowlinson model: two equivalent formulations

References:

- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation.
- L. Šamaj, Widom-Rowlinson model (continuum and lattice), arXiv:0709.0617, 2007.
- B. Widom and J.S. Rowlinson, New model for the study of liquid-vapor phase transitions, J. Chem. Phys. 52, 1670-1684, 1970.

Widom-Rowlinson model: 1 species

- Target: to study a model exhibiting phase transitions of the type "condensation from a vapour to a liquid" in the continuum.
- We focus on the Widom-Rowlinson model of interacting discs in $\mathbb{R}^d$ with $d \geq 2$.
- Remark: In the continuum, all questions about phase transitions and critical behaviours turn out to be much more challenging than on lattices or graphs.

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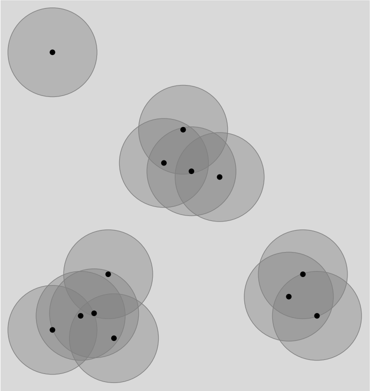
- Remark: In the continuum, all questions about phase transitions and critical behaviours turn out to be much more challenging than on lattices or graphs.
- In 1970 Widom and Rowlinson introduced a simple model of a classical fluid in thermodynamic equilibrium.
- In the Widom-Rowlinson model, the interactions are purely geometric, which makes it more tractable.
- Two equivalent formulations: 1 species-WR and 2 species-WR.

Widom-Rowlinson model: 1 species

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

$$\Omega = \{\omega \subset \mathbb{T}\colon\ N(\omega) \in \mathbb{N}_0\}, \quad N(\omega):\ \text{cardinality of } \omega$$



Choose a configuration ω.
Draw a disc of radius 1 around each point $x \in \omega$.

Definition: halo of a configuration

$$h(\omega) = \bigcup_{x \in \omega} B_1(x)$$

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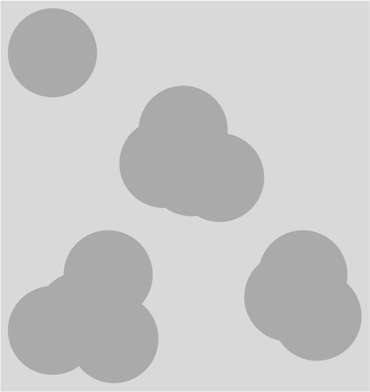

Definition: halo of a configuration

$$h(\omega) = \bigcup_{x\in\omega} B_1(x)$$

Hamiltonian:

$$H(\omega) = \left|\bigcup_{x\in\omega} B_1(x)\right| - \sum_{x\in\omega} |B_1(\omega)|$$

$$= V(\omega) - N(\omega)V_0$$

where $|\cdot|$ is the Lebesgue measure, $V(\omega) = |h(\omega)|$ and $V_0 = |B_1(0)| = \pi$.

Widom-Rowlinson model: 1 species

- The interaction Hamiltonian is given by

$$H(\omega) = |h(\omega)| - N(\omega)V_0$$

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

$$-(N(\omega) - 1)V_0 \leq H(\omega) \leq 0$$

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- We work in the grand-canonical ensemble. The equilibrium Gibbs measure is the probability measure on Ω given by

$$\mu_{\lambda,\mathbb{T},\beta}(\mathrm{d}\omega) = \frac{1}{\Xi}\mathrm{e}^{-\beta(H(\omega)-\lambda N(\omega))}\mathbb{Q}(\mathrm{d}\omega),$$

where

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

Widom-Rowlinson model: 1 species

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$$\mu_{z,\mathbb{T},\beta}(\mathrm{d}\omega) = \frac{1}{\Xi} z^{N(\omega)}\, \mathrm{e}^{-\beta H(\omega)} \mathbb{Q}(\mathrm{d}\omega),$$

where

  - $\mathbb{Q}$ is the Poisson point process with intensity 1,
  - $z = \mathrm{e}^{\lambda\beta}$ is called the activity
  - $\beta \in (0, \infty)$ is the inverse temperature,
  - Ξ is the normalization,

Remark: $\Xi = \Xi_{\mathbb{T},z,\beta}$ is the normalisation constant

$$\Xi = \int_\Omega \mathbb{Q}(\mathrm{d}\omega)\, z^{N(\omega)}\, \mathrm{e}^{-\beta H(\omega)}.$$

Note that $\bar{\Xi} = \Xi\, \mathrm{e}^{|\mathbb{T}|}$ is the grand-canonical partition function

$$\bar{\Xi} = \sum_{n \in \mathbb{N}_0} \frac{z^n}{n!} \int_{\mathbb{T}^n} \mathrm{d}\omega\ \mathrm{e}^{-\beta H(\omega)},$$

because of the normalisation

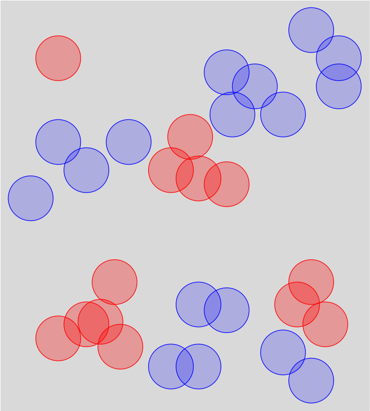
$$1 = \int_\Omega \mathbb{Q}(\mathrm{d}\omega) = \mathrm{e}^{-|\mathbb{T}|} \sum_{n \in \mathbb{N}_0} \frac{1}{n!} \int_{\mathbb{T}^n} \mathrm{d}\omega$$

with $|\mathbb{T}| = L^2$.

Widom-Rowlinson model: 2 species

The set of finite particle configurations in $\mathbb{T}$ is:

$$\tilde{\Omega} = \left\{(\omega^R, \omega^B) \colon \omega^R, \omega^B \subset \mathbb{T},\, N(\omega^R), N(\omega^B) \in \mathbb{N}_0\right\}.$$



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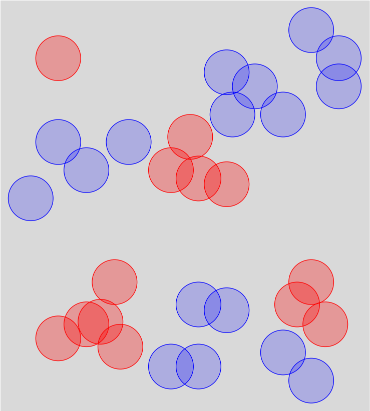

Particles of the same color/type do not interact, i.e., for two particles located at x_1 and x_2 the energy is

$$U_{R,R}(x_1, x_2) = U_{B,B}(x_1, x_2) = 0$$

The set of finite particle configurations in $\mathbb{T}$ is:

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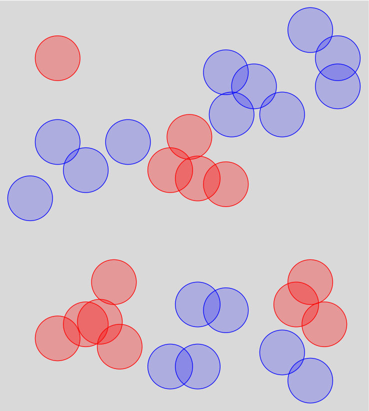


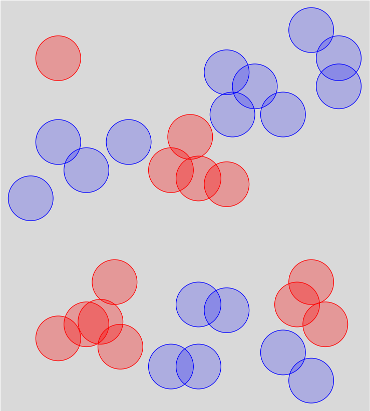
Particles of different color/type interact pairwise via hard-core repulsion, i.e., for two particles located at x_1 and x_2 the energy is

$$U_{R,B}(x_1, x_2) = \begin{cases} \infty, & \text{if } |x_1 - x_2| < 1, \\ 0, & \text{otherwise} \end{cases}$$

Widom-Rowlinson model: 2 species

The set of finite particle configurations in $\mathbb{T}$ is:

$$\tilde{\Omega} = \left\{(\omega^R, \omega^B) \colon \omega^R, \omega^B \subset \mathbb{T},\, N(\omega^R), N(\omega^B) \in \mathbb{N}_0\right\}.$$



We can draw circles of radius $1/2$ around each center and discs of different color can not overlap.

Define the Hamiltonian $\tilde{H} = \tilde{H}_{\mathbb{T}}$ as

$$\tilde{H}(\omega^R, \omega^B) = \sum_{\substack{x_i \in \omega^R \\ x_j \in \omega^B}} U_{R,B}(x_i, x_j)$$

Widom-Rowlinson model: 2 species

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The grand-canonical Gibbs measure for the 2 species model is:

$$\mathrm{d}\tilde{\mu}(\omega^R, \omega^B) = \mathrm{d}\tilde{\mu}_{\mathbb{T}, z_R, z_B}(\omega^R, \omega^B) = \frac{1}{\tilde{\Xi}} \chi(\omega^R, \omega^B)\, z_R^{N(\omega^R)} z_B^{N(\omega^B)} \mathrm{d}\mathbb{Q}(\omega^R)\, \mathrm{d}\mathbb{Q}(\omega^B)$$

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where

- $z_i = \mathrm{e}^{\lambda_i \beta}$ is the activity of particle of type i,
- NO temperature,
- $\chi(\omega^R, \omega^B)$ is the indicator variable that equals 0, if $|x_1 - x_2| < 1$ for the configuration (ω^R, ω^B), and equals 1 otherwise,
- $\mathbb{Q}$ is the Poisson point process with intensity 1,
- $\tilde{\Xi}$ is the normalisation.

Remark (same as before): The normalisation $\tilde{\Xi} = \tilde{\Xi}_{\mathbb{T},z_R,z_B}$ is

$$\tilde{\Xi} = \int_{\tilde{\Omega}} \chi(\omega^R, \omega^B)\, z_R^{N(\omega^R)} z_B^{N(\omega^B)} \mathrm{d}\mathbb{Q}(\omega^R)\, \mathrm{d}\mathbb{Q}(\omega^B).$$

Note that $\hat{\Xi} = \tilde{\Xi}\, \mathrm{e}^{2|\mathbb{T}|}$ is the grand-canonical partition function

$$\hat{\Xi} = \sum_{m,n\in\mathbb{N}_0} \frac{{z_R}^m {z_B}^n}{m!n!} \int_{\mathbb{T}^m \times \mathbb{T}^n} \mathrm{d}\omega^R \mathrm{d}\omega^B\, \chi(\omega^R, \omega^B) \mathbf{1}_{\{N(\omega^R)=m, N(\omega^B)=n\}}$$

because of the normalisation

$$1 = \int_\Omega \mathbb{Q}(\mathrm{d}\omega^R) = \int_\Omega \mathbb{Q}(\mathrm{d}\omega^B) = \mathrm{e}^{-|\mathbb{T}|} \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \int_{\mathbb{T}^n} \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

Equivalence of the 1-species and 2-species

Take the 2-species equilibrium density:

$$\frac{1}{\tilde{\Xi}}\,\chi(\omega^R,\omega^B)\,z_R^{N(\omega^R)}\,z_B^{N(\omega^B)}$$

Equivalence of the 1-species and 2-species

Fix the red and integrate over the blue:

$$\int_{\Omega} \mathrm{d}\mathbb{Q}(\omega^B) \frac{1}{\tilde{\Xi}} \chi(\omega^R, \omega^B) \, z_R^{N(\omega^R)} z_B^{N(\omega^B)}$$

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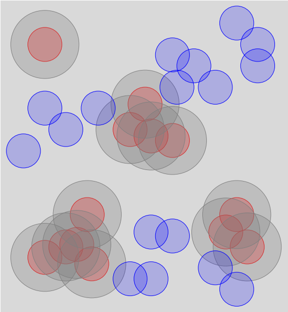
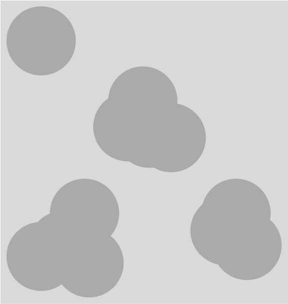




The hard-core repulsion in the 2-species model implies that the centers of the blue discs must stay outside the halo of radius 1 around the centers of the red discs.
$\Rightarrow$ When we integrate out over the blue ones, we precisely get the 1-species Widom-Rowlinson interaction for the red ones.

Equivalence of the 1-species and 2-species

Duality: There exist choices for the parameters z_R, z_B such that the marginal distribution in the 2-species model equals the distribution in the 1-species model.

