Statistics of histories
an application to systems with glassy dynamics

Vivien Lecomte[1,2], Cécile Appert-Rolland[1], Estelle Pitard[3], Kristina van Duijvendijk[1,2], Frédéric van Wijland[1,2]

Juan P. Garrahan[4], Robert L. Jack[5,6]

[1]Laboratoire de Physique Théorique, Université d'Orsay
[2]Laboratoire Matière et Systèmes Complexes, Université Paris 7
[3]Laboratoire Colloïdes, Verres et Nanomatériaux, Université Montpellier 2
[4]School of physics and astronomy, University of Nottingham
[5]Rudolf Peierls Centre for Theoretical Physics, University of Oxford
[6]Department of Chemistry, University of California

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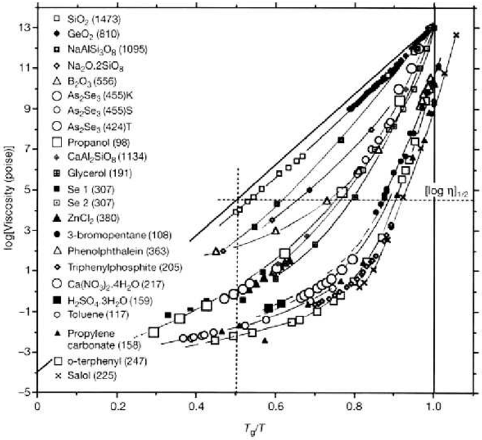
Glasses



from Martinez and Angell, *Nature* **410** 663 (2001)

Glasses: characterization

Distinctive features

- huge increase of relaxation time as $T \searrow$
- stretched exponential time-relaxation of correlations
- ageing
- dynamical heterogeneities

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Static Boltzmann-Gibbs thermodynamics

$$P(\mathcal{C}) = \mathrm{e}^{-\beta E(\mathcal{C})}$$

Can't be used in any situation!

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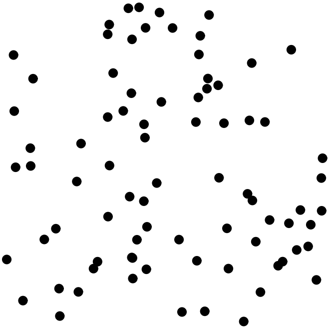
Static Boltzmann-Gibbs thermodynamics

$$P(\mathcal{C}) = \mathrm{e}^{-\beta E(\mathcal{C})}$$

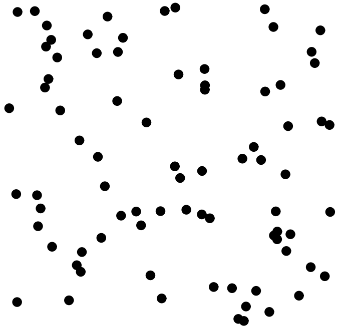
$\longrightarrow$ Need for a dynamical description

From configurations to histories



fluctuations of configurations

From configurations to histories



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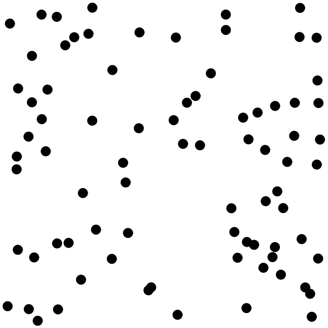

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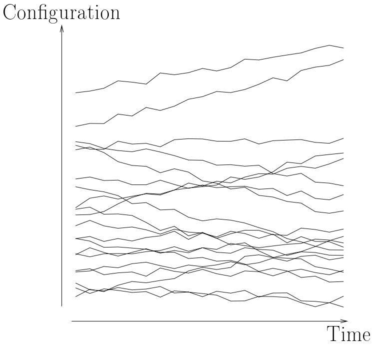

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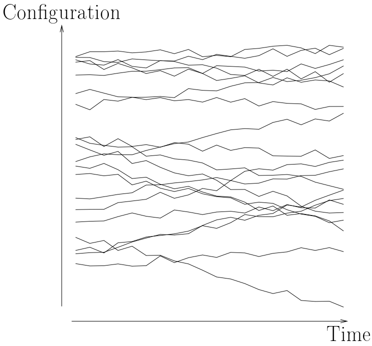

