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

Takahiro Nemoto\textsuperscript{1}, Shin-ichi Sasa\textsuperscript{1}, Frédéric van Wijland\textsuperscript{2}

\textsuperscript{1}Kyoto University \hspace{1cm} \textsuperscript{2}MSC, Paris 7 University

Tel-Aviv \hspace{1cm} 22th October 2014
Dynamical excitations in glass-forming liquids

Can we model this simply?

From: Keys et. al PRX 1 021013 (2011)
Example 0: (in 1D for simplicity)

Independent sites

- L sites \( n = \{ n_i \} \) with \[
\begin{aligned}
    n_i &= 0 \quad \text{unexcited site} \\
    n_i &= 1 \quad \text{excited site} \\
\end{aligned}
\]

- Transition rates in each site:
  - excitation with rate \( W(0_i \rightarrow 1_i) = c \)
  - unexcitation with rate \( W(1_i \rightarrow 0_i) = 1 - c \)
Example 0: (in 1D for simplicity)

Independent sites

- $L$ sites $\mathbf{n} = \{n_i\}$ with

\[
\begin{cases}
  n_i = 0 & \text{unexcited site} \\
  n_i = 1 & \text{excited site} \\
\end{cases}
\]

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

Unconstrained model

Equilibrium distribution: 

\[
P_{eq}(\mathbf{n}) = \prod_i c^{n_i} (1 - c)^{1-n_i}
\]

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

unexcitation: \[ 1 - c \quad 1 - c \]

excitation: \[ c \quad c \quad c \quad c \]

same equilibrium distribution $P_{eq}(n)$ with and without the constraint

BUT [for some KCMs]: ageing, super-Arrhenius slowing down, dynamical heterogeneity

static free-energy landscape not useful here

need for a genuinely dynamical description
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

unexcitation:

excitation:

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

\[\longrightarrow\text{ static free-energy landscape not useful here}\]
\[\longrightarrow\text{ need for a genuinely dynamical description}\]
Space-time “bubbles” of inactivity

From: Merolle, Garrahan and Chandler, PNAS 102, 10837 (2005)
Space-time “bubbles” of inactivity

[Fig. by A. Leos Zamorategui]
Questions

Active and inactive histories having a probability of the same order

\[ \uparrow \]

Coexistence of \textit{dynamical} phases?

→ Need for tools

- How to describe a \textit{dynamical} 1\textsuperscript{st} order phase transition?
- Dynamical Landau free-energy landscape? (\textit{i.e.} competition between different optima)
Questions

Active and inactive histories having a probability of the same order

Coexistence of dynamical phases?

→ Need for tools

- How to describe a dynamical 1st 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

- \( \beta \) conjugated to energy \((\text{statics})\)
- \( s \) conjugated to activity \( K \) \((\text{dynamics})\)

\[ P(K \approx kt, t) \sim e^{t\pi(k)} \quad \psi(s) = \max_k \{\pi(k) - sk\} \]
Dynamical phase transition: FA model \((d=1)\)

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

\[
\rho(0) = c
\]

Comparison between constrained and unconstrained dynamics

more active \((K > \bar{K})\)  
less active \((K < \bar{K})\)
Dynamical Landau free-energy landscape $\mathcal{F}(\rho, s)$

Dynamical free energy: $\psi(s) = -\min_{\rho} \mathcal{F}(\rho, s)$

reached at $\rho = \rho(s)$
Dynamical free energy picture: in “mean-field”

“Mean-field” version of the FA model:

\[ A + A \xrightleftharpoons[c\leftrightarrow_1]{} A \]

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

\[ W(n) + W(n) = c(Ln) \]
\[ W(n) = (1 - c) \]

Kinetic constraint/number of excited neighbours
Dynamical free energy picture: in “mean-field”

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

\[ A + A \xrightarrow{c}{1-c} A \]

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
Dynamical free energy picture: in “mean-field”

Extremalization principle:

\[ \psi(s) = - \min_{P \neq 0} \frac{\langle P \rvert - \mathcal{W}_{K}^{\text{sym}}(s) \rvert P \rangle}{\langle P \rvert P \rangle} \]
Dynamical free energy picture: in “mean-field”

Extremalization principle:

\[ \psi(s) = - \min_{P \neq 0} \frac{\langle P \mid - W_{\text{sym}}^{K}(s) \mid P \rangle}{\langle P \mid P \rangle} \]

Thermodynamic limit (finite density \( \rho = \frac{n}{L} \)):

\[ P(n) \sim e^{-Lf(n/L)} \]