Lemma 1 (Equivalence of one and two species, dHJKP)

Fix $z_R, z_B > 0$. Let $\pi_R, \pi_B \colon \tilde{\Omega} \to \Omega$ be the projections that map (ω^R, ω^B) to ω^R and ω^B, respectively. Define β, z, β', z' by

$$(\beta, z\,\mathrm{e}^{\beta V_0}) = (z_R, z_B) = (z'\,\mathrm{e}^{\beta' V_0}, \beta'),$$

and let $\mu_{\beta,z}$ and $\mu_{\beta',z'}$ be the associated 1-species Gibbs measures. Then

$$\tilde{\mu} \circ \pi_B^{-1} = \mu_{\beta,z}, \quad \tilde{\mu} \circ \pi_R^{-1} = \mu_{\beta',z'}.$$

Equivalence of the 1-species and 2-species

Proof:

$$
\begin{aligned}
\int_\Omega \mathrm{d}\mathbb{Q}(\omega^B)\frac{1}{\tilde\Xi}\,\chi(\omega^R,\omega^B)\,z_R^{N(\omega^R)} z_B^{N(\omega^B)} &= \frac{1}{\tilde\Xi}\,z_R^{N(\omega^R)}\,\mathrm{e}^{-|\mathbb{T}|}\sum_{n\in\mathbb{N}_0}\frac{z_B^n}{n!}\left[|\mathbb{T}|-V(\omega^R)\right]^n \\
&= \frac{1}{\tilde\Xi}\,z_R^{N(\omega^R)}\,\mathrm{e}^{-|\mathbb{T}|}\,\mathrm{e}^{z_B[|\mathbb{T}|-V(\omega^R)]} \\
&= \frac{\Xi}{\tilde\Xi}\,\mathrm{e}^{(\beta-1)|\mathbb{T}|}\,\frac{1}{\Xi}\left(ze^{-\beta V_0}\right)^{N(\omega^R)}\mathrm{e}^{-\beta V(\omega^R)}.
\end{aligned}
$$

- $z_B=\beta, z_R = z\mathrm{e}^{-\beta V_0}$,
- the green part is the Radon-Nikodým derivative of the Gibbs measure with respect to the Poisson measure $\mathbb{Q}$ on Ω,
- integrating the identity against $\mathbb{Q}(\mathrm{d}\omega^R)$, we have $\tilde\Xi = \Xi\,\mathrm{e}^{(\beta-1)|\mathbb{T}|}$.

Phase transition for the Widom-Rowlinson model

References:

- J.T. Chayes, L. Chayes and R. Kotecký, The analysis of the Widom-Rowlinson model by stochastic geometric methods, Commun. Math. Phys. 172, 551-569, 1995.
- H.-O. Georgii and O. Häggström, Phase transition in continuum Potts models, Commun. Math. Phys. 181 (1996) 507–528.
- D. Ruelle, Existence of a phase transition in a continuous classical system, Phys. Rev. Lett. 27, 1040-1041, 1971.
- B. Widom and J.S. Rowlinson, New model for the study of liquid-vapor phase transitions, J. Chem. Phys. 52, 1670-1684, 1970.
- L. Šamaj, Widom-Rowlinson model (continuum and lattice), arXiv:0709.0617, 2007.

Symmetry:

The mixture of red and blue particles is symmetric with respect to an interchange of the colors of the particles. This means that

$$\tilde{\mathcal{P}}(z_R, z_B) = \tilde{\mathcal{P}}(z_B, z_R),$$

where

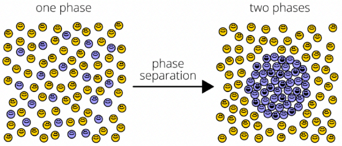
$$\tilde{\mathcal{P}}(z_B, z_R) = -\lim_{|\mathbb{T}|\to\infty} \frac{1}{|\mathbb{T}|} \log \hat{\Xi}(z_B, z_R)$$

is the thermodynamic pressure.

The phase diagram of the 2-species model is a function of the activities, z_R and z_B, of the two species. Since there is a symmetry between red and blue particles, $z_R = z_B = z$ is a line of symmetry of the phase diagram.

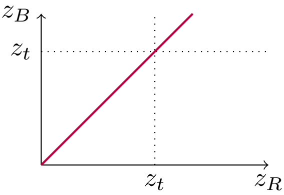
Phase transition for the Widom-Rowlinson model

Symmetry breaking:



- For z small enough the system behaves like an ideal gas: there is one mixed phase with equivalent particle densities $z_R = z_B$,
- For z large enough the symmetry is spontaneously broken and there are two phases: a R-rich phase and a B-rich phase.
- In the language of phase transitions: in the R-rich phase we observe a sea of red particles with small islands of blue particles.
- Why? Different species of particles repel each other infinitely strongly, and therefore a mixed phase would suffer from packing restrictions when z is large.

Phase transition for the Widom-Rowlinson model



Coexistence line for the 1-species model:

$$z_B = z_R$$

$z_B = z_R < z_t$ mixed phase
$z_B = z_R > z_t$ two phases: red/blue

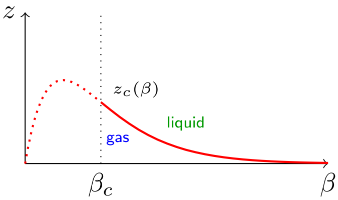
The following theorem is taken from Georgii and Häggström.

Theorem 2 (Phase transition in the two-species model)

There exists a value of the activity z_t such that for $z > z_t$ the 2-species model on the line $z_R = z_B = z$ has at least two Gibbs measures (with different densities of the particles), while for $z < z_t$ it has a unique Gibbs measure.

Phase transition for the Widom-Rowlinson model

- The critical line $z_R = z_B$ in the 2-species model becomes the critical curve $z = \beta e^{-\beta V_0}$ in the 1-species model,
- the critical point $z_R = z_B = z_t$ becomes the critical point $\beta_c = z_t, z_c = z_t\, e^{-z_t V_0}$.



Coexistence line for the 2-species model:

$$z_c(\beta) = \beta e^{-V_0 \beta}$$

$\beta < \beta_c$ single phase
$\beta > \beta_c$ two phases: gas/liquid

Phase transition for the Widom-Rowlinson model

For $\beta < \beta_c$ there is a single phase, while for $\beta > \beta_c$ the curve $z = \beta e^{-\beta V_0}$ is the coexistence curve of the gas phase and the liquid phase, with densities $\rho_{\text{gas}} < \rho_{\text{liquid}}$.
How is the liquid-gas phase transition linked to the red-blue phase transition?

Phase transition for the Widom-Rowlinson model

For $\beta < \beta_c$ there is a single phase, while for $\beta > \beta_c$ the curve $z = \beta e^{-\beta V_0}$ is the coexistence curve of the gas phase and the liquid phase, with densities $\rho_{\text{gas}} < \rho_{\text{liquid}}$.

How is the liquid-gas phase transition linked to the red-blue phase transition?

In the two-phase region with the help of a virial expansion, we obtain that, for large β, $\rho_{\text{gas}} \sim z$ (ideal gas):

$$\rho_{\text{gas}} \sim \beta\, \mathrm{e}^{-\beta V_0}, \quad \rho_{\text{liquid}} \sim \beta - \beta^2 \mathrm{e}^{-\beta} + \ldots, \qquad \beta \to \infty.$$

In the two-species model

$$\rho_{\text{gas}} \sim z_B\, \mathrm{e}^{-z_R V_0}, \quad \rho_{\text{liquid}} \sim z_R, \qquad z_R, z_B \to \infty.$$

Phase transition at the thermodynamic limit, i.e. $|\mathbb{T}| \to \mathbb{R}^d$!!!

Two proofs: Ruelle ('71, Peierls argument) and Chayes, Chayes and Kotecký ('95, percolation argument)

Proof of phase transition: a sketch of the percolation argument

References:

- J.T. Chayes, L. Chayes and R. Kotecký, The analysis of the Widom-Rowlinson model by stochastic geometric methods, Commun. Math. Phys. 172, 551-569, 1995.
- H.-O. Georgii and O. Häggström, Phase transition in continuum Potts models, Commun. Math. Phys. 181 (1996) 507–528.
- H.-O. Georgii and O. Häggström, C. Maes, The random geometry of equilibrium phases, Phase Transitions and Critical Phenomena, Editor(s): C. Domb, J.L. Lebowitz, Academic Press, Volume 18,1-142, 2001.

Proof of phase transition

- CCK: Stochastic-geometric approach using random cluster representation.
- The Gray representation of the Widom-Rowlinson model:

  Take $\Lambda \subset \mathbb{R}^d$ (hypercube). Denote by $\omega_N = (x_1, ..., x_N)$ any configuration of N points in Λ and by s_N any of the 2^N conceivable colorings (i.e. assignments of the red and blue labels) of the N given particles. The canonical partition function is

$$Z^{G,\eta}_{\Lambda,N} = \frac{1}{N!} \int \mathrm{d}\omega_N \mathrm{d}s_N \chi^{\eta}_N(\omega_N, s_N)$$

  where

$$\chi^{\eta}_N(\omega_N, s_N) = \begin{cases} 1, & \text{if the configuration } (\omega_N, s_N) \text{ is allowed,} \\ 0, & \text{if the configuration } (\omega_N, s_N) \text{ is forbidden} \end{cases}$$

  with given boundary condition η.

Proof of phase transition

- If ω_N is a configuration, the set

$$c(\omega_N) = \bigcup_{x \in \omega_N} B_{1/2}(x)$$

consists of distinct components.

- if $B_{1/2}(x_i)$ and $B_{1/2}(x_j)$ overlap for some i and j, then $\chi_N^\eta(\omega_N, s_N)$ will vanish unless i and j belong to the same species $\Rightarrow$ each separate cluster of ω_N must be composed of a single species.
- The number of ways in which this can be arranged is $2^{\mathcal{C}(\omega_N)}$ where

$$\mathcal{C}(\omega_N) = \{\text{number of components of } c(\omega_N) \text{ with boundary condition } \eta\}.$$

Proof of phase transition

- Therefore we can rewrite the canonical partition function as

$$Z^{G,\eta}_{\Lambda,N} = \frac{1}{N!}\int_{\Omega_\Lambda} 2^{\mathcal{C}(\omega_N)}\,\mathrm{d}\omega_N$$

- The grand-canonical gray measure at activity z is

$$\mu^G_{\Lambda,z}(\mathrm{d}\omega) = \frac{1}{\Xi^G_{z,\Lambda}} 2^{\mathcal{C}(\omega)}\mathbb{Q}_z(\mathrm{d}\omega)$$

  where $\mathbb{Q}_z$ is the Poisson point process in Λ with intensity z.

- Advantage of the grey representation: it allows a “comparison” between WR and the ideal gas.

- The ideal gas (Poisson point process) percolates when the activity (intensity) is big enough.

Proof of phase transition

- Let $\mathbb{Q}$ be a Poisson process with intensity z and $\bar{\mathbb{Q}} = \bigcup_{x \in \mathbb{Q}} B_R(x)$ be a random set. Such random subsets are widely known as Boolean models. Fix $R = 1/2$ for simplicity.
- Two points $x, y \in \mathbb{Q}$ are connected to each other if they are connected in $\bar{\mathbb{Q}}$, meaning that there exists a continuous path from x to y in $\bar{\mathbb{Q}}$.
- Let $\theta(z)$ denote the probability that the origin belongs to an unbounded connected component of $\bar{\mathbb{Q}}$.

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- Let $\theta(z)$ denote the probability that the origin belongs to an unbounded connected component of $\bar{\mathbb{Q}}$.
- Boolean continuum percolation:

Theorem 3

There exists a critical value $z_c = z_c(d) \in (0, \infty)$ such that $\theta(z) = 0$ if $z < z_c$ and $\theta(z) > 0$ if $z > z_c$.

[For mathematical theory of continuum percolation: Meester and Roy]

Proof of phase transition

Let us go back to the grey representation of the WR model.

- We take advantage of stochastic monotonicity properties.
- Let us define a partial order $\preceq$ on $\Omega_\Lambda \times \Omega_\Lambda$ by setting: $(x, y) \preceq (x', y')$ if $x \subseteq x'$ and $y \supseteq y'$.

  $\Rightarrow$ a configuration increases with respect to $\preceq$ if red points are added and blue points are deleted.
- An event A is said to be increasing if, for any $\omega \in A$, it is the case that $\eta \in A$ for all $\eta \preceq \omega$.

  $\Rightarrow$ the event is never destroyed by adding particles to a configuration in which it occurs.
- If μ and ν are two (grand-canonical) measures, we say that $\mu(\cdot) \geq_{FKG} \nu(\cdot)$ if $\mu(A) \geq \nu(A)$ whenever A is an increasing event.
- Then the grey distributions have positive correlations relative to this order (FKG-like inequalities)!

