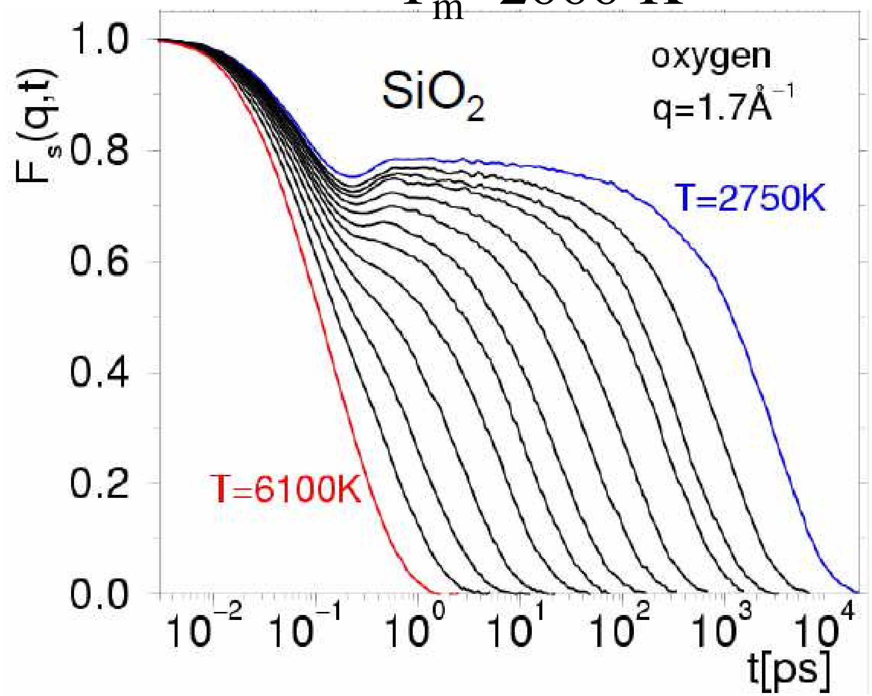
Activated Dynamics in High-Dimensional Rugged Landscapes

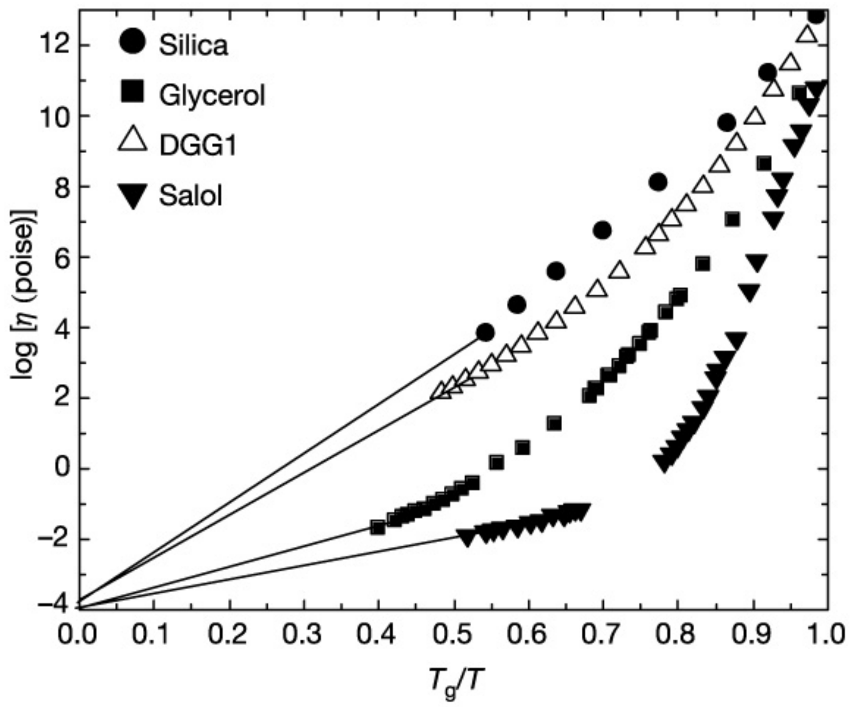
Marco Baity-Jesi (Columbia University)
Chiara Cammarota (King’s College London)

KITP program: The Rough High-Dimensional Landscape Prblem
UCSB, Jan 29th 2019

Slow glassy dynamics

T_m=2000 K



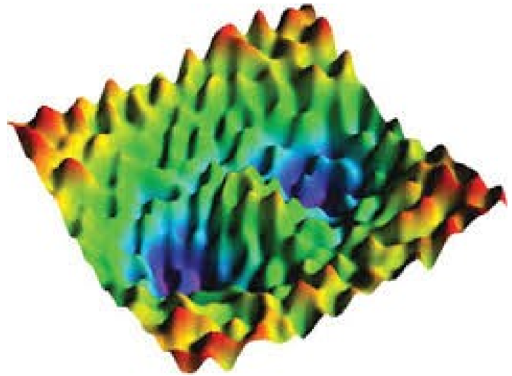


Viscosity grows steeply upon supercooling a liquid

The glass problem: what is the mechanism behind this phenomenon?

Landscape of glasses:

- High-dimensional
- Non-convex
- Rugged



Similar to landscape of most problems treated in this program.

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 51, NUMBER 9 1 NOVEMBER 1969

Viscous Liquids and the Glass Transition: A Potential Energy Barrier Picture

MARTIN GOLDSTEIN

Belfer Graduate School of Science, Yeshiva University, New York, New York 10033

(Received 20 November 1968)

