

Metastability for the Widom-Rowlinson model

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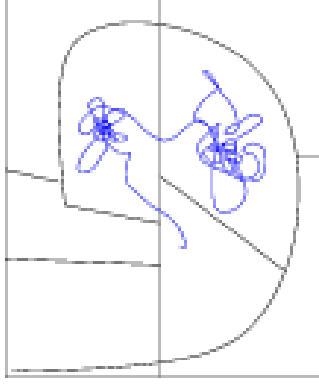
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Joint work with S. Jansen (Bochum), R. Kotecký (Prague & Warwick)
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§ WHAT IS METASTABILITY?

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



- **Fast time scale:** rapid transitions within a single subregion.
- **Slow time scale:** slow transitions between different subregions.

§ WHY IS METASTABILITY IMPORTANT ?

Metastability is **universal**: it manifests itself in a wide variety of systems coming from physics, chemistry, biology, economics.

The mathematical challenge is to understand metastability in **quantitative terms**.

MONOGRAPHS:

Olivieri & Vares 2005

Bovier & den Hollander 2015



§ METASTABILITY IN STATISTICAL PHYSICS

Metastability is the dynamical manifestation of a **first-order phase transition**. An example is condensation:

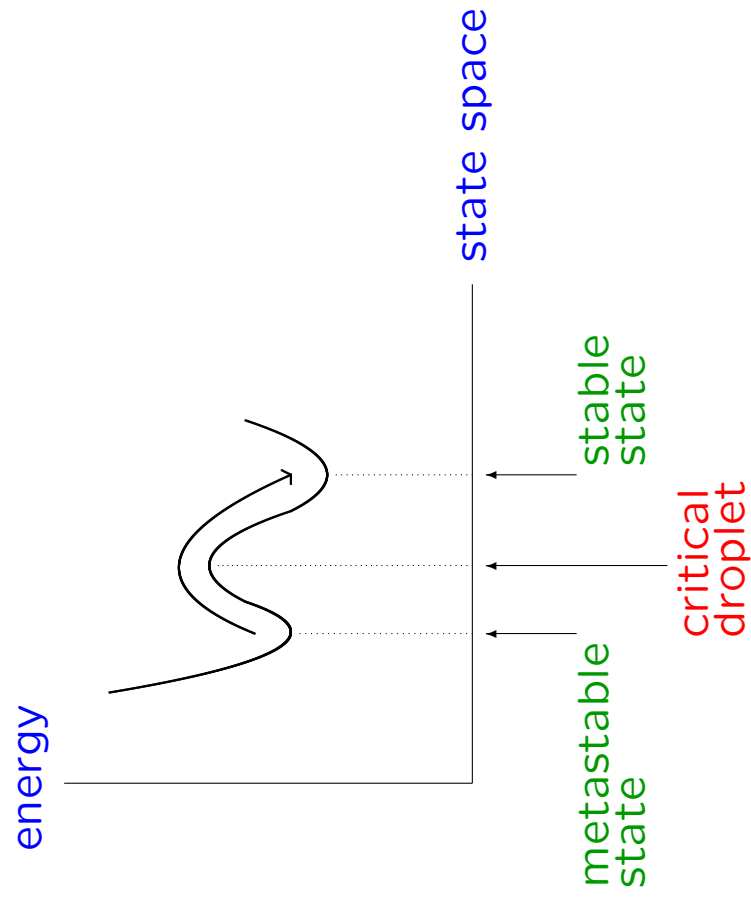


When a vapour is **cooled down**, it persists for a very long time in a **metastable vapour state**, before transitioning to a **stable liquid state** under the influence of **random fluctuations**.

The crossover occurs after the system manages to create a **critical droplet** of liquid inside the vapour, which subsequently grows and invades the whole system.

While in the **metastable vapour state**, the system makes many **unsuccessful attempts** to form a **critical droplet**.