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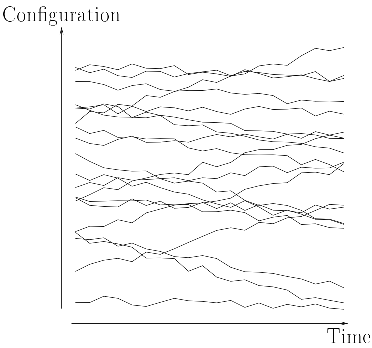
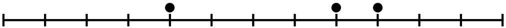


fluctuations of histories

Outline

1. Motivations
   - Glasses
   - statics vs dynamics
2. Models of glass formers
   - example
   - statistics of histories
   - results
   - dynamical phase coexistence
3. Perspective

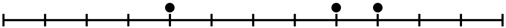
Example



Independent particles

- L sites $\boldsymbol{n} = \{n_i\}$ with $\begin{cases} n_i = 0 & \text{inactive site} \\ n_i = 1 & \text{active site} \end{cases}$

Example



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- Transition rates in each site:
  - activation with rate $W(0_i \to 1_i) = c$
  - inactivation with rate $W(1_i \to 0_i) = 1 - c$

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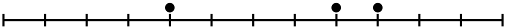

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Equilibrium distribution: $P_{\text{eq}}(\boldsymbol{n}) = \prod_i c^{n_i}(1-c)^{1-n_i}$

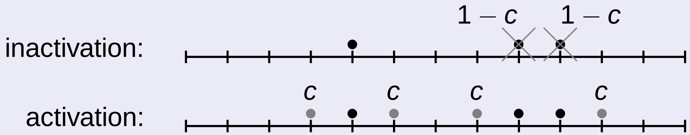
Mean density of active sites: $\langle n \rangle = \frac{1}{L}\sum_i \langle n_i \rangle = c$

Kinetically constrained models (KCM)

Constrained dynamics: changes occur only around active sites.

Fredrickson Andersen model in 1D

at least one neighbor of *i* must be active to allow *i* to change



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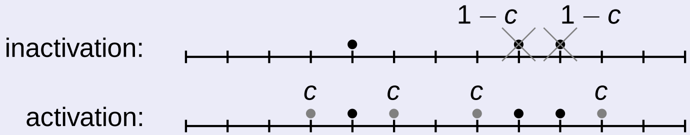

- *same* equilibrium distribution $P_{\text{eq}}(\boldsymbol{n})$
- *same* mean density $\langle n \rangle = c$

BUT:

- ageing, super-Arrhenius slowing down, dynamical heterogeneity

Fluctuation of a dynamical observable

$$\rho(t) = \frac{1}{Lt}\sum_{i=1}^{L}\int d\tau\, n_i(\tau) = \left|\begin{array}{l}\text{space- \& time-averaged}\\ \text{density of active sites}\end{array}\right.$$

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$$\text{Prob}_{[0,t]}(\rho) \sim e^{-t\,L\,\mathcal{F}(\rho)}$$

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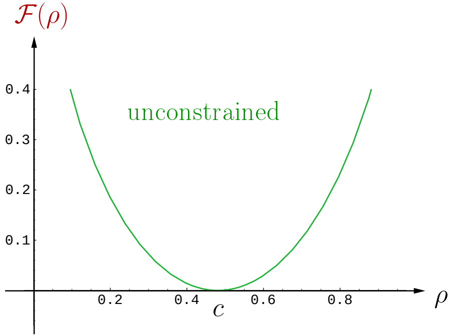

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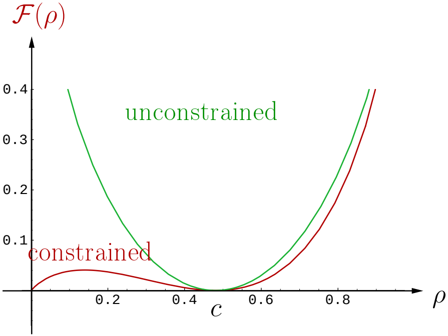

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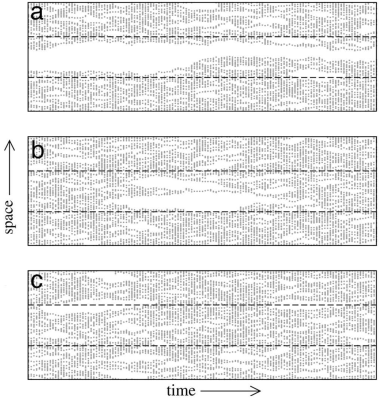
Dynamical coexistence



from Merolle, Garrahan and Chandler, *PNAS* **102** 10837 (2005)

Questions

Equal probability for active and inactive histories

$\updownarrow$

Coexistence of dynamical phases?

