Finite size scaling of the dynamical free-energy in the interfacial regime of a kinetically constrained model

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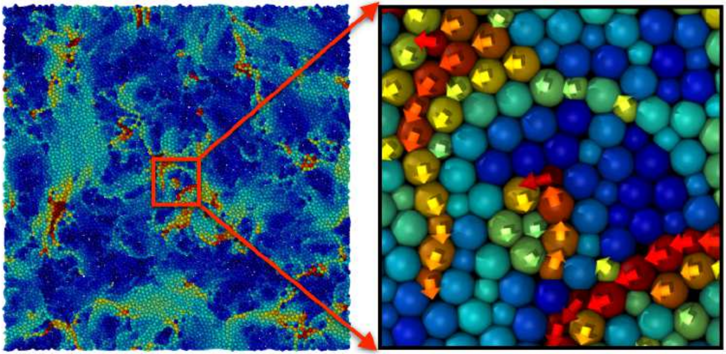
Dynamical excitations in glass-forming liquids



From: Keys *et. al* PRX **1** 021013 (2011)

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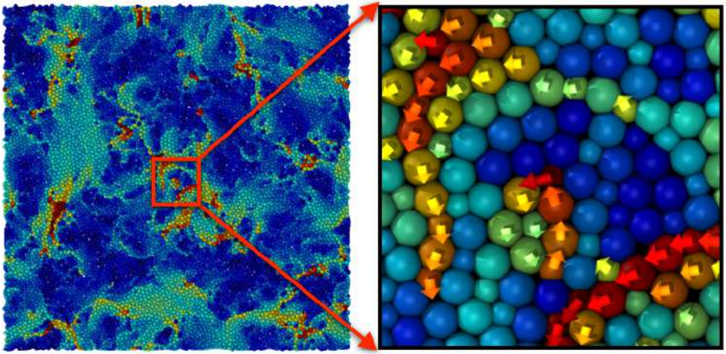

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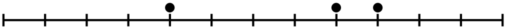
Can we model this simply?

Example 0: (in 1D for simplicity)



Independent sites

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

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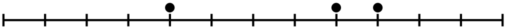

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- Transition rates in each site:
  - excitation with rate $W(0_i \to 1_i) = c$
  - unexcitation with rate $W(1_i \to 0_i) = 1 - c$

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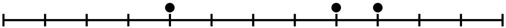

Independent sites — **Unconstrained model**

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

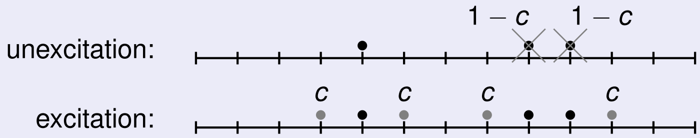
Mean density of excited sites: $\langle n \rangle = \frac{1}{L}\sum_i \langle n_i \rangle = c$

Kinetically constrained models (KCM)

Constrained dynamics: changes occur only around excited sites.

Fredrickson Andersen model in 1D

at least one neighbor of i must be excited to allow i to change



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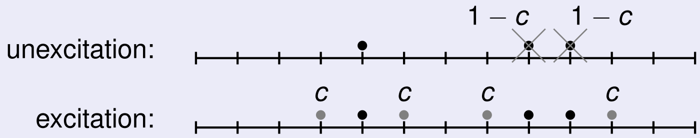
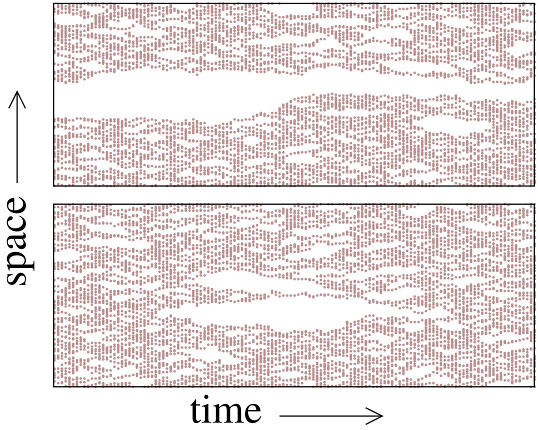


- *same* equilibrium distribution $P_{\text{eq}}(\boldsymbol{n})$ with&without the constraint
- BUT: ageing, super-Arrhenius slowing down, dynamical heterogeneity

$\longrightarrow$ static free-energy landscape not useful
$\longrightarrow$ need for a dynamical description

Space-time "bubbles" of inactivity



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

Questions

Active and inactive histories
having a probability of the same order
$\updownarrow$
Coexistence of dynamical phases?

- How to describe a dynamical 1^{st} order phase transition?
- Dynamical Landau free-energy landscape?

