LECTURE 1

Statistical physics and beyond.
Motivation, targets and examples.

§ WHAT IS METASTABILITY?

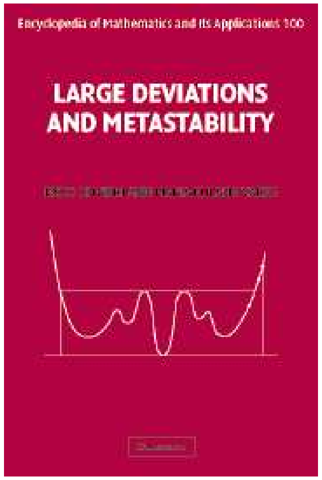
Metastability is the phenomenon where a system, under the influence of a stochastic dynamics, undergoes slow transitions between different phases. It is observed in a variety of physical, chemical and biological settings.

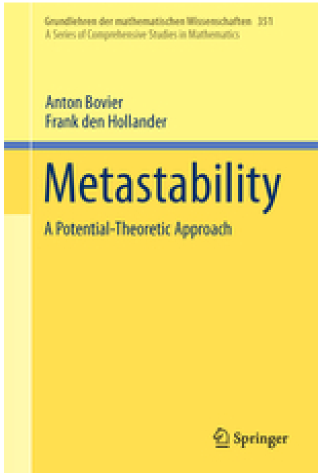
The challenge is to propose mathematical models and to explain the experimentally observed universality.

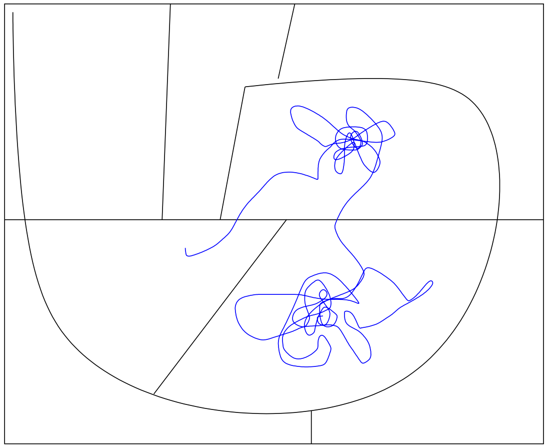
MONOGRAPHS:

Olivieri, Vares 2005

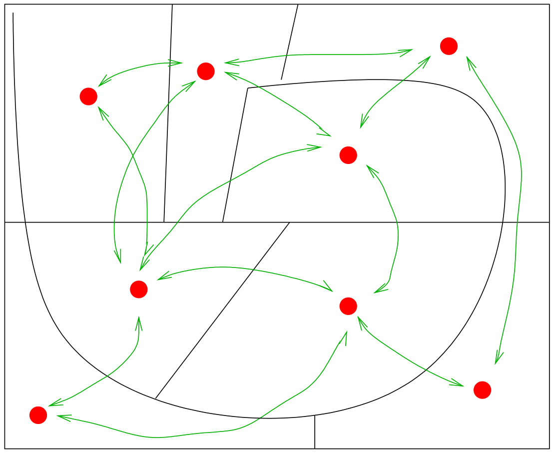
Bovier, den Hollander 2015







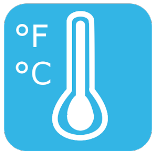
Fast transitions within phases.



Slow transitions between phases.

§ METASTABILITY IN STATISTICAL PHYSICS

Within the narrower perspective of statistical physics, the phenomenon of metastability is a dynamical manifestation of a first-order phase transition. A well-known example is condensation:

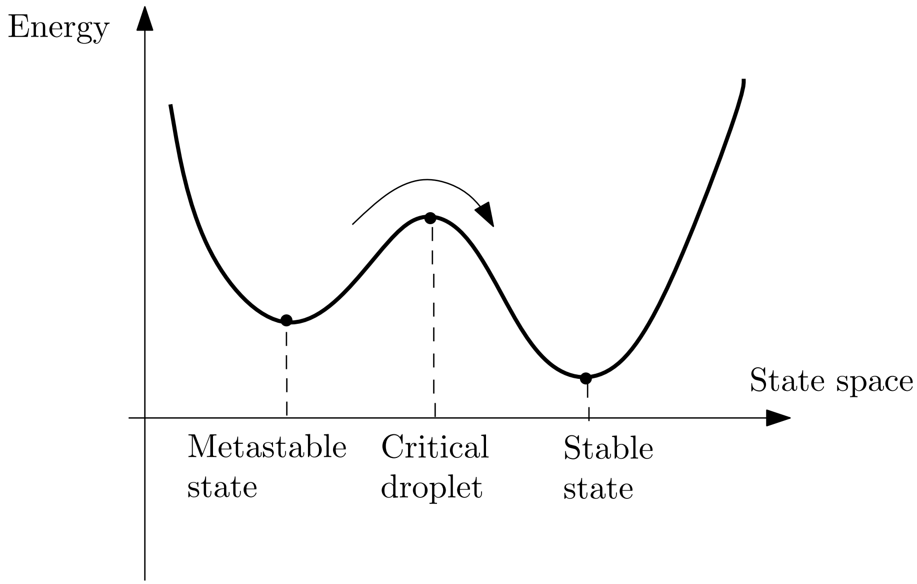


> When a vapour is cooled down slowly, it persists for a long time in a metastable vapour state, before transiting to a stable liquid state under the influence of random fluctuations.

