Metastability for interacting particle systems

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outline

Lecture 1
Introduction: history, questions, approaches.
Lecture 2
Key results and key challenges.

Lecture 3
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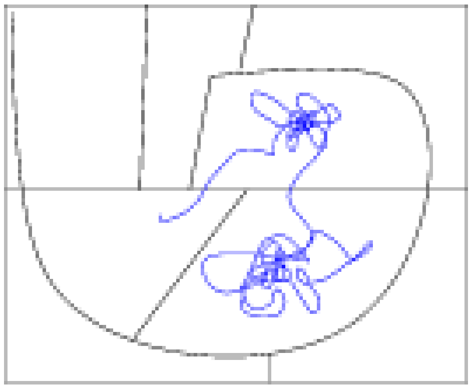
Glauber dynamics: Ising spins with random flips.
Lecture 5
Kawasaki dynamics: lattice gas with random hopping.

LECTURE 1

Introduction: history, questions, approaches

§ 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.

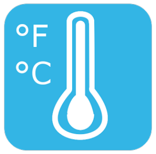
§ WHY IS METASTABILITY IMPORTANT?

Metastability is universal: it is encountered in a rather wide variety of stochastic systems, in physics, chemistry, biology, economics, ...

> The mathematical challenge is to describe metastability in qualitative and quantitative terms.

§ METASTABILITY IN STATISTICAL PHYSICS

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

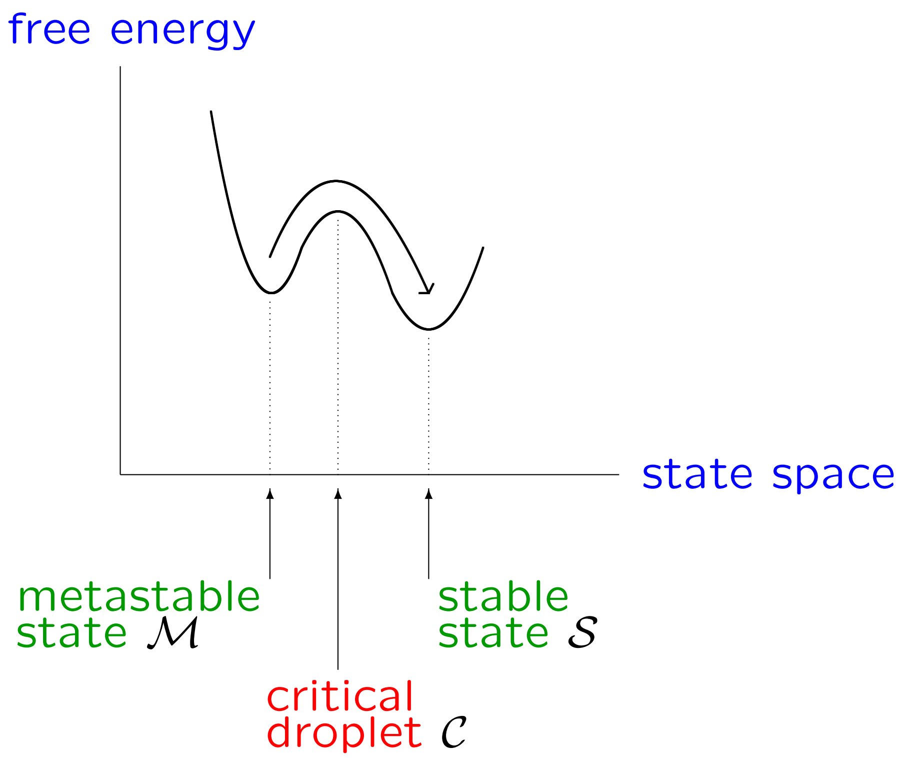


When a vapour is cooled down, it persists for a very long time in a metastable vapour state, before transiting to a stable liquid state under the influence of random fluctuations.

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



KEY QUESTION:

Let $\omega = (\omega_t)_{t \geq 0}$ denote the evolution of the system on an appropriate configuration space Ω. Typically, ω is some reversible Markov process. Write P to denote the law of ω.

Let $\mathcal{M}, \mathcal{S} \subset \Omega$ denote the subset of configurations that correspond to the metastable state, respectively, the stable state of the system.

- Start the system in the metastable state, i.e., $\omega_0 \in \mathcal{M}$.
- Wait for the first time when the system reaches the stable state, i.e.,

$$\tau_{\mathcal{S}} = \inf\{t \geq 0 \colon\ \omega_t \in \mathcal{S}\}.$$

$\boxed{\text{What can we say about the law of } \tau_{\mathcal{S}}\text{?}}$

METASTABLE REGIME:

In order to see sharp metastable behaviour, the system has to be driven into a metastable regime, for instance, small noise, small magnetic field, low temperature, high density.

The metastable regime corresponds to the situation where $\mathcal{M}$ is a local minimum of the free energy and $\mathcal{S}$ is the global minimum of the free energy, separated by a saddle point $\mathcal{C}$ representing the critical droplet.

In what follows, we will characterise this regime with the help of a metastability parameter $\rho \to \infty$.

Later we will see specific examples.

§ THREE TYPICAL THEOREMS

THEOREM 1 [Arrhenius formula]

$$\lim_{\rho\to\infty} \mathrm{e}^{-\rho\Gamma} E_{\mathcal{M}}(\tau_{\mathcal{S}}) = K.$$

THEOREM 2 [Exponential law]

$$\lim_{\rho\to\infty} P_{\mathcal{M}}\Big(\tau_{\mathcal{S}}/E_{\mathcal{M}}(\tau_{\mathcal{S}}) > t\Big) = \mathrm{e}^{-t} \qquad \forall\, t \geq 0.$$

THEOREM 3 [Critical droplet]

$$\lim_{\rho\to\infty} P_{\mathcal{M}}\Big(\tau_{\mathcal{C}} < \tau_{\mathcal{S}} \mid \tau_{\mathcal{M}} > \tau_{\mathcal{S}}\Big) = 1.$$

Here, Γ, K are the free energy, respectively, the (inverse of the) entropy of the critical droplet.

INTERPRETATION:

- The Arrhenius formula is the classical formula coming from reaction rate theory.
- The exponential law is typical for metastable crossover times: the critical droplet only appears after a large number of unsuccessful attempts.
- On its way from $\mathcal{M}$ to $\mathcal{S}$ the system must pass through $\mathcal{C}$, i.e., the critical droplet is the gate for the metastable crossover.