Proof of phase transition

- Suppose μ is a probability measure on Ω_Λ absolutely continuous with density $f(\omega)$ relative to the unit intensity Poisson process $\mathbb{Q}$.
- For $x \in \Lambda$ and a point configuration $\omega \in \Omega_\Lambda$ not containing x, the Papangelou intensity of μ at x given x is,

$$\zeta(x|\omega) = \frac{f(\omega \cup \{x\})}{f(\omega)}$$

  Heuristically, $\zeta(x|\omega)\mathrm{d}x$ is the probability density of finding a point inside an infinitesimal region $\mathrm{d}x$ around x, given that the point configuration outside this region is ω.
- The Poisson process $\mathbb{Q}_z$ has Papangelou intensity z.

Proof of phase transition

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- The Poisson process $\mathbb{Q}_z$ has Papangelou intensity z.

Theorem 4

Suppose μ and μ' are probability measures on Ω_Λ with Papangelou intensities $\zeta(\cdot|\cdot)$ and $\zeta'(\cdot|\cdot)$ satisfying $\zeta(x|\omega) \leq \zeta'(x|\omega')$, whenever $x \in \Lambda$ and $\omega, \omega' \in \Omega_\Lambda$ are such that $\omega \subseteq \omega'$. Then $\mu(\cdot) \leq_{FKG} \mu'(\cdot)$

Proof of phase transition

- The grey representation grand-canonical measure μ^G, has Papangelou intensity $\zeta(x|\omega) = z2^{1-k(x,\omega)}$, where $k(x,\omega)$ is the number of connected components of $\bigcup_{y\in\omega} B_{1/2}(y)$ intersecting $B_{1/2}(x)$.
- $k(x,\omega) \leq k_{\text{max}}$ for all x and ω. For $d = 2$ we take $k_{\text{max}} = 5$.
- It follows that
$$z2^{1-k_{\text{max}}} \leq \zeta(x|\omega) \leq 2z$$
- Hence applying Theorem 4 we have that $\mu^G \leq_{FKG} \mathbb{Q}_{2z}$, i.e. the grey measure is stochastically dominated by the ideal gas.
- Corollary: For $z < z_c/2$ we obtain the absence of unbounded connected components
- $\Rightarrow$ **Uniqueness** of Gibbs measures for the WR model iff we **do not** have any infinite connected component in the grey model.
- And viceversa...

Proof of phase transition

- The grey representation grand-canonical measure μ^G, has Papangelou intensity $\zeta(x|\omega) = z2^{1-k(x,\omega)}$, where $k(x,\omega)$ is the number of connected components of $\bigcup_{y\in\omega} B_{1/2}(y)$ intersecting $B_{1/2}(x)$.
- $k(x,\omega) \leq k_{\text{max}}$ for all x and ω. For $d = 2$ we take $k_{\text{max}} = 5$.
- It follows that
$$z2^{1-k_{\text{max}}} \leq \zeta(x|\omega) \leq 2z$$
- Hence applying Theorem 4 we have that $\mu^G \geq_{FKG} \mathbb{Q}_{z2^{1-k_{\text{max}}}}$, i.e. the grey measure stochastically dominates the ideal gas.
- Corollary: For $z > z_c 2^{k_{\text{max}}-1}$ we have the presence of unbounded connected components
- $\Rightarrow$ **Non uniqueness** of Gibbs measures for the WR model.

Summary

In this lecture we have seen:

- Equilibrium statistical mechanics: micro and macro states, statistical ensembles, thermodynamic potentials, thermodynamic limit, phase transitions.
- Widom-Rowlinson model: the 1-species and the 2-species formulation, equivalence of the two models, phase transition.
- Proof of phase transition: the grey measure, percolation for a Boolean model, stochastic monotonicity, percolation of the grey measure via FKG-type inequalities.

Thank you for your attention!

References 1

Equilibrium statistical mechanics:

- S. Friedli, Y. Velenik, Statistical Mechanics of Lattice Systems: A Concrete Mathematical Introduction Cambridge: Cambridge University Press, 2017.
- G. Gallavotti, Statistical Mechanics: A Short Treatise, Springer Verlag, Berlin, 1999.
- E. Presutti, Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics, Theoretical and Mathematical Physics, Springer, 2009.

References 2

Widom-Rowlinson model:

- J.T. Chayes, L. Chayes and R. Kotecký, The analysis of the Widom-Rowlinson model by stochastic geometric methods, Commun. Math. Phys. 172, 551-569, 1995.
- H.-O. Georgii and O. Häggström, Phase transition in continuum Potts models, Commun. Math. Phys. 181 (1996) 507–528.
- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation.
- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Mesoscopic fluctuations for the critical droplet, preprint arXiv: 1907.00453.
- F. den Hollander, S. Jansen, R. Kotecky, E. Pulvirenti, The Widom-Rowlinson model: Microscopic fluctuations for the critical droplet and effective interface model, manuscript in preparation.
- D. Ruelle, Existence of a phase transition in a continuous classical system, Phys. Rev. Lett. 27, 1040-1041, 1971.

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The Widom-Rowlinson model: from phase transition to metastability. Lecture 2

Elena Pulvirenti

TU Delft

"DFG SPP2265 Summer School on
Probability and geometry on configuration spaces"
Berlin, July 17-21, 2023

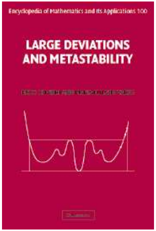
Plan of the mini-course

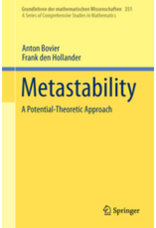
- Lecture 1:
  - Introduction and basic notions of equilibrium statistical mechanics
  - Widom-Rowlinson model: two equivalent formulations
  - Phase transition for the WR model
- Lecture 2:
  - Introduction to metastability and potential theory
  - Dynamic WR model
- Lecture 3:
  - Metastability for the WR model
  - Mesoscopic fluctuations of the critical droplet
  - Microscopic fluctuations and the parabolic interface model

Introduction to metastability

References:

- E. Olivieri and M.E. Vares, *Large Deviations and Metastability*, Encyclopedia of Mathematics and its Applications, Vol. 100, Cambridge University Press, Cambridge, 2005.
- A. Bovier, F. den Hollander, *Metastability - A Potential-Theoretic Approach*, Grundlehren der mathematischen Wissenschaften, Volume 351, Springer, 2015.





What is metastability?

Super-saturated vapour

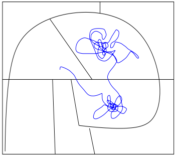
Super-cooled water

Snow avalanche

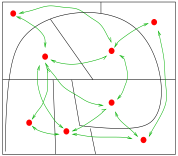
What is metastability?

Metastability is a phenomenon where a system, under the influence of a stochastic dynamics, moves between different regions of its state space on different time scales.

Fast time scale: quasi-equilibrium within single subregion

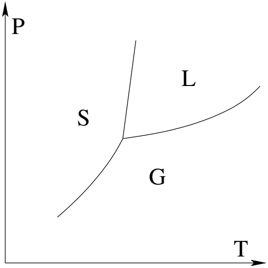


Slow time scale: transitions between different subregions



It is observed in a variety of physical, chemical and biological settings. The challenge is to propose mathematical models and to explain the experimentally observed universality.

Metastable behaviour is the dynamical manifestation of a first-order phase transition, for instance: condensation.

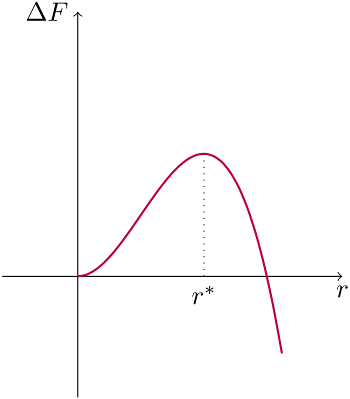


When vapour is cooled rapidly below the critical temperature, we see that the system will persist for long time in a metastable vapour state before transiting (rapidly) to the new stable liquid state under some random fluctuations.

Why?

Metastability in Statistical Physics

Metastable behaviour is the dynamical manifestation of a first-order phase transition, for instance: condensation.



The system has to form a critical droplet of liquid to trigger the crossover, which then will grow and invade the whole space. But many unsuccessful attempts because forming small droplets results in an increasing of free energy...

State of the art

Statistical physics has been very successful in describing discrete particle systems. Over the years a broad and deep understanding of critical phenomena has emerged:

- spin-flip systems
- particle-hop systems
- cellular automata
- ...

Much less is known for continuous interacting particle systems, which are very hard to analyse. In fact, a rigorous proof of the presence of a phase transition has so far been achieved for very few models only (see Lecture 1).

Goal: we focus on the continuum Widom-Rowlinson model of fluids. This is the first study of metastability for continuum interacting particle systems.

Hystorical perspective

Early work on metastability was done by van 't Hoff and Arrhenius in the 1880s, to develop a theory for chemical reaction rates. Mathematically, metastability took off with the work of Kramers in the 1940s.

Since then, various approaches to metastability have been developed, with different pros and cons.

- Lebowitz, Penrose 1960-1970, van der Waals
- Freidlin, Wentzell 1960-1970, SDE
- Cassandro, Galves, Olivieri, Vares 1980-1985, path LDP
- Davies 1980-1985, spectra

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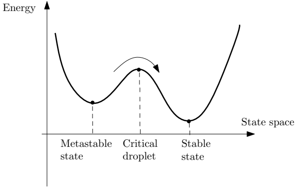
Our approach:
With the help of potential theory, the problem of understanding metastability of Markov processes translates into the study of capacities in electric networks.

- Bovier, Eckhoff, Gayrard and Klein, 2001;
- Bovier and den Hollander, 2015

How to study metastability?

Given F the free energy, the quantities of interest are

1. Metastable parameter regime $\rightarrow$ multiple minima of F
2. Critical points of F:
   - local minima (metastable states)
   - global minimum (stable state)
   - local maxima/saddle points



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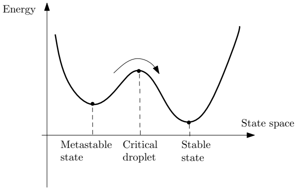

3. **Mean hitting time**: the mean time the system (subject to a stochastic dynamics) needs to "hit" the stable state starting from a metastable state. Arrhenius law: $\mathbb{E}(\tau) \sim \exp(N\Delta F^*)$, in the limit $N \to \infty$.
4. **Critical droplet**: typical configuration of the system on the saddle point.

Potential theoretic approach

References:

- Chapter 7 of A. Bovier, F. den Hollander, *Metastability - A Potential-Theoretic Approach* 2015, and references therein.
- A. Gaudillière, *Condenser physics applied to Markov chains: a brief introduction to potential theory*, Notes from the XII. Brazilian school of probability, 2009.

Setting

- Discrete-time Markov process $X = (X_n)_{n \in \mathbb{N}_0}$ on a countable state space S with transition kernel
$$P = (p(x,y))_{x,y \in S}$$
and a (discrete-time) generator $L = P - \mathbb{I}$.
- L is given by
$$(Lf)(x) = \sum_{y \in S} p(x,y)\,[f(y) - f(x)]$$
- We assume that X is irreducible and reversible, i.e. there exists μ such that
$$\mu(x)p(x,y) = \mu(y)p(y,x) = c(x,y), \quad \forall x, y \in S.$$
where c is the conductance.

The Dirichlet problem

- A fundamental object in potential theory is the Dirichlet problem, where $A, B \subset S$ are two non-empty disjoint subsets:

$$
\begin{aligned}
(-Lh)(x) &= 0, \qquad x \in S \setminus (A \cup B),\\
h(x) &= 1 \qquad x \in A,\\
h(x) &= 0 \qquad x \in B.
\end{aligned}
$$

- Boundary conditions: $h \equiv 1$ on A (target set) and $h \equiv 0$ on B (killing set).
- If S is finite, then the Dirichlet problem has always a unique solution, denoted by $h_{A,B}(x)$ and called the equilibrium potential.

The Dirichlet form

- The following probabilistic representation of the equilibrium potential holds:

$$h_{A,B}(x) = \mathbb{P}_x(\tau_A < \tau_B), \qquad x \in S \setminus (A \cup B)$$

where $\tau_C = \inf\{n \in \mathbb{N} : X_n \in C\}$.

The Dirichlet form

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  where $\tau_C = \inf\{n \in \mathbb{N} : X_n \in C\}$.