letters to nature

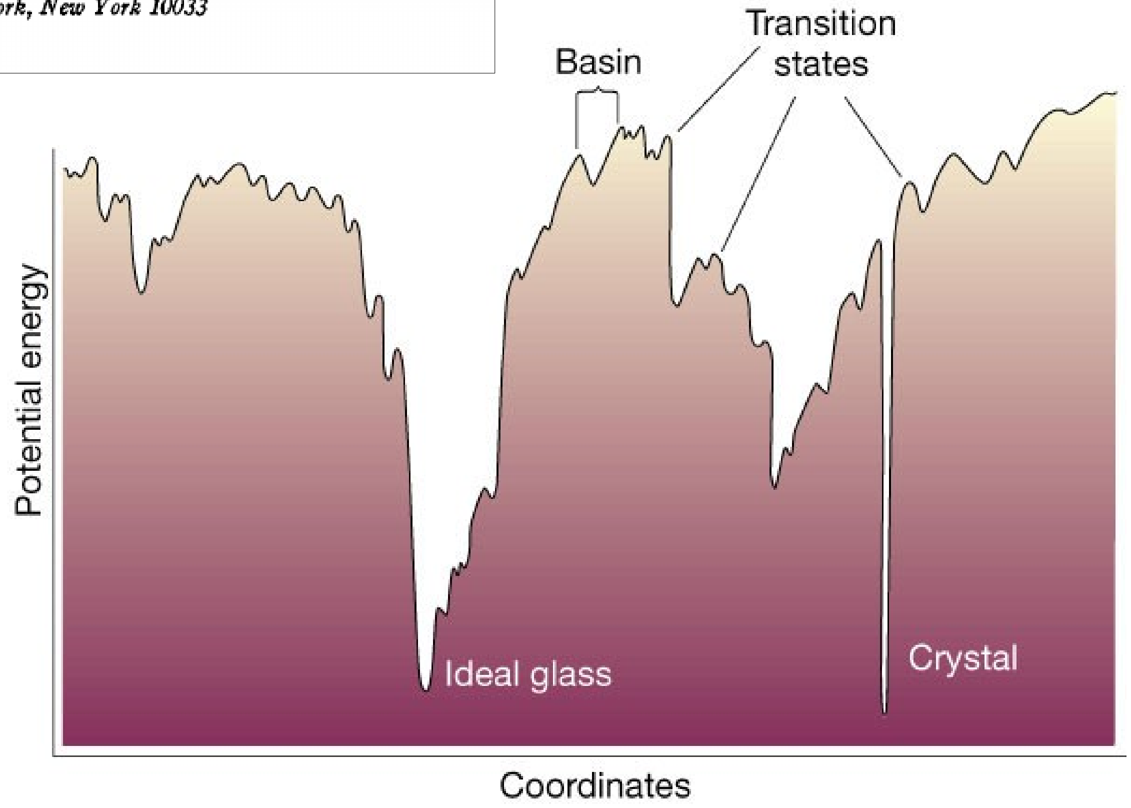
Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid

Srikanth Sastry*†, Pablo G. Debenedetti* & Frank H. Stillinger‡§

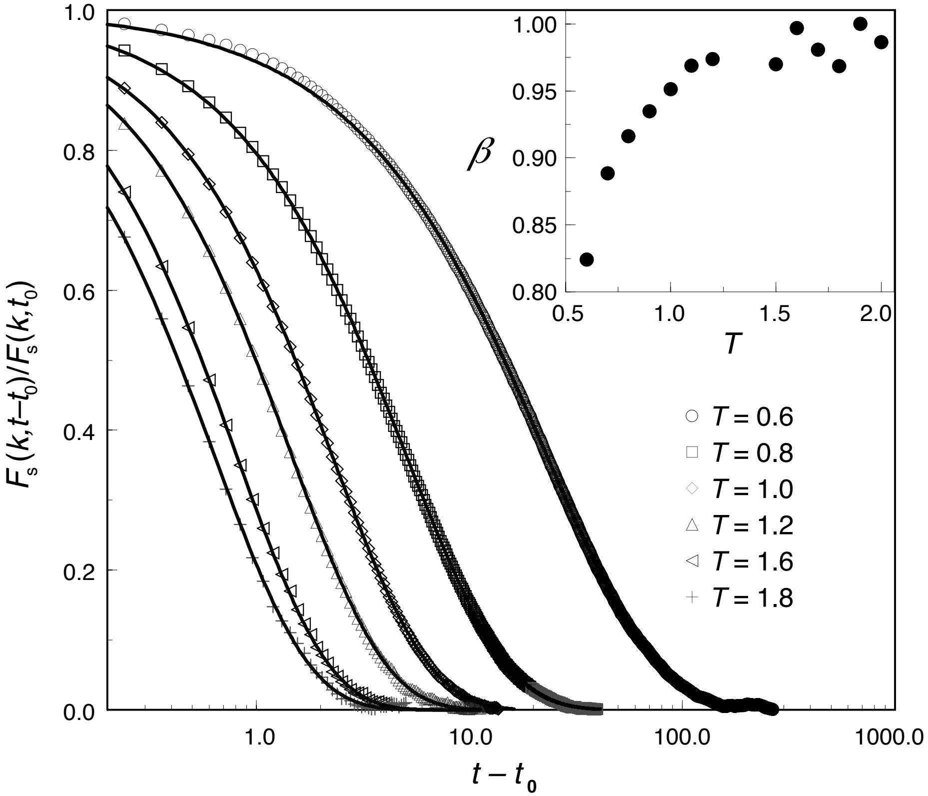
* *Department of Chemical Engineering,* ‡ *Princeton Materials Institute, Princeton University, Princeton, New Jersey 08544, USA*

§ *Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974, USA*

† *Permanent address: Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore 560064, India.*