van 't Hoff 1884

Arrhenius 1889

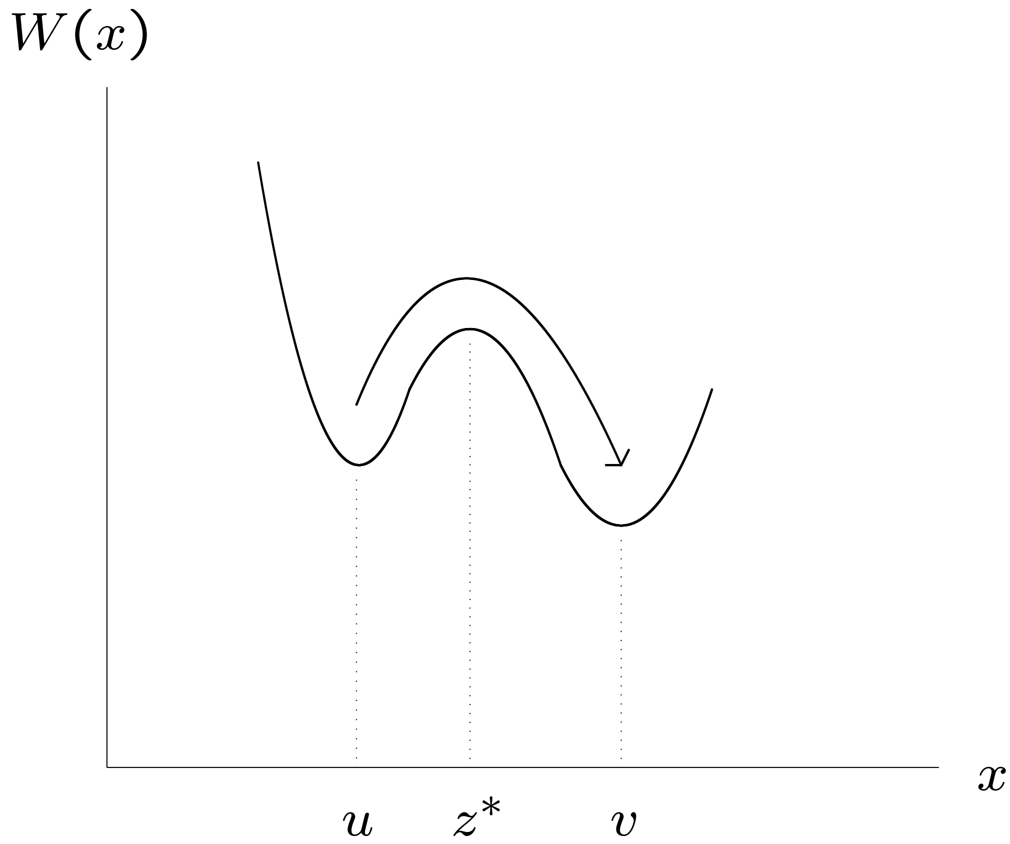
§ KRAMERS FORMULA

Kramers

The very first mathematical model for metastability was proposed in 1940 by Kramers and consists of the one-dimensional diffusion equation

$$dX_t = -W'(X_t)\,dt + \sqrt{2\epsilon}\,dB_t.$$

Here, X_t is the position at time t of a particle diffusing in a drift field $-W'$, with $W\colon \mathbb{R} \to \mathbb{R}$ a double-well potential, B_t is the position at time t of a standard Brownian motion, and ϵ is a noise parameter.



Double-well potential with local minimum at u, global minimum at v and saddle point at z^*.

Kramers showed that the average transition time is given by

$$E_u[\tau_v] = [1 + o(1)]\, \mathrm{e}^{[W(z^*)-W(u)]/\epsilon} \times \frac{2\pi}{\sqrt{[-W''(z^*)]W''(u)}}, \qquad \epsilon \downarrow 0.$$

This formula fits the classical Arrhenius law with threshold $\Gamma = W(z^*) - W(u)$, amplitude $K = 2\pi/\sqrt{[-W''(z^*)]W''(u)}$ and metastability parameter $\rho = 1/\epsilon$. He also proved the exponential law.

Note that the flatter W near z^* and u, the larger the amplitude: flatness slows down the crossover at z^* and increases the number of returns to u.

Kramers formula has become the paradigm of metastability!

In Lecture 2 we will encounter various models each of which exhibits similar metastable behaviour.

In each of these models, results of the type as stated in the three typical theorems have been derived, with an explicit identification of the quadruple

$$(\mathcal{M}, \mathcal{S}, \mathcal{C}, \rho).$$

§ APPROACHES

Several approaches have been developed to deal with issues around metastability:

- Pathwise:
  Freidlin, Wentzell 1970
  Cassandro, Galves, Olivieri, Vares 1984

- Spectral:
  Davies 1982
  Gaveau, Moreau, Schulman 1998

- Potential-theoretic:
  Bovier, Eckhoff, Gayrard, Klein 2000

- Computational:
  E, Ren, Schütte, Vanden-Eijnden 2006

MONOGRAPHS:

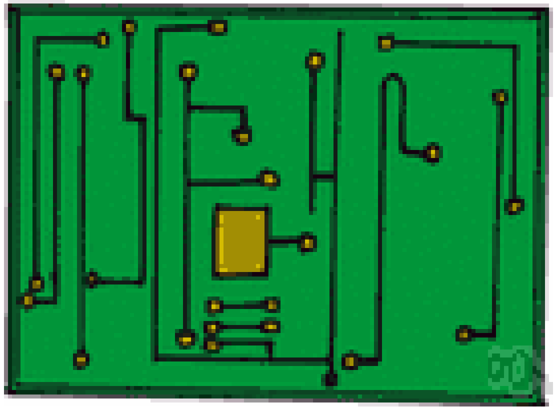
Olivieri, Vares 2005

Pathwise approach

Bovier, den Hollander 2015

Potential-theoretic approach

§ POTENTIAL-THEORETIC APPROACH TO METASTABILITY

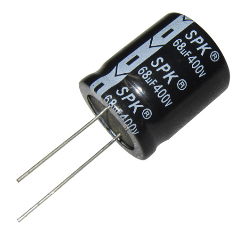


With the help of potential theory, the problem of how to understand metastability of reversible Markov processes translates into the study of capacities in electric networks.

The key formula for the average metastable crossover time provided by potential theory is

$$\boxed{E_{\mathcal{M}}(\tau_{\mathcal{S}}) = \frac{\int_{\Omega} \mu(\mathrm{d}\omega) P_{\omega}(\tau_{\mathcal{M}} < \tau_{\mathcal{S}})}{\mathrm{cap}(\mathcal{M}, \mathcal{S})}}$$

where μ is the reversible equilibrium distribution of the dynamics on Ω, and $\mathrm{cap}(\mathcal{M}, \mathcal{S})$ is the capacity of the pair $\mathcal{M}, \mathcal{S}$.



In most examples, the numerator simplifies in the limiting metastable regime, namely,

$$\int_{\Omega} \mu(\mathrm{d}\omega) P_{\omega}(\tau_{\mathcal{M}} < \tau_{\mathcal{S}}) = \mu(\mathcal{M})\,[1 + o(1)], \qquad \rho \to \infty,$$

so that it remains to identify the scaling of the capacity.

The capacity satisfies the Dirichlet principle

$$\mathrm{cap}(\mathcal{M},\mathcal{S}) = \inf_{\substack{f:\ \Omega\to[0,1] \\ f|_{\mathcal{M}}=1,\, f|_{\mathcal{S}}=0}} \mathcal{E}(f,f),$$

where

$$\begin{aligned}\mathcal{E}(f,f) &= \int_\Omega \mu(\mathrm{d}\omega)\, f(\omega)(-Lf)(\omega) \\ &= \int_{\Omega\times\Omega} \mu(\mathrm{d}\omega)\, c(\omega,\omega')\,[f(\omega')-f(\omega)]^2\end{aligned}$$

is the Dirichlet form associated with the generator L of the Markovian dynamics, and $c(\omega,\omega')$ is the rate of the transition from ω to ω'.

