Thermodynamics of histories: application to systems with glassy dynamics

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Outline

1. Motivations
   - glassy systems
   - a thermodynamic phase transition?
2. Thermodynamics of histories
   - historical background
   - histories versus configurations
3. A picture of phase coexistence
   - kinetically constrained models
   - dynamical free-energy

Glassy systems: a picture

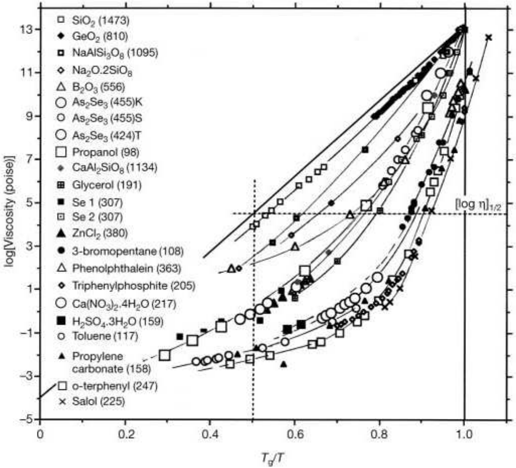

Fig.1 from Martinez and Angell, *Nature* **410** 663 (2001)

Glassy systems: experimental characterisation

Real systems

- glasses obtained from supercooled liquids
- colloids
- magnetic spin glasses
- polydisperse gases of hard spheres

Dramatic slow-down of the dynamics

- viscosity strongly depends on temperature
- large relaxation times τ , heuristic fits:

Glassy systems: experimental characterisation

Real systems

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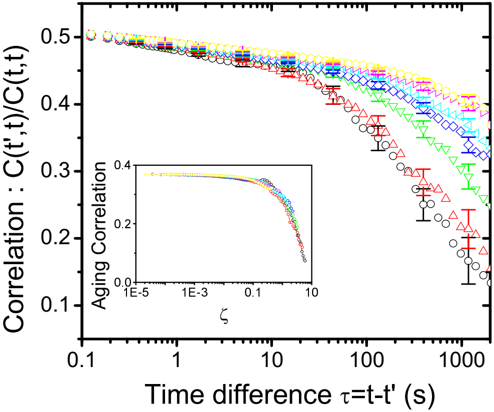
Dramatic slow-down of the dynamics

- viscosity strongly depends on temperature
- large relaxation times τ , heuristic fits:

$$\tau \sim \exp\left(\frac{A}{T - T_0}\right) \quad \text{or} \quad \tau \sim \exp\left(\frac{A}{T^b}\right) \quad \text{or} \ldots$$

Anomalous decay of correlation function: aging

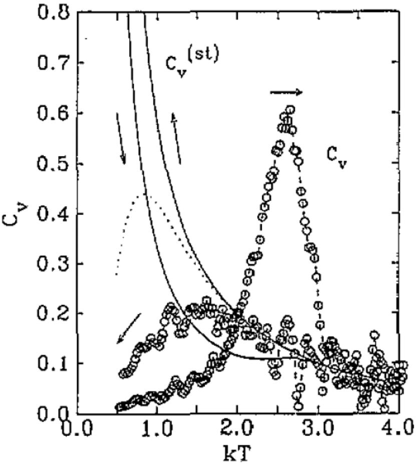
experimental data
(magnetic spin glass)



from Hérisson and Ocio, *PRL* **88** 257202 (2002)

Hysteresis

specific heat in a kinetically constrained model



from Graham, Piché and Grant, *J. Phys. Cond. Matt.*, **5** L349 (1993)

Diverging length

Direct Experimental Evidence of a Growing Length Scale Accompanying the Glass Transition

L. Berthier,[1*] G. Biroli,[2] J.-P. Bouchaud,[3,4] L. Cipelletti,[1]
D. El Masri,[1] D. L'Hôte,[4] F. Ladieu,[4] M. Pierno[1]

Understanding glass formation is a challenge, because the existence of a true glass state, distinct from liquid and solid, remains elusive: Glasses are liquids that have become too viscous to flow. An old idea, as yet unproven experimentally, is that the dynamics becomes sluggish as the glass transition approaches, because increasingly larger regions of the material have to move simultaneously to allow flow. We introduce new multipoint dynamical susceptibilities to estimate quantitatively the size of these regions and provide direct experimental evidence that the glass formation of molecular liquids and colloidal suspensions is accompanied by growing dynamic correlation length scales.