Onset of glassiness

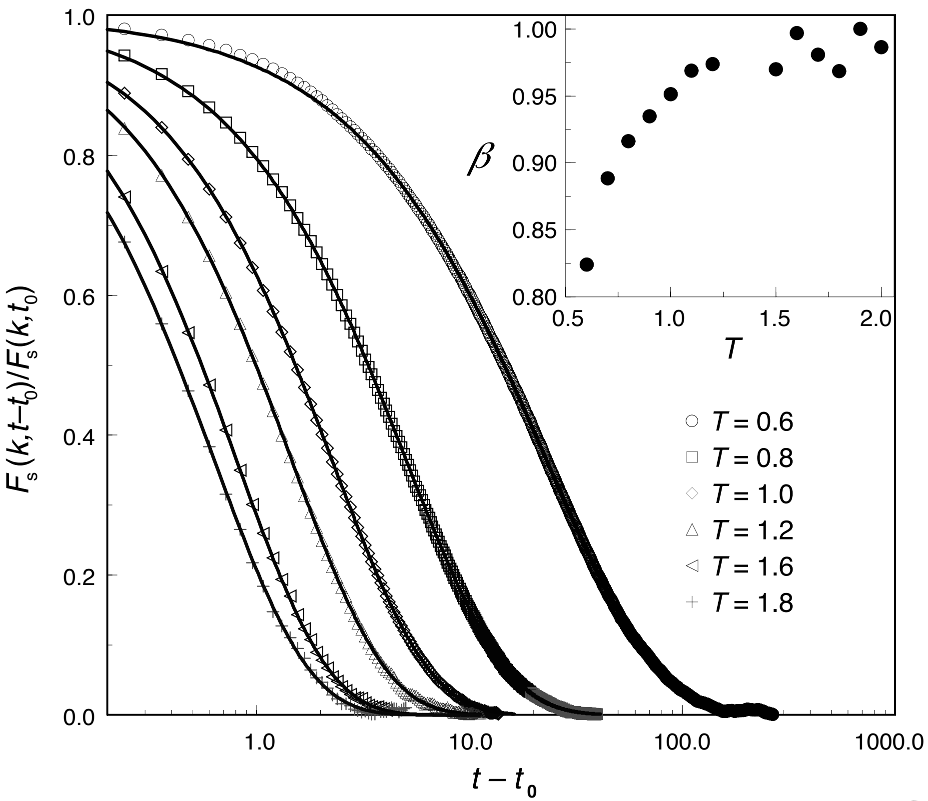


Dynamic correlation functions develop a plateau
-> slow dynamics

Inherent Structure: bottom of minimum visited by dynamics

Explored landscape changes structure
-> deep down in the region with many minima

Onset of glassiness



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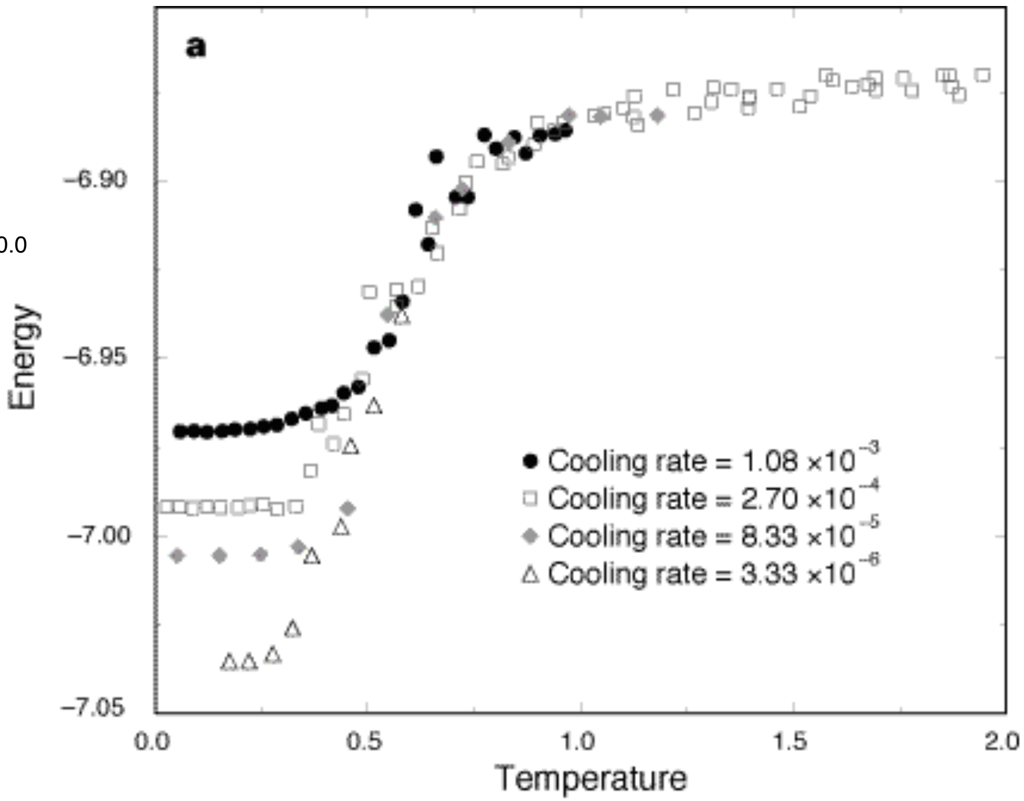