- L defines a quadratic form called Dirichlet form, which is non-negative-definite

$$\mathcal{E}(f,g) := \sum_{x \in S} \mu(x) f(x)(-Lg)(x), \qquad f, g \in L^2(S, \mu)$$

- In the discrete case it is easy to write down $\mathcal{E}(f,g)$ explicitly

$$\mathcal{E}(f,g) = \frac{1}{2} \sum_{x,y \in S} \mu(x) p(x,y)[f(x) - f(y)][g(x) - g(y)]$$

A key equation

Let $\nu_{A,B}$ be the last-exit biased distribution on A for the transition from A to B:

$$\nu_{A,B}(x) = \frac{\mu(x)\mathbb{P}_x\big[\tau_B < \tau_A\big]}{\sum_{x\in A}\mu(x)\mathbb{P}_x\big[\tau_B < \tau_A\big]}, \qquad x \in A.$$

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Theorem 1 (Cor. 7.11 BdH)

Let $A, B \subset S$ be non-empty and disjoint. For reversible MP,

$$\mathbb{E}_{\nu_{A,B}}\left[\tau_B\right] = \sum_{x\in A}\nu_{A,B}(x)\mathbb{E}_x[\tau_B] = \frac{1}{\mathrm{cap}(A,B)}\sum_{y\in S}\mu(y)h_{A,B}(y),$$

where

$$\mathrm{cap}(A,B) = \sum_{x\in A}\mu(x)\mathbb{P}_x(\tau_B < \tau_A).$$

In particular, for $A = \{x\}$,

$$\mathbb{E}_x\left[\tau_B\right] = \frac{1}{\mathrm{cap}(x,B)}\sum_{y\in S}\mu(y)h_{x,B}(y),$$

Dirichlet principle

$$\mathrm{cap}(A,B) = \inf_{f \in \mathcal{H}_{AB}} \mathcal{E}(f,f)$$

where

$$\mathcal{H}_{AB} := \{f : S \to [0,1] : f|_A = 1, f|_B = 0\}$$

and

$$\mathcal{E}(f,f) = \frac{1}{2} \sum_{x,y \in S} \mu(x) p(x,y) [f(x) - f(y)]^2.$$

Variational principles for capacity estimates

Let E be the set of pairs (x, y) such that $p(x, y) \neq 0$, $x, y \in S$.
Then a unit flow is a map $\varphi : E \to \mathbb{R}$ such that

$$\sum_{\substack{y \in V: \\ (y,x) \in E}} \varphi(y, x) = \sum_{\substack{w \in V: \\ (x,w) \in E}} \varphi(x, w) \qquad \text{(Kirchhoff's law)}$$

$$\sum_{a \in A} \sum_{\substack{y \in V: \\ (a,y) \in E}} \varphi(a, y) = 1 = \sum_{b \in B} \sum_{\substack{y \in V: \\ (y,b) \in E}} \varphi(y, b).$$

$\mathcal{U}_{AB}$ is the space of all unit flows from A to B

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$\mathcal{U}_{AB}$ is the space of all unit flows from A to B

Thomson principle

$$\mathrm{cap}(A, B) = \sup_{\phi \in \mathcal{U}_{AB}} \frac{1}{\mathcal{D}(\phi, \phi)},$$

where

$$\mathcal{D}(\phi, \phi) = \sum_{(x,y) \in E} \frac{\phi(x, y)^2}{\mu(x) p(x, y)}$$

Potential theoretic approach

- Instead of computing hitting times, we have to estimate capacities. Facilitated by variational principles: Dirichlet, Thomson, Berman-Konsowa,...
- configuration $\to$ vertex of the network,
- transition $\to$ edge of the network,
- transition probability $\to$ conductance of the associated edge,
- average hitting time $\to$ inverse of capacity (effective restistance),
- Random walk $\to$ electric networks: network of resistors, $c(x,y) = 1/r(x,y)$ conductance, $f(x)$ voltage at node x, then $\mathcal{E}(f,f)$ is the power of dissipated energy: $P = RI^2 = CU^2$

A. Gaudillière, *Condenser physics applied to Markov chains: a brief introduction to potential theory*, Notes from the XII. Brazilian school of probability, 2009.

Definition of metastability

Consider a **simple case** where $\mathcal{M} = \{m_1, ..., m_k\} \subset \mathcal{S}$ is a **set of points**, e.g. minima of F. Suppose $|\mathcal{S}| < \infty$.
Let $X = \{X(t) : t \geq 0\}$ be a Markov process and

$$\tau_{\mathcal{A}} := \inf\big\{t > 0 : X(t) \in \mathcal{A}, X(t-) \notin \mathcal{A}\big\}$$

be the first return time to $\mathcal{A}$.

Then X is said to be ρ-**metastable** with respect to the set of metastable points $\mathcal{M}$ if

$$|\mathcal{S}| \frac{\sup_{x \in \mathcal{M}} \mathbb{P}_x \Big[\tau_{\mathcal{M}\setminus x} < \tau_x\Big]}{\inf_{y \notin \mathcal{M}} \mathbb{P}_y \Big[\tau_{\mathcal{M}} < \tau_y\Big]} \leq \rho \ll 1.$$

Here ρ is a small intrinsic parameter that characterises the degree of metastability. Definition from Bovier - den Hollander.

The dynamic WR model

References:

- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation
- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Mesoscopic fluctuations for the critical droplet, preprint arXiv: 1907.00453.
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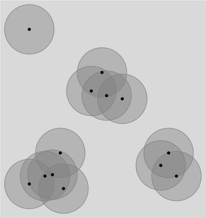
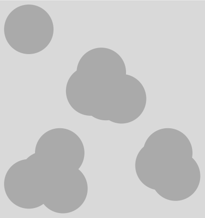
Let $\mathbb{T} \subset \mathbb{R}^2$ be a finite torus. The set of finite particle configurations in $\mathbb{T}$ is $\Omega = \{\omega \subset \mathbb{T}\colon\ N(\omega) \in \mathbb{N}_0\}$, $\quad N(\omega)$: cardinality of ω





Halo of a configuration

$$h(\omega) = \bigcup_{x\in\omega} B_1(x)$$

Notation: $V(\omega) := |h(\omega)|$

Hamiltonian

$$H(\gamma) = V(\omega) - N(\omega)\pi$$

Note that is attractive

$$-(N(\gamma)-1)\pi \le H(\gamma) \le 0$$

Dynamic 1-species WR model

Particle configuration is a continuous-time Markov process $(\omega_t)_{t\geq 0}$ with state space Ω and with generator

$$(Lf)(\omega) = \int_{\mathbb{T}} \mathrm{d}x \; b(x,\omega)\,[f(\omega \cup x) - f(\omega)] + \sum_{x\in\omega} d(x,\omega)\,[f(\omega\backslash x) - f(\omega)]$$

where particles are added at rate b (birth) and removed at rate d (death).
The grand-canonical Gibbs measure is reversible with respect to this dynamics when b and d satisfy the relation

$$b(x,\omega)\,\mathrm{e}^{-\beta H(\omega)} = d(x,\omega\cup x)\,\mathrm{e}^{-\beta H(\omega\cup x)}, \qquad x\notin\omega, \quad \omega\in\Omega.$$

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$$b(x,\omega)\,\mathrm{e}^{-\beta H(\omega)} = d(x,\omega\cup x)\,\mathrm{e}^{-\beta H(\omega\cup x)}, \qquad x\notin\omega, \quad \omega\in\Omega.$$

The heat bath dynamics corresponds to the choice

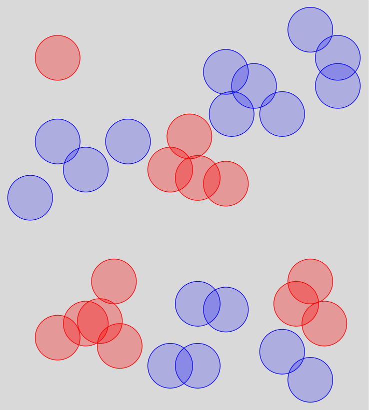
$$b(x,\omega) = z\mathrm{e}^{-\beta[H(\omega\cup x)-H(\omega)]}, \quad x\notin\omega, \qquad d(x,\omega)=1, \quad x\in\omega, \qquad \omega\in\Omega,$$

i.e., particles are added at rate corresponding to the change of the Gibbs weight, but are removed at a rate that is independent of their location and the location of the other particles. Once inside $\mathbb{T}$, particles do *not* move.

Recall: 2-species Widom-Rowlinson model

The set of finite particle configurations in $\mathbb{T}$ is:

$$\tilde{\Omega} = \left\{(\omega^R, \omega^B) \colon \omega^R, \omega^B \subset \mathbb{T},\, N(\omega^R), N(\omega^B) \in \mathbb{N}_0\right\}.$$



$$\tilde{H}(\omega^R, \omega^B) = \sum_{\substack{x_i \in \omega^R \\ x_j \in \omega^B}} U_{R,B}(x_i, x_j),$$

$$U_{R,B}(x_1, x_2) = \begin{cases} \infty, & \text{if } |x_1 - x_2| < 1, \\ 0, & \text{otherwise} \end{cases}$$

Dynamic 2-species WR model

Particle configuration is a continuous-time Markov process $(\omega_t)_{t\geq 0} = (\omega_t^R, \omega_t^B)_{t\geq 0}$ with state space $\tilde{\Omega}$ and with generator

$$(\tilde{\mathcal{L}}f)(\omega) = \sum_{i=R,B} \int_{\mathbb{T}} b^i(x^i,\omega)\,[f(\omega\cup x^i) - f(\omega)]\,\mathrm{d}x^i \\ + \sum_{i=R,B} \sum_{x^i\in\omega^i} d^i(x^i,\omega)\,[f(\omega\setminus x^i) - f(\omega)], \qquad \omega\in\tilde{\Omega},$$

where $\omega = (\omega^R, \omega^B)$, $b^i(x^i,\omega)$ is the birth rate of type i and $d^i(x^i,\omega)$ is the death rate of type i.

Dynamic 2-species WR model

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where $\omega = (\omega^R, \omega^B)$, $b^i(x^i,\omega)$ is the birth rate of type i and $d^i(x^i,\omega)$ is the death rate of type i. The grand-canonical Gibbs measure is reversible with respect to the dynamics when b^i, d^i, $i = R, B$, satisfy

$$\sum_{i=R,B} b^i(x^i,\omega)\,\mathrm{e}^{-\beta\tilde{H}(\omega)} = \sum_{i=R,B} d^i(x^i,\omega\cup x^i)\,\mathrm{e}^{-\beta\tilde{H}(\omega\cup x^i)}.$$

The heat bath dynamics corresponds to the choice

$$b^R(x^R,\omega) = z_R\,\chi(\omega^R\cup x^R,\omega^B), \quad b^B(x^B,\omega) = z_B\,\chi(\omega^R,\omega^B\cup x^B), \\ d^R(x^R,\omega) = d^B(x^B,\omega) = 1.$$

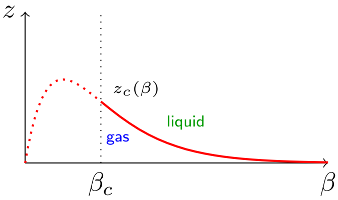
Dynamic link of 1-and 2-species WR model

- In analogy with Lemma 1 (of Lecture 1) for the models at equilibrium, there is a dynamic duality property linking the generators of the dynamic 1 and 2-species WR model.
- *At equilibrium* we can project the 2-species model onto the 1-species model (by integrating out the configurations of one of the colors).
- We can do it again and obtain the one-step dynamics for the 1-species model. However, by projecting the full 2-species dynamics, we **do not** get the full 1-species dynamics: through the projection the Markov property is lost.

Key questions

Let $\square = \emptyset$ and $\blacksquare = \{\omega \in \Omega : h(\omega) = \mathbb{T}\}$ be the set of configurations where $\mathbb{T}$ is empty, respectively, full.

- Start with $\mathbb{T}$ empty, i.e. $\omega_0 = \square$ (preparation in vapour state)
- Choose $z = \kappa\, z_c(\beta)$, $\kappa \in (1, \infty)$ (reservoir is super-saturated vapour)
- Wait for the first time $\tau_\blacksquare$ when the system fills $\mathbb{T}$ (condensation to liquid state)



Coexistence line for the 2-species model:

$$z_c(\beta) = \beta e^{-V_0 \beta}$$

Key questions

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- Wait for the first time $\tau_{\blacksquare}$ when the system fills $\mathbb{T}$ (condensation to liquid state)

Questions:
In the limit as $\beta \to \infty$ for fixed $\mathbb{T}$ and κ:

- What are the asymptotics of the mean hitting time

$$\mathbb{E}_{\square}(\tau_{\blacksquare})?$$

- What is the law of $\tau_{\blacksquare}$?
- What does the critical droplet look like?