Berthier *et al.*, *Science* **310** 1797 (2005)

($n \geq 4$)-point correlator

BUT...

Absence of thermodynamic phase transition in a model glass former

Ludger Santen & Werner Krauth

CNRS-Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

The glass transition can be viewed simply as the point at which the viscosity of a structurally disordered liquid reaches a universal threshold value[1]. But this is an operational definition that circumvents fundamental issues, such as whether the glass transition is a purely dynamical phenomenon[2]. If so, ergodicity gets broken (the system becomes confined to some part of its phase space), but the thermodynamic properties of the liquid remain unchanged across the transition, provided they are determined as thermodynamic equilibrium averages over the whole phase space. The opposite view[3–6] claims that an underlying thermodynamic phase transition is responsible for the pronounced slow-down in the dynamics at the liquid–glass boundary.

Santen and Krauth, *Nature* **405** 550 (2000)

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   - a thermodynamic phase transition?

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Thermodynamic of histories for glassy systems

Chaotic Properties of Systems with Markov Dynamics

VL, Appert-Rolland and van Wijland, *PRL* **91** 010601 (2005)

Space–time thermodynamics of the glass transition

Mauro Merolle[†], Juan P. Garrahan[‡], and David Chandler[†§]

[†]Department of Chemistry, University of California, Berkeley, CA 94720-1460; and [‡]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom

Contributed by David Chandler, June 15, 2005

We consider the probability distribution for fluctuations in dynamical action and similar quantities related to dynamic heterogeneity. We argue that the so-called "glass transition" is a manifestation of low action tails in these distributions where the entropy of trajectory space is subextensive in time. These low action tails are a consequence of dynamic heterogeneity and an indication of phase coexistence in trajectory space. The glass transition, where the system falls out of equilibrium, is then an order–disorder phenomenon in space–time occurring at a temperature T_g, which is a weak function of measurement time. We illustrate our perspective ideas with facilitated lattice models and note how these ideas apply more generally.

dynamic heterogeneity | entropy | phase transition | supercooled liquids

A glass transition, where a supercooled fluid falls out of equilibrium, is irreversible and a consequence of experimental protocols, such as the time scale over which the system is prepared and the time scale over which its properties are observed (for reviews, see refs. 1–3). It is thus not a transition in

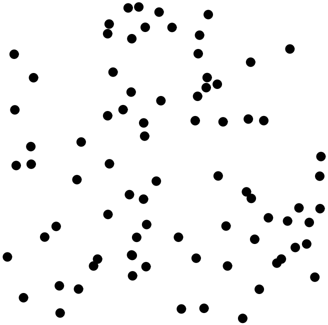
22). In both cases, there is an energy function $J\Sigma_i n_i$, where $J >$ 0 sets the equilibrium temperature scale, n_i is either 1 or 0, indicating whether lattice site i is excited or not, and the sum over i extends over lattice sites. The system moves stochastically from one microstate to another through a sequence of single-cell moves. In the FA model, the state of cell i at time slice $t + 1$, $n_{i,t+1}$, can differ from that at time slice t, $n_{i,t}$, only if at least one of two nearest neighbors, $i \pm 1$, is excited at time t. In the East model the condition is that $n_{i+1,t}$ must be excited. These dynamic constraints affect the metric of motion, confining the space–time volume available for trajectories (23). This mimics the effects of complicated intermolecular potentials in a dense nearly jammed material. Excitations in this picture are regions of space–time where molecules are unjammed and exhibit mobility. As such, we refer to $n_{i,t}$ as the mobility field. For both models, the dynamics is time-reversal symmetric and obeys detailed balance. The equilibrium concentration of excitations, $c \equiv \langle n \rangle = 1/(1 + e^{J/T})$, is the relevant control parameter. The average distance between excitations sets the characteristic length scale for relaxation, $\ell \approx$