Explored landscape changes structure
-> deep down in the region with many minima

Two dynamical regimes

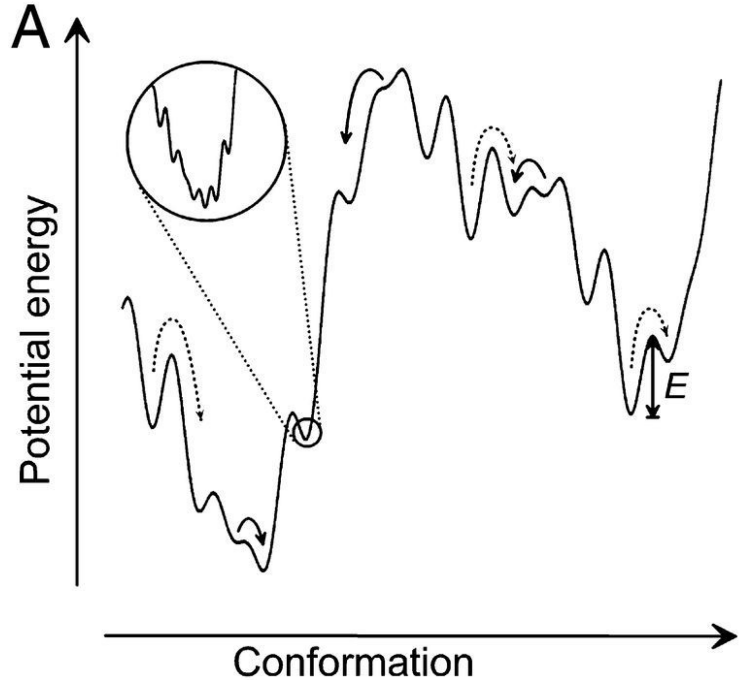
T

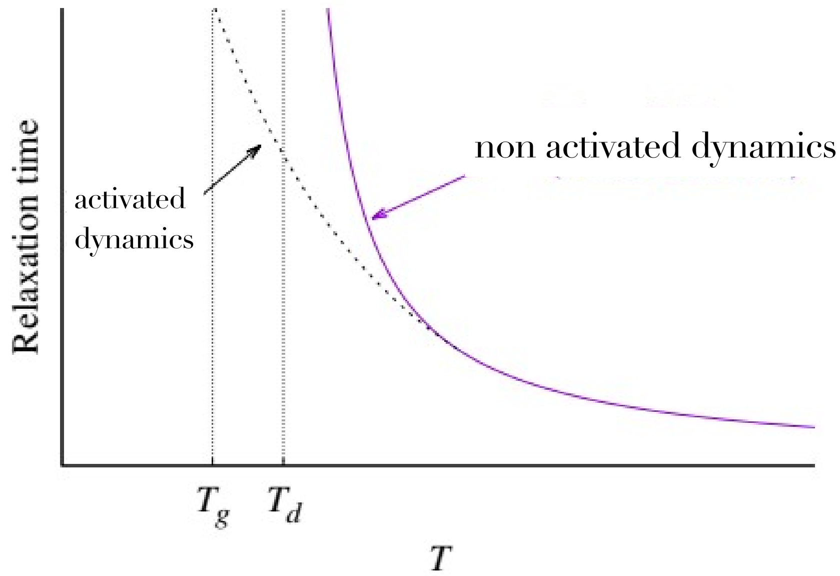
(liquid behaviour)

slow dynamics without barrier crossing

slow dynamics with barrier crossing

$$\tau \sim \exp(\Delta E / k_B T)$$





Mean Field (dense networks)

Barriers are proportional to the number of variables (extensive) $t \sim \exp[N]$

The two dynamical regimes are well separated:

- Short times: $\lim_{t \to \infty} \lim_{N \to \infty}$: $t \leq N$
- Long times: $\lim_{N \to \infty} \lim_{t \to \infty}$: $t >> N$

Results exist essentially in the short-time regime*

This talk is about the long-time regime

✻ VOLUME 71, NUMBER 1 PHYSICAL REVIEW LETTERS 5 JULY 1993

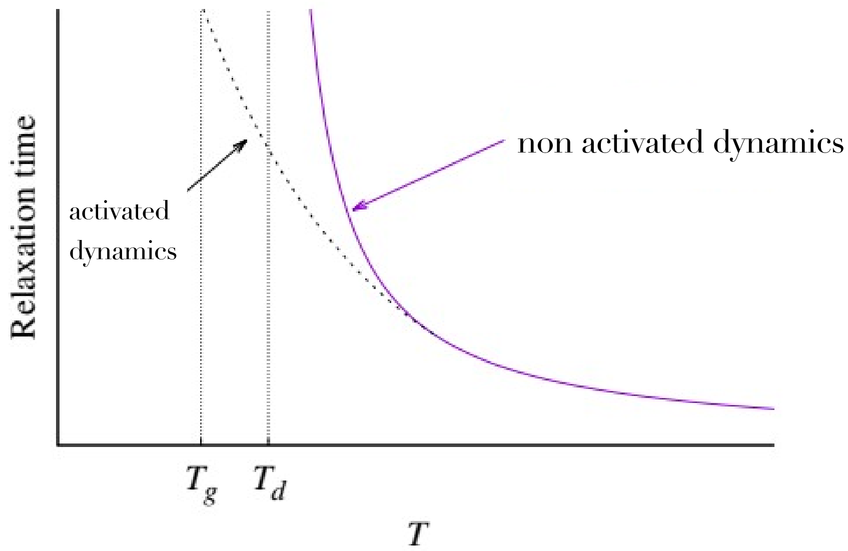
Analytical Solution of the Off-Equilibrium Dynamics of a Long-Range Spin-Glass Model

L. F. Cugliandolo and J. Kurchan
Dipartimento di Fisica, Università di Roma, La Sapienza, I-00185 Roma, Italy
and Istituto Nazionale di Fisica Nucleare, Sezione di Roma I, Roma, Italy
(Received 8 March 1993)

Finite dimension (sparse networks)

The two dynamical regimes are NOT well separated

see Patrick-Grzegorz talk, last week



How can we disentangle them?

Can we rely on simple solvable models to describe activated dynamics?

Low T glass dynamics as Random Walk

PHYSICAL REVIEW E **67**, 030501(R) (2003)

Hopping in a supercooled Lennard-Jones liquid: Metabasins, waiting time distribution, and diffusion

B. Doliwa[1] and A. Heuer[2]
[1]*Max Planck Institute for Polymer Research, 55128 Mainz, Germany*
[2]*Institute of Physical Chemistry, University of Münster, Münster, Germany*

(Received 14 May 2002; published 12 March 2003)

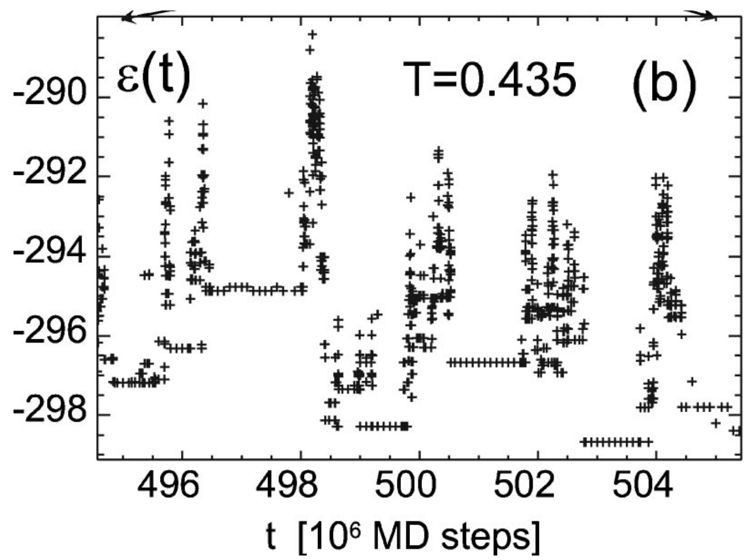
We investigate the jump motion among potential energy minima of a Lennard-Jones model glass former by extensive computer simulation. From the time series of minima energies, it becomes clear that the energy landscape is organized in superstructures called metabasins. We show that diffusion can be pictured as a random walk among metabasins, and that the whole temperature dependence resides in the distribution of waiting times. The waiting time distribution exhibits algebraic decays: $\tau^{-1/2}$ for very short times and $\tau^{-\alpha}$ for longer times, where $\alpha \approx 2$ near T_c. We demonstrate that solely the waiting times in the very stable basins account for the temperature dependence of the diffusion constant.