Key questions

- These questions are delicate!
- We want to obtain a detailed description of metastability for a model of interacting particles in the continuum.
- There are many challenges in: understanding the details behind the droplet formation and computing sharp asymptotics of the mean hitting time.
- In Lecture 3, I will state the main results and show various properties of the critical droplet.

Summary

In this lecture we have seen:

- Metastability: general description out of equilibrium;
- Potential theoretic approach to metastability for a general Markov process: Dirichlet problem, Dirichlet forms, equilibrium potential;
- Dynamic version of the 1-species WR model (and link to the dynamic 2-species WR model);
- Key questions for the study of metastability for the 1-species WR model with birth/death.

References

- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation.
- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Mesoscopic fluctuations for the critical droplet, preprint arXiv: 1907.00453.
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- A. Gaudillière, *Condenser physics applied to Markov chains: a brief introduction to potential theory*, Notes from the XII. Brazilian school of probability, 2009.
- E. Olivieri and M.E. Vares, *Large Deviations and Metastability*, Encyclopedia of Mathematics and its Applications, Vol. 100, Cambridge University Press, Cambridge, 2005.
- A. Bovier, F. den Hollander, *Metastability - A Potential-Theoretic Approach*, Grundlehren der mathematischen Wissenschaften, Volume 351, Springer, 2015.

The Widom-Rowlinson model: from phase transition to metastability. Lecture 3

Elena Pulvirenti

TU Delft

“DFG SPP2265 Summer School on Probability and geometry on configuration spaces”
Berlin, July 17-21, 2023

Plan of the mini-course

- Lecture 1:
  - Introduction and basic notions of equilibrium statistical mechanics
  - Widom-Rowlinson model: two equivalent formulations
  - Phase transition for the WR model
- Lecture 2:
  - Introduction to metastability and potential theory
  - Dynamic WR model
- Lecture 3:
  - Metastability for the WR model
  - Mesoscopic fluctuations of the critical droplet
  - Microscopic fluctuations and the parabolic interface model

Metastability for the WR model

References:

- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation.
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Frank den Hollander, Leiden

Sabine Jansen, Munich

Roman Kotecký, Warwick/Prague

Key questions for the study of metastability

Recall the 1-species WR model with birth/death dynamics.
Let $\square = \emptyset$ and $\blacksquare = \{\omega \in \Omega : h(\omega) = \mathbb{T}\}$ be the set of configurations where $\mathbb{T}$ is empty, respectively, full.

- Start with $\mathbb{T}$ empty, i.e. $\omega_0 = \square$ (preparation in vapour state)
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In the limit as $\beta \to \infty$ for fixed $\mathbb{T}$ and κ:

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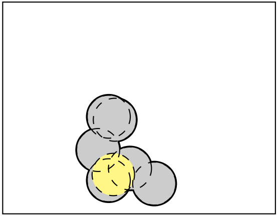
$$\mathbb{E}_\square(\tau_\blacksquare)?$$

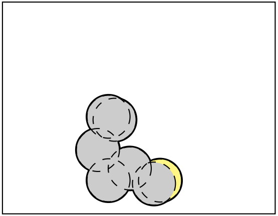
- What is the law of $\tau_\blacksquare$?
- What does the critical droplet look like?

Heuristics for the dynamics of particles

In the metastable regime $z = \kappa z_c(\beta)$, $z_c(\beta) = \beta e^{-\pi\beta}$, the birth rate is

$$b(x,\omega) = z\mathrm{e}^{-\beta[H(\omega\cup x)-H(\omega)]} = \kappa\beta\, e^{-\beta[V(\omega\cup x)-V(\omega)]}$$





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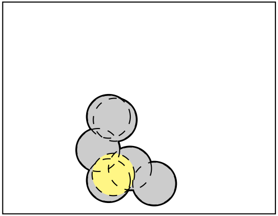
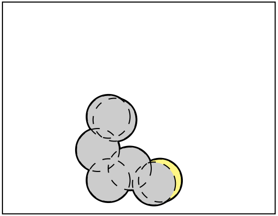
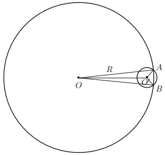


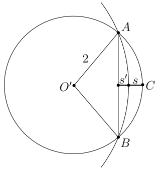


- Particles inside a cluster are created at a rate $\kappa\beta$. $\Rightarrow$ Inside a droplet Poisson point process with intensity $\kappa\beta \gg 1$
- Particles sticking out are created at a rate exponentially small in the area "sticking out" of the cluster (yellow area), which is function of the local curvature.

Heuristics: an elementary calculation

Suppose that a particle is sticking out by a *radial distance* s from a big cluster of perfect circular shape.





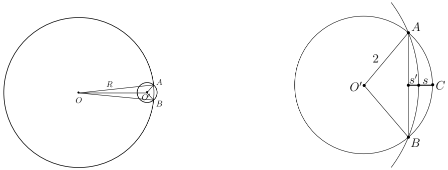
$$\Delta V = V(\omega \cup x) - V(\omega) \asymp s^{3/2}, \qquad \text{when } s \downarrow 0.$$

- The typical *volume* is $\Delta V \asymp \beta^{-1}$, because the birth rate is $\asymp \mathrm{e}^{-\beta \Delta V}$.
- Therefore, the typical *radial distance* s by which the particle sticks out is of the order $\beta^{-2/3}$.
- The *length* ℓ of the arc on the boundary of the disc that is taken away by the particle is of the order $s^{1/2}$ and therefore of order $\beta^{-1/3}$.

$\Rightarrow$ The typical number of particles sticking out of the critical droplet is of order...

Heuristics: an elementary calculation

Suppose that a particle is sticking out by a *radial distance* s from a big cluster of perfect circular shape.



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$$\boxed{N \asymp \beta^{1/3}, \qquad \beta \to \infty}$$

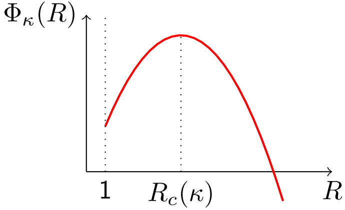
Summary of heuristics

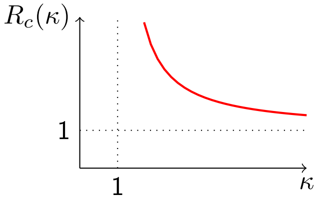
- Since particles have a tendency to stick together, they form a droplet that is close to a large disc, say of radius R.
- Inside the droplet, particles are distributed according to a Poisson process with intensity $\kappa\beta \gg 1$
- Near the perimeter of the droplet, particles are born at a rate that depends on how much they stick out.
- For small R the droplet tends to shrink, for large R it tends to grow. The curvature of the droplet determines which of the two prevails.
- There are approximately $\beta^{1/3}$ particles on the boundary of the droplet.

Three target theorems

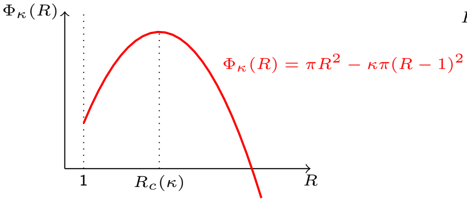
For $R \in [1, \infty)$ and $\kappa \in (1, \infty)$, let

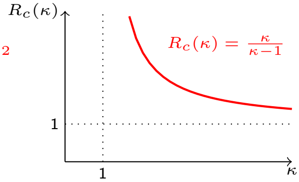
$$\Phi_\kappa(R) = \pi R^2 - \kappa\pi(R-1)^2, \qquad R_c(\kappa) = \frac{\kappa}{\kappa - 1}$$





Three target theorems





Target Theorem 1 [Mean hitting time - Arrhenius formula]

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

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

where

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

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

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

The second theorem shows that the crossover time divided by its mean is distributed according to an exponential law.

Target Theorem 2 [Exponential law]
For every $\kappa \in (1, \infty)$ and $L > R_c(\kappa)$,

$$\lim_{\beta \to \infty} P_{\square}\big(\tau_{\blacksquare}/E_{\square}(\tau_{\blacksquare}) > t\big) = \mathrm{e}^{-t} \qquad \forall\, t \geq 0.$$

The exponential law is typical for metastable crossover times: the critical droplet appears after many unsuccessful attempts.

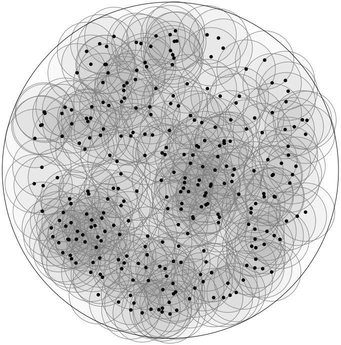
Three target theorems

For $\kappa \in (1,\infty)$, $L > R_c(\kappa)$ and $\delta > 0$ small enough, let

$$\mathcal{C}_\delta(\kappa) = \Big\{\omega \in \Omega\colon\ B_{R_c(\kappa)-\delta}(x) \subset h(\gamma) \subset B_{R_c(\kappa)+\delta}(x) \text{ for some } x \in \mathbb{T}\Big\}.$$

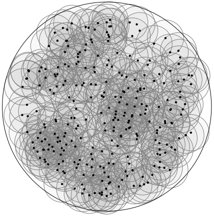
Target Theorem 3 [Critical droplet]
For every $\kappa \in (1,\infty)$, $L > R_c(\kappa)$ and $\delta > 0$,

$$\lim_{\beta\to\infty} P_\square\big(\tau_{\mathcal{C}_\delta(\kappa)} < \tau_\blacksquare \mid \tau_\blacksquare < \tau_\square\big) = 1.$$



The critical droplet in the metastable regime is close to a disc of radius $R_c(\kappa)$ and has a random boundary.
$\asymp \beta$ discs in the interior,
$\asymp \beta^{1/3}$ discs on the boundary.

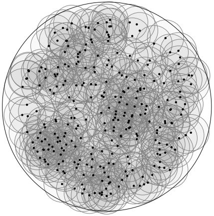
Three target theorems: comments



The critical droplet is close to a disc $B_{R_c(\kappa)}$ and has a random boundary that fluctuates within a narrow annulus whose width shrinks to zero as $\beta \to \infty$. There are $\approx \beta$ discs in the interior and $\approx \beta^{1/3}$ discs on the boundary.

- $\Phi(\kappa)$ scales with β and is the volume free energy of the critical droplet
- $\Psi(\kappa)$ scales with $\beta^{1/3}$ and is the surface free energy of the critical droplet.
- The analysis relies on an identification of the large deviation and moderate deviation properties of the volume and the surface of the critical droplet.

Three target theorems: comments



The critical droplet is close to a disc $B_{R_c(\kappa)}$ and has a random boundary that fluctuates within a narrow annulus whose width shrinks to zero as $\beta \to \infty$. There are $\approx \beta$ discs in the interior and $\approx \beta^{1/3}$ discs on the boundary.

- We first analyse the mesoscopic fluctuations of the surface of the critical droplet
- We then analyse the microscopic fluctuations of the locations of the discs in the boundary layer of the critical droplet
- These are both needed to obtain the sharp asymptotics for the metastable crossover time.
- In the physics literature, density fluctuations at the surface of macroscopic droplets in the continuum are studied in terms of capillary waves (see Stillinger and Weeks). The results to be describes provide a rigorous foundation for capillary waves.

Potential theoretic approach to metastability

For the choice $z = \kappa\, z_c(\beta) = \kappa\, \beta\, \mathrm{e}^{-\beta\pi}$ the grand-canonical Gibbs measure reads

$$\mu(\mathrm{d}\omega) = \frac{1}{\Xi}\, (\kappa\beta)^{N(\omega)}\, \mathrm{e}^{-\beta V(\omega)}\, \mathbb{Q}(\mathrm{d}\omega)$$

and the Dirichlet form associated with the dynamics reads

$$\mathcal{E}(f,f) = \frac{1}{\Xi} \int_\Omega \mathbb{Q}(\mathrm{d}\omega) \int_\Lambda \mathrm{d}x\, (\kappa\beta)^{N(\omega\cup x)}\, e^{-\beta V(\omega\cup x)}\, \big[f(\omega\cup x) - f(\omega)\big]^2.$$

where $N(\omega)$ is the cardinality of ω and $V(\omega)$ is the volume of the halo of ω. Both quantities play a crucial role for the computation of capacities that underpin the potential-theoretic approach to metastability.