- Dynamical Landau free-energy landscape?
- First order phase transition?
- How can we escape the critical point?

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More generally

Can we find an analogous dynamical free energy characterizing glassiness?

Ruelle formalism in one slide

(Dynamical) canonical ensemble

- β conjugated to energy (Boltzmann)
- s conjugated to activity K (Ruelle)

Ruelle formalism in one slide

s-ensemble:
- $s < 0$: more active histories ("large" activity K)
- $s = 0$: equilibrium state
- $s > 0$: less active histories ("small" activity K)

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Dynamical partition function

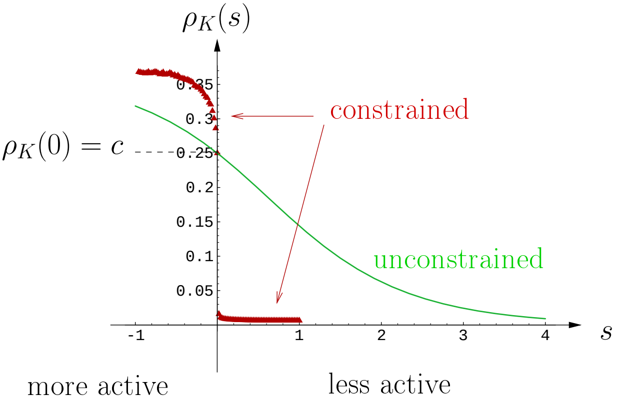
- Thermodynamics of configurations

$$Z(\beta, L) = \sum_{E} \sum_{\substack{\text{configurations}\\ \text{of energy } E}} e^{-\beta E} = e^{-L f(\beta)} \qquad \text{(large } L\text{)}$$

- Thermodynamics of histories [*à la* Ruelle]

$$Z_K(s, t) = \sum_{K} \sum_{\substack{\text{histories}\\ \text{of activity } K}} e^{-sK} = e^{-t L f_K(s)} \qquad \left(\begin{matrix}\text{large } t\\ \text{large } L\end{matrix}\right)$$

Dynamical phase transition: FA model (d=1)



Comparison between constrained and unconstrained dynamics

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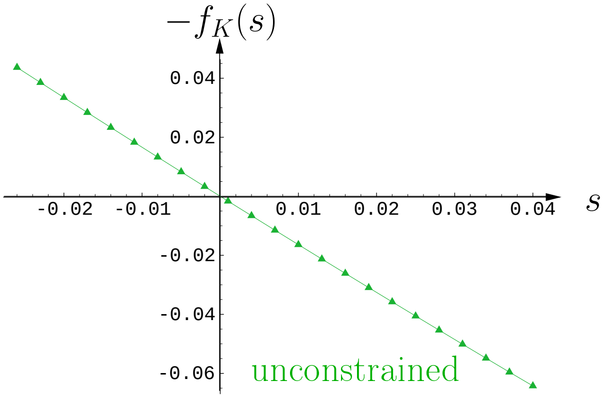

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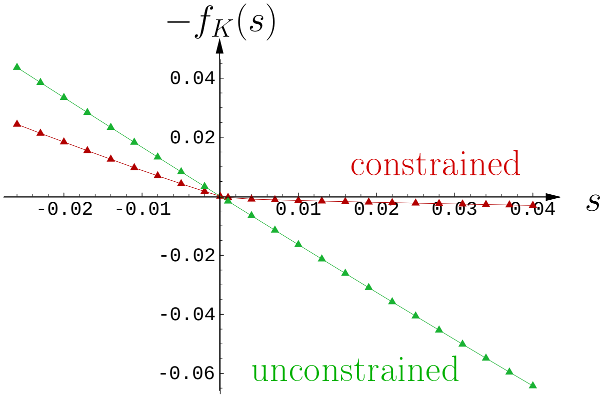

