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

Complexity Summer School
Warwick University
2013

→ 1st lecture, very descriptive.

utline:

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

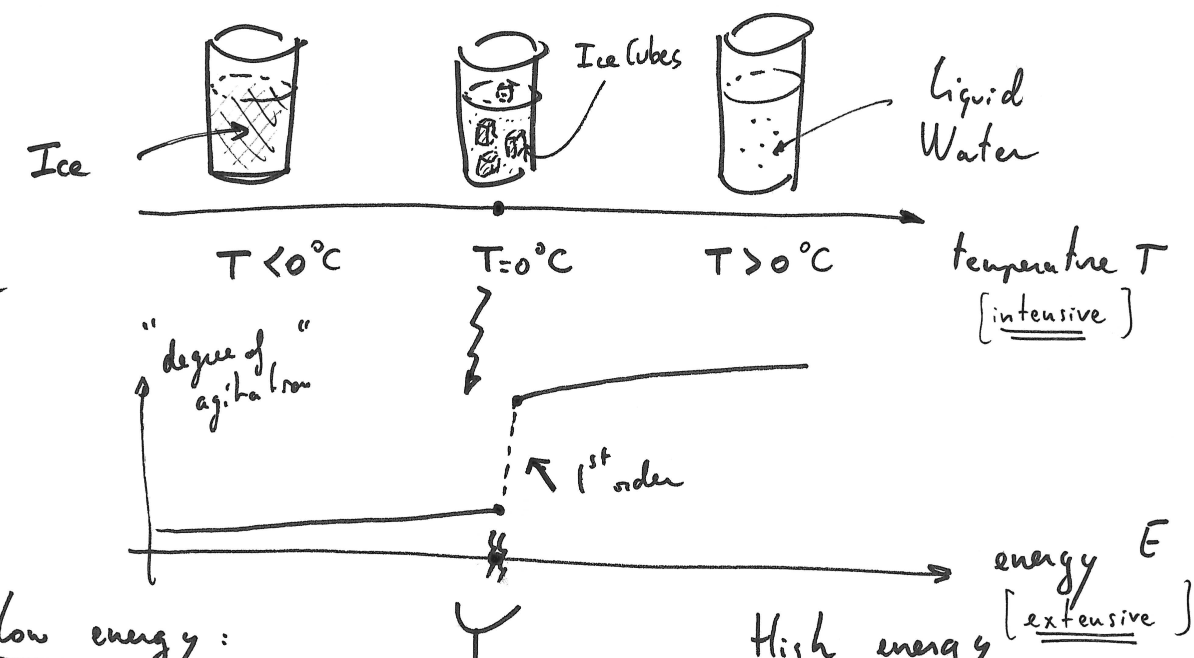
. Examples of Phase Transitions . Static & Dynamical Coexistence

1. a (Static) liquid-solid phase coexistence

canonical "ensemble"

