Finite-size effects in a mean-field kinetically constrained model

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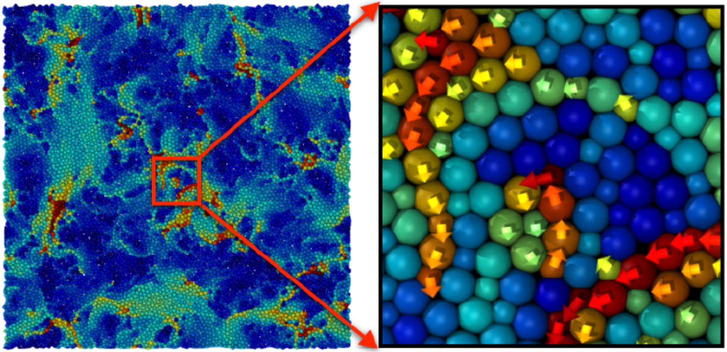
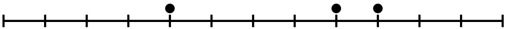
Dynamical excitations in glass-forming liquids



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

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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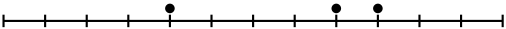

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  - excitation with rate $W(0_i \to 1_i) = c$
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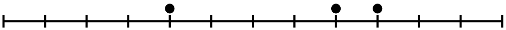

Independent sites — Unconstrained model

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- Transition rates in each site:
  - excitation with rate $W(0_i \to 1_i) = c$
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Equilibrium distribution: $$P_{\text{eq}}(\boldsymbol{n}) = \prod_i c^{n_i}(1-c)^{1-n_i}$$

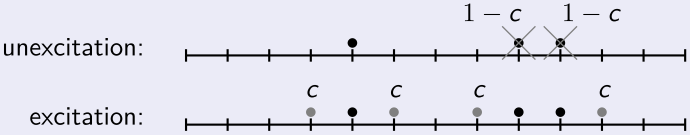
Mean density of excited sites: $$\langle n \rangle = \frac{1}{L}\sum_i \langle n_i \rangle = c$$

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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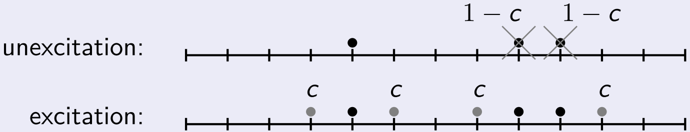
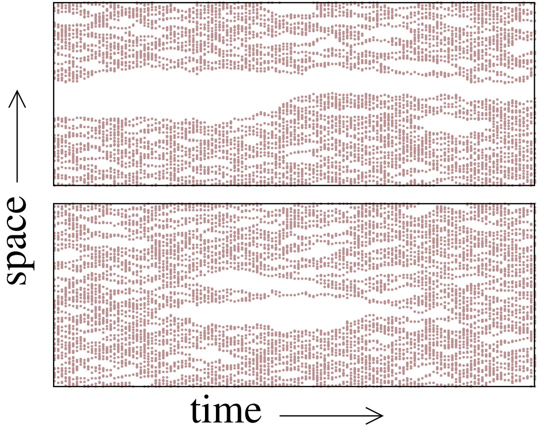


- *same* equilibrium distribution $P_{\mathrm{eq}}(\boldsymbol{n})$ with&without the constraint
- BUT: ageing, super-Arrhenius slowing down, dynamical heterogeneity

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

Space-time "bubbles" of inactivity



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

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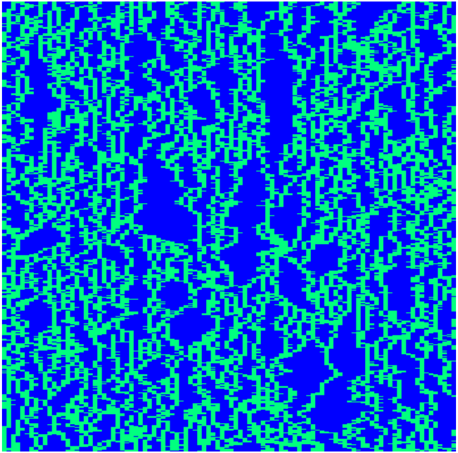

[Fig. by A. Leos Zamorategui]

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?
  (*i.e.* competition between different optima)