Recall that the capacity of $\square, \blacksquare \subset \Omega$ is defined as

$$\mathrm{cap}(\square, \blacksquare) = \mu(\square)\, \mathbb{P}_{\square}(\tau_{\blacksquare} < \tau_{\square}).$$

The capacity is given by two dual variational principles: the Dirichlet principle and the Thomson principle.

$$\mathrm{cap}(\square, \blacksquare) = \inf_{\substack{f:\ \Gamma \to [0,1] \\ f|_{\square}=1,\ f|_{\blacksquare}=0}} \mathcal{E}(f,f) = \sup_{\substack{f:\ \Gamma \to [0,1] \\ Lf \le 0 \text{ on } \Gamma \setminus (\square, \blacksquare)}} \frac{\mathcal{E}(\mathbf{1}_{\square}, f)^2}{\mathcal{E}(f,f)},$$

Recall the link between **mean metastable time** and **capacity**

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) := \frac{\int_{\Omega} \mu(\mathrm{d}\omega)\, h_{\square\blacksquare}(\omega)}{\mathrm{cap}(\square, \blacksquare)} = \frac{[1+o(1)]\mathbb{Q}(\square)}{\Xi \mathrm{cap}(\square, \blacksquare)}$$

where we skip the proof of the second equality (technical Proposition). Note that $\mathbb{Q}(\square) = \mathrm{e}^{-|\mathbb{T}|}$ does not depend on the relevant parameters κ, β.

Choice of the test function

We want to approximate the unique minimiser $h_{\square,\blacksquare}$ of

$$\mathcal{E}(f,f)\Xi = \int_\Omega \mathbb{Q}(\mathrm{d}\omega) \int_\Lambda \mathrm{d}x\, (\kappa\beta)^{N(\omega\cup x)}\, e^{-\beta V(\omega\cup x)} \left[f(\omega\cup x) - f(\omega)\right]^2,$$

by picking a test function f as follows

$$f_\eta(\omega) = \begin{cases} 1, & \omega \in \mathcal{V}_{\square,\eta}, \\ f_\eta^*(\omega), & \omega \in \Omega \setminus (\mathcal{V}_{\square,\eta} \cup \mathcal{V}_{\blacksquare,\eta}), \\ 0, & \omega \in \mathcal{V}_{\blacksquare,\eta}, \end{cases}$$

$$\mathcal{V}_{\square,\eta} = \{\omega \in \Omega\colon\ V(\omega) \le \pi R_c^2 - \eta\}, \qquad \mathcal{V}_{\blacksquare,\eta} = \{\omega \in \Omega\colon\ V(\omega) \ge \pi R_c^2 + \eta\}.$$

Note: $\square \in \mathcal{V}_{\square,\eta}, \blacksquare \in \mathcal{V}_{\blacksquare,\eta}$.
$\mathcal{V}_{\square,\eta}$ and $\mathcal{V}_{\blacksquare,\eta}$ are the valleys around $\square$ and $\blacksquare$, which are separated by a neighbourhood of the critical droplet. f on that neighbourhood depends on both the volume and the surface of the critical droplet.

Approximation of the capacity

From heuristics: fix $C \in (0, \infty)$ and choose $\eta = C\beta^{-2/3}$.
Therefore from variational principles we get:

$$[\mathbb{E}_{\square}(\tau_{\blacksquare})]^{-1} \mathrm{e}^{-|\mathbb{T}|} \asymp \Xi \,\mathrm{cap}(\square, \blacksquare) \asymp O(\beta)\, \mathcal{I}(\kappa, \beta, C)$$

where

$$\begin{aligned} \mathcal{I}(\kappa, \beta, C) &= \int_{\Omega} \mathbb{Q}(\mathrm{d}\omega)\, (\kappa\beta)^{N(\omega)}\, \mathrm{e}^{-\beta V(\omega)}\, \mathbf{1}_{\{|V(\omega) - \pi R_c^2(\kappa)| \le C\beta^{-2/3}\}} \\ &= \Xi\, \mu(|V(\omega) - \pi R_c^2(\kappa)| \le C\beta^{-2/3}) \end{aligned}$$

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where

$$\begin{aligned} \mathcal{I}(\kappa, \beta, C) &= \int_{\Omega} \mathbb{Q}(\mathrm{d}\omega) \, (\kappa\beta)^{N(\omega)} \, \mathrm{e}^{-\beta V(\omega)} \, \mathbf{1}_{\{|V(\omega) - \pi R_c^2(\kappa)| \leq C\beta^{-2/3}\}} \\ &= \Xi \, \mu(|V(\omega) - \pi R_c^2(\kappa)| \leq C\beta^{-2/3}) \end{aligned}$$

$\Rightarrow$ The dominant contribution to the capacity comes from the configurations where the volume of the halo is close to the volume of the critical disc.
$\Rightarrow$ The special role played by the critical disc $B_{R_c(\kappa)}$ becomes apparent through the fact that the set

$$\{\omega \in \Omega \, : \, |V(\omega) - \pi R_c^2(\kappa)| \leq C\beta^{-2/3}\}$$

is the gate for the metastable transition from the vapour phase (empty $\mathbb{T}$) to the liquid phase ($\mathbb{T}$ full).

Approximation of the capacity

Throughout the sequel, $\kappa \in (1, \infty)$ is fixed. Recall

$$\Phi(\kappa) := \Phi_\kappa(R_c(\kappa)) = \frac{\pi\kappa}{\kappa - 1}, \qquad \Psi(\kappa) = s_* \, \frac{\kappa^{2/3}}{\kappa - 1}$$

where s_* is a constant that will be identified later and does not depend on κ. The crucial ingredient is now the following sharp asymptotics

TARGET

For C large enough and $\beta \to \infty$

$$\mathcal{I}(\kappa, \beta; C) = \mathrm{e}^{-\beta\, \Phi(\kappa) + \beta^{1/3}\Psi(\kappa) + o(\beta^{1/3})}.$$

Proof via:

- Large deviation principles for the halo shape and the halo volume
- Moderate deviations for the halo volume close to the critical droplet

Mesoscopic fluctuations of the critical droplet

References:

- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Metastability, manuscript in preparation.
- F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Mesoscopic fluctuations for the critical droplet, preprint arXiv: 1907.00453.
- F. den Hollander, S. Jansen, R. Kotecky, E. Pulvirenti, The Widom-Rowlinson model: Microscopic fluctuations for the critical droplet and effective interface model, manuscript in preparation.

Admissible sets

- Let $\mathcal{F}$ be a family of non-empty closed subsets of the torus $\mathbb{T}$.
- Equip $\mathcal{F}$ with the Hausdorff metric

$$d_{\mathrm{H}}(F_1, F_2) = \max\Big\{\max_{x\in F_1} \mathrm{dist}(x, F_2), \max_{x\in F_2} \mathrm{dist}(x, F_1)\Big\}$$

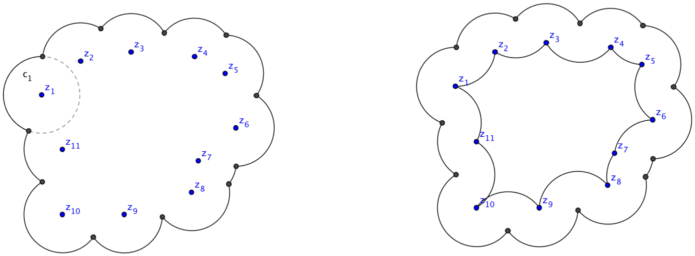
  where $\mathrm{dist}(x, F) = \min_{y\in F} \mathrm{dist}(x, y)$.
- This turns $\mathcal{F}$ into a compact metric space.
- Let $\mathcal{S} \subset \mathcal{F}$ be the collection of all sets that are *admissible*, i.e.,

$$\mathcal{S} = \{S \subset \mathbb{T}\colon\ \exists\, F \text{ such that } h(F) = S\},$$

  where $h(F) = \cup_{x\in F} B(x)$ is the halo of F.

Admissible sets

There is a unique maximal F such that $h(F) = S$, which we denote by S^- and which equals $S^- = \{x \in S\colon\ B(x) \subset S\}$, the 1-interior of S.



Note: Not every closed set is admissible. For example, when we form 1-halos we round off corners, and so a shape with sharp corners cannot be in $\mathcal{S}$. Also note that $S^- \neq \emptyset$ whenever S is admissible: S necessarily contains at least one unit disc $B(x)$ with $x \in S$.

Large Deviation Principle: setting

Define

$$J(S) = |S| - \kappa |S^-|, \qquad S \in \mathcal{S},$$

and

$$I(S) = J(S) - \inf_{\mathcal{S}} J.$$

We view the halo $h(\omega)$ as a random variable with values in the space $\mathcal{S}$, topologized with the Hausdorff distance.
Note that

$$\inf_{\mathcal{S}} J = -(\kappa - 1)|\mathbb{T}|.$$

Large Deviation Principle for the halo

Theorem 1 (Large deviation principle for the halo shape)

The family of probability measures

$$(\mu_\beta(h(\omega) \in \cdot\,))_{\beta \geq 1}$$

satisfies the LDP on $\mathcal{S}$ with rate β and with rate function I.

Informally, Theorem 1 says that

$$\mu_\beta\big(h(\omega) \approx S\big) \approx \exp\big(-\beta I(S)\big), \qquad \beta \to \infty.$$

The contraction principle suggests that an LDP also holds for the halo volume. To formulate this LDP, we first state a minimisation problem for

$$J(S) = |S| - \kappa |S^-|, \qquad S \in \mathcal{S}.$$

Large Deviation Principle: minimisers

Theorem 2 (Minimisers of the rate function for the halo shape)

For every $R \in (1, \frac{L}{\pi} + \frac{1}{2})$,

(1)

$$\min\left\{|S| - \kappa|S^-| \colon\ S \in \mathcal{S}, |S| = |B_R|\right\} = |B_R| - \kappa|B_R^-|$$

and the minimisers are the discs of radius R.

(2) *The minimisers are stable in the following sense: There exists an* $\varepsilon_0 > 0$ *such that if* $R - 1 \geq \epsilon_0$ *and* $S \in \mathcal{S}$ *satisfies*

$$\left(|S| - \kappa|S^-|\right) - \left(|B_R| - \kappa|B_R^-|\right) \leq \pi\kappa\varepsilon \text{ with } |S| = |B_R| \text{ and } \varepsilon \in (0, \varepsilon_0),$$

then S^- *and* $\mathbb{T} \setminus S^-$ *are connected and*

$$d_{\mathrm{H}}(\partial S, \partial B_R) \leq \sqrt{5R\varepsilon},$$

where d_{H} *denotes the Hausdorff distance.*

Large Deviation Principle: minimisers

Theorem 2 is a powerful tool because it shows that *the near-minimers of the halo rate function are close to a disc and have no holes inside*. In particular, it tells us that

$$\begin{aligned} I(B_R) :=& J(B_R) - \inf_{\mathcal{S}} J \\ =& |B_R| - \kappa |B_R^-| + (\kappa - 1)|\mathbb{T}| \\ =& \Phi_\kappa(R) + (\kappa - 1)|\mathbb{T}|, \end{aligned}$$

and allows us, via the contraction principle, to deduce the LDP for the halo volume, which we state next.

Recall

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

Large Deviation Principle for the halo volume

Theorem 3 (Large deviation principle for the halo volume)

The family of probability measures

$$(\mu_\beta(V(\omega) \in \cdot\,))_{\beta \geq 1}$$

satisfies the LDP on $[0,\infty)$ *with rate* β *and with rate function* I^* *given by*

$$I^*(A) = \inf\{I(S)\colon\ |S| = A\}, \qquad A \in [0,\infty).$$

Informally, Theorem 3 says that

$$\mu_\beta\big(V(\omega) \approx A\big) \approx \exp\big(-\beta I^*(A)\big).$$

For every $R \in (1, \frac{L}{\pi} + \frac{1}{2})$, we have

$$I^*(\pi R^2) = I(B_R) = \Phi_\kappa(R) + (\kappa - 1)|\mathbb{T}|.$$

Fluctuations of the critical droplet: moderate deviations

To reach our target, we need to zoom in on a neighborhood of the critical droplet, i.e. $R = R_c$. The large deviation principle implies

$$\mu_\beta\Big(|V(\omega) - \pi R_c^2| \le \varepsilon\Big) = \exp\Big(-\beta \min_{\substack{A\in[0,\infty):\\ |A-\pi R_c^2|\le\varepsilon}} I^*(A) + o(\beta)\Big), \qquad \beta \to \infty,$$

for $\varepsilon > 0$ fixed. We would like to take $\varepsilon = \varepsilon(\beta) \downarrow 0$, for which we need a refined analysis. We would like to capture the term of order $\beta^{1/3}$.

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In particular, we want to compute the asymptotics of

$$\frac{1}{\beta^{1/3}} \log\Big\{ e^{\beta I(B_{R_c})} \mu_\beta\Big(|V(\omega) - \pi R_c^2| \le C\beta^{-2/3}\Big)\Big\}, \qquad \beta \to \infty.$$

This is done by controlling the mesoscopic fluctuations of the surface of the critical droplet.