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

\[ = - \min_{\rho} \mathcal{F}(\rho, s) \]
Dynamical phase transition model on a complete graph

Dynamical free energy picture: in “mean-field”

Extremalization principle:

\[ \psi(s) = - \min_{P \neq 0} \frac{\langle P \rangle - \mathbb{W}^{\text{sym}}_K(s) \mid P \rangle}{\langle P \mid P \rangle} \]

Thermodynamic limit (finite density \( \rho = \frac{n}{L} \)):

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

\[ = - \min_{\rho} \mathcal{F}(\rho, s) \]

One can also use Donsker-Varadhan

\[ \langle e^{-sK \delta\left( \frac{1}{Lt} \int_0^t dt' \ n(t') = \rho \right)} \rangle \sim e^{-tL\mathcal{F}(\rho, s)} \]
Dynamical free energy picture: in “mean-field”

Mean-field version of the FA model:

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

\[ \mathcal{F}(\rho, s) \]

\[ s > s_{sp} \]
\[ s > 0 \]
\[ s = 0 \]
\[ s < 0 \]
Dynamical phase transition model on a complete graph

Dynamical free energy picture: in “mean-field”

Mean-field version of the FA model:

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

\[
\mathcal{F}(\rho, s)
\]

the steady state \((s = 0)\)

is critical

\[
\rho
\]

\[
s = 0
\]
Dynamical free energy picture: in “mean-field”

Mean-field version of the FA model:

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

\[ \mathcal{F}(\rho, s = 0) \]

\[ \rho \]

unconstrained

constrained
Rounding of the first-order transition

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

[same picture for $-\frac{1}{L} \psi' (\lambda / L) = \frac{1}{Lt} \langle K \rangle_{s=\lambda / L}$]

(transition at $\lambda_c > 0$)
Finite-size effects: required to understand $P(K, t)$

Scale of fluctuations: $s = \frac{\lambda}{L}$

(transition at $\lambda_c > 0$)

\[
\rho(\lambda L) = \frac{1}{L} \psi'(\lambda/L) = \frac{1}{Lt} \langle K \rangle_{s=\lambda/L}
\]
Finite-size effects: required to understand $P(K, t)$

Scale of fluctuations: $s = \frac{\lambda}{L}$

(transition at $\lambda_c > 0$)

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

[same picture for $-\frac{1}{L} \psi'(\lambda/L) = \frac{1}{Lt} \langle K \rangle_{s=\lambda/L}$]
Idea of the method

Extremalization principle:

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

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

- infinite-size limit: one only needs \( \rho = \arg\min f \)
- in a window around \( \lambda_C \): one needs more
Idea of the method

Extremalization principle:

\[ \psi(s) = - \min_{P \neq 0} \frac{\langle P | - W_{K}^{\text{sym}}(s) | P \rangle}{\langle P | P \rangle} \]

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 \( \lambda_c \): one needs more

Equation for \( f(\rho) \) (from extremalization)
Idea of the method

**Extremalization principle:**

\[
\psi(s) = - \min_{P \neq 0} \frac{\langle P | - W_{K}^{\text{sym}}(s) | P \rangle}{\langle P | P \rangle}
\]

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

- infinite-size limit: one only needs \( \rho = \arg\min f \)
- in a window around \( \lambda_c \): one needs more

**Equation for \( f(\rho) \) (from extremalization)**

**Exactly at coexistence \( (\lambda = \lambda_c) \): non-analyticity of \( f(\rho) \)**

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

**Around coexistence \( (\lambda \approx \lambda_c) \):**

\[
P(n) = (1 + a(s)) P_{\text{inactive}}^{n < n_c}(n) + (1 - a(s)) P_{\text{active}}^{n \geq n_c}(n)
\]
Idea of the method

Extremalization principle:

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

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

- infinite-size limit: one only needs $\rho = \arg\min f$
- in a window around $\lambda_c$: one needs more

Equation for $f(\rho)$ (from extremalization)

Exactly at coexistence ($\lambda = \lambda_c$): non-analyticity of $f(\rho)$

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

Around coexistence ($\lambda \approx \lambda_c$): [in a good basis]

$$
P(n) = (1 + a(s))P^{n < n_c}_{\text{inactive}}(n) + (1 - a(s))P^{n \geq n_c}_{\text{active}}(n)
$$
Idea of the method

Extremalization principle:

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

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

- infinite-size limit: one only needs $\rho = \arg\min f$
- in a window around $\lambda_c$: one needs more

Equation for $f(\rho)$ (from extremalization)