PNAS PNAS PNAS

PHYSICS

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

Histories vs configurations



fluctuation of configurations

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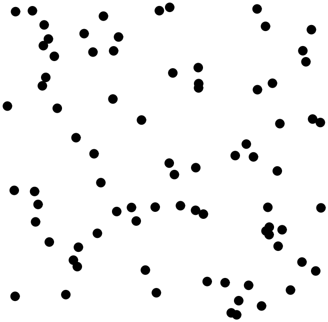

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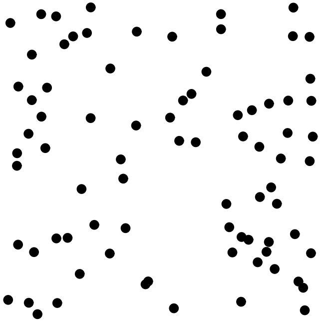

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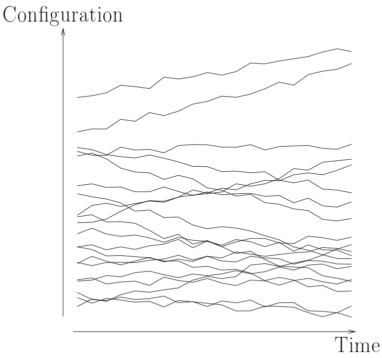

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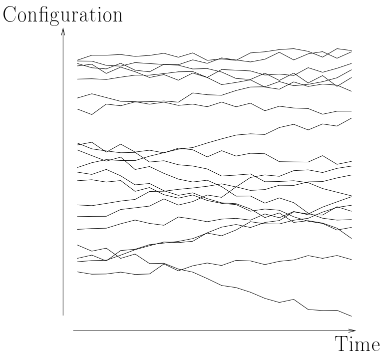

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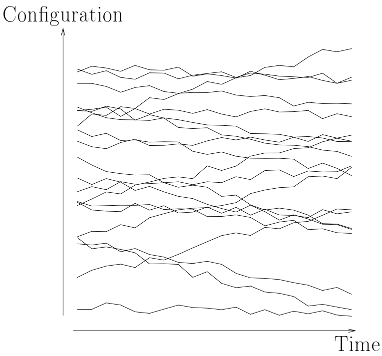

fluctuation of histories

Historical perspective

Historical background in mathematics

- Ruelle's thermodynamic formalism: deterministic dynamics
- work of Kolmogorov, Sinai, Shannon

In physics

- Gaspard: *discrete* time stochastic dynamics
- our contribution: *continuous* time stochastic dynamics

Historical perspective

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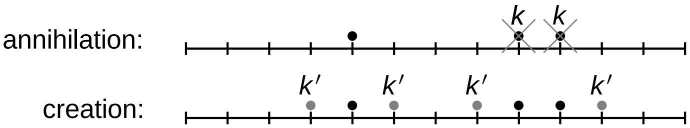
Kinetically Constrained Models (KCM)

Fredrickson Andersen model in 1D

- L sites $\boldsymbol{n} = \{n_i\}$ with $n_i = 1$ or 0 in one dimension
- Constraint: at least one neighbor is alive to allow an event
- Transition rates:
  - annihilation with rate $W(1_i \to 0_i) = k$
  - creation with rate $W(0_i \to 1_i) = k'$