Fluctuations of the critical droplet: rough result

Theorem 4 (Moderate deviation: rough asymptotics)

For C large enough,

$$\limsup_{\beta\to\infty} \frac{1}{\beta^{1/3}} \log\Big\{ \mathrm{e}^{\beta I(B_{R_c})} \mu_\beta\Big(|V(\omega) - \pi R_c^2| \le C\beta^{-2/3} \Big)\Big\} \le 2\pi G_\kappa \tau_*,$$

$$\liminf_{\beta\to\infty} \frac{1}{\beta^{1/3}} \log\Big\{ \mathrm{e}^{\beta I(B_{R_c})} \mu_\beta\Big(|V(\omega) - \pi R_c^2| \le C\beta^{-2/3} \Big)\Big\} \ge 2\pi G_\kappa (\tau_* - c),$$

with $c \in (0,\infty)$ some constant, $\tau_* \in \mathbb{R}$ solution of the equation

$$\int_0^\infty \sqrt{2\pi u}\, \exp\Big(-\tau_* u - \frac{u^3}{24} \Big)\, \mathrm{d}u = 1,$$

and

$$G_\kappa = \frac{(2\kappa)^{2/3}}{\kappa - 1}.$$

In order to have sharp asymptotics, we need to do better!

Fluctuations of the critical droplet: sharp result

Theorem 5 (Moderate deviation: sharp asymptotics)

Under "certain assumptions", for C large enough and $\beta \to \infty$,

$$\mu_\beta\Big(|V(\omega) - \pi R_c^2| \le C\beta^{-2/3}\Big) = e^{-\beta I(B_{R_c}) + \beta^{1/3}\Psi(\kappa) + o(\beta^{1/3})},$$

where, for some $\tau_{**} > 0$ that does not depend on κ,

$$I(B_{R_c}) = \Phi(\kappa) - (1-\kappa)|\mathbb{T}|, \qquad \Psi(\kappa) = 2\pi G_\kappa(\tau_* - \tau_{**}).$$

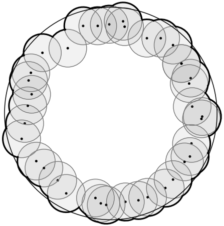
These "certain assumptions" are related to the microscopic fluctuations of the surface of the critical droplet and come from an effective microscopic interface model. This model is of independent interest and will be analysed in the last part of this lecture.

Main ingredients of the proof of sharp asymptotics

References: mainly

F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Mesoscopic fluctuations for the critical droplet, preprint arXiv: 1907.00453.

Step 1: Parametrisation of the halo by boundary points



Let $S = h(\omega)$ be the halo of some configuration ω. The boundary of S consists of a union of arcs of unit circles that are disjoint except for their endpoints. We call the centres

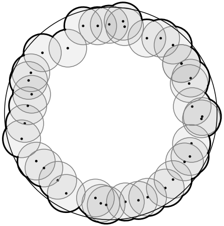
$$z_1, ..., z_n \qquad n = n(\omega)$$

of these circles the boundary points of S.

We say that $z(\omega) = (z_1, ..., z_n)$ is a connected outer contour if there exists a halo $S(z)$ with a simply connected 1-interior S^- having precisely these points as boundary points.

The set of connected outer contours is denoted by $\mathcal{O}$

Step 1: Parametrisation of the halo by boundary points



Idea: Given $S(z)$, $z_1, \dots, z_n$ are the boundary points. We would like to:

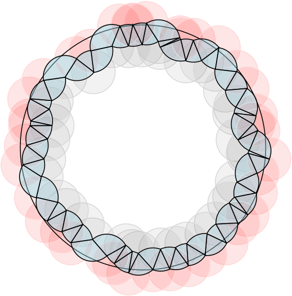
$$\mu_\beta(\omega\ :\ \dots) \longrightarrow \int_{\mathbb{T}^n} \mathrm{d}z_1 \cdots \mathrm{d}z_n \mathbf{1}_{\{z\in\mathcal{O}\}}$$

Reduction to a surface integral

$$\mu_\beta\Big(h(\gamma)\in A\Big) \asymp e^{-\beta I^*(\pi R_c^2)} \sum_{n\in\mathbb{N}_0} \frac{(\kappa\beta)^n}{n!} \int_{\mathbb{T}^n} \mathrm{d}z\, \mathrm{e}^{-\beta\Delta(z)}\, \mathbf{1}_{\{S(z)\in A, z\in\mathcal{O}\}},$$

with $\Delta(z) = |S(z)| - \kappa|S^-(z)| - I^*(\pi R_c^2)$ a surface term.

Step 2: Approximation of the surface term



The second step is to approximate

$$\Delta(z) = |S(z)| - \kappa|S^{-}(z)| - I^{*}(\pi R_c^2)$$

$\Delta(z)$ looks like the blue “sausage”.

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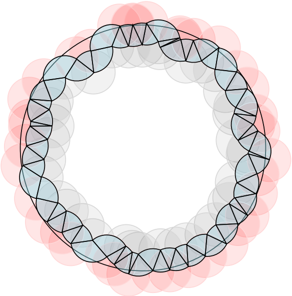

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$$\Delta(z) = |S(z)| - \kappa |S^-(z)| - I^*(\pi R_c^2)$$

$\Delta(z)$ looks like the blue "sausage".

We use polar coordinates $z_i = (r_i \cos t_i, r_i \sin t_i)$, where we may think of

- the angular coordinates $t_1, ..., t_n$ as the points of an angular point process
- the radii $r_1, ..., r_n$ as the values of a Gaussian process evaluated at the random angles.

We then expand $\Delta(z)$ and all the constraints A in terms of r_i and t_i and write the integral in terms of an expectation of functionals of random variables. To make this picture more precise, we need to introduce auxiliary processes.

Step 3: Auxiliary random variables

- Let $(W_t)_{t\geq 0}$ be the standard Brownian motion starting in 0, and let

$$(\widetilde{W}_t)_{t\in[0,2\pi]}, \qquad \widetilde{W}_t = W_t - \frac{t}{2\pi}W_{2\pi},$$

  be the standard Brownian bridge on $[0,2\pi]$.The process

$$(B_t)_{t\in[0,2\pi]}, \qquad B_t = \widetilde{W}_t - \frac{1}{2\pi}\int_0^{2\pi}\widetilde{W}_s \mathrm{d}s,$$

  is called the *mean-centred Brownian bridge*.

- Set

$$\lambda(\beta) = G_\kappa \beta^{1/3}, \quad G_\kappa = \frac{(2\kappa)^{2/3}}{\kappa - 1}.$$

  and let

$$\mathcal{T} = \text{Poisson point process on } [0,2\pi) \text{ with intensity } \lambda(\beta),$$
$$N = |\mathcal{T}| = \text{cardinality of } \mathcal{T}.$$

Step 3: Auxiliary random variables

- Note that N is a Poisson random variable with mean $2\pi\lambda(\beta) = 2\pi G_\kappa \beta^{1/3}$.
- Conditional on the event $\{N = n\}$, we may write

$$\mathcal{T} = \{T_i\}_{i=1}^n, \qquad \text{with } 0 \leq T_1 < \cdots < T_n < 2\pi$$

  and define

$$\Theta_i = T_{i+1} - T_i,\ 1 \leq i \leq n, \qquad \Theta_n = (T_1 + 2\pi) - T_n.$$

  Note that $\Theta_i \geq 0$, $1 \leq i \leq n$, and $\sum_{i=1}^n \Theta_i = 2\pi$.
- We assume that $(B_t)_{t\in[0,2\pi]}$ and $\mathcal{T}$ are defined on a common probability space $(\Omega, \mathsf{F}, \mathcal{P})$ and they are independent.

Step 3: Auxiliary random variables

The boundary points can be represented as random variables:

For $m \in \mathbb{R}$, set

$$Z^{(m)} = \{Z_i^{(m)}\}_{i=1}^N$$

with

$$Z_i^{(m)} = \left(r_i^{(m)} \cos T_i, r_i^{(m)} \sin T_i\right),$$
$$r_i^{(m)} = (R_c - 1) + \frac{m + B_{T_i}}{\sqrt{(\kappa - 1)\beta}}, \qquad 1 \leq i \leq N.$$

This formula constitutes a convenient representation of the probability measure for the boundary points in terms of the auxiliary processes.

Remark: the parameter m play the role of a dilation and will turn out to be insignificant. Think of $m = 0$.

Step 4: Asymptotics of surface integrals

Therefore the quantity (recall)

$$\mu_\beta\Big(h(\gamma)\in A\Big) \asymp e^{-\beta I^*(\pi R_c^2)} \sum_{n\in\mathbb{N}_0} \frac{(\kappa\beta)^n}{n!} \int_{\mathbb{T}^n} \mathrm{d}z\, \mathrm{e}^{-\beta\Delta(z)}\, \mathbf{1}_{\{S(z)\in A, z\in\mathcal{O}\}},$$

with $\Delta(z) = |S(z)| - \kappa|S^-(z)| - I^*(\pi R_c^2)$, can be rewritten in terms of a new tilted probability measure. Set

$$\widehat{Y}_0 = \frac{1}{2}\sum_{i=1}^N \log\big(2\pi\beta^{1/3} G_\kappa \Theta_i\big), \quad \widehat{Y}_1 = \frac{1}{24}\sum_{i=1}^N \big(\beta^{1/3} G_\kappa \Theta_i\big)^3,$$

and consider the tilted probability measure $\widehat{\mathbb{P}}$ on $(\Omega, \mathsf{F}, \mathbb{P})$ defined by

$$\widehat{\mathbb{P}}(A) = \frac{\mathbb{E}[\exp(\widehat{Y}_0 - \widehat{Y}_1)\mathbf{1}_A]}{\mathbb{E}[\exp(\widehat{Y}_0 - \widehat{Y}_1)]}, \qquad A \subset \Omega \text{ measurable.}$$

The somewhat baroque quantities Y_0 and Y_1 arise from a Taylor expansion of $\Delta(z)$, i.e. the difference between the volume of the halo and the volume of the critical disc.

Other technical steps

Via stochastic geometry, analysis, LDP, ...

- Show a number of a priori estimates on the radial and the angular coordinates of the boundary points;
- Show a local characterisation of the boundary points, in the sense that being a boundary point depends only on the centre of the two neighbouring discs;
- Show that contribution to the free energy coming from halos that are not close to a critical disc either in volume or in Hausdorff distance is negligible;
- Show that the centre of the critical disc can be placed at the origin;
- Estimate integrals via controlling exponential moments and discretisation errors;
- ...

What have we done:

We analysed the mesoscopic fluctuations of the surface of the critical droplet and obtained sharp asymptotics for the capacity. The result was subject to three "technical conditions".

Microscopic fluctuations of the critical droplet

References: mainly

F. den Hollander, S. Jansen, R. Kotecký, E. Pulvirenti, The Widom-Rowlinson model: Microscopic fluctuations for the critical droplet and effective interface model, manuscript in preparation.

Microscopic fluctuations of the critical droplet

What we do next:

- The proof of the "technical conditions" relies on a closer analysis of the microscopic fluctuations of the surface of the critical droplet.
- In particular, it relies on a detailed study of a certain Gibbs modification of what in stochastic geometry is known as the *paraboloid hull process* (references of stochastic geometry at the end).
- This modification, which we refer to as the parabolic interface model (PIM), arises as the scaling limit of the surface of the critical droplet in the WR model when $\beta \to \infty$.
- PIM is of special interest because it provides a rigorous microscopic foundation for the notion of surface tension in statistical physics

The parabolic interface model

The PIM is a variant of a standard (1+1)-dimensional interface model built on the discrete Gaussian Free Field (see e.g. Friedli and Velenik).
The principal differences are:

- The lattice $\mathbb{Z}$ of the one-dimensional discrete GFF is replaced by a random point configuration on the halfline $\mathbb{R}_+$.
- There is a cubic interaction that favours even spacings.
- There is a hard-core interaction that comes from a geometric constraint: the points of the interface have to be extremal (definition in the next slide).
  This geometric constraint is equivalent to the constraint of z being a connected outer contour in the WR model.

Think of the "interface" as what we see when we zoom in on the boundary points of the critical droplet until the scale of their separation is of order 1. On that scale the interface looks flat.