Activity of histories: order parameter

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

(Dynamical) canonical ensemble

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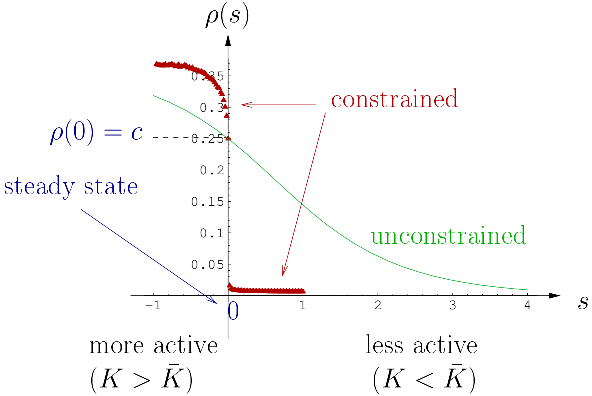
s-ensemble:
$$\begin{cases} s < 0 : & \text{more active histories} \quad (\text{“large” activity } K > \bar{K}) \\ s = 0 : & \text{equilibrium state} \quad (\text{equilib. activity } K = \bar{K}) \\ s > 0 : & \text{less active histories} \quad (\text{“small” activity } K < \bar{K}) \end{cases}$$

$$\langle \mathcal{O} \rangle_s = \frac{\langle \mathcal{O} e^{-sK} \rangle}{\langle e^{-sK} \rangle} \qquad \langle e^{-sK} \rangle \sim e^{t\psi(s)}$$

$$P(K \simeq kt, t) \sim e^{t\pi(k)} \qquad \psi(s) = \max_k \{\pi(k) - sk\}$$

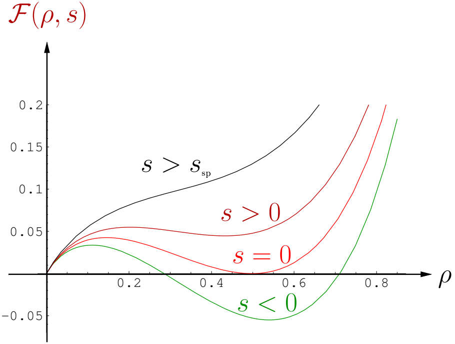
Dynamical phase transition: FA model (d=1)

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



Comparison between constrained and unconstrained dynamics

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



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

Dynamical free energy picture: in "mean-field"

"Mean-field" version of the FA model: (on a complete graph)

$$A + A \underset{1-c}{\overset{c}{\rightleftharpoons}} A$$

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Rates for number n of excitations (with L sites):

$$W_+(n) \equiv W(n \to n+1) = c(L-n)\frac{n}{L}$$
$$W_-(n) \equiv W(n \to n-1) = (1-c)n\frac{n-1}{L}$$

Kinetic constraint $\propto$ number of excited neighbours

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Extremalization principle:

$$\psi(s) = -\min_{P\neq 0} \frac{\langle P| - \mathbb{W}_K^{\mathsf{sym}}(s)|P\rangle}{\langle P|P\rangle}$$

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Thermodynamic limit (finite density $\rho = \frac{n}{L}$): $P(n) \sim e^{-Lf(n/L)}$

$$\frac{1}{L}\psi(s) = -\min_{\rho}\left\{-2e^{-s}\sqrt{W_+W_-} + W_+ + W_-\right\}$$

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One can also use Donsker-Varadhan

$$\left\langle \mathrm{e}^{-sK}\delta\Big(\frac{1}{Lt}\int_0^t dt'\ n(t') = \rho\Big)\right\rangle \sim \mathrm{e}^{-tL\mathcal{F}(\rho,s)}$$

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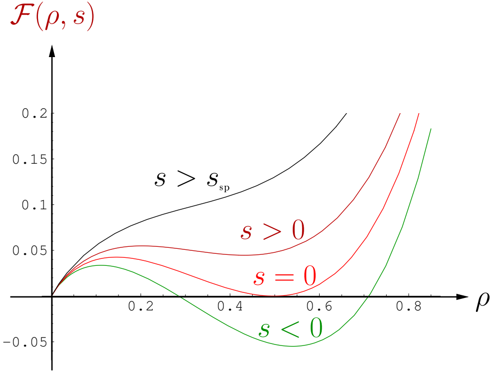
$$f_K(s) = \min_\rho \mathcal{F}(\rho, s) = \mathcal{F}(\rho(s), s)$$



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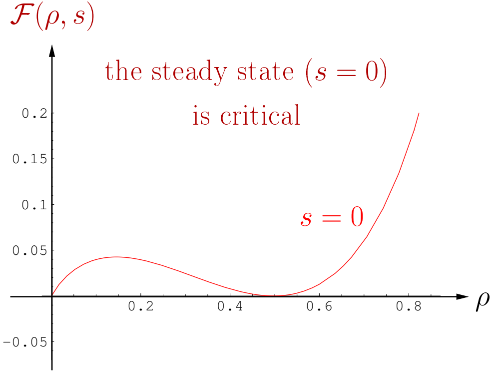