Outline

Classification of histories using time-extensive parameters on $[0, t]$

- number of *configuration change*: K
- *"dynamical complexity"*: Q_+

$$Q_+[\textit{history}] = \ln \mathrm{Prob}[\textit{history}] = \sum_{k=1}^{K} \ln \frac{W(\boldsymbol{n}_k \to \boldsymbol{n}_{k+1})}{r(\boldsymbol{n}_k)} \qquad \text{with} \quad r(\boldsymbol{n}) = \sum_{\boldsymbol{n}' \neq \boldsymbol{n}} W(\boldsymbol{n} \to \boldsymbol{n}')$$

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Probing the space of histories: particle density $\rho(K)$, $\rho(Q_+)$

$$\rho(K) = \sum_{\substack{\text{histories} \\ \text{from } 0 \text{ to } t}} \delta\big(K - K[\textit{hist}]\big)\,\rho(t)$$

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Dynamical entropy

Kolmogorov Sinai entropy

$$h_{\mathrm{KS}} = -\lim_{t\to\infty} \frac{1}{t} \sum_{\text{histories}} \mathrm{Prob}\{\text{history}\} \ln \mathrm{Prob}\{\text{history}\} = -\lim_{t\to\infty} \frac{1}{t} \langle Q_+ \rangle$$

Lyapunov exponents for deterministic dynamics

Pesin theorem: $$h_{\mathrm{KS}} = \sum_{\lambda_i > 0} \lambda_i$$

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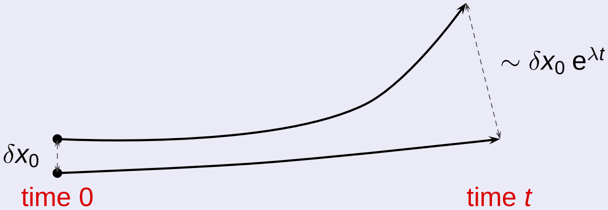
Lyapunov exponents for deterministic dynamics



Pesin theorem:

$$h_{KS} = \sum_{\lambda_i > 0} \lambda_i$$

Dynamical partition function

Probing fluctuations (1): the micro-canonical way

- Thermodynamics of configurations

$$Z(E,N) = \sum_{\boldsymbol{n}} \delta\big(E - \mathcal{H}(\boldsymbol{n})\big) \qquad \text{(large } N\text{)}$$

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- Thermodynamics of histories [Ruelle]

$$Z_{\text{dyn}}(Q_+, t) = \sum_{\substack{\text{histories}\\ \text{from 0 to } t}} \delta\big(Q_+ - Q_+[\mathit{history}]\big) \qquad \text{(large } t\text{)}$$

Dynamical partition function

Probing fluctuations (2): the canonical way

- Thermodynamics of configurations

$$Z(\beta, N) = \sum_{\boldsymbol{n}} e^{-\beta\,\mathcal{H}(\boldsymbol{n})} = e^{-N\,f(\beta)} \qquad \text{(large } N\text{)}$$

- Thermodynamics of histories [Ruelle]

$$Z_{\text{dyn}}(s, t) = \sum_{\substack{\text{histories}\\ \text{from 0 to } t}} \text{Prob}\{\text{history}\}^{1-s} = e^{-t\,f_{\text{dyn}}(s)} \qquad \text{(large } t\text{)}$$

Canonical (dynamical) ensemble

- β conjugated to energy
- s conjugated to dynamical complexity Q_+

Dynamical partition function

Probing fluctuations (2): the canonical way

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Canonical (dynamical) ensemble

$$\rho_+(s) = \frac{1}{Z_{\mathrm{dyn}}(s,t)} \sum_{Q_+} \mathrm{e}^{-s\,Q_+} \rho(Q_+)$$

