I. Dynamical Phase Transitions: Introduction & Examples. Large Deviations Functions

Complexity Summer School
Warwick University
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→ 1st lecture, very descriptive.

<u>Outline</u>:

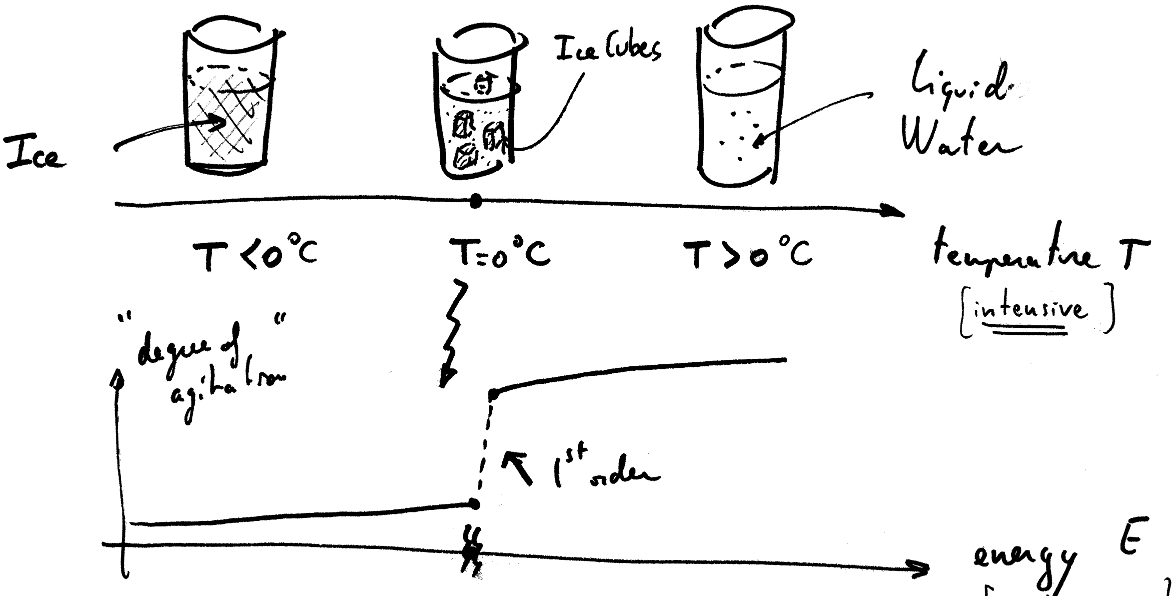
1. Examples of Phase Transitions: static & dynamical coexistence
2. Fluctuations of Dynamical Observables; Large Deviation Functions

1. Examples of Phase Transitions. Static & Dynamical Coexistence

1. a (<u>Static</u>) liquid-solid phase coexistence

"canonical ensemble"

Thermostated system



Isolated system

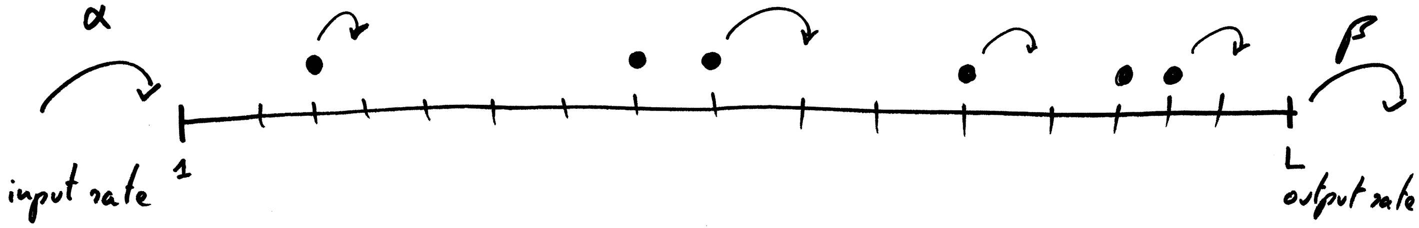
<u>Low energy</u>:
most probable configurations are crystallyzed
→ Ice