DOI: 10.1103/PhysRevE.67.030501 PACS number(s): 64.70.Pf, 61.43.Fs, 61.20.Ja, 66.30.−h

Inherent structures along the dynamics

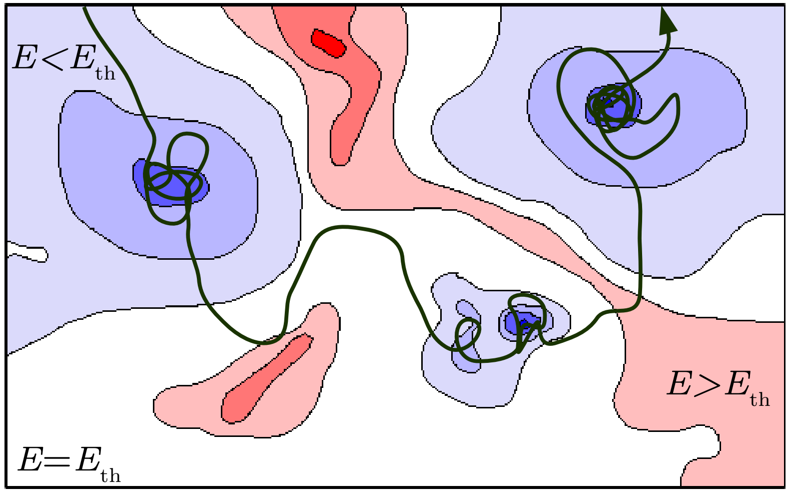
Dynamics seems

- trapped for a long time
- suddenly moving away

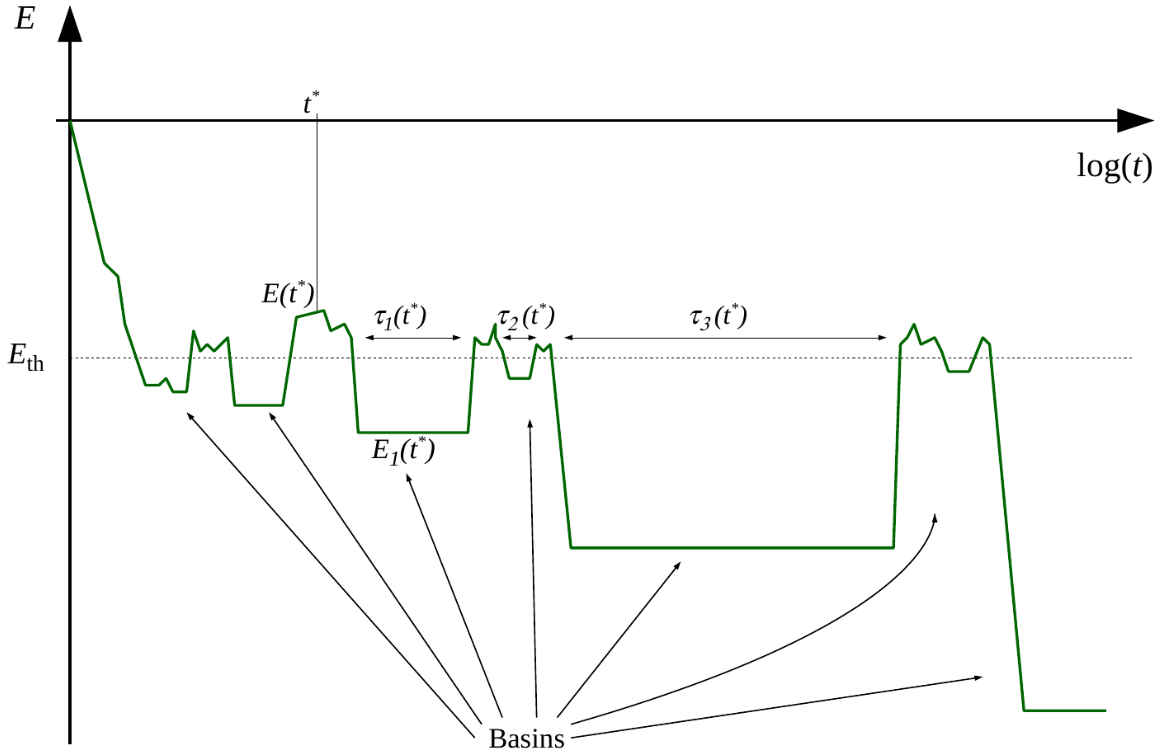


From large-d **to** 1d **description**

Phase space dynamics in Generic Model



Times series of the energy



Bouchaud, 1992

Trap Model (TM)

- Random walk on M-state fully-connected graph

- State i has random energy E_i *from*

$$\rho(E) = \exp(E)\,\Theta(-E)$$

$$E<0$$

- Transitions allowed between <u>any</u> two states. Do **not** depend on final state:

$$p_{i,j} = \exp[-\beta(E_i - E_{th})]\,/M$$

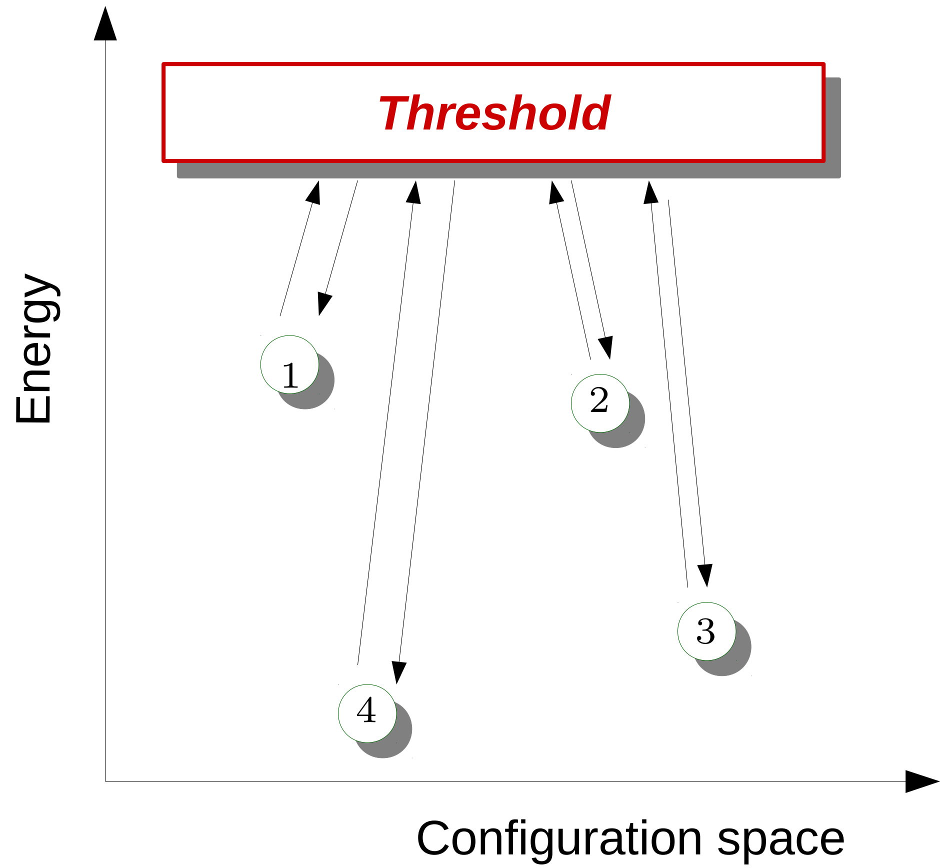
Threshold Energy

$$E_{th} = 0$$

$$\beta = 1/k_B T$$

Renewal process
each time threshold is reached, memory is lost

Static Landscape



Bouchaud, 1992

Some features of the Trap Model

Distribution of Trapping Times τ

$$\psi(\tau) \sim 1/\tau^{1+x} \quad ; \quad x = T/T_c$$

x depends on distribution ρ

Logarithmic Energy

$$<E> \sim -T\log(t)$$

Weak Ergodicity breaking

When $T<T_c$, $\langle \tau \rangle = \infty$

(full phase space can still be visited)

Aging function $\Pi(t_w, t_w+t)$

Probability of remaining in trap between t_w and t_w+t

$$\Pi(t_w, t_w(1+\omega)) \rightarrow H_x(\omega)$$

$$\omega = t/t_w$$

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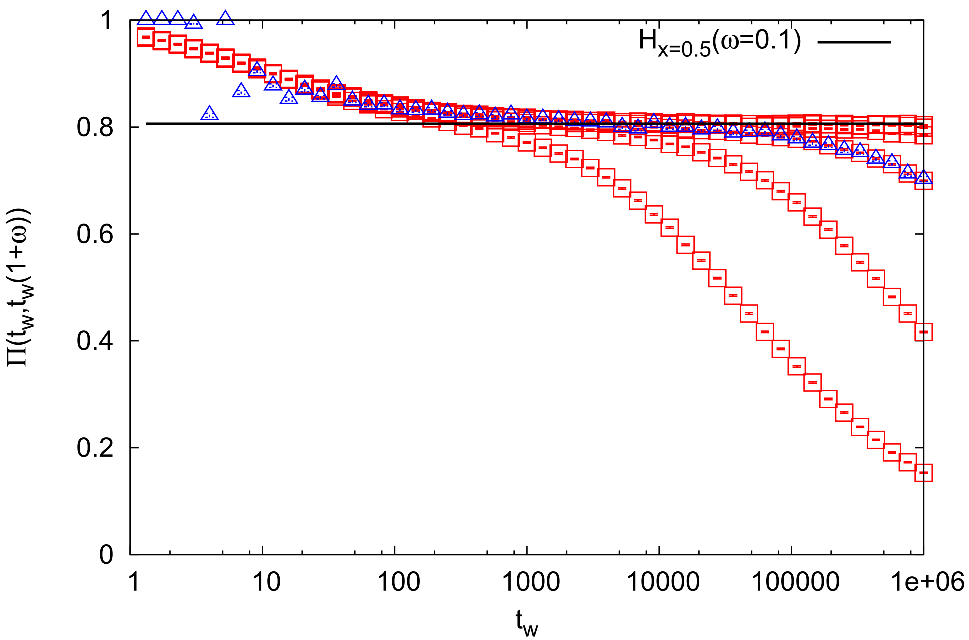

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$$\omega = t/t_w$$

Can the TM be useful?

Use Trap as *null model* for the understanding of activated processes (in any context)

- Can we use the TM to understand activated dynamics in generic models?
- Can it help us to understand their landscape?

Inference -> spiked tensor

Even Deep Neural Networks?

Follow Learning Dynamics

Dynamics not blocked by barriers

<u>In the following:</u>

Barriers not needed

Landscape from activated dynamics

From spiked tensor to REM

Reconstructing from $T_{i_1,\ldots,i_p} = W_{i_1,\ldots,i_p} + v_{i_1}\ldots v_{i_p}$

equivalent to minimising $H = -\sum_{(i_1,\ldots,i_p)} J_{i_1,\ldots,i_p} x_{i_1}\ldots x_{i_p} - rN\left(\sum_i \frac{x_i v_i}{N}\right)^p$

When dynamics starts, signal is small: $\sum_i \frac{x_i v_i}{N} \sim \frac{1}{\sqrt{N}}$

$$H = -\sum_{(i_1,\ldots,i_p)} J_{i_1,\ldots,i_p} x_{i_1}\ldots x_{i_p}$$ p-spin model

(a.k.a. spin MF paradigm for supercooled liquids)

In the large-p limit, p-spin simplifies in the Random Energy Model (REM)

Derrida, 1980

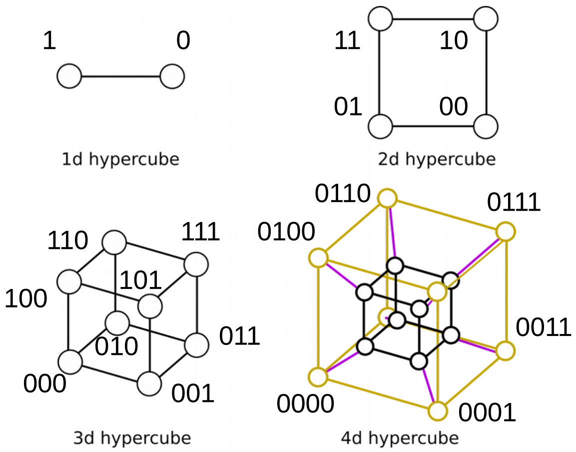
Derrida, 1980

The simplest glass model

Random Energy Model (REM)