Thermostated system

Isolated system



Low energy: most probable configurations are crystallyzed → Ice

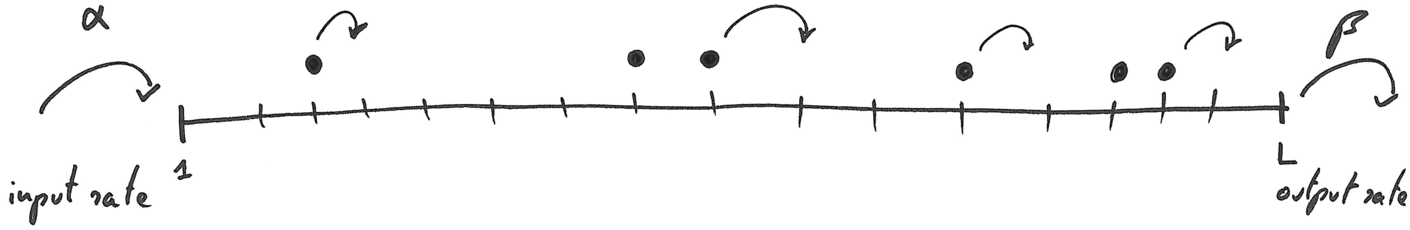
phase coexistence

High energy most probable configurations are "agitated" → Liquid

1.b. 1D transport : a traffic model

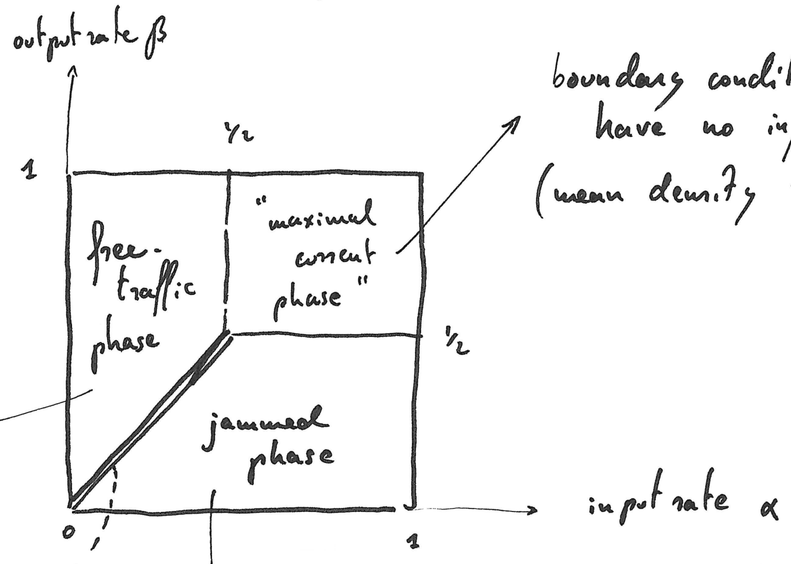
(Driving in dense traffic : one observes large fluctuations of jamming

. Very simple model ("Ising model of non-equilibrium"): TASEP
[Totally Asymmetric Simple Exclusion Process]



- each site either occupied • or not
- jump to the rate occurs with rate 1 provided the target site is empty ("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)

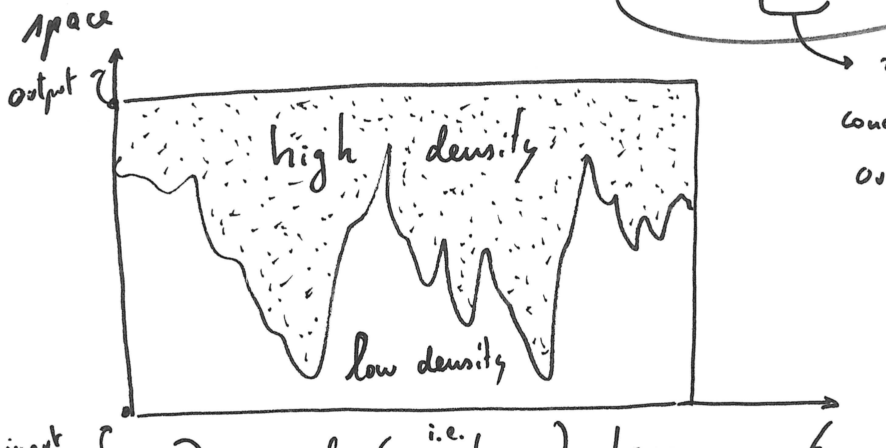
input rate > output rate
⇒ full system conditionned by the output boundary
(complete jam)

1^{st} order coexistence line

1_b' Coexistence between jammed & free traffic.

$0 < \underbrace{\alpha = \beta}_{} < 1/2$ → represents realistic conditions where output ≈ input

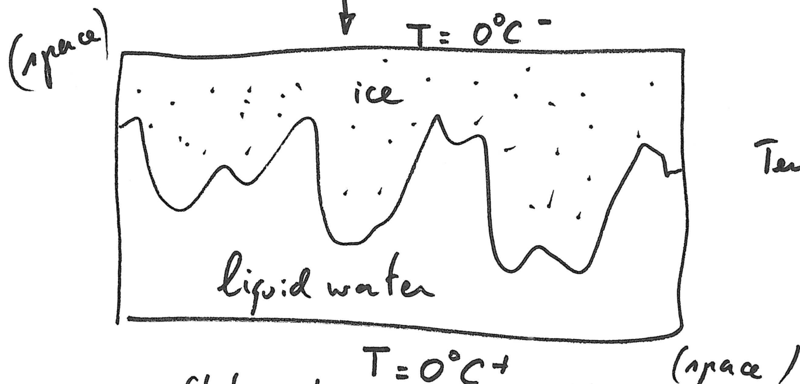
TASEP



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: $\boxed{\text{Large Deviation Functions}}$.