Dirichlet

The idea is that the capacity is dominated by those f that rapidly drop from 1 to 0 in the vicinity of the critical droplet. The estimation of capacity therefore proceeds via

- Upper bound:
  Estimate $\mathrm{cap}(\mathcal{M}, \mathcal{S}) \leq \mathcal{E}(f, f)$ for a test function f that is guessed via physical insight.

- Lower bound:
  Restrict the integral over $\Omega \times \Omega$ in $\mathcal{E}(f, f)$ to only those configurations ω that are in the vicinity of the critical droplet.

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

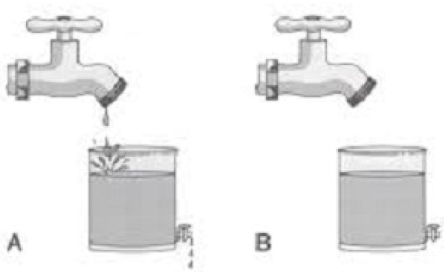
Other variational principles for capacity complement the Dirichlet principle:

- Thomson principle
- Berman-Konsowa principle

Together they make capacity into a powerful tool.

In essence, understanding capacity is part of equilibrium statistical physics, since it deals with acquiring the relevant knowledge about the free energy landscape of the system.

Potential theory links this knowledge to the metastable dynamics of the system, which is part of non-equilibrium statistical physics.



§ WHAT HAS BEEN ACHIEVED?

The mathematical theory of metastability has made rapid progress in the past 20 years. In Lecture 2 we look at various examples, listing key results and formulating key challenges.

In Lecture 2 we will focus on four classes of examples:

[1] Diffusions with small noise: SDEs and SPDEs.

[2] The Curie-Weiss model of ferromagnetism with small magnetic field: hysteresis.

[3] Lattice systems at low temperature: Glauber dynamics and Kawasaki dynamics.

[4] Continuum systems at high density: Widom-Rowlinson model.

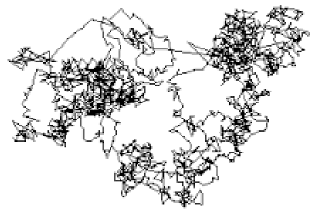
For each class we identify the quadruple $(\mathcal{M}, \mathcal{S}, \mathcal{C}, \rho)$ and the key quantities in the Arrhenius law.

In Lectures 3+4+5 we will discuss techniques and provide proofs for class [3].

LECTURE 2

Key results and key challenges

[1] DIFFUSIONS WITH SMALL NOISE



Kramers formula for one-dimensional Brownian motion in a double-well potential can be extended to higher dimension.

The setting is the SDE

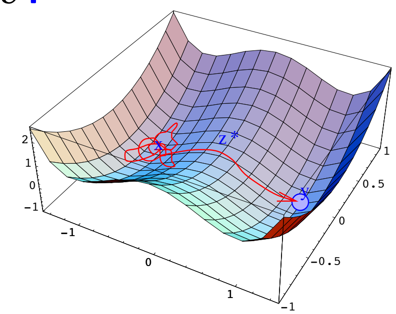
$$dX_t = -\nabla W(X_t)\, dt + \sqrt{2\epsilon}\, dB_t$$

on a regular domain $\Omega \subset \mathbb{R}^d$, where the drift $-\nabla W$ is generated by a potential function W that is sufficiently regular.

> Metastability occurs when W has two minima and the noise parameter ϵ is small.

The diffusion is killed as soon as it exits Ω.

Suppose that W is smooth, with a local minimum at u and a global minimum at v, separated by a saddle point z^*. Let $B_\delta(v)$ denote the ball of radius δ around v.



THEOREM 1 Bovier, Eckhoff, Gayrard, Klein 2004

For δ small enough and $\epsilon \downarrow 0$,

$$E_u\Big[\tau_{B_\delta(v)}\Big] = [1 + o(1)]\, \mathrm{e}^{[W(z^*)-W(u)]/\epsilon} \times \frac{2\pi}{[-\lambda^*(z^*)]} \frac{\sqrt{-\det(\nabla^2 W(z^*))}}{\sqrt{\det(\nabla^2 W(u))}}.$$

where $\nabla^2 W$ is the Hessian of W, det *is the determinant, and $\lambda^*(z^*)$ is the negative eigenvalue of the Hessian of W at z^*.*

THEOREM 2 Bovier, Eckhoff, Gayrard, Klein 2004

For δ small enough and $\epsilon \downarrow 0$,

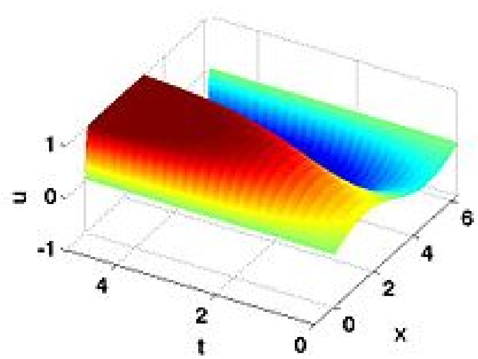
$$\lim_{\epsilon \downarrow 0} P_u\Big(\tau_{B_\delta(z^*)} < \tau_{B_\delta(v)} \mid \tau_{B_\delta(u)} > \tau_{B_\delta(v)}\Big) = 1.$$

(This result actually already follows from Freidlin-Wentzell theory.)

$$\boxed{\text{A similar formula holds when there are several local minima, in which case certain non-degeneracy assumptions need to be made.}}$$

The results can be pushed to infinite dimension. An example is the stochastic Allen-Cahn equation, which is the SPDE

$$\frac{\partial}{\partial t} u(x,t) = \frac{1}{2} D \frac{\partial^2}{\partial x^2} u(x,t) - W'(u(x,t)) + \sqrt{2\epsilon} \frac{\partial^2}{\partial x \partial t} B(x,t).$$



Space-time plot $(x,t) \mapsto u(x,t)$.

Here, $\Omega = C[0,1]$ and

$x \in [0,1]$	space-coordinate
$t \in [0,\infty)$	time-coordinate
$D > 0$	diffusion constant
$W: \mathbb{R} \to \mathbb{R}$	potential function
$\epsilon > 0$	noise-strength

and B is the space-time Brownian sheet, i.e., the centred Gaussian process indexed by $[0,1] \times [0,\infty)$ with covariance

$$E\left[B(x,t)B(y,s)\right] = (x \wedge y)(t \wedge s).$$

The SPDE may start from any function in $C[0,1]$, and the boundary condition may be either periodic, Dirichlet or von Neumann.

Again we assume that W has a local minimum u, a global minimum v, and a saddle point z^*. We start from the constant function $\equiv u$ and wait until a neighbourhood of the constant function $\equiv v$ is hit.