PARADIGM PICTURE OF METASTABILITY:



Continuum systems are particularly difficult to analyse. A rigorous proof of the presence of a phase transition has been achieved for very few models only:

- Widom-Rowlinson model.
Ruelle 1971
- One-dimensional models with long-range interaction.
Johansson 1995
- Kac models with 2-body attraction and 4-body repulsion.
Lebowitz, Mazel & Presutti 1999

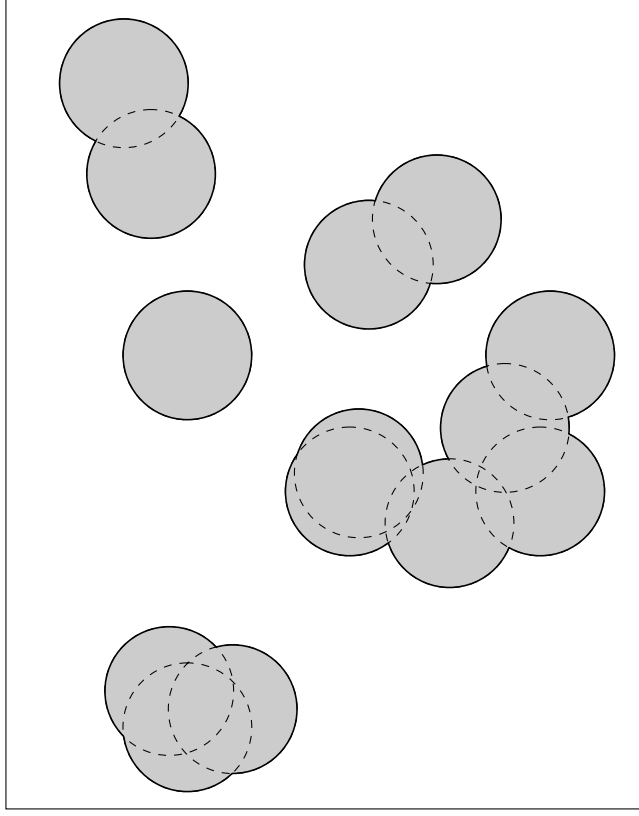
Metastability for continuum systems: crystallisation of two-dimensional particles interacting via a soft-disk potential.
Jansen & den Hollander, in preparation

In this talk we focus on the Widom-Rowlinson model.

§ THE STATIC WIDOM-ROWLINSON MODEL

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

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



The grand-canonical Gibbs measure is

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

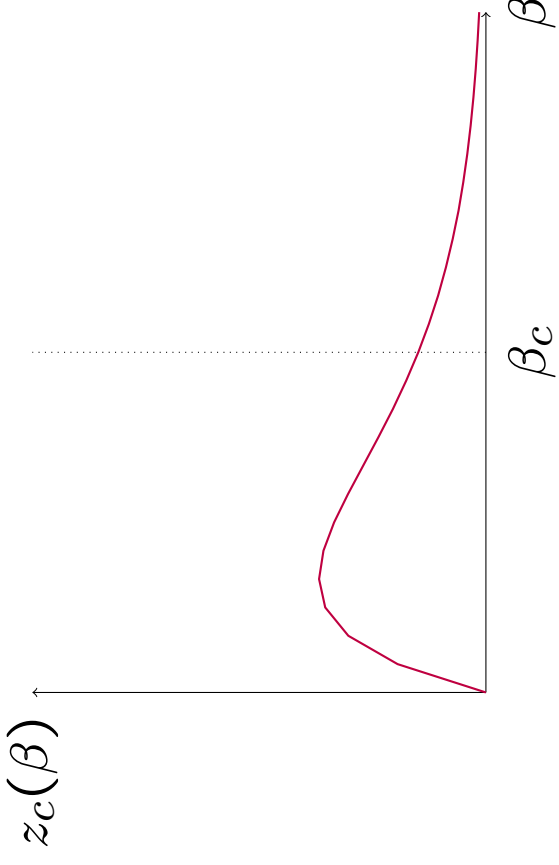
where

- Q is the Poisson point process with intensity 1,
- z is the chemical activity,
- $\beta \in (0, \infty)$ is the inverse temperature,

$H(\omega)$ is the interaction Hamiltonian

$$H(\omega) = - \text{total volume of the overlap of the 2-spheres around } \omega,$$

and Ξ is the normalising partition function.