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:



Energy $\rightarrow$ Free energy

metastable crossover: super-saturated vapour

metastable crossover: super-cooled water

metastable crossover: snow avalanche

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 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.

§ HISTORICAL 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.

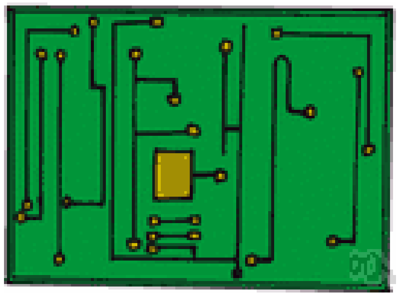
Since then, various approaches to metastability have been developed, with different pros and cons.

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

§ POTENTIAL-THEORETIC APPROACH TO METASTABILITY

Bovier, Eckhoff, Gayrard, Klein 2000

Bovier, den Hollander 2015



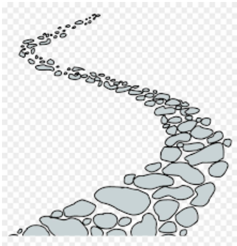
With the help of potential theory, the problem of how to understand metastability of Markov processes translates into the study of capacities in electric networks.

Dictionary:

state	$\longrightarrow$	vertex
transition	$\longrightarrow$	edge
rate	$\longrightarrow$	conductance
hitting time	$\longrightarrow$	effective resistance

§ DIFFERENT APPROACHES TO METASTABILITY

- Pathwise approach



The pathwise approach to metastability was initiated in the late 1960's and early 1970's by Freidlin and Wentzell. They introduced the theory of large deviations on path space to analyse the long-term behaviour of dynamical systems under the influence of weak random perturbations.

The idea that metastable behaviour is controlled by large deviations of the random processes driving the dynamics has permeated most of the mathematical literature on the subject since.

M. Freidlin, A. Wentzell,

Random Perturbations of Dynamical Systems 1984

The application of these ideas in statistical physics was pioneered in the early 1980's by Cassandro, Galves, Olivieri and Vares. They realised that the theory put forward by Freidlin and Wentzell could be applied to study metastable behaviour of interacting particle systems.

Cassandro, Galves, Olivieri and Vares 1984

This paper in turn led to a flurry of results for a variety of Markovian lattice models, summarised in:

E. Olivieri and M.E. Vares,

Large Deviations and Metastability 2005

> This monograph describes the cross-fertilisation between statistical physics, large deviation theory and the study of metastable phenomena.

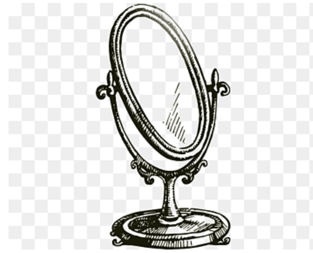
• The advantage of the pathwise approach is that it gives very detailed information on the metastable behaviour of the system. By identifying the most likely path between metastable states,

typically the minimiser of some action integral representing the rate function on path space,

information is obtained on what the system does before and after the crossover, i.e., the tube of typical trajectories.

•The drawback of the pathwise approach is that it is in general hard to identify the rate function, especially for systems with a spatial interaction, for which the dynamics is non-local. Consequently, the pathwise approach typically leads to relatively crude results on the crossover time.

- Spectral approach



In the early 1980's, Davies proposed an axiomatic approach to metastability based on spectral properties of generators of reversible Markov processes. He showed that metastable behaviour arises when the spectrum of the generator of the Markov process consists of a cluster of very small real eigenvalues, separated by a comparatively wide gap from the rest of the spectrum.

> The associated eigenfunctions allow for a decomposition of the state space into metastable sets. The motion of the Markov process between these sets is slow, with time-scales that are given by the inverses of the corresponding eigenvalues.

Davies 1982–1983

In the late 1990's the above ideas were developed further by Gaveau and Schulman and Gaveau and Moreau.

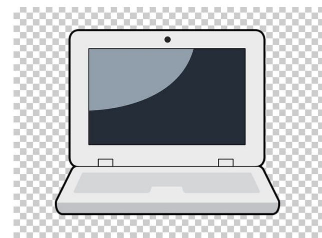
> While the spectral approach to metastability certainly is conceptually nice and natural, it is typically very difficult to carry through in detail mathematically.