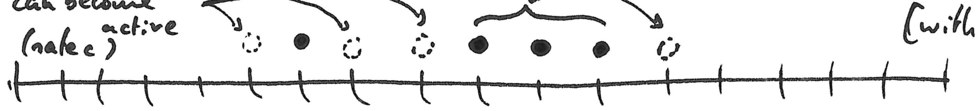
c. Glass Formers ; Kinetically Constrained Models

- 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 :

can become active (rate c)

can become inactive [with rate ∝ (1-c)]



1 $\qquad$ i $\qquad$ L $\qquad$ (periodic boundary conditions)

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

Dynamics :

transition rates are:

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

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

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 :

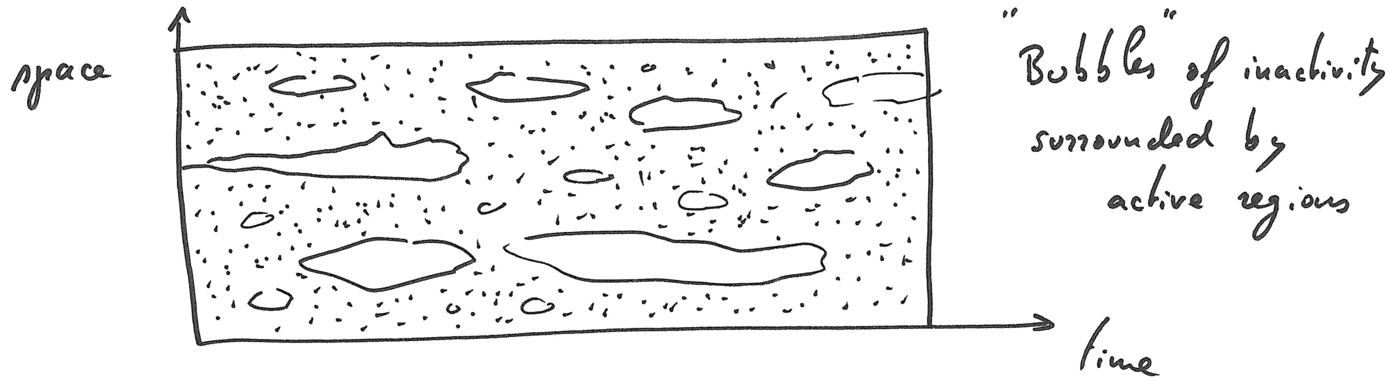
$$\boxed{P_{eq}(\{n_i\}) = \prod_i c^{n_i} (1-c)^{1-n_i}}$$
→ uncorrelated ; same as WITHOUT CONSTRAINT

↕ ◐

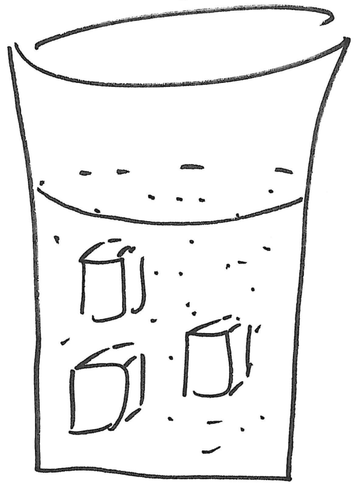
Non-trivial Dynamics :

Slow decay of correlation functions
Hysterisis & Ageing
→ Glassy-like properties

• Space-time diagramm :



analogy



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 : $\nearrow [\text{cf } e^{-\beta E}]$

weight histories by A $\quad e^{-sA}$

2.6 Large Deviation functions:

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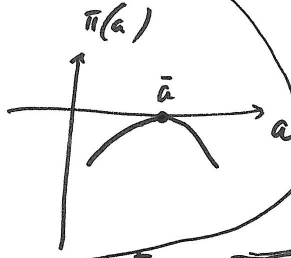
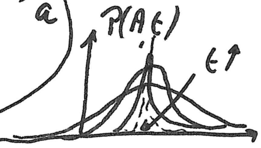
P(A): $P(A,t) \underset{t\to\infty}{\sim} e^{t\,\pi(A/t)}$