phase coexistence

<u>High energy</u>
most probable configurations are "agitated"
→ Liquid

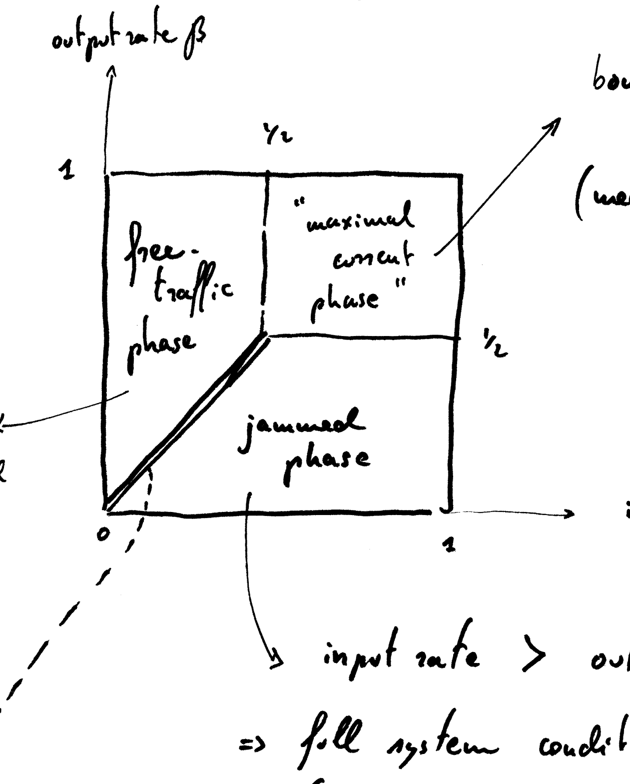
1.b. 1D transport: a traffic model

(Driving in dense traffic: one observes large fluctuations of jamming
Very simple model ("Ising model of non-equilibrium"): TASEP
[Totally Asymmetric Simple Exclusion Process]



- each site either occupied ● or not
- jumps to the rate occurs with rate 1 <u>provided the target site is empty</u>
("Exclusion rule")

Phase diagram (in the large-size limit $L \to \infty$)



boundary condition have no influence (mean density 1/2)

output rate > input rate
⇒ full system conditionned by the input boundary
(~ free traffic)

input rate > output rate
⇒ full system conditionned by the output boundary
(complete jam)

1st order coexistence line

1.b' Coexistence between jammed & free traffic.

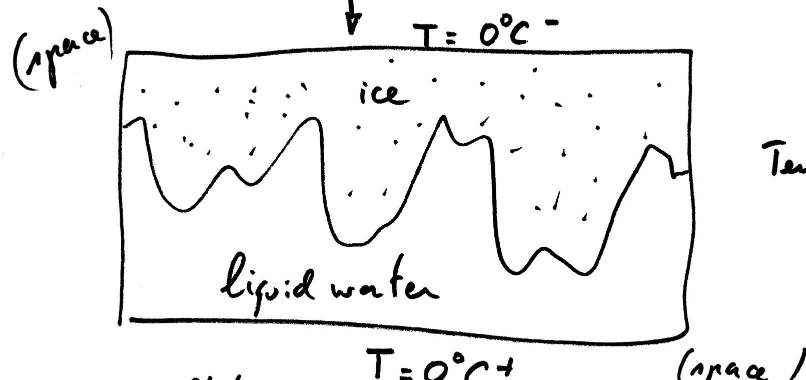
$0 < \alpha = \beta < 1/2$ → represents realistic conditions where output ≃ input

TASEP

Dynamical (i.e. space-time) phase coexistence b/w high & low density

analogy with static (1st order) phase coexistence

Water



Temperature = 0°C

Static phase coexistence b/w ice & liquid water

⚠ **However**, this is only an analogy: there is no exact mapping (time → ∞ ; long-range correlations in TASEP)

Question: for the TASEP

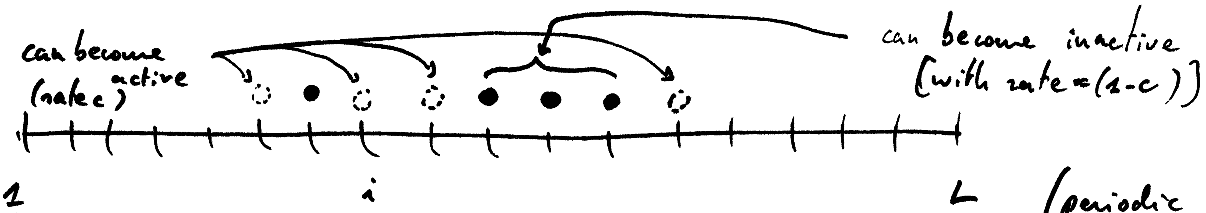
- How can one quantify the dynamical phase coexistence?
- Can it explain the large fluctuations of the density?
- Can one "isolate" the coexisting phases & characterize their properties?