Let F be the functional on $C^1[0,1]$ given by

$$F(\phi) = \frac{1}{2} D \int_{[0,1]} \Big[|\phi'(x)|^2 + W(\phi(x)) \Big] \mathrm{d}x.$$

The Hessian of F at $\phi \in C^1([0,1])$ is the Sturm-Liouville operator $\mathcal{H}_\phi F$ given by

$$(\mathcal{H}_\phi F)[\psi](x) = -D\psi''(x) + W''(\phi(x))\psi(x), \quad \psi \in C^2([0,1]).$$

The determinant of $\mathcal{H}_\phi F$ *is* $\det(\mathcal{H}_\phi F) = \psi(1)$ *with* ψ *the solution of the initial value problem*

$$(\mathcal{H}_\phi F)[\psi](x) = 0, \quad \psi(0) = 1, \quad \psi'(0) = 0.$$

THEOREM 3 Barret, Bovier, Méléard 2010

Under certain regularity assumptions on W*, the analogue of Kramers formula holds for the stochastic Allen-Cahn equation with* F *as the energy functional and* $\det(\mathcal{H}_{\equiv u})F$ *and* $\det(\mathcal{H}_{\equiv z^*})F$ *as the Hessians of* F *at* $\equiv u$ *and* $\equiv z^*$*.*

[2] CURIE-WEISS WITH SMALL MAGNETIC FIELD

The Curie-Weiss model of a ferromagnet has state space $\Omega = \{-1, +1\}^\Lambda$ with $\Lambda = \{1, \ldots, N\}$, $N \in \mathbb{N}$. The Hamiltonian is given by

$$H_N(\sigma) = -\frac{1}{2N} \sum_{i,j \in \Lambda} \sigma_i \sigma_j - h \sum_{i \in \Lambda} \sigma_i, \qquad \sigma \in \Omega,$$

and is mean-field because it depends on σ only through the empirical magnetisation $m_N(\sigma) = \frac{1}{N} \sum_{i \in \Lambda} \sigma_i$, namely,

$$H_N(\sigma) = -N \left(\tfrac{1}{2} m_N^2(\sigma) + h m_N(\sigma) \right).$$

Curie

Weiss

We choose a discrete-time dynamics on Ω with Metropolis transition probabilities

$$p(\sigma,\sigma') =$$
$$\begin{cases} N^{-1}\,\mathrm{exp}\left[-\beta\left[H_N(\sigma') - H_N(\sigma)\right]_+\right], & \sigma \sim \sigma', \\ 1 - \sum_{\sigma''\neq\sigma} p(\sigma,\sigma''), & \sigma = \sigma', \\ 0, & \text{otherwise}, \end{cases}$$

where the middle line takes care of the normalisation. This dynamics is reversible w.r.t. the Gibbs measure

$$\mu_{\beta,N}(\sigma) = \frac{1}{Z_{\beta,N}}\,\mathrm{e}^{-\beta H_N(\sigma)}\,2^{-N}, \qquad \sigma \in \Omega,$$

with $Z_{\beta,N}$ the normalising partition function and β the inverse temperature.

The empirical magnetisation performs a random walk on the state space

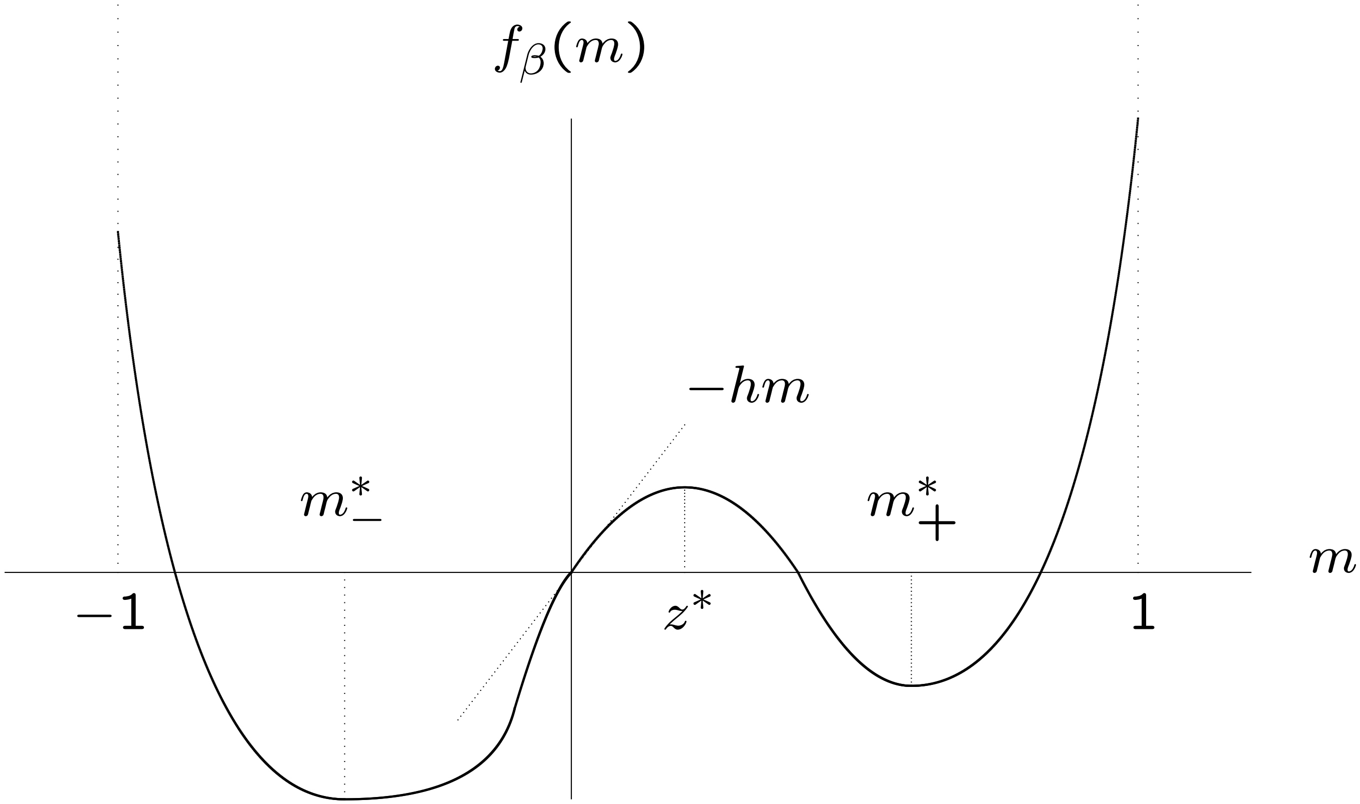
$$\bar{\Omega} = \left\{ -1, -1 + 2N^{-1}, \ldots, 1 - 2N^{-1}, 1 \right\}.$$

In the limit as $N \to \infty$ this random walk converges to a diffusion on $[-1, 1]$ with potential βf_β,where

$$\begin{aligned} f_\beta(m) &= -\tfrac{1}{2}m^2 - hm + \beta^{-1} I(m), \\ I(m) &= \tfrac{1}{2}(1+m)\log(1+m) + \tfrac{1}{2}(1-m)\log(1-m). \end{aligned}$$

This potential is a double well when $\beta > 1$ and h is small enough. The stationary points are the solutions of the equation

$$m = \tanh[\beta(m+h)].$$



Plot of f_β on $[-1, 1]$ when $\beta > 1$ and $h < 0$.

Let $m_-^* < m_+^*$ be the two local minima of f_β, and z^* the saddle point in between. Let $m_-^*(N), m_+^*(N)$ denote the points in Γ_N that are closest to m_-^*, m_+^*.