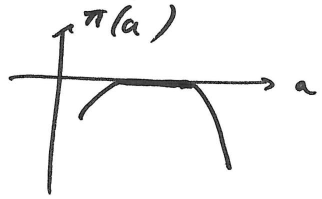


"normal" case $\pi(a)$ analytic

$$\pi(a) = \frac{(\bar{a}-a)^2}{2\sigma} + \dots$$ 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

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

$\langle e^{-sA}\rangle \simeq \int da\, P(a)\, e^{-sat} \sim \int da\, e^{t(\pi(a)-sa)}$ dominated by the max

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

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

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

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

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

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

biased statistics over histories

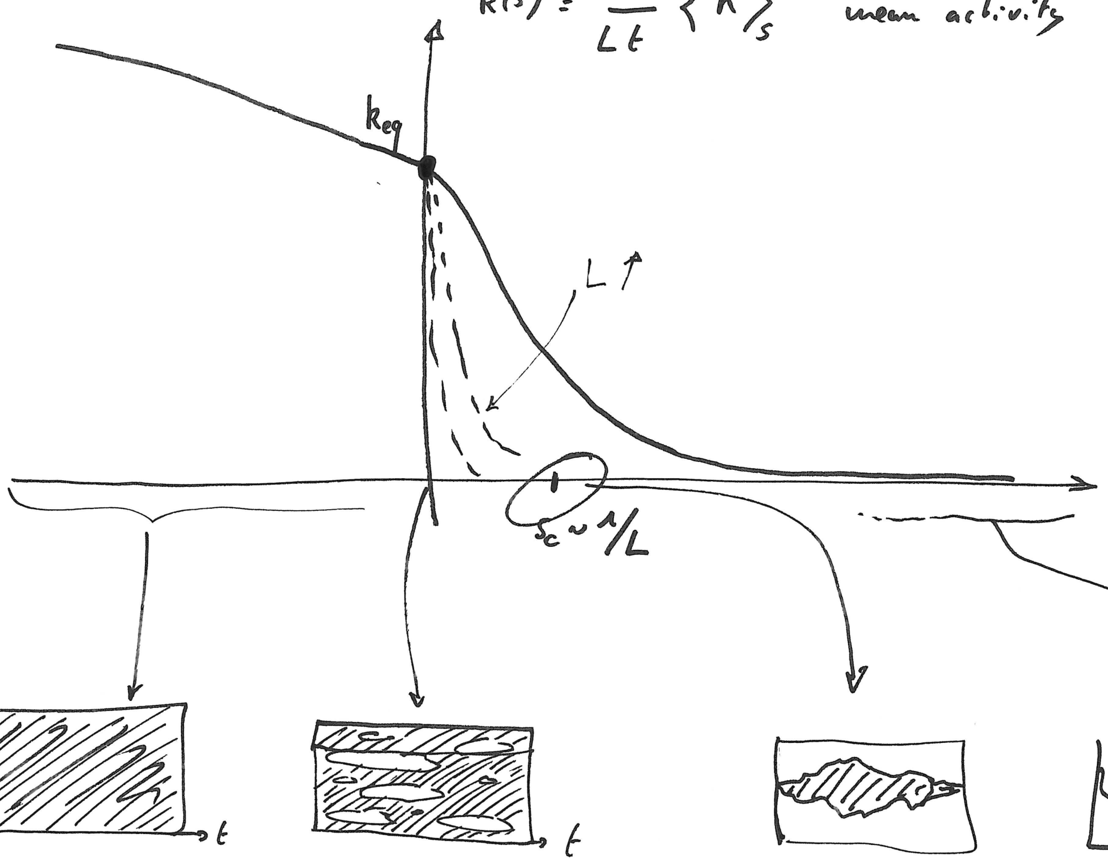
↳ In practice: $\boxed{\text{biasing histories with } s \text{ allows to track down dynamical phase transitions}}$

* Preview of the results for KCMs

(Our aim in the next lectures: provide details & algorithms)

L: system size

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



fully active system

bubbles of inactivity

one active bubble of size $L^{1/3}$

a few / a single active site

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

i.e. very close to