Exactly at coexistence ($\lambda = \lambda_c$): non-analyticity of $f(\rho)$

$$P(n) = P_{inactive}^{n tuple} + P_{active}^{n tuple}$$

Around coexistence ($\lambda \simeq \lambda_c$): [in a good basis] [sub-finite-size effects]

$$P(n) = (1 + a(s)) P_{inactive}^{n tuple} + (1 - a(s)) P_{active}^{n tuple}$$
Finite size: comparison to 1D

\[ \psi(\lambda/L) = \varphi(\lambda) = -\Sigma + C \left( \frac{\lambda}{L} \right)^{2/3} + \ldots \]
Finite size: comparison to 1D

\[ \pi_L(k) = -L \frac{(k - K)^2}{2K^2} \]

\[ \pi_L(k) = -\Sigma - \frac{4A^3}{27L^2} k^{-2} \]

\[ \pi_L(k) = -r_\infty + Lk \left(1 - \log \frac{Lk}{2\epsilon}\right) \]
Conclusion

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 and geometrical features

Perspectives:

- Finite dimension? [T Bodineau, VL, C Toninelli, JSP 2012]
- Finite time? (Gap, spectral density)
- Other models?
Questions for you

Finite time / finite-size
- Cut-off phenomenon in time $\leftrightarrow s_c \to 0$? [Fabio Martinelli]
- Structure of the left/right eigenvector @ $s > 0$ (i.e. $\nu < 0$)? [Peter Sollich, Rob Jack]

Closeness to critical point
- Mixed-order phase transition also varying $s$, boundary conditions? [Giulio Biroli]
- Spectral density $\leftrightarrow$ finite-time moments of $K$?[JuanP Garrahan]

Relation to quantum models:
- *Link to 1st order quantum phase transition* [Guilhem Semerjian]
  What is the classical $\leftrightarrow$ quantum dictionary?
- Dynamical Landau approach for MBL? [JuanP Garrahan]
Thank you for your attention!

- **Takahiro Nemoto**, VL, Shin-ichi Sasa, Frédéric van Wijland
  arxiv:1405.1658 (2014)
Appendix: operators

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

Maximization principle:

$$\psi(s) = \max_P \frac{\langle P| W^{sym}_K(s) | P \rangle}{\langle P| P \rangle}$$
Appendix: operators

We assume detailed balance: \( P_{eq}(C) W(C \rightarrow C') = P_{eq}(C') W(C' \rightarrow C) \)

Maximization principle:

\[
\psi(s) = \max_P \frac{\langle P|W^{sym}_K(s)|P\rangle}{\langle P|P\rangle}
\]

What is \( W^{sym} \)?

\[
W_{C'C} = W(C \rightarrow C') - r(C)\delta_{CC'}
\]

Symetrization by \( R = \frac{1}{2} P_{eq}(C) \delta_{CC'} \) : \( W^{sym} = R^{-1}WR \)
Appendix: operators

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

Maximization principle:

\[
\psi(s) = \max_P \frac{\langle P | \mathcal{W}_{sym}^k(s) | P \rangle}{\langle P | P \rangle}
\]

What is \( \mathcal{W}_{sym} \)?

\[
\mathcal{W}_{C'C} = \mathcal{W}(C \rightarrow C') - r(C) \delta_{CC'}
\]

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

\[
(\mathcal{W}_{sym})_{C'C} = [\mathcal{W}(C \rightarrow C') \mathcal{W}(C' \rightarrow C)]^{\frac{1}{2}} - r(C) \delta_{CC'}
\]

we have

\[
(\mathcal{W}_{sym})^\dagger = \mathcal{W}_{sym}
\]
Appendix: operators

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

Maximization principle:

\[
\psi(s) = \max_P \frac{\langle P | W_{\text{sym}}^K(s) | P \rangle}{\langle P | P \rangle}
\]

What is \( W_{\text{sym}}^K \)?

\[
(W_{\text{sym}}^K)_{CC'} = e^{-s} W(C \to C') - r(C) \delta_{CC'}
\]

Symetrisation by

\[
R = P_{eq}^{\frac{1}{2}}(C) \delta_{CC'} : \quad W_{\text{sym}}^K = R^{-1} W^K R
\]

\[
(W_{\text{sym}}^K)_{CC'} = e^{-s} [W(C \to C') W(C' \to C)]^{\frac{1}{2}} - r(C) \delta_{CC'}
\]

we have

\[
(W_{\text{sym}}^K)^\dagger = W_{\text{sym}}^K
\]