↳ A tool: $\boxed{\text{Large Deviation Functions}}$.

1.c. Glass Formers; Kinetically Constrained Models

- **Motivation**: from realistic glassy phenomena / models
  [See Keys et al, PRX 1 021013 (2011)] for binary mixtures
  → physical picture: $\boxed{\text{active regions enhance activity in their vicinity}}$

- An example of 'Kinetically Constrained Model' (KCM)
  a 1D Fredrickson-Anderson (FA) model:



(periodic boundary conditions)

On each site: $\begin{cases} n_i = 0 & : \text{inactive site} \\ \text{or } n_i = 1 & : \text{active site} \end{cases}$

KINETIC CONSTRAINT

Dynamics:
transition rates are:

$$\begin{cases} \text{activation} & W(n_i=0 \to n_i=1) = c \cdot \underbrace{(n_{i-1}+n_{i+1})}_{\text{KINETIC CONSTRAINT}} \\ \text{inactivation} & W(n_i=1 \to n_i=0) = (1-c) \cdot (n_{i-1}+n_{i+1}) \end{cases}$$

Each site follows a death & birth process, conditionned by the number of neighbors & $n_i \in \{0,1\}$

Link with discrete time: during a small time interval dt:

$$\text{prob}(n \to n') = \begin{cases} dt\, c\, (n_{i-1}+n_{i+1}) & \text{activat}^{\circ} \\ dt\,(1-c)(n_{i-1}+n_{i+1}) & \text{inactivation} \\ 1 - dt[\cdot + \cdot] & \text{nothing happens} \end{cases}$$

- **Remarkable Feature**:

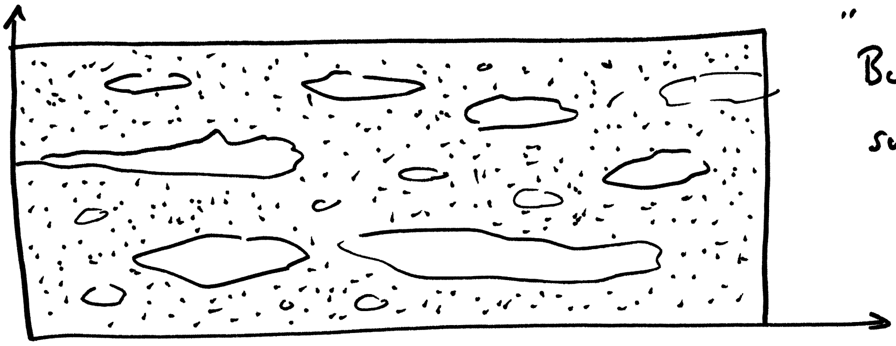
Trivial Equilibrium Distribution:
$$P_{eq}(\{n_i\}) = \prod_i c^{n_i}(1-c)^{1-n_i}$$
→ uncorrelated; same as WITHOUT CONSTRAINT

↕ ⦶

Non-trivial Dynamics:
Slow decay of correlation functions
Hysterisis & Ageing
→ Glassy-like properties

• Space-time diagramm:

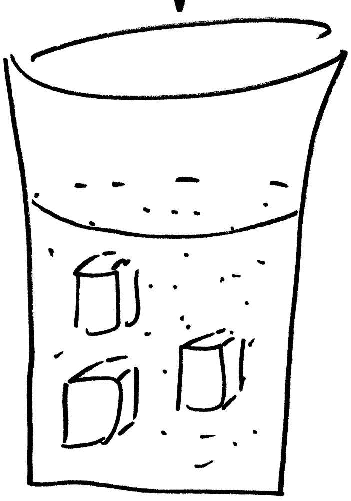
space



"Bubbles" of inactivity surrounded by active regions

time

analogy



ice cubes in liquid water @ T = 0°C

Again: there is no exact mapping

However, this suggest a picture in terms of a dynamical phase coexistence btw active & inactive regions

→ Questions: . how can one formalize/quantify this observation?