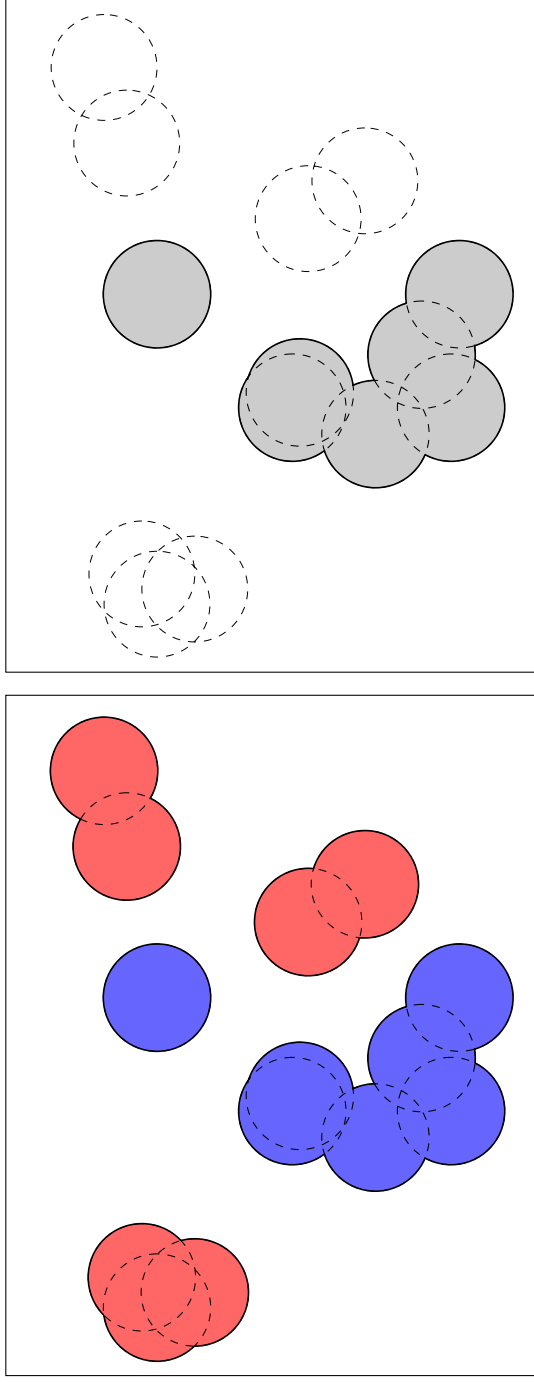


For $\beta > \beta_c$ a phase transition occurs at $z = z_c(\beta) = \beta e^{-4\pi\beta}$ in the thermodynamic limit, i.e., $\Lambda \rightarrow \mathbb{R}^2$.

Ruelle 1971

Chayes, Chayes & Kotecký 1995

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



§ THE DYNAMIC WIDOM-ROWLINSON MODEL

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

$$(Lf)(\omega) = \int_{\Lambda} dx \, b(x, \omega) [f(\omega \cup x) - f(\omega)] \\ + \sum_{x \in \omega} d(x, \omega) [f(\omega \setminus x) - f(\omega)],$$

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

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

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

KEY QUESTION:

Let $\square$ and $\blacksquare$ denote the set of configurations where Λ is empty, respectively, full.



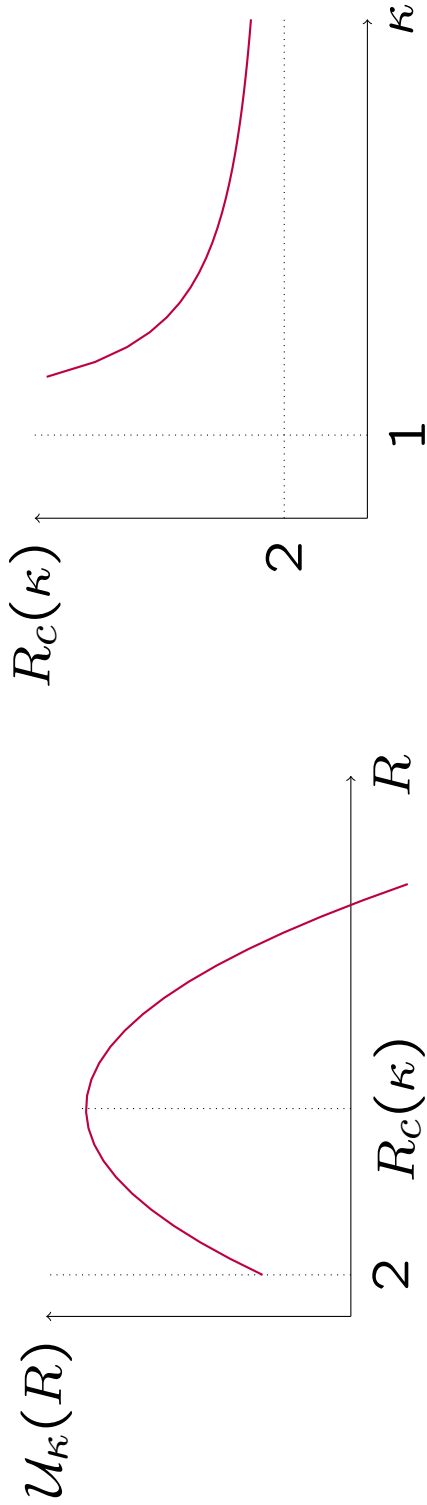
- Start with Λ empty, i.e., $\omega_0 = \square$.
[vapour]
- Choose $z > \kappa z_c(\beta)$, $\kappa \in (1, \infty)$.
[super-saturated vapour]
- Wait for the first time $\tau_{\blacksquare}$ when the system fills Λ .
[condensation]

What can we say about the law of $\tau_{\blacksquare}$ in the limit as $\beta \rightarrow \infty$ for fixed Λ and κ ?

