# Metastability for interacting particle systems

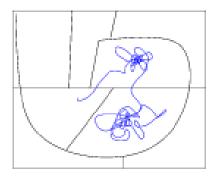
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P.C. Mahalanobis Lectures 2015–2016, Indian Statistical Institute, Delhi & Bangalore & Kolkata.

# $\S$ what is metastability?

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



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

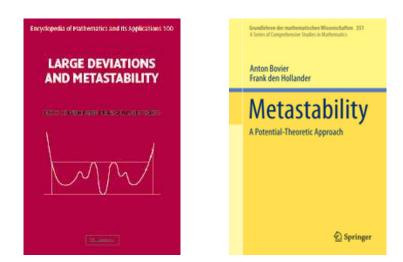
# $\S$ WHY IS METASTABILITY IMPORTANT?

Metastability is universal: it is encountered in a very wide variety of stochastic systems.

The mathematical challenge is to propose computable models and analyse metastability in quantitative terms.

MONOGRAPHS:

Olivieri & Vares 2005 Bovier & den Hollander 2015



# $\S$ METASTABILITY IN STATISTICAL PHYSICS

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

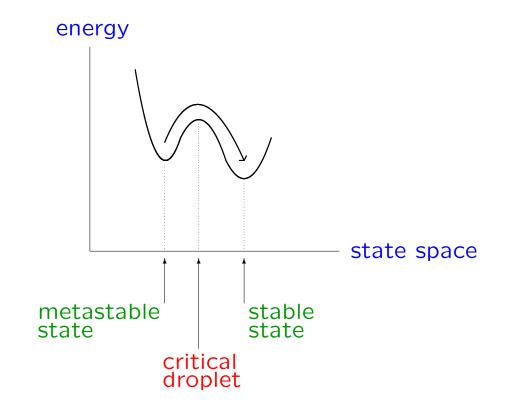
When a vapour is cooled down, it persists for a very long time in a metastable vapour state, before transiting to a stable liquid state under the influence of random fluctuations.



The crossover occurs after the system manages to create a critical droplet of liquid inside the vapour, which once present 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:



Particle systems in the continuum are particularly difficult to analyse, but they give rise to new phenomena. A rigorous proof of the presence of a phase transition has been achieved for very few models only.

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

In this model, the interactions are purely geometric, which makes it more amenable to a detailed analysis.

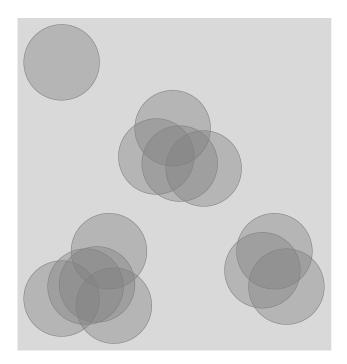
The results described in the sequel are joint work with:

- S. Jansen (Bochum)
- R. Kotecký (Prague & Warwick)
- E. Pulvirenti (Leiden)

#### $\S$ THE STATIC WIDOM-ROWLINSON MODEL

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

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



disks of radius 2 around  $\omega$ 

The grand-canonical Gibbs measure is

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

where

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

 ${\boldsymbol{H}}$  is the interaction Hamiltonian given by

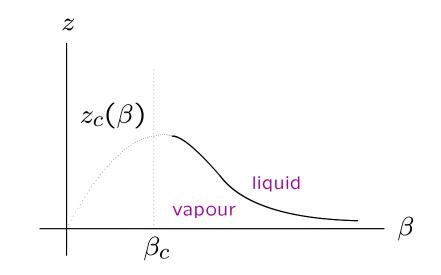
$$H(\omega) = -\sum_{\substack{x,y\in\omega\\x< y}} |B_2(x) \cap B_2(y)|,$$

i.e., minus the sum of the pairwise overlaps of the 2-disks around  $\omega$ .