Extremality

Let $\mathbf{x} = \{(s_i, y_i)\}_{i \in I}$ be a sequence of points in $\mathbb{R}^2$ indexed by a countable set of successive indices $I \subseteq \mathbb{Z}$. Consider the union of downward parabolas

$$\mathcal{A}(\mathbf{x}) = \bigcup_{i \in I} \left\{(s, y) \in \mathbb{R}^2 \colon\ y \leq y_i - \tfrac{1}{2}(s - s_i)^2\right\}.$$

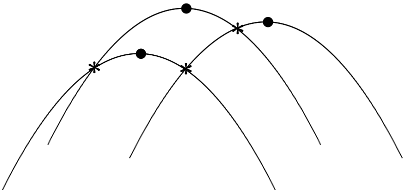
- A point $(s_i, y_i) \in \mathbf{x}$ is said to be *extremal* when

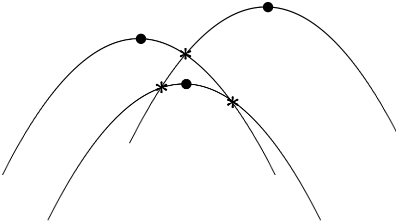
$$\mathcal{A}(\mathbf{x} \setminus \{(s_i, y_i)\}) \subsetneq \mathcal{A}(\mathbf{x}).$$

- $\mathbf{x} = \{(s_i, y_i)\}_{i \in I}$ is said to be *extremal* if every $(s_i, y_i) \in \mathbf{x}$ is extremal.

We use $\mathcal{E}$ to denote the set of all extremal $\mathbf{x}$. These will be referred to as sequences of boundary points.

The parabolic interface model: extremality





Two examples of triplets of parabolas. The $\bullet$'s mark the tips of the parabolas, the $*$'s mark the pairwise intersection points.

The left picture is extremal, and the two outer $*$'s appear in the same order as the associated pairs of $\bullet$'s. The right picture is not extremal, and the two outer $*$'s appear in the opposite order as the associated pairs of $\bullet$'s.

The parabolic interface model: partition function

The following partition function associated with the PIM, called the grand-canonical pinned partition function, will be the key object in our analysis of the WR model

$$
\begin{aligned}
\mathcal{Z}_{L,M} = & 1 + \sum_{n=2}^{\infty} \int_{\mathbb{R}_+^{n-1}} \mathrm{d}s_2 \cdots \mathrm{d}s_n \int_{\mathbb{R}^{n-1}} \mathrm{d}y_2 \cdots \mathrm{d}y_n \\
& \times \mathbf{1}_{\{s_1 < s_2 < \cdots < s_n < s_{n+1}\}} \mathbf{1}_{\mathcal{E}}\left(\{(s_i, y_i)\}_{i=1}^{n+1}\right) \\
& \times \exp\Big(- \sum_{i=1}^{n} \frac{(s_{i+1} - s_i)^3}{24} - \sum_{i=1}^{n} \frac{(y_{i+1} - y_i)^2}{2(s_{i+1} - s_i)} \Big),
\end{aligned}
$$

with pinned first and last parabola,

$$
(s_1, y_1) = (0, 0), \quad (s_{n+1}, y_{n+1}) = (L, M).
$$

The appropriate choice to link PIM and WRM is:

$$
L = 2\pi G_\kappa \beta^{1/3} \qquad M = 0.
$$

Later we have to replace the “pinned” boundary condition by a circular boundary condition, appropriate for the circular interface of the critical droplet in the WR moel.

The parabolic interface model: two key theorems

Theorem 6 (Interface free energy)

Let $\lambda(p,q)$ *be the principal eigenvalue of the operator* $\mathbf{K}_{p,q}$ *(defined later). Then, for any* $\alpha \in (-\pi, \pi)$*,*

$$\lim_{L\to\infty} \frac{1}{L} \log \mathcal{Z}_{L, L\tan\alpha} = -p_\alpha - q_\alpha \tan\alpha,$$

where $(p_\alpha, q_\alpha) \in \mathbb{R}\times\mathbb{R}$ *is the unique solution of the set of equations*

$$\log \lambda(p,q) = 0, \qquad \frac{\frac{\partial}{\partial q}\log\lambda(p,q)}{\frac{\partial}{\partial p}\log\lambda(p,q)} = \tan\alpha.$$

If $\alpha = 0$ *(flat interface), then* $(p_\alpha, q_\alpha) = (p_*, 0)$ *with* $p_* \in \mathbb{R}$ *the unique solution of the equation* $\lambda(p,0) = 1$*.*

The parabolic interface model: two key theorems

Given $\mathbf{x} = \{(s_i, y_i)\}_{i=1}^{n+1}$, define a path $X_L \colon [0,1] \to \mathbb{R}$ by putting

$$X_L(0) = 0, \qquad X_L\left(\frac{s_i}{L}\right) = \frac{y_i}{\sqrt{L}}, \quad 2 \le i \le n, \qquad X_L(1) = 0,$$

and applying piecewise affine interpolation.

Theorem 7 (Invariance principle)

As $L \to \infty$, $(X_L(t))_{t\in[0,2\pi]}$ under the Gibbs measure $\mathcal{P}_{L,0}$ (associated to $\mathcal{Z}_{L,0}$) converges in distribution to σB for some $\sigma^2 \in (0,\infty)$, with $(B_t)_{t\in[0,2\pi]}$ mean-centered Brownian bridge.

- These two theorems are crucial to prove the three "technical conditions" and therefore prove the sharp asymptotics for the capacity of the WR model.
- The key observation in proving these results is that the extremality constraint is not really a hard-core multy-body interaction as it seems...

The parabolic interface model: extremality is local

Lemma 8

Let $\mathbf{x} = \{(s_i, y_i)\}_{i\in I} \in \mathcal{X}$. *Assume that* $s_i < s_{i+1}$ *for all* $i \in I$ *and define linear spacings* ϑ_i *and height increments* φ_i *by*

$$\vartheta_i = s_{i+1} - s_i, \quad \varphi_i = y_{i+1} - y_i.$$

Then

- $\mathbf{x} \in \mathcal{E}$ *if and only if all triplets* (x_{i-1}, x_i, x_{i+1}) *are extremal;*
- $\mathbf{x} \in \mathcal{E}$ *if and only if*

$$\frac{2}{\vartheta_i + \vartheta_{i-1}}\left(\frac{\varphi_i}{\vartheta_i} - \frac{\varphi_{i-1}}{\vartheta_{i-1}}\right) < 1 \qquad \forall\, i \in I.$$

This lemma shows that:

Extremality constraint is local $\Rightarrow$ it can be expressed in terms of increments $\Rightarrow$ and as a product of nearest-neighbour constraints.

The parabolic interface model: transfer operator

Because of the locality of the constraint, we can rewrite the Gibbs measure in terms of a transfer operator.

Let p, q be some parameters to weigh the endpoints. Put $\mathbb{S} = \mathbb{R}_+ \times \mathbb{R}$. For $(p, q) \in \mathbb{R} \times \mathbb{R}$ define the integral kernel $K_{p,q} \colon \mathbb{S}^2 \to [0, \infty)$ given by

$$\begin{aligned} &K_{p,q}\big((\vartheta_1, \varphi_1), (\vartheta_2, \varphi_2)\big) \\ &= \exp\Big(\frac{1}{2}\Big[p\vartheta_1 + q\varphi_1 - \frac{\vartheta_1^3}{24} - \frac{\varphi_1^2}{2\vartheta_1}\Big]\Big)\, \mathbf{1}_{\left\{\frac{2}{\vartheta_1+\vartheta_2}\left(\frac{\varphi_2}{\vartheta_2} - \frac{\varphi_1}{\vartheta_1}\right) < 1\right\}} \\ &\quad \times \exp\Big(\frac{1}{2}\Big[p\vartheta_2 + q\varphi_2 - \frac{\vartheta_2^3}{24} - \frac{\varphi_2^2}{2\vartheta_2}\Big]\Big). \end{aligned}$$

Let $\mathbf{K}_{p,q} : L^2(\mathbb{S}) \to L^2(\mathbb{S})$ be the integral operator given by

$$(\mathbf{K}_{p,q} f)(\xi) = \int_{\mathbb{S}} \mathrm{d}\xi'\, K_{p,q}(\xi, \xi') f(\xi').$$

The parabolic interface model: unpinned measure

For fixed n, we drop the constraint $(s_{n+1}, y_{n+1}) = (L, M)$, but use the parameters $p, q \in \mathbb{R}$ to weigh the endpoint instead. This represents a free boundary condition. We define the canonical unpinned partition function as

$$\mathsf{Z}_n(p,q) = \int_{\mathbb{R}_+^n} \mathrm{d}s_2 \dots \mathrm{d}s_{n+1} \int_{\mathbb{R}^n} \mathrm{d}y_2 \dots \mathrm{d}y_{n+1} \, \mathbf{1}_{\{0<s_2<\cdots<s_{n+1}\}} \, \mathbf{1}_{\mathcal{E}}\big(\{(s_i, y_i)\}_{i=1}^{n+1}\big)$$

$$\times \exp\Big(p\, s_{n+1} + q\, y_{n+1} - \sum_{i=1}^{n} \frac{(s_{i+1}-s_i)^3}{24} - \sum_{i=1}^{n} \frac{(y_{i+1}-y_i)^2}{2(s_{i+1}-s_i)} \Big)$$

For fixed n, we drop the constraint $(s_{n+1}, y_{n+1}) = (L, M)$, but use the parameters $p, q \in \mathbb{R}$ to weigh the endpoint instead. This represents a free boundary condition. We define the canonical unpinned partition function as

$$
\begin{aligned}
\mathsf{Z}_n(p,q) &= \int_{\mathbb{R}_+^n} \mathrm{d}s_2 \ldots \mathrm{d}s_{n+1} \int_{\mathbb{R}^n} \mathrm{d}y_2 \ldots \mathrm{d}y_{n+1} \, \mathbf{1}_{\{0<s_2<\cdots<s_{n+1}\}} \, \mathbf{1}_{\mathcal{E}}\big(\{(s_i,y_i)\}_{i=1}^{n+1}\big) \\
&\qquad \times \exp\Big(p\, s_{n+1} + q\, y_{n+1} - \sum_{i=1}^{n} \frac{(s_{i+1}-s_i)^3}{24} - \sum_{i=1}^{n} \frac{(y_{i+1}-y_i)^2}{2(s_{i+1}-s_i)} \Big) \\
&= \int_{\mathbb{R}_+^n} \mathrm{d}\vartheta_1 \ldots \mathrm{d}\vartheta_n \int_{\mathbb{R}^n} d\varphi_1 \ldots \mathrm{d}\varphi_n \, \mathbf{1}_{\mathcal{E}}\big(\{(\vartheta_i,\varphi_i)\}_{i=1}^{n}\big) \\
&\qquad\qquad \times \exp\Big(p \sum_{i=1}^{n} \vartheta_i + q \sum_{i=1}^{n} \varphi_i - \sum_{i=1}^{n} \frac{\vartheta_i^3}{24} - \sum_{i=1}^{n} \frac{\varphi_i^2}{2\vartheta_i} \Big).
\end{aligned}
$$

The parabolic interface model: free energy

We can write the canonical unpinned partition function in terms of the scalar product

$$\mathsf{Z}_n(p,q) = (F_{p,q}, \mathbf{K}_{p,q}^{n-1} F_{p,q}).$$

where F is a suitably chosen function encoding the boundary condition

$$F_{p,q}(\vartheta, y) = \exp\Big(\frac{1}{2}\Big[p\vartheta + q\varphi - \frac{\vartheta^3}{24} - \frac{\varphi^2}{2\vartheta}\Big]\Big).$$

Lemma 9

For every $(p,q) \in \mathbb{R} \times \mathbb{R}$,

$$\lim_{n\to\infty} \frac{1}{n} \log \mathsf{Z}_n(p,q) = \log \lambda(p,q),$$

where $\lambda(p,q)$ is the principal eigenvalue of $\mathbf{K}_{p,q}$. Moreover, $(p,q) \mapsto \lambda(p,q)$ is analytic, strictly increasing and strictly convex on $\mathbb{R} \times \mathbb{R}$.

The parabolic interface model: Conclusion

- Link the free energy associated with the unpinned PIM to the one associated with the pinned PIM,
- Link the pinned PIM to a version of the PIM on the circle (instead of on the line),
- Link the PIM on the circle to the WR model.

All these models are thermodynamically equivalent and are approximating tools to analyse WR.

The transfer operator of the WR is a perturbation of the transfer operator of the PIM.
For the PIM we found that the free energy equals p^*, with p^* the unique solution of the equation

$$\lambda(p, 0) = 1.$$

Recalling that the average number of discs touching the boundary of the critical droplet in the WRM is $2\pi G_\kappa \beta^{1/3}$, we get that the surface free energy of the WRM equals $\Psi(\kappa) = 2\pi G_\kappa p^*$.

Summary

In this last lecture we have seen:

- Key questions for the study of metastability for the 1-species WR model with birth/death;
- Heuristics for the formation of the critical droplet;
- Three target theorems for the analysis of metastability;
- Potential theoretic approach for the WR model: approximation of the capacity;
- Mesoscopic fluctuations of the critical droplet: LDPs, isoperimetric inequalities, MDs;
- Strategy of the proof;
- Microscopic fluctuations of the critical droplet: the PIM;
- Two key theorems for the PIM, link to WR and conclusions.

Thank you for your attention!

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