§ THREE THEOREMS

For $R \in [2, \infty)$, let

$$\mathcal{U}_\kappa(R) = \pi R^2 - \kappa \pi (R - 2)^2, \qquad R_c(\kappa) = \frac{2\kappa}{\kappa - 1}.$$



THEOREM 1 [Arrhenius formula]

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

$$\lim_{\beta \rightarrow \infty} \beta^{-1/6} \mathrm{e}^{-\beta \Gamma(\kappa)} E_{\square}(\tau_{\blacksquare}) = \frac{1}{|\Lambda|} K(\kappa)$$

with

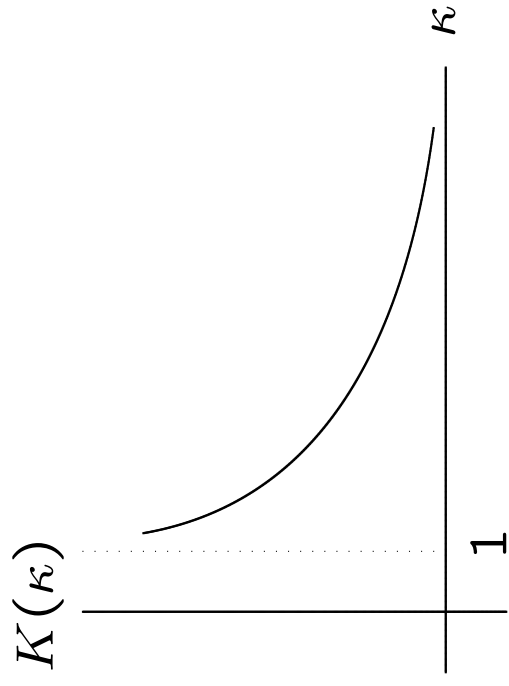
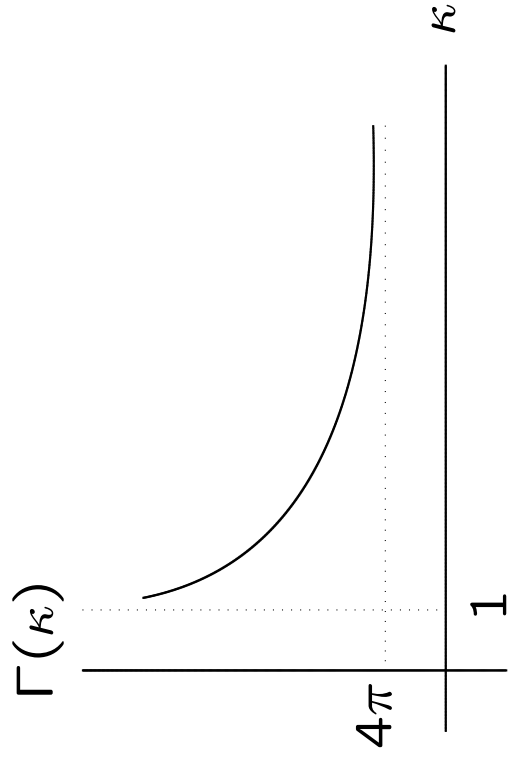
$$\Gamma(\kappa) = \mathcal{U}_{\kappa}(R_c(\kappa)) = \frac{4\pi\kappa}{\kappa-1}$$

and

$$K(\kappa) = L(\kappa) \sqrt{\frac{2\pi}{-\mathcal{U}_{\kappa}''(R_c(\kappa))}} = L(\kappa) \sqrt{\frac{1}{\kappa-1}},$$

where $L(\kappa) = \frac{1}{C} \kappa^{1/3}$ with $C = \frac{5}{3^{7/3}} \Gamma(\frac{2}{3})$.