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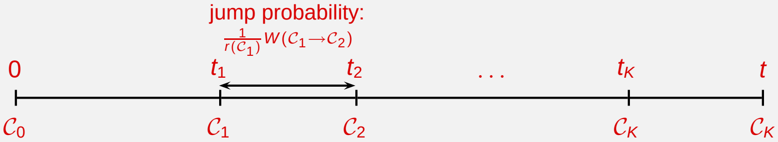
$$Z_{\text{dyn}}(s,t) = \sum_{\substack{\text{histories}\\ \text{from 0 to } t}} \text{Prob}\{\text{history}\}^{1-s} = \mathrm{e}^{-t\,f_{\text{dyn}}(s)} \qquad \text{(large } t\text{)}$$

Canonical (dynamical) ensemble

$$\rho_K(s) = \frac{1}{Z_{\text{K}}(s,t)} \sum_K \mathrm{e}^{-s\,K}\,\rho(K)$$

Explicit construction (1)

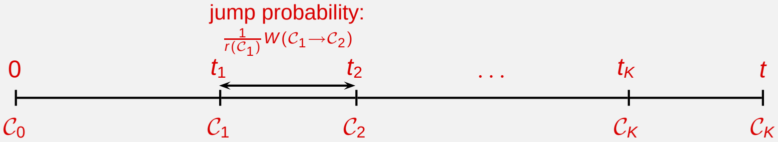


Markov process

- probabilities → rates: $w(\mathcal{C} \to \mathcal{C}') = \tau\, W(\mathcal{C} \to \mathcal{C}')$
- master equation (limit $\tau \to 0$)

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

Explicit construction (1)



Which configurations will be visited?

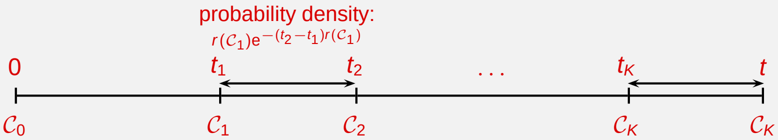
Configurational part of the trajectory: $\mathcal{C}_0 \to \ldots \to \mathcal{C}_K$

$$\text{Prob}\{\text{history}\} = \prod_{n=0}^{K-1} \frac{W(\mathcal{C}_n \to \mathcal{C}_{n+1})}{r(\mathcal{C}_n)}$$

where

$$r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}')$$

Explicit construction (2)



When shall the system jump from one configuration to the next one?

- probability density for the time interval $t_n - t_{n-1}$

$$r(\mathcal{C}_{n-1})e^{-(t_n-t_{n-1})r(\mathcal{C}_{n-1})}$$

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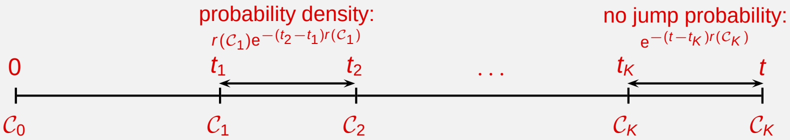

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- probability density for the time interval $t_n - t_{n-1}$

$$r(\mathcal{C}_{n-1})e^{-(t_n-t_{n-1})r(\mathcal{C}_{n-1})}$$

- probability not to leave $\mathcal{C}_K$ during the time interval $t - t_K$

$$e^{-(t-t_K)r(\mathcal{C}_K)}$$

Results

Explicit expression

$$Z_{\text{dyn}}(s,t|\mathcal{C}_0,t_0) = \sum_{K=0}^{+\infty} \sum_{\mathcal{C}_1,\ldots,\mathcal{C}_K} \int_{t_0}^{t} dt_1 \int_{t_{K-1}}^{t} dt_K$$

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$$\int_{t_{K-1}}^{t} dt_K \, r(\mathcal{C}_{K-1}) e^{-(t_K-t_{K-1})r(\mathcal{C}_{K-1})}$$
$$e^{-(t-t_K)r(\mathcal{C}_K)}$$

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$$
\begin{aligned}
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&\quad \int_{t_{K-1}}^{t} dt_K\, r(\mathcal{C}_{K-1}) e^{-(t_K-t_{K-1}) r(\mathcal{C}_{K-1})} \\
&\quad e^{-(t-t_K) r(\mathcal{C}_K)} \left[\prod_{n=1}^{K} \frac{W(\mathcal{C}_{n-1}\to\mathcal{C}_n)}{r(\mathcal{C}_{n-1})} \right]^{1-s} \\
&= \left\langle e^{-s\, Q_+} \right\rangle
\end{aligned}
$$