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

$$z = z_c(\beta) = \beta \,\mathrm{e}^{-4\pi\beta}$$

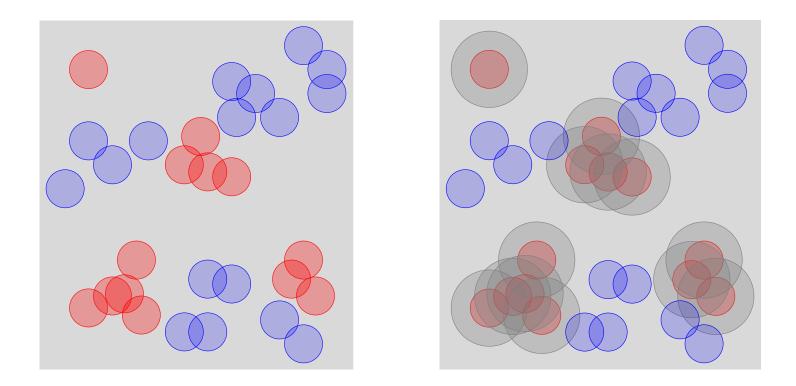
in the thermodynamic limit, i.e.,  $\Lambda \to \mathbb{R}^2$ . No closed form expression is known for  $\beta_c$ .



# 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:



disks of radius 1 around  $\omega^{\rm red}$  and  $\omega^{\rm blue}$ 

#### § THE DYNAMIC WIDOM-ROWLINSON MODEL

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

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

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

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

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

### KEY QUESTION:

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

• Start with  $\Lambda$  empty, i.e.,  $\omega_0 = \Box$ . [preparation in vapour state]



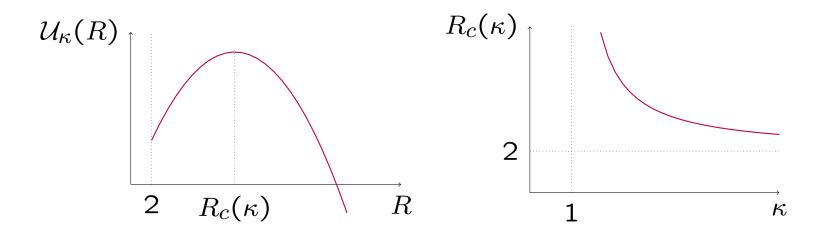
Arrhenius

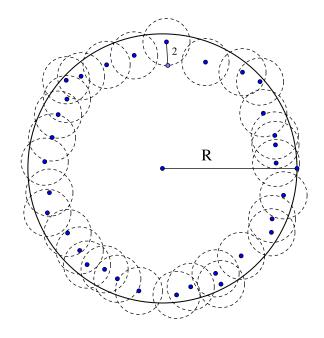
- Choose  $z = \kappa z_c(\beta)$ ,  $\kappa \in (1, \infty)$ . [reservoir is super-saturated vapour]
- Wait for the first time τ<sub>■</sub> when the system fills Λ.
   [condensation to liquid state]

What can we say about the law of  $\tau_{\blacksquare}$  in the limit as  $\beta \to \infty$  for fixed  $\Lambda$  and  $\kappa$ ?

### $\S$ THREE THEOREMS

For  $R \in [2, \infty)$ , let  $\mathcal{U}_{\kappa}(R) = \pi R^2 - \kappa \pi (R-2)^2$ ,  $R_c(\kappa) = \frac{2\kappa}{\kappa - 1}$ .





A droplet of radius R filled with 2-disks:  $\asymp\beta$  disks in the interior,  $\asymp\beta^{1/3}$  disks on the boundary

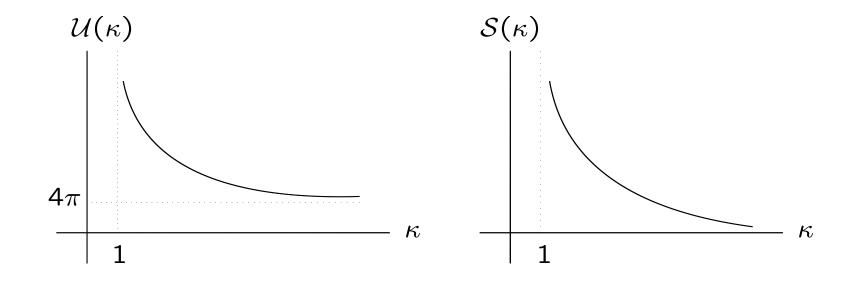
#### THEOREM 1 [Arrhenius formula]

For every 
$$\kappa \in (1, \infty)$$
,  
 $E_{\Box}(\tau_{\blacksquare}) = \exp\left[\beta \mathcal{U}(\kappa) - \beta^{1/3} \mathcal{S}(\kappa) + O(\log \beta)\right], \qquad \beta \to \infty,$ 

#### where

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

and  $S(\kappa)$  is given by an intricate variational formula that involves a large deviation rate function for the positions of the particles near the boundary of the critical droplet. Plots of the key quantities in the Arrhenius formula:



U(κ) is the energy of the critical droplet.
S(κ) is the entropy associated with the surface fluctuations of the critical droplet.