THEOREM 4 Bovier, Eckhoff, Gayrard, Klein 2001

As $N \to \infty$,

$$E_{m_+^*(N)}\left[\tau_{m_-^*(N)}\right] = [1 + o(1)]\, \mathrm{e}^{\beta N\left(f_\beta(z^*) - f_\beta(m_+^*)\right)}$$

$$\times \frac{\pi N}{1 - z^*}\sqrt{\frac{1 - z^{*2}}{1 - m_+^{*2}}}\, \frac{1}{\beta\sqrt{[-f_\beta''(z^*)]f_\beta''(m_+^*)}}.$$

The result matches with what was found for the Kramers model, with $W = \beta f_\beta$ and $\epsilon = N^{-1}$.

The prefactor has a small discrepancy, due to the fact that the dynamics is discrete rather than continuous in time.

[3] LATTICE SYSTEMS AT LOW TEMPERATURE

Let $\Lambda \subset \mathbb{Z}^2$ be a large square torus, centred at the origin. With each site $x \in \Lambda$ we associate a spin variable $\sigma(x)$ assuming the values -1 or $+1$, indicating whether the spin at x is pointing down or up.

A configuration is denoted by $\sigma \in \Omega = \{-1,+1\}^\Lambda$. Each configuration $\sigma \in \Omega$ has an energy that is given by the Hamiltonian

$$H_\Lambda(\sigma) = -\frac{J}{2} \sum_{\substack{x,y \in \Lambda \\ x \sim y}} \sigma(x)\sigma(y) - \frac{h}{2} \sum_{x \in \Lambda} \sigma(x).$$

This interaction consists of a ferromagnetic pair potential $J > 0$ and a magnetic field $h > 0$.

−	−	+	−	−
+	−	−	−	+
+	−	−	+	−
−	+	+	+	−
+	−	−	+	−

An Ising-spin configuration.

GLAUBER DYNAMICS:

Consider the continuous-time Markov process on Ω with transition rates

$$c_{\beta,\Lambda}(\sigma,\sigma') = \begin{cases} \mathrm{e}^{-\beta[H_\Lambda(\sigma')-H_\Lambda(\sigma)]_+}, & \sigma \sim \sigma', \\ 0, & \text{otherwise.} \end{cases}$$

This is the Metropolis dynamics with respect to H_Λ at inverse temperature β with single-spin flips as allowed moves.

The Gibbs measure

$$\mu_{\beta,\Lambda}(\sigma) = \frac{1}{Z_{\beta,\Lambda}}\,\mathrm{e}^{-\beta H_\Lambda(\sigma)}, \qquad \sigma \in \Omega,$$

is the reversible equilibrium of the Glauber dynamics, i.e.,

$$\mu_{\beta,\Lambda}(\sigma)c_{\beta,\Lambda}(\sigma,\sigma') = \mu_{\beta,\Lambda}(\sigma')c_{\beta,\Lambda}(\sigma',\sigma) \qquad \forall\, \sigma,\sigma' \in \Omega.$$

We consider the parameter range

$$h \in (0, 2J), \qquad \beta \to \infty,$$

which turns out to correspond to the metastable regime. We will see that the linear size of the critical droplet is

$$\ell_c = \left\lceil \frac{2J}{h} \right\rceil.$$

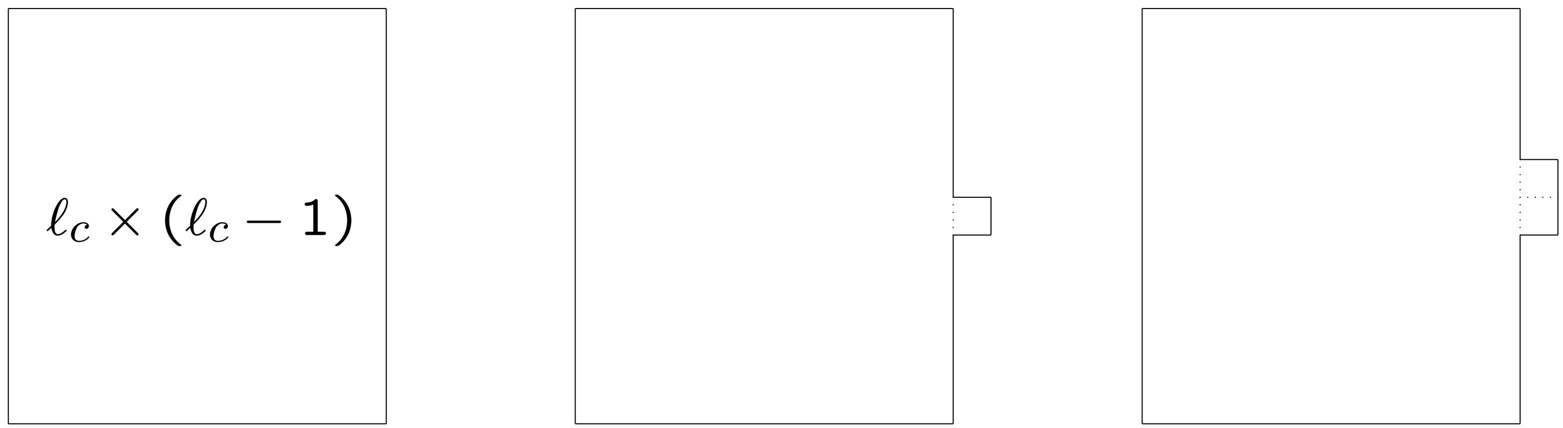
Thus, an $(\ell_c - 1) \times (\ell_c - 1)$ droplet will be subcritical while an $\ell_c \times \ell_c$ droplet will be supercritical.

Let

$$\boxminus = \{\sigma \in \Omega \colon\ \sigma(x) = -1\ \forall\, x \in \Lambda\},$$
$$\boxplus = \{\sigma \in \Omega \colon\ \sigma(x) = +1\ \forall\, x \in \Lambda\},$$

denote the configurations where all spins in Λ are all down, respectively, all up.

Let $\mathcal{Q}$ be the set of configurations where the up-spins form a single $(\ell_c - 1) \times \ell_c$ quasi-square anywhere in Λ. Let $\mathcal{Q}^{\mathsf{1pr}}$ and $\mathcal{Q}^{\mathsf{2pr}}$ be the set of configurations obtained from $\mathcal{Q}$ by attaching a single protuberance or a double protuberance anywhere to one of the longest sides of the quasi-square.



Configurations in $\mathcal{Q}$, $\mathcal{Q}^{1\text{pr}}$ and $\mathcal{Q}^{2\text{pr}}$. Inside the contours sit the up-spins, outside the contours sit the down-spins.