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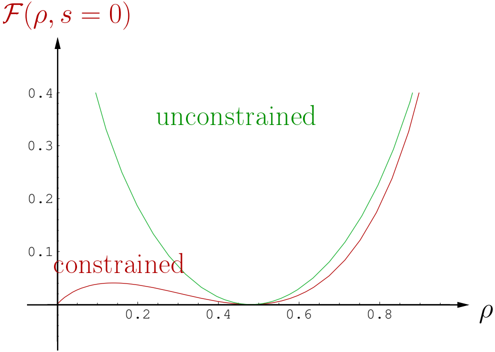

Rounding of the first-order transition

Finite-size effects: required to understand $P(K,t)$
Scale of fluctuations: $s = \frac{\lambda}{L}$ (transition at $\lambda_c > 0$)

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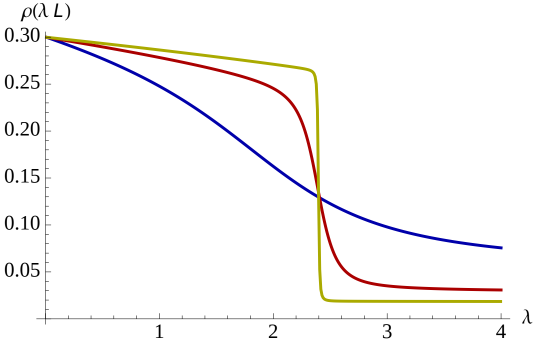

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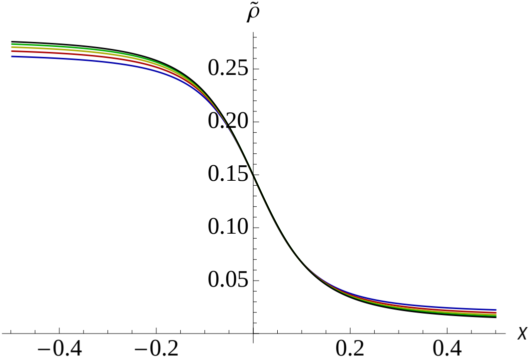

Fine finite-size scaling: $\lambda = \lambda_c + e^{-\alpha L} x$

Idea of the method

Extremalization principle:

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Large-deviation form for the eigenvector: $P(n) \sim e^{-Lf(n/L)}$

- ⋆ infinite-size limit: one only needs $\rho = \text{argmin } f$
- ⋆ in a window around λ_c: one needs more

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$$P(n) = P_{\text{inactive}}^{n<n_c}(n) + P_{\text{active}}^{n\geq n_c}(n)$$

Around coexistence ($\lambda \simeq \lambda_c$):

$$P(n) = \big(1 + a(s)\big) P_{\text{inactive}}^{n<n_c}(n) + \big(1 - a(s)\big) P_{\text{active}}^{n\geq n_c}(n)$$

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Summary

First-order dynamical phase transition

- competition between active and inactive region in space-time
- dynamical heterogeneities

"Mean-field" model (complete graph)

- Dynamical Landau free-energy landscape
- finite-size effects

Perspectives:

- Finite dimension? [T Bodineau, VL, C Toninelli, JSP 2012]
- Finite time? (Gap, spectal density)
- Other models?
- *Link to 1st order quantum phase transition*

Thank you for your attention!

References:

- **Takahiro Nemoto, Vivien Lecomte, Shin-ichi Sasa, Frédéric van Wijland**
  `arxiv:1405.1658` (2014)
  Accepted for publication in J. Stat. Mech.
- Juan P. Garrahan, Robert L. Jack, Vivien Lecomte, Estelle Pitard, Kristina van Duijvendijk and Frédéric van Wijland, J. Phys. A **42** 075007 (2009)

Appendix: operators

We assume detailed balance: $P_{\text{eq}}(\mathcal{C})W(\mathcal{C}\to\mathcal{C}') = P_{\text{eq}}(\mathcal{C}')W(\mathcal{C}'\to\mathcal{C})$

Maximization principle:

$$\psi(s) = \max_P \frac{\langle P|\mathbb{W}_K^{\text{sym}}(s)|P\rangle}{\langle P|P\rangle}$$

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$$\mathbb{W}_{\mathcal{C}'\mathcal{C}} = W(\mathcal{C}\to\mathcal{C}') - r(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'}$$

Symetrization by $R = P_{\text{eq}}^{\frac{1}{2}}(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'}$: $\mathbb{W}^{\text{sym}} = R^{-1}\mathbb{W}R$

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$$(\mathbb{W}^{\text{sym}})_{\mathcal{C}'\mathcal{C}} = \left[W(\mathcal{C}\to\mathcal{C}')W(\mathcal{C}'\to\mathcal{C})\right]^{\frac{1}{2}} - r(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'}$$

we have

$$(\mathbb{W}^{\text{sym}})^\dagger = \mathbb{W}^{\text{sym}}$$

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