Results

Canonical (dynamical) s-state

- micro-canonical: fixed value of Q_+
- canonical: fixed value of s

$s > 0$: more active state ("high" Q_+)
$s = 0$: steady state
$s < 0$: less active state ("low" Q_+)

Of practical interest

- $f_{\text{dyn}}(s)$ = smallest eigenvalue of some operator
- corresponding eigenvector = s-state

$\rightarrow$ exact results, numerical approach

Numerical method (with J. Tailleur)

Evaluation of large deviation functions

$$Z_{\text{dyn}}(s,t) = \left\langle e^{-s\,Q_+} \right\rangle \sim e^{t f_{dyn}(s)}$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: J. Tailleur, VL [*work in progress*]

Cloning dynamics

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t) - r_s(\mathcal{C}) P(\mathcal{C},t)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C}) P(\mathcal{C},t)}_{\text{cloning term}}$$

- numerical evaluation of $f_{dyn}(s)$
- direct visualization of s-states

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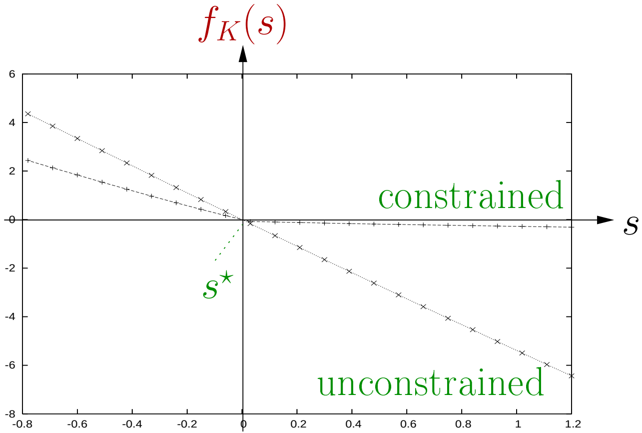
Dynamical phase transition: FA model (d=1)



Comparison between constrained and unconstrained model

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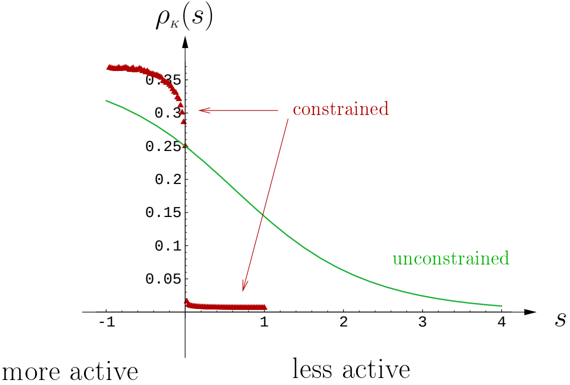
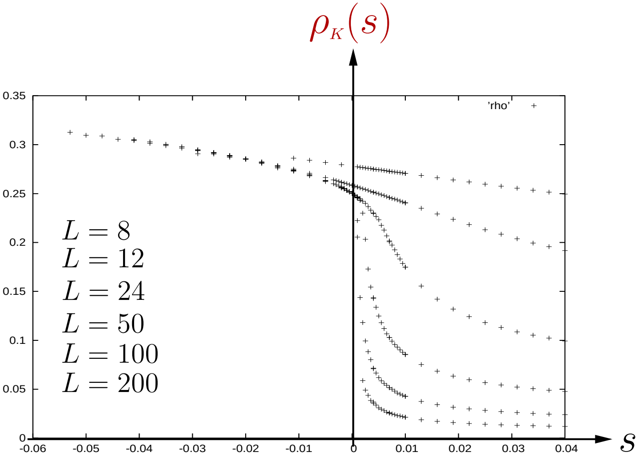