#### THEOREM 2 [Exponential law]

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

$$\lim_{\beta \to \infty} P_{\Box} \left( \tau_{\blacksquare} / E_{\Box} (\tau_{\blacksquare}) > t \right) = \mathrm{e}^{-t} \qquad \forall t \ge 0.$$

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

For 
$$\delta > 0$$
, let

$$\mathcal{C}_{\delta}(\kappa) = \Big\{ \omega \in \Omega \colon \exists x \in \Lambda \text{ such that} \\ B_{R_{c}(\kappa) - \delta}(x) \subset \mathsf{halo}(\omega) \subset B_{R_{c}(\kappa) + \delta}(x) \Big\}.$$

#### THEOREM 3 [Critical droplet]

For every  $\kappa \in (1, \infty)$ ,  $\lim_{\beta \to \infty} P_{\Box} \Big( \tau_{\mathcal{C}_{\delta(\beta)}(\kappa)} < \tau_{\blacksquare} \mid \tau_{\Box} > \tau_{\blacksquare} \Big) = 1$ 

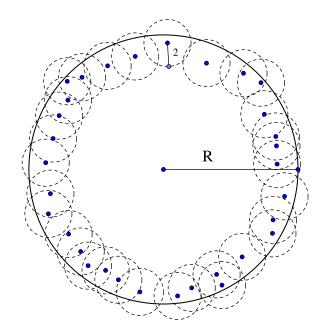
whenever

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

# $\S$ HEURISTICS

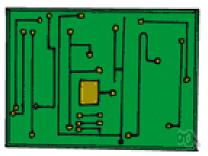
- Since particles have a tendency to stick together, they form some sort of droplet.
- Inside the droplet, particles are distributed according to a Poisson process with intensity  $\kappa\beta \gg 1$ .
- Near the perimeter of the droplet, particles are born at a rate that depends on how much they stick out.
- For  $R < R_c(\kappa)$  the droplet tends to shrink, while for  $R > R_c(\kappa)$  the droplet tends to grow. The curvature of the droplet determines which of the two prevails.

A droplet with a rough boundary: energy controlled by the interior, entropy controlled by the boundary.



# § POTENTIAL-THEORETIC APPROACH TO METASTABILITY

Bovier & den Hollander 2015



With the help of potential theory, the problem of how to understand 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 the relation

$$E_{\Box}(\tau_{\blacksquare}) = [1 + o(1)] \frac{\mu(\Box)}{\operatorname{cap}(\Box, \blacksquare)}, \qquad \beta \to \infty.$$

The capacity between □ and ■ satisfies the Dirichlet principle

$$\operatorname{cap}(\Box, \blacksquare) = \inf_{\substack{f \colon \Omega \to [0,1] \\ f|_{\Box} = 1, f|_{\blacksquare} = 0}} \mathcal{E}(f, f),$$



Dirichlet

where

$$\mathcal{E}(f,f) = \int_{\Omega} f(\omega)(-Lf)(\omega) \,\mu(\mathrm{d}\omega)$$
  
=  $\frac{1}{\Xi} \int_{\Omega} \mathbb{Q}(\mathrm{d}\omega) \int_{\Lambda} \mathrm{d}x \, z^{N(\omega \cup x)} \,\mathrm{e}^{-\beta H(\omega \cup x)} \left[ f(\omega \cup x) - f(\omega) \right]^2.$ 

The estimation of capacity proceeds via physical insight:

- Upper bound: Estimate cap(□, ■) ≤ E(f, f) for a cleverly chosen test function f that jumps from 1 to 0 in the vicinity of the critical droplet.
- Lower bound: Restrict  $\int_{\Omega} \mathbb{Q}(d\omega)$  to those configurations  $\omega$  that are in the vicinity of the critical droplet in order to get a reduced variational formula.

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

# $\S$ CONCLUSION

We have obtained a detailed description of metastability for a model of interacting particles in the continuum.

The Arrhenius formula for the average of the condensation time involves both the energy and the entropy of the critical droplet.

There are still many challenges in understanding metastability of interacting particle systems.



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A Potential-Theoretic Approach

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