Plots of the condensation energy and
the prefactor in the Arrhenius formula:



THEOREM 2 [Exponential law]

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

$$\lim_{\beta \rightarrow \infty} P_{\square}(\tau_{\blacksquare} / E_{\square}(\tau_{\blacksquare}) > t) = e^{-t} \quad \forall t \geq 0.$$

THEOREM 3 [Critical droplet]

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

$$\lim_{\beta \rightarrow \infty} P_{\square}(\tau_{\mathcal{C}_{\delta}(\kappa)} < \tau_{\blacksquare} \mid \tau_{\square} > \tau_{\blacksquare}) = 1 \quad \forall \delta > 0,$$

where

$$\begin{aligned} & \mathcal{C}_{\delta}(\kappa) \\ &= \left\{ \omega \in \Omega : B_{R_c(\kappa) - \delta}(x) \subset h(\omega) \subset B_{R_c(\kappa) + \delta}(x) \exists x \in \Lambda \right\}. \end{aligned}$$

§ HEURISTICS

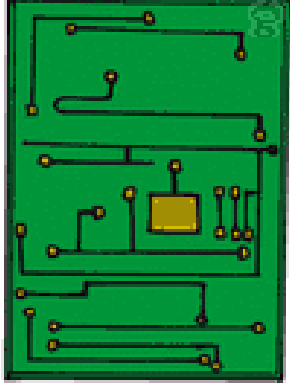
- Since particles have a tendency to stick together, they form some sort of droplet.
- Inside the droplet, particles are distributed as a Poisson process with intensity $\kappa\beta \gg 1$.



- Near the perimeter of the droplet, particles are born at a rate that depends on how much they stick out.
- For $R < R_c(\kappa)$ the droplet tends to shrink, while for $R > R_c(\kappa)$ it tends to grow.

§ POTENTIAL-THEORETIC APPROACH TO METASTABILITY

Bovier & den Hollander 2015



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

The key link between the average metastable crossover time and capacity is

$$E_{\square}(\tau_{\blacksquare}) = [1 + o(1)] \frac{1}{\Xi e^{|\Lambda|} \text{cap}(\square, \blacksquare)}, \quad \beta \rightarrow \infty.$$

The capacity of two disjoint subsets $A, B \subset \Omega$ is defined as

$$\text{cap}(A, B) = \int_A \mu(d\omega) P_\omega(\tau_B < \tau_A),$$

where $\tau_C = \inf\{t > 0: X_t \in C, X_{t-} \notin C\}$ is the first return time to $C \subset \Omega$.

The capacity satisfies the Dirichlet principle

$$\text{cap}(\square, \blacksquare) = \inf_{\substack{f: \Omega \rightarrow [0,1] \\ f|_{\square} = 1, f|_{\blacksquare} = 0}} \mathcal{E}(f, f),$$

where

$$\begin{aligned} \mathcal{E}(f, f) &= \int_{\Omega} f(\omega)(-L f)(\omega) \mu(d\omega) \\ &= \frac{1}{2} \int_{\Omega} \mathbb{Q}(d\omega) \int_{\Lambda} dx \, e^{-\beta H(\omega \cup x)} [f(\omega \cup x) - f(\omega)]^2. \end{aligned}$$



The estimation of capacity proceeds via

- **Upper bound:** Estimate $\text{cap}(\square, \blacksquare) \leq \mathcal{E}(f, f)$ for a test function f that needs to be guessed from intuition.
- **Lower bound:** Restrict the integral over $\mathcal{Q}$ to those configurations in the vicinity of the critical droplet.

The details of the computation are rather delicate and need to be precise enough in order to produce the prefactor in the Arrhenius formula.

The large-deviation approach to metastability does not allow for such a precision.

§ LINK WITH KRAMERS FORMULA

Let $(\bar{\omega}_t)_{t \geq 0}$ be the dynamics obtained by removing the time intervals during which the system resides at $\square$. Let $(R_\tau)_{\tau \geq 0}$ be the radial process defined by

$R_\tau =$ radius of halo of $\bar{\omega}_{L(\kappa)_\tau}$.

It turns out that this process approximately evolves according to the diffusion equation

$$dR_\tau = -\mathcal{U}'_\kappa(R_\tau) d\tau + \sqrt{2/\beta} dW_\tau,$$

with a reflecting boundary at $R = 2$, where $(W_\tau)_{\tau \geq 0}$ is a standard Brownian motion on $\mathbb{R}$.



The scaling formula we found for $E_\square(\tau_\blacksquare)$ coincides with the classical Kramers formula for the average metastable crossover time for this diffusion.

There are many remaining challenges to understand
metastability for continuum systems !