THEOREM 5 Bovier, Manzo 2002

For $h \in (0, 2J)$ *and* $\beta \to \infty$,

$$E_{\boxminus}\left[\tau_{\boxplus}\right] = [1 + o(1)]\, K \mathrm{e}^{\beta\Gamma}$$

with

$$\Gamma = J[4\ell_c] - h[\ell_c(\ell_c - 1) + 1],$$

$$K = \frac{3}{4(2\ell_c - 1)} \frac{1}{|\Lambda|}.$$

THEOREM 6 Bovier, Manzo 2002

For $h \in (0, 2J)$ *and* $\beta \to \infty$,

$$\lim_{\beta \to \infty} P_{\boxminus}\Big(\tau_{\mathcal{Q}^{1\mathrm{pr}}} < \tau_{\boxplus} \mid \tau_{\boxminus} > \tau_{\boxplus}\Big) = 1.$$

KAWASAKI DYNAMICS:

Once again consider the box $\Lambda \subset \mathbb{Z}^2$, but this time with an open boundary. With each site $x \in \Lambda$ we associate an occupation variable $\eta(x)$ assuming the values 0 or 1. A configuration is denoted by $\eta \in \Omega = \{0,1\}^\Lambda$.

Each configuration $\eta \in \Omega$ has an energy given by the Hamiltonian

$$H_\Lambda(\eta) = -U \sum_{\substack{x,y \in \Lambda \\ x \sim y}} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x),$$

This interaction consists of a binding energy $-U < 0$ and an activation energy $\Delta > 0$.

0	0	1	0	0
0	0	0	1	0
0	1	1	0	0
0	1	1	0	0
0	0	0	0	0

A lattice-gas configuration.

We are interested in Kawasaki dynamics on Ω with an open boundary. This is the Metropolis dynamics with respect to H_Λ at inverse temperature β with two types of allowed moves:

(1) particle hop: 0 and 1 interchange at a pair of neighbouring sites in Λ.

(2) particle creation or annihilation: 0 changes to 1 or 1 changes to 0 at a single site in $\partial\Lambda$.

We may think of $\mathbb{Z}^2 \backslash \Lambda$ as an infinite reservoir that keeps the particle density inside Λ fixed at $e^{-\beta\Delta}$.

The Gibbs measure μ_β is again the reversible equilibrium of the Kawasaki dynamics.

We consider the parameter range

$$\Delta \in (U, 2U), \qquad \beta \to \infty,$$

which corresponds to the metastable regime. The linear size of the critical droplet is

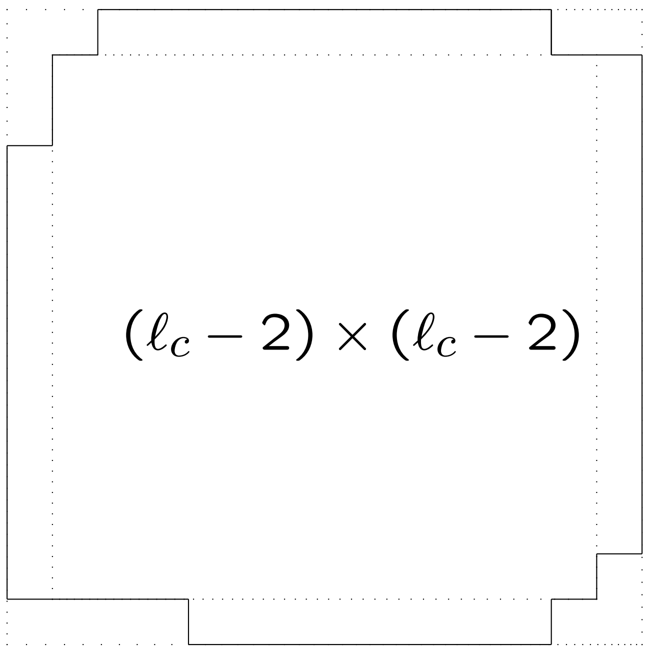
$$\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil .$$

Let

$$\square = \{\eta \in \Omega \colon\ \eta(x) = 0\ \forall\, x \in \Lambda\},$$
$$\blacksquare = \{\eta \in \Omega \colon\ \eta(x) = 1\ \forall\, x \in \Lambda\},$$

denote the configurations where Λ is empty, respectively, full.

Let $\mathcal{D}$ be the set of configurations with a single cluster anywhere in Λ consisting of an $(\ell_c - 2) \times (\ell_c - 2)$ square with four bars attached to its four sides of total length $3\ell_c - 3$. Let $\mathcal{D}^{\mathrm{fp}}$ denote the set of configurations obtained from $\mathcal{D}$ by adding a free particle anywhere in $\partial\Lambda$.



A configuration in $\mathcal{D}$.

The configurations in $\mathcal{D}$ arise from each other via motion of particles along the border of the droplet, a phenomenon that is specific to Kawasaki dynamics.

THEOREM 7 Bovier, den Hollander, Nardi 2006

For $\Delta \in (U, 2U)$ *and* $\beta \to \infty$*,*

$$E_{\square}\left[\tau_{\blacksquare}\right] = [1 + o(1)]\, K \mathrm{e}^{\beta\Gamma}$$

with

$$\Gamma = -U[(\ell_c - 1)^2 + \ell_c(\ell_c - 2) + 1] + \Delta[\ell_c(\ell_c - 1) + 2]$$

and $K = K(\Lambda)$ *a complicated prefactor that scales like*

$$\lim_{\Lambda \to \mathbb{Z}^2} \frac{|\Lambda|}{\log |\Lambda|} K(\Lambda) = \frac{1}{4\pi N(\ell_c)}$$

with

$$N(\ell_c) = \sum_{k=1,2,3,4} \binom{4}{k} \left[\binom{\ell_c + k - 2}{2k - 1} + 2\binom{\ell_c + k - 3}{2k - 1}\right],$$

which is the cardinality of $\mathcal{D}$ *modulo shifts.*

THEOREM 8 Bovier, den Hollander, Nardi 2006

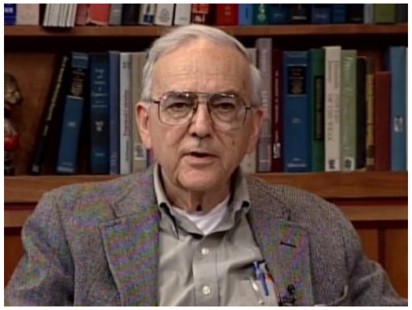
For $\Delta \in (U, 2U)$ *and* $\beta \to \infty$,

$$\lim_{\beta\to\infty} P_{\square}\Big(\tau_{\mathcal{D}} < \tau_{\blacksquare} \mid \tau_{\square} > \tau_{\blacksquare}\Big) = 1.$$

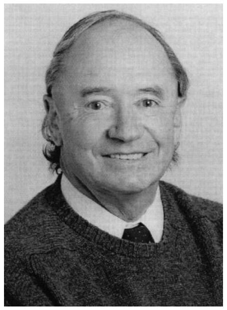
[4] CONTINUUM SYSYEMS AT HIGH DENSITY

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

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.