- N *spins* $s_i = 0, 1,\ M = 2^N$ states
- Each state has N neighbors
- States i have independent random energy E_i from Gaussian $\rho(E)$
- "Metropolis" rate, only between neighboring states:

$$p_{i,j} = \frac{1}{N} \exp[-\beta\ (E_i - E_j)]$$



Thermodynamics:

$$REM = \lim_{p \to \infty} p - spin$$

Paradigmatic glass model

Derrida, 1980

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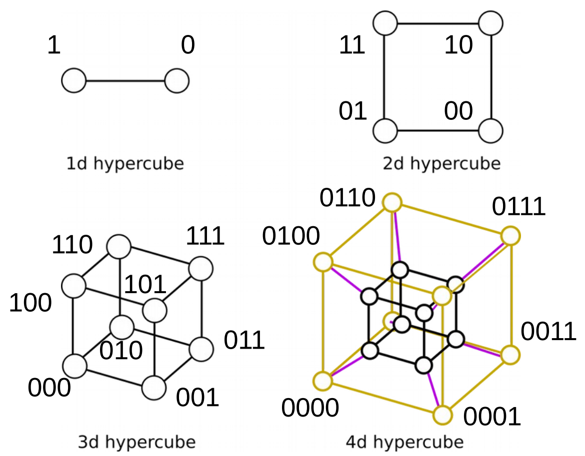
Paradigmatic glass model

N neighbors have $E \in [-\sqrt{2N\log N}, \sqrt{2N\log N}]$

$$E_{th} = -\sqrt{2N\log N} \quad , \quad \lim_{N\to\infty} \frac{E_{th}}{N} = 0$$

Deep basins made of 1 configuration



Derrida, 1980

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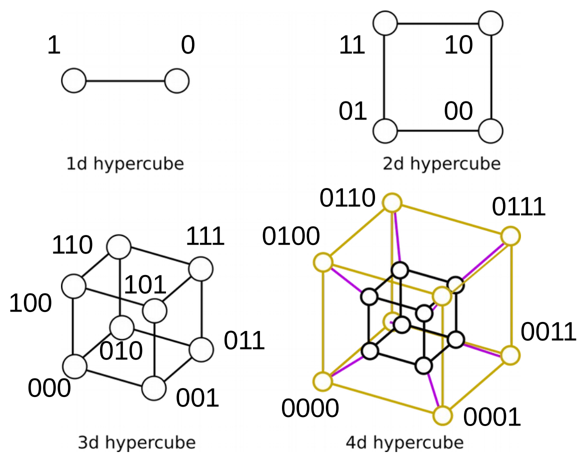


Candidate for trap dynamics

We can study activated dynamics at finite N

Does the system loose memory when $E > E_{\mathrm{th}}$?

Are trap predictions recovered?

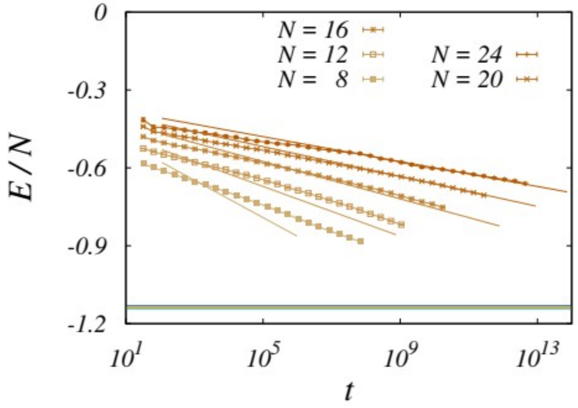
Gayrard, 2017
MBJ, Cammarota & Biroli, 2018

Trap behavior in the REM

Trap predictions are fullfilled

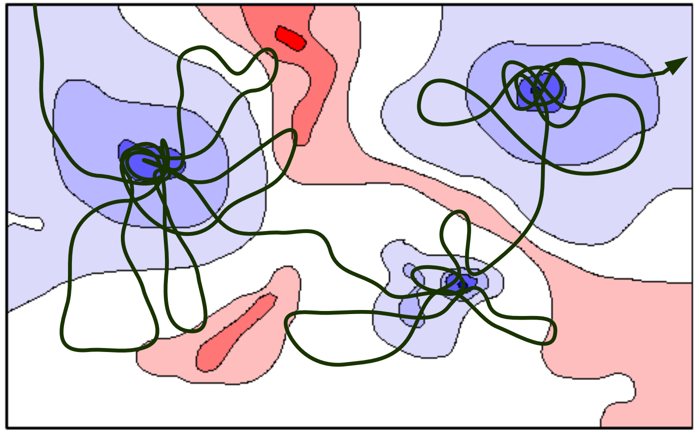
- $E \sim -T\,\log(t)$
- $\psi(\tau) \sim 1/\tau^{1+x}$
- $\Pi(t_w, t_w+t) = H_x(\omega)$
- Renewal