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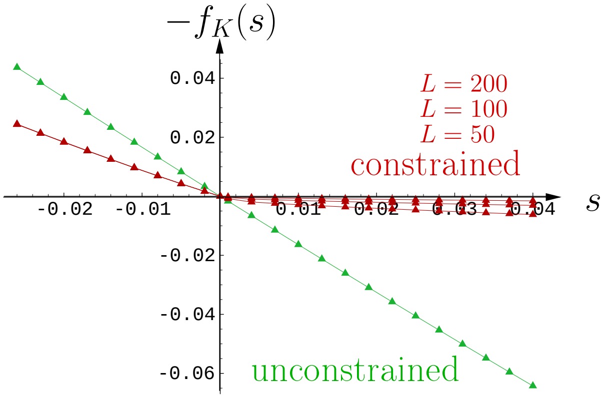
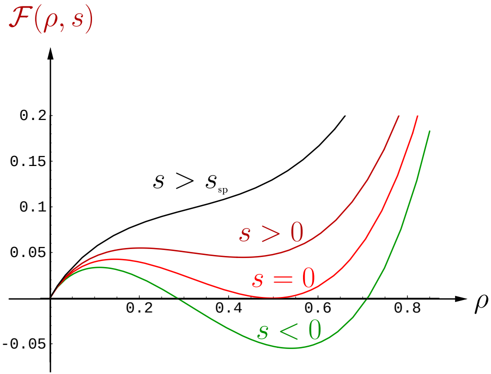


Comparison between constrained and unconstrained dynamics

Dynamical Landau free-energy landscape



$\text{Prob}_{[0,t]}(\rho, s) \sim e^{-t\,L\,\mathcal{F}(\rho, s)}$ in the s-ensemble

Statistics over histories: summary

Results

- s-ensemble $\equiv$ tools to study dynamics
- Description of dynamical phase coexistence
  $\longrightarrow$ Dynamical Landau free energy $\mathcal{F}(\rho, s)$ $\longleftarrow$

Dynamical phase transition

- Criticality in a (dynamical) "hidden" dimension
- Dynamical heterogeneity

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Perspective

Perspective

- Link with dynamical growing lengths

References

- *PRL* **95** 010601 (2005)
- *J. Stat. Phys.* **127** 51 (2007)
- *PRL* **98** 195702 (2007)
- *JSTAT* P03004 (2007)

Perspective

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- Link with dynamical growing lengths
- Systems without phase coexistence?
- Other glassy systems
  - structural glasses (Lennard-Jones)
  - disordered systems

References

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- Link with dynamical growing lengths
- Systems without phase coexistence?
- Other glassy systems
  - structural glasses (Lennard-Jones)
  - disordered systems
- Experimental realization of $s(\simeq 0)$-states

References

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s-modified dynamics

- Markov processes:

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},t)}_{\text{loss term}} \Big\}$$

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- More detailed dynamics for $P(\mathcal{C},K,t)$:

$$\partial_t P(\mathcal{C},K,t) = \sum_{\mathcal{C}'} \Big\{ W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',K-1,t) - W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},K,t) \Big\}$$

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- Canonical description: s conjugated to K

$$P(\mathcal{C},s,t) = \sum_K e^{-sK} P(\mathcal{C},K,t)$$

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Numerical method (with J. Tailleur)

Evaluation of large deviation functions

$$Z(s,t) = \sum_{\mathcal{C}} P(\mathcal{C},s,t) = \left\langle e^{-sK} \right\rangle \sim e^{-t f_K(s)}$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: Lecomte, Tailleur [JSTAT P03004 (2007)]

Cloning dynamics

$$\partial_t P(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',s) - r_s(\mathcal{C}) P(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C}) P(\mathcal{C},s)}_{\text{cloning term}}$$

- $W_s(\mathcal{C}' \to \mathcal{C}) = e^{-s} W(\mathcal{C}' \to \mathcal{C})$
- $r_s(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W_s(\mathcal{C} \to \mathcal{C}')$
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