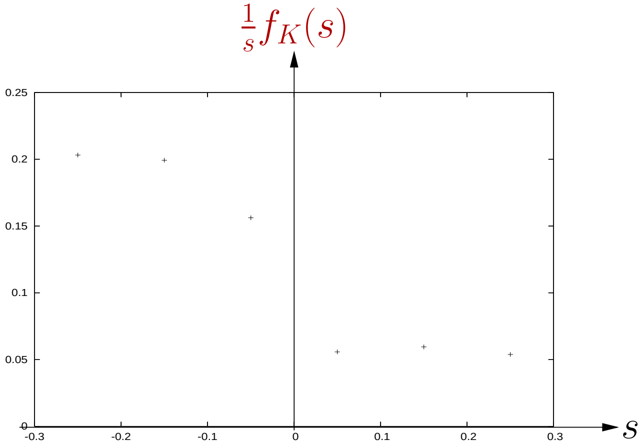
Comparison between constrained and unconstrained model

Dynamical phase transition: EAST model (d=1)



Large size scaling

Dynamical phase transition: TLG



$f_K(s)$ for the triangular lattice gas

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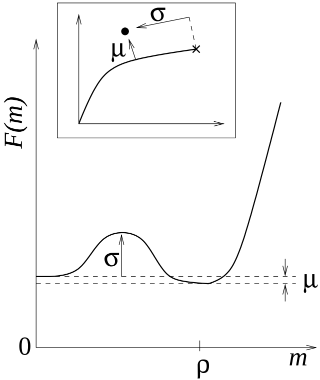
   - dynamical free-energy

Dynamical free energy picture (1)



From Jack, Garrahan and Chandler, [cond-mat/0604068]

Dynamical free energy picture (2)

Mean-field version of the FA model:

$$A + A \underset{\zeta}{\overset{1}{\rightleftharpoons}} A$$

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Rates for occupation number n (with N sites):

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

Dynamical free energy picture (2)

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:

$$f_{\text{dyn}}(s) = \max_Q \frac{\langle Q|\mathbb{W}_K^{\text{sym}}(s)|Q\rangle}{\langle Q|Q\rangle}$$

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What is $\mathbb{W}^{\text{sym}}$?

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

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

we have

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

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Maximization principle:

$$f_K(s) = \max_{Q} \frac{\langle Q | \mathbb{W}_K^{\mathrm{sym}}(s) | Q \rangle}{\langle Q | Q \rangle}$$

Dynamical free energy picture (2)

Maximization principle:

$$f_{\mathrm{K}}(s) = \max_{Q} \frac{\langle Q|\mathbb{W}_K^{\mathrm{sym}}(s)|Q\rangle}{\langle Q|Q\rangle}$$

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

$$\frac{1}{N} f_{\mathrm{K}}(s) = \max_{\rho} \Big\{ 2e^{-s}\sqrt{W_+ W_-} - W_+ - W_- \Big\}$$

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The result holds whenever detailed balance is satisfied.

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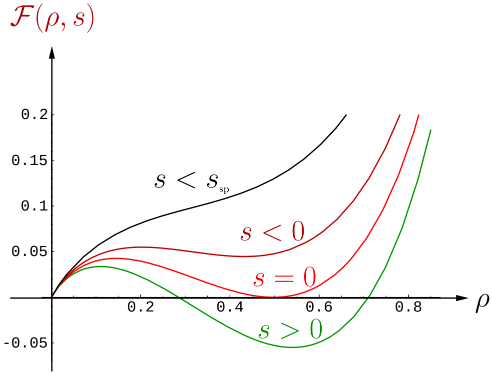