Widom

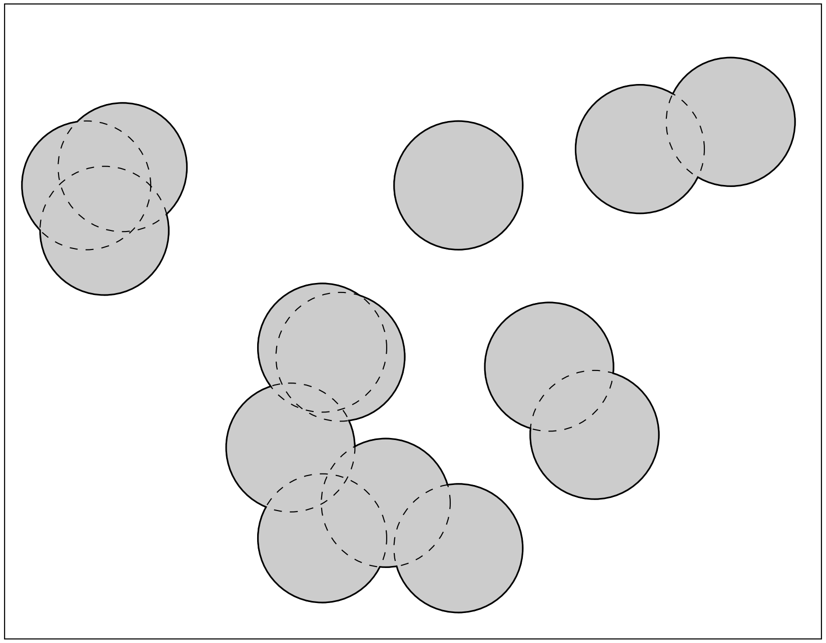


Rowlinson

THE STATIC WIDOM-ROWLINSON MODEL:

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

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



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,

H is the interaction Hamiltonian given by

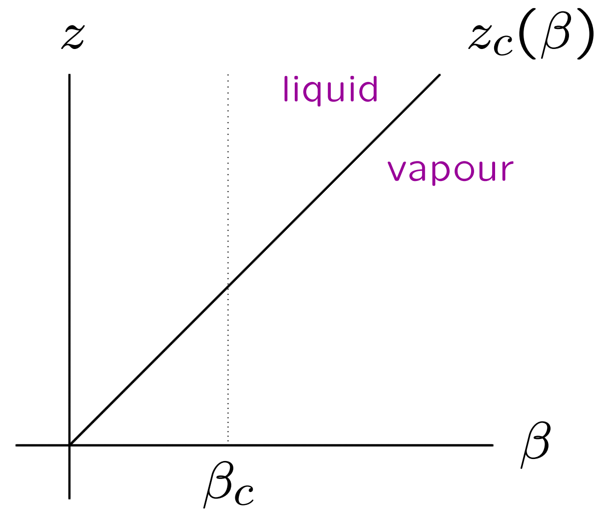
$$H(\omega) = \text{volume of the halo of the 2-spheres around } \omega,$$

and Ξ is the normalising partition function.

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

$$z = z_c(\beta) = \beta$$

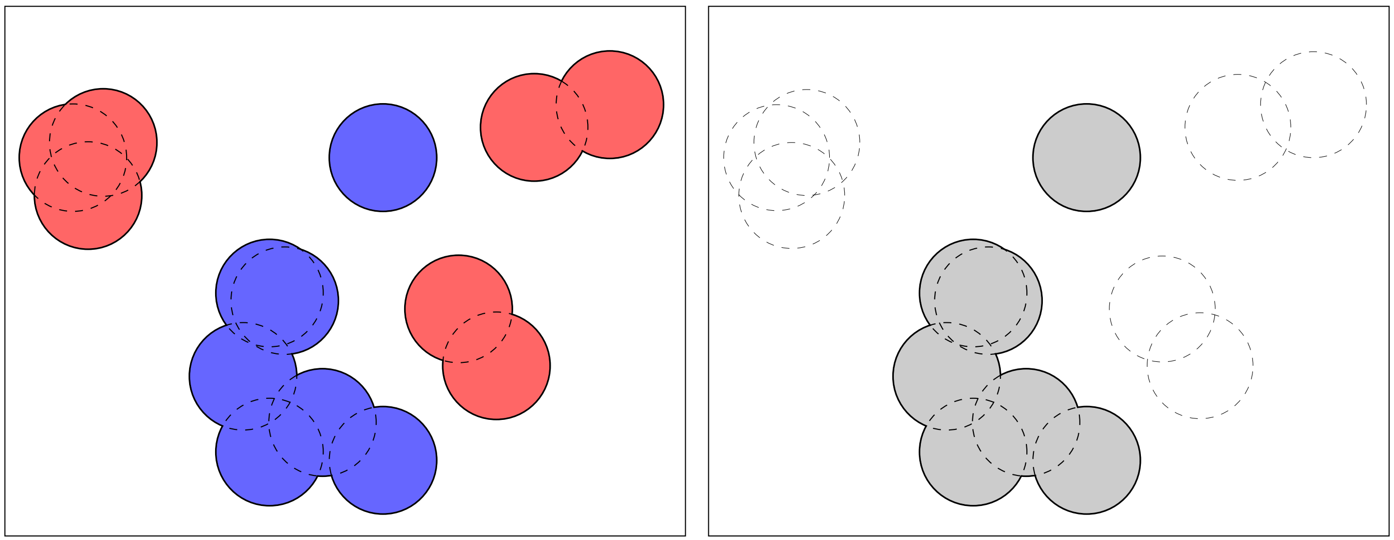
in the thermodynamic limit, i.e., $\Lambda \to \mathbb{R}^2$. No closed form expression is known for β_c.



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:



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

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

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

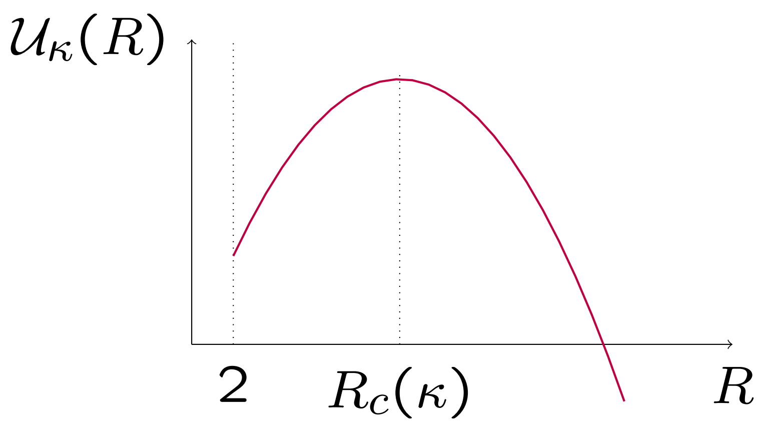
$$\begin{aligned} b(x,\omega) &= z\,\mathrm{e}^{-\beta[H(\omega\cup x)-H(\omega)]}, & x\notin\omega,\\ d(x,\omega) &= 1, & x\in\omega. \end{aligned}$$

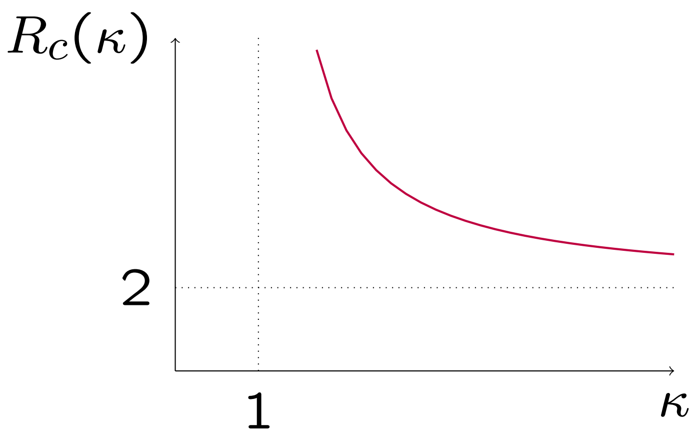
The grand-canonical Gibbs measure is the unique reversible equilibrium of this stochastic dynamics.