. can one study the properties of the active/the inactive phase?

. can this be used to explain the slow dynamics?

↪ use large deviation functions.

2 - Fluctuation of Dynamical Observables Large Deviation Functions

2. a - Dynamical order parameters

	Static phase transition	Dynamical Phase Transition
extensive order parameter	energy E (volume-extensive)	. activity $K = \#\{\text{events}\}$. current $Q = \#\{\text{jump} \nearrow\} - \#\{\text{jumps} \nwarrow\}$. integrated density $\int_0^t n(\tau)\,d\tau$ → "time-extensive", ie $\propto t =$ duration of the history
intensive conjugated variable	$\beta = 1/\text{Temperature}$ fixes the mean energy	s

One focuses on histories followed by the system btw 0 & time t.

× Dynamical order parameters : $A = K$ or Q or $\int_0^t n(\tau)d\tau$ or ....

- depend on (the realization of) the history followed by the system
- "time-exensive", ie on average $\propto \left\{ \begin{array}{l} \text{duration } t \text{ of the} \\ \text{considered histories} \end{array} \right\}$
- allow to classify histories and detect phase coexistence (or phase transition in general), in a dynamical sense.

× Equivalent of the microcanonical → canonical : $\left[\text{cf } e^{-\beta E}\right]$

weight histories by A e^{-sA}

2.b Large Deviation Functions:

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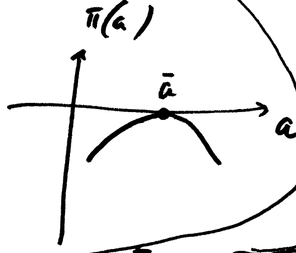
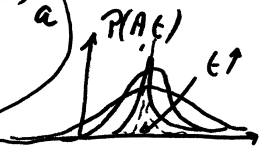
* ~~Pa~~ $P(A)$: $\quad P(A,t) \underset{t\to\infty}{\sim} e^{t\,\pi(A/t)}$

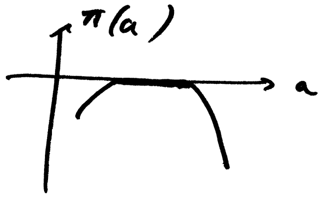




"normal" case $\pi(a)$ analytic

$$\pi(a) = \frac{(\bar{a}-a)^2}{2\sigma} + \dots$$ Gaussian fluctuations of the observable A.

"atypical case" $\pi(a)$ non analytic: non convex



↳ corresponds to different cases of phase-transitions → 'Ensemble inequivalence' which arises in the $L\to\infty$ limit in our case

→ Good tool to probe dynamical phase transitions.

(!) However: difficult to understand.

* Conjugated variable s: ["s-ensemble"]

s will fix the mean value of A for (slightly or not) atypical histories

$$\langle e^{-sA}\rangle \underset{t\to\infty}{\sim} e^{t\,\psi(s)}$$

$\psi(s)$ cumulant generating function

$$\psi(s) = \max_a \{\pi(a) - sa\}$$

$\langle e^{-sA}\rangle = \int da\, P(a)\, e^{-sat} \sim \underbrace{\int da\, e^{t[\pi(a)-sa]}}_{\text{dominated by the max}}$

$$\psi^{(k)}(s)\big|_{s=0} = \langle A^k\rangle_c$$ k-th cumulant

Physical interpretation $[\lim_{t\to\infty}]$

$$\boxed{\langle O\rangle_{\left\{\substack{\text{histories with}\\ A\approx at}\right\}} = \langle O\rangle_{s^*(a)} \qquad \text{with } \langle O\rangle_s \equiv \frac{\langle O e^{-sA}\rangle}{\langle e^{-sA}\rangle}}$$