Activity of histories: order parameter

Activity K = number of events = (# excitations) + (# unexcitations)

(Dynamical) canonical ensemble

- β conjugated to energy (statics)
- s conjugated to activity K (dynamics)

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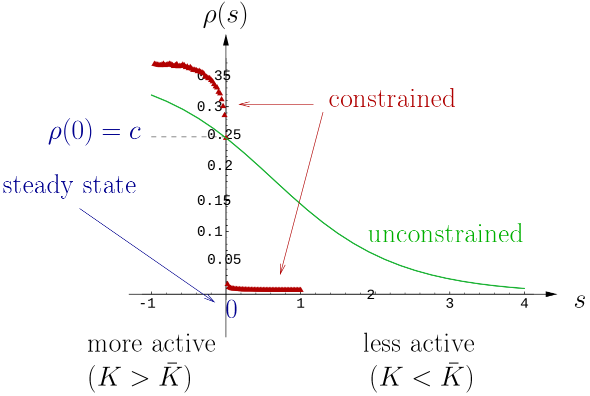
s-ensemble:
$$\begin{cases} s < 0 : & \text{more active histories} \quad (\text{“large” activity } K > \bar{K}) \\ s = 0 : & \text{equilibrium state} \quad (\text{equilib. activity } K = \bar{K}) \\ s > 0 : & \text{less active histories} \quad (\text{“small” activity } K < \bar{K}) \end{cases}$$

Dynamical phase transition: FA model (d=1)

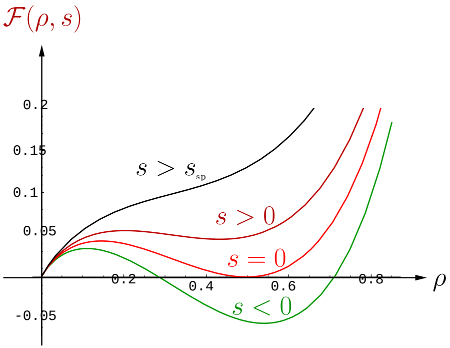
Density of excitations $\rho(s)$ depending on histories.



Comparison between constrained and unconstrained dynamics

Dynamical Landau free-energy landscape $\mathcal{F}(\rho, s)$

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

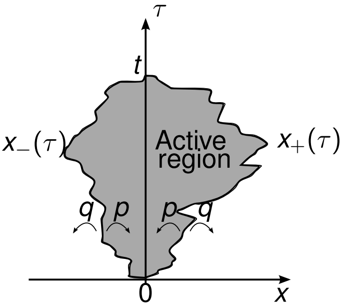


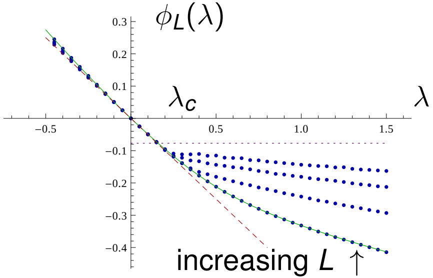
Dynamical free energy: $f(s) = \underbrace{\min_{\rho}}_{\text{reached at } \rho=\rho(s)} \mathcal{F}(\rho, s)$

Scaling of the free energy in the interfacial regime

Finite-size scaling of the free energy f: $\phi_L(\lambda) = f\left(\frac{\lambda}{L}\right)$

$$s = \frac{\lambda}{L}$$





Interfacial model $\longleftrightarrow$ finite-size scaling

Surface tension Σ

$$\phi_L(\lambda) = -\Sigma - A\left(\frac{\lambda}{L}\right)^{\frac{2}{3}}$$

Scaling function

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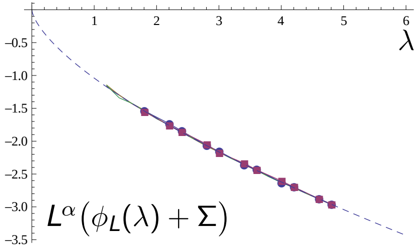

Summary and outlook

- Correspondence $\left\{ \begin{array}{c} \text{finite-size scaling} \\ \text{of dyn. free-energy } f(s) \end{array} \right\} \longleftrightarrow \left\{ \begin{array}{c} \text{geometrical features} \\ \text{of active excitations} \end{array} \right\}$:

$$\underbrace{\phi_L(\lambda)}_{\substack{\text{finite-size} \\ \phi_L(\lambda)=f\left(\frac{\lambda}{L}\right)}} = \underbrace{-\Sigma}_{\substack{\text{surface tension} \\ \text{(excitations} \\ \text{are bubbles)}}} - \underbrace{A\left(\frac{\lambda}{L}\right)^{\alpha}}_{\substack{\alpha=\frac{2}{3} \\ \text{(boundaries are} \\ \text{Brownian)}}}$$

- Questions:
  - ⋆ How to link $\left\{ \begin{array}{l} \text{the } (s>0) \text{ bubbles of excitation to} \\ \text{the } (s=0) \text{ bubbles of inactivity} \end{array} \right.$?
  - ⋆ How to write the correspondence in more realistic models?
  - ⋆ Link dynamical phase transition and glassy features.
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