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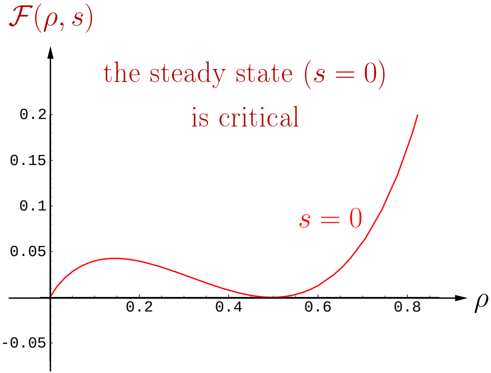

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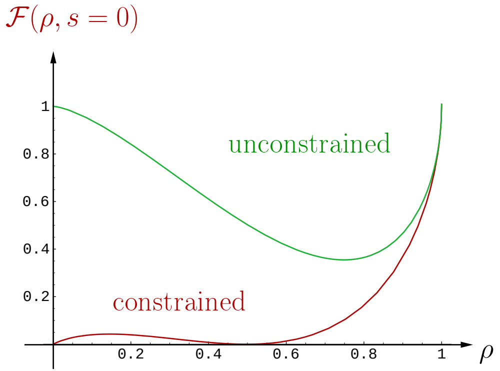


Conclusions

Framework

- Unified picture
- Criticality in a "hidden" dynamical direction

Main results

- s-states $\equiv$ probe of dynamical aspects of the steady state
- Efficient tools to find dynamical phase transition in physical models
- glassiness in KCM's $\leftrightarrow$ $s = 0$ is a critical point

Conclusions

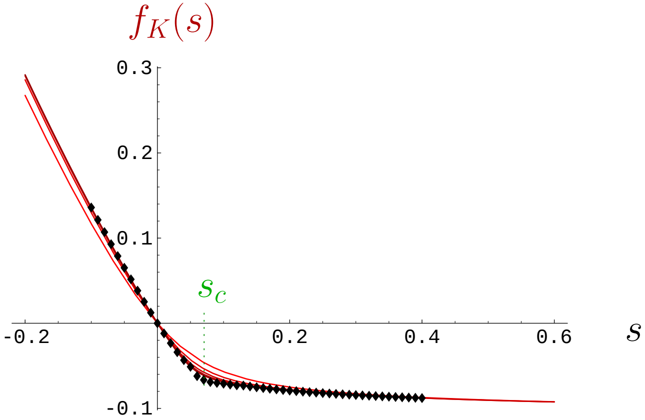
Perspectives – Open questions

- Relations between $\langle K^2 \rangle_c$ and $(n \geq 4)$-correlators?
- Measurement of the h_{KS} entropy jump at $s = 0$?
- Quantitative behaviour of time relaxation?
- Experimental predictions?
- Experimental realization of s-states?

References:

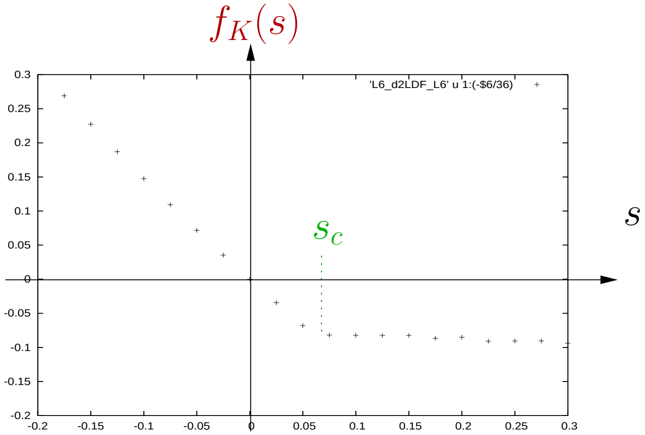
- *PRL* **91** 010601 (2005)
- `cond-mat/0606211` (to appear in *J. Stat. Phys.*)

Dynamical phase transition: contact process (d=1)



Dynamical critical point at $s_c > 0$

Dynamical phase transition: contact process (d=2)



Dynamical critical point at $s_c > 0$