Let $\square$ and $\blacksquare$ denote the set of configurations where Λ is empty, respectively, full. Choose $z > \kappa z_c(\beta)$, $\kappa \in (1, \infty)$.

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 9 den Hollander, Jansen, Kotecký, Pulvirenti 2015

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

$$E_{\square}(\tau_{\blacksquare}) = \exp\left[\beta\,\mathcal{U}(\kappa) - \beta^{1/3}\,\mathcal{S}(\kappa) + h.o.\right], \qquad \beta \to \infty,$$

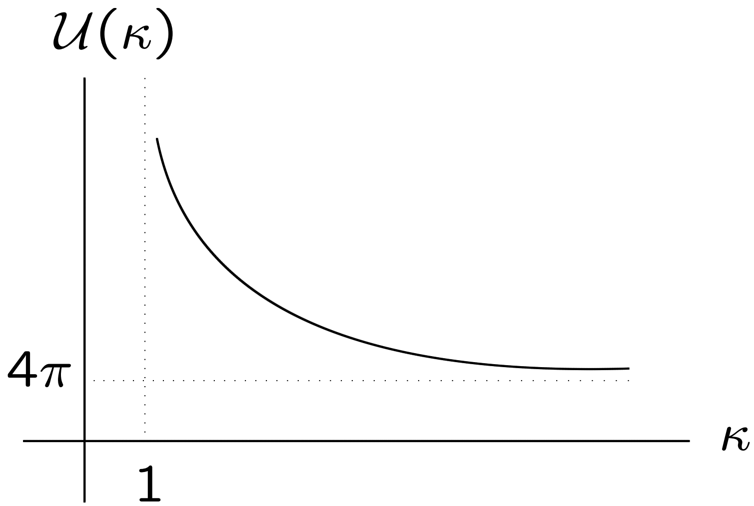
where

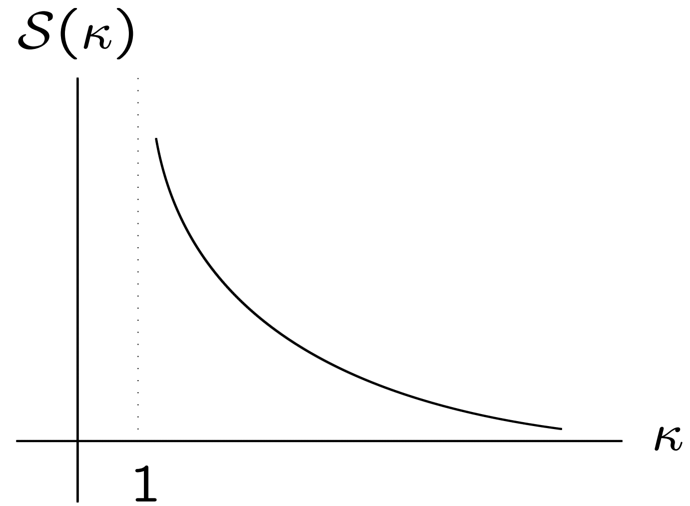
$$\mathcal{U}(\kappa) = \mathcal{U}_{\kappa}(R_c(\kappa)) = \frac{4\pi\kappa}{\kappa-1},$$

$$\mathcal{S}(\kappa) = \frac{A\kappa^{2/3}}{\kappa-1}\,\mathrm{e}^{-B(2\kappa-1)},$$

with $A = \pi\Gamma(\frac{4}{3})/\Gamma(\frac{2}{3})$ *and* $B = \frac{1}{3}$*.*

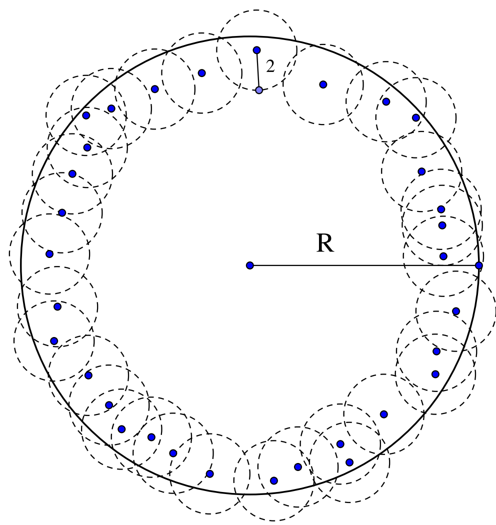
Plots of the key quantities in the Arrhenius formula:





- $\mathcal{U}(\kappa)$ is the energy of the critical droplet.
- $\mathcal{S}(\kappa)$ is the entropy associated with the surface fluctuations of the critical droplet.

A droplet with a rough boundary:



For $\delta > 0$, let

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

THEOREM 10 den Hollander, Jansen, Kotecký, Pulvirenti 2015

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

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

whenever

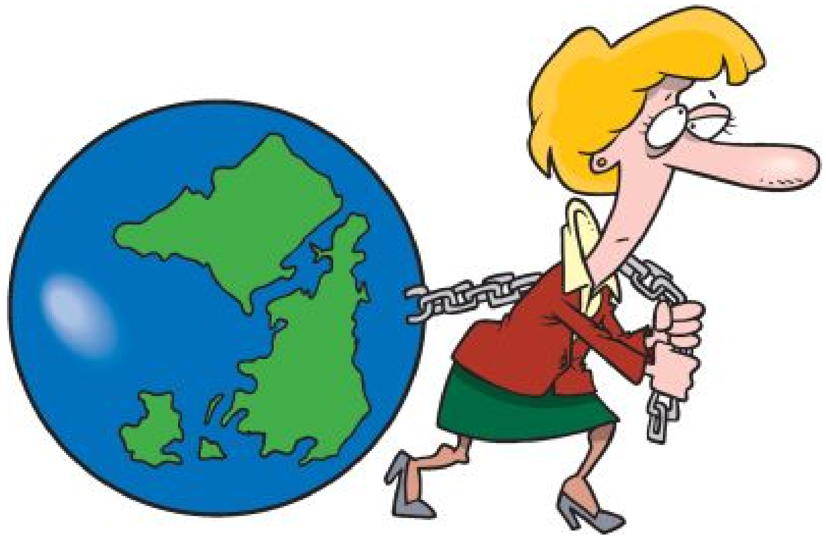
$$\lim_{\beta\to\infty} \delta(\beta) = 0, \qquad \lim_{\beta\to\infty} \beta^{1/3}\delta(\beta) = \infty.$$

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 $\kappa z_c(\beta) = \kappa\beta \gg 1$.
- 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.

§ SOME KEY CHALLENGES FOR METASTABILITY

- Lattice systems at low temperature in large volume:
  spatial entropy.
- Weak metastability and large critical droplets:
  Wulff shapes.
- Droplet growth beyond metastability:
  Becker-Döring theory.



Lectures 3+4+5 discuss techniques and provide proofs for Glauber dynamics and Kawasaki dynamics!