Gaveau and Schulman 1998

Gaveau and Moreau 2000

- Computational approach

There is interest in quantitative numerical computations for specific systems that exhibit metastable phenomena. Since metastability is driven by rare events and involves very long time-scales, doing a simulation is challenging and requires highly sophisticated techniques.



Some of the methods developed for the computational approach have links to the spectral approach. The so-called transition path theory relies on numerical methods to compute harmonic functions.

Ren and Vanden-Eijnden 2002

E and Vanden-Eijnden 2006

Metzner, Schütte and Vanden-Eijnden 2008

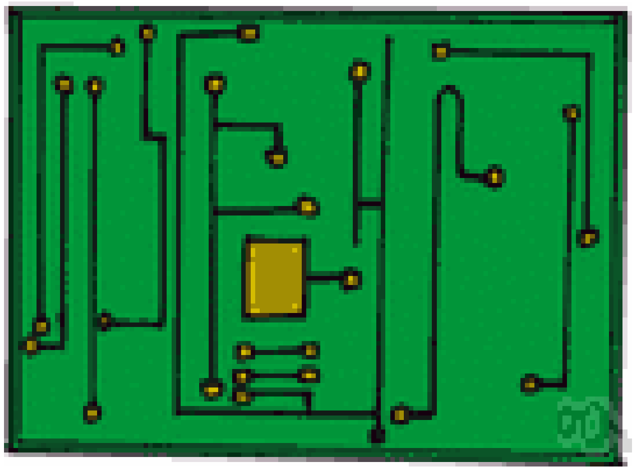
- Potential-theoretic approach

The potential-theoretic approach to metastability initiated in 2001 with the work of Bovier, Eckhoff, Gayrard and Klein.

Instead of identifying the most likely paths that realise a metastable crossover and estimating their probabilities, this work

> interprets the metastability phenomenon as a sequence of visits of the path to different metastable sets, and focuses on a precise analysis of the respective hitting probabilities and hitting times of these sets with the help of potential theory.

Put differently, the problem of understanding metastable behaviour of Markov processes is translated into the study of equilibrium potentials and capacities of some associated electric networks.



Dictionary:

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• The configurations of the system are represented by the vertices of the network and the transitions between pairs of configurations as the edges of the network. The transition probabilities are represented by the conductances of the associated edges.

• The hitting probabilities of a set of configurations as a function of the starting configuration can be expressed in terms of the equilibrium potential on the network when the potential is set to 1 on the vertices of the target set and to 0 on the starting vertex.

• The average hitting time of the set can be expressed in terms of the equilibrium potential and capacity associated with the target set and the starting vertex. For metastable sets it turns out that the average hitting time is essentially the inverse of the capacity.

1. A key observation in the potential-theoretic approach is that capacities can be estimated by exploiting powerful variational principles. In fact, dual variational principles are available that express the capacity as a supremum over potentials and as an infimum over flows.

This opens up the possibility to derive sharp lower bounds and upper bounds on the capacity via a judicious choice of test functions.

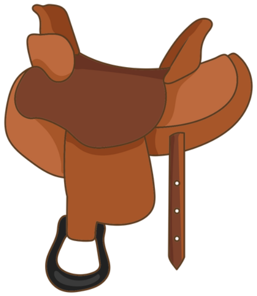
In fact, with the proper physical insight, test functions can be found for which the lower bounds and the upper bounds are asymptotically equivalent, in some appropriate limit corresponding to a metastable regime.

2. Another key observation is that the relevant equilibrium potentials can in turn be bounded from above and below by capacities with the help of renewal equations. This is crucial, as it avoids the formidable problem of solving the boundary value problems through which the equilibrium potentials are defined.

> Consequently, estimates of the average crossover time can be derived that are much sharper than those obtained via the pathwise approach.

Capacities are expressed with the help of Dirichlet forms, which have the dimension of the configuration space. It turns out that the high-dimensional variational principles for the capacity often can be reduced to low-dimensional variational principles when the system is metastable.

The dimensional reduction comes from the fact that typical metastable crossovers occur near saddles connecting metastable sets of configurations. The equilibrium potential is very close to 1 or to 0 away from these saddles, so that only the configurations close to the saddles are relevant.



3. The success of the potential-theoretic approach rest on the fact that it applies to reversible Markov processes. While variational characterisations of capacities are known also for non-reversible Markov processes, these are far more complicated and far more difficult to use.

A. Bovier and F. den Hollander,

Metastability: A Potential-Theoretic Approach, 2015

LITERATURE:

Chapter 1 of Bovier and den Hollander 2015, and references therein.