$\langle \dots \rangle$ = average for histories of duration t

$$\pi(a) = \min_s \; \psi(s) + sa$$

$$s^*(a) = \underset{a}{\mathrm{argmax}} \{\pi(a) - sa\}$$

biased statistics over histories

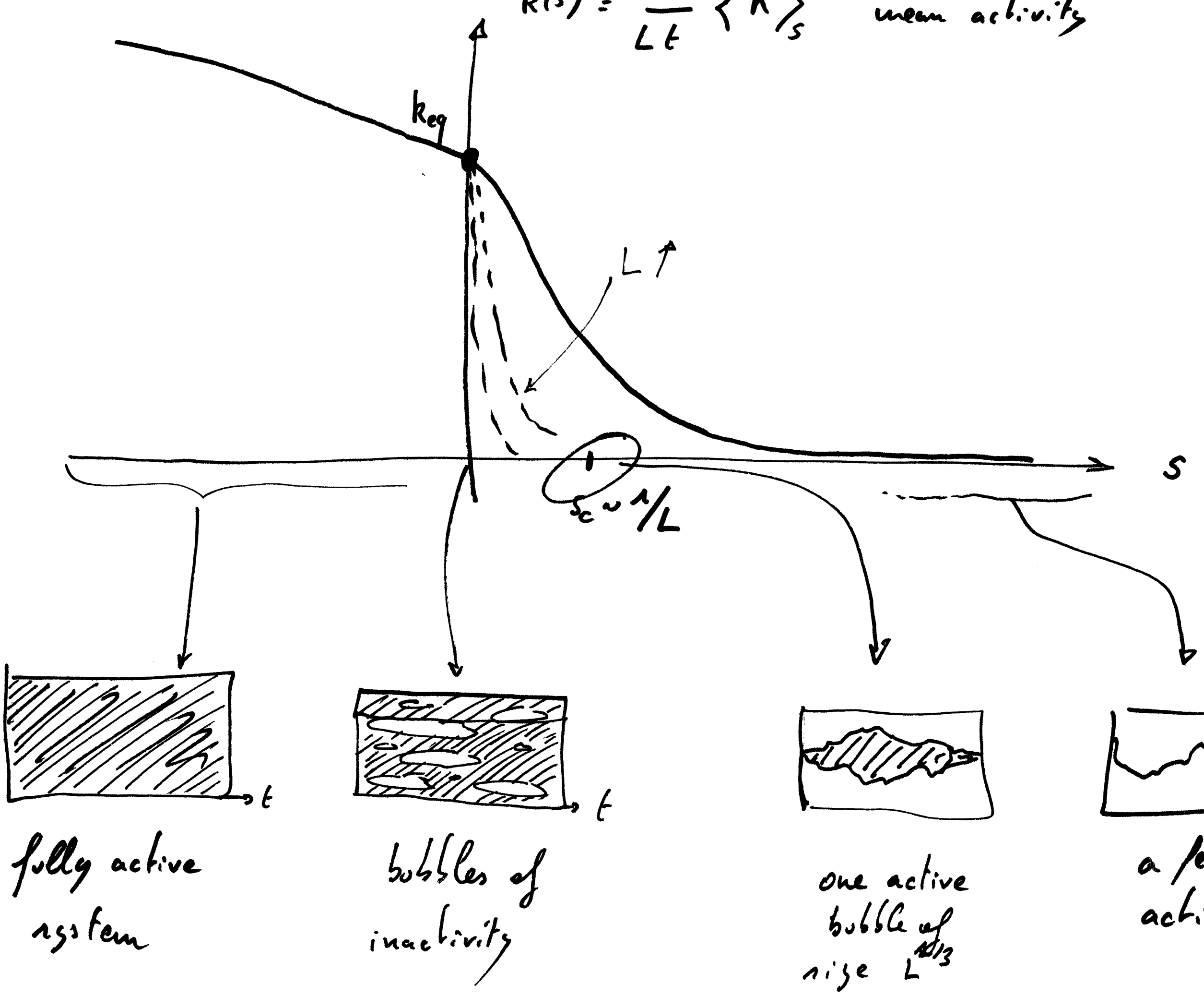
↳ In practice: $\boxed{\text{biasing histories with } s \text{ allows to track down dynamical phase transitions}}$

* Preview of the results for KCMs

[As aim in the next lectures: provide details & algorithms]

L: system size

$k(s) = \frac{1}{Lt} \langle K \rangle_s$ mean activity



→ $s=0$ lies closeby to a ~~critical~~ dynamical coexistence point $s_c \sim 1/L$

i.e. very close to