Logarithmic energy

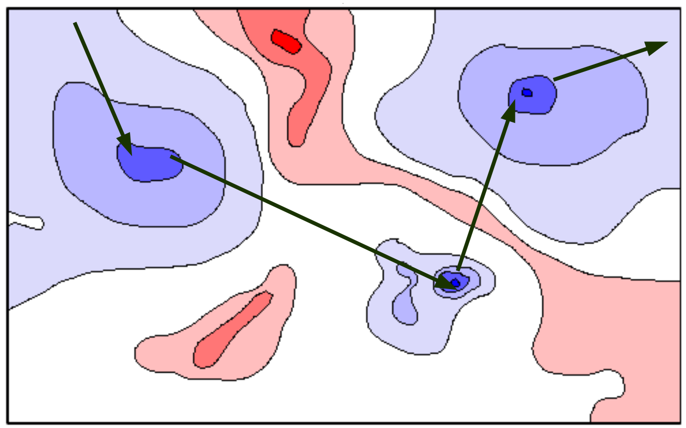


Renewal process

Actual dynamics

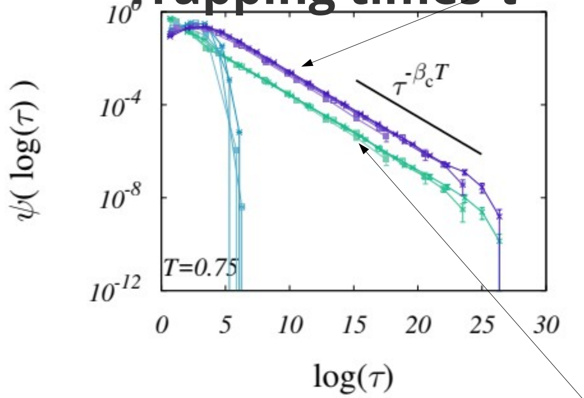


Renormalized dynamics

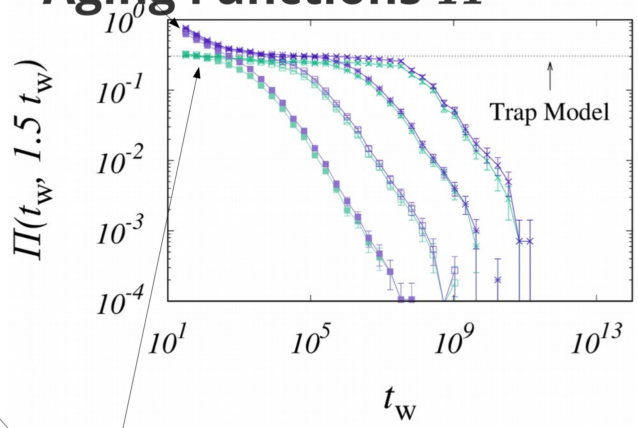


basins

Trapping times τ



Aging Functions Π



configurations

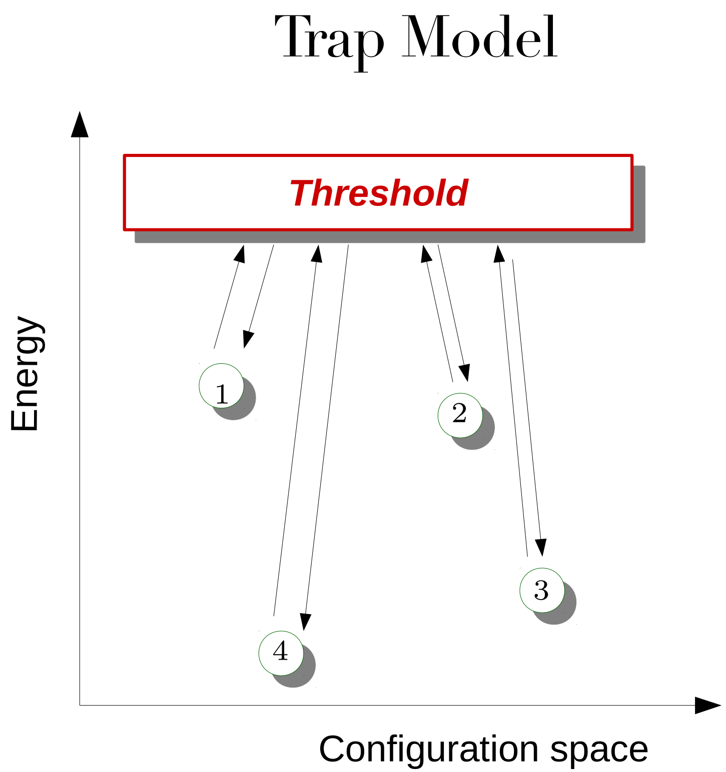
Cammarota & Marinari, 2018

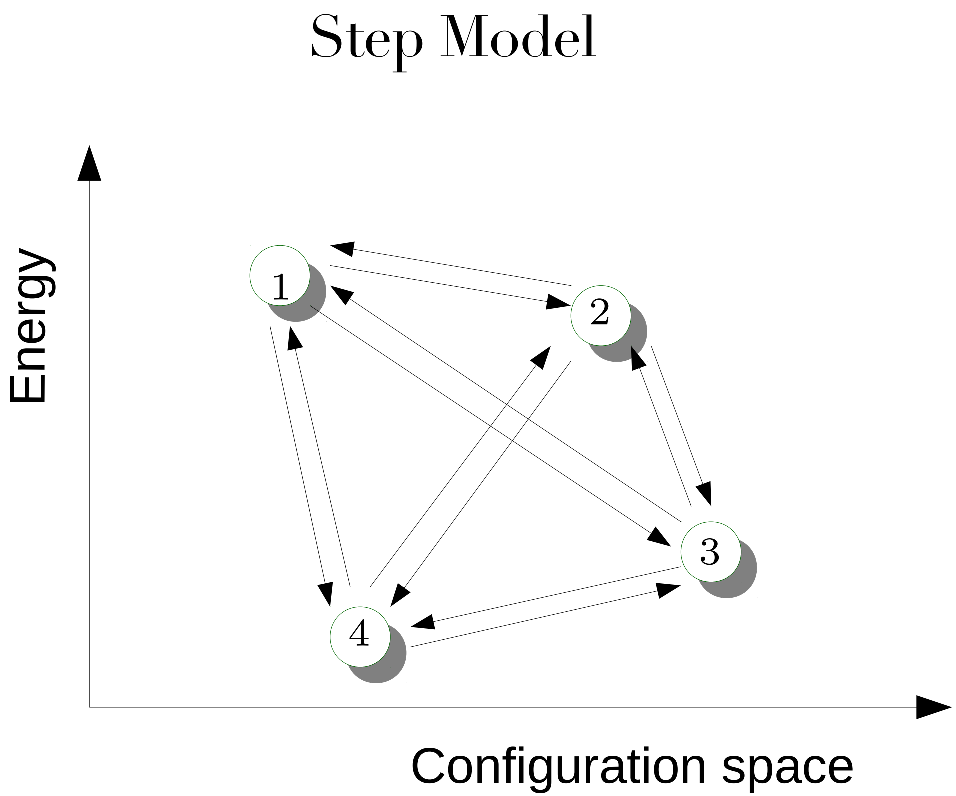
Notes:

- Plots are for exponential $\rho(E)$.*
- Gaussian $\rho(E)$: more involved analysis of $\Pi(t_w, t_w+t)$.
- Exact proof by V. Gayrard for Π with Gaussian $\rho(E)$. Gayrard, 2017
- Other models were shown to be trap (e.g. number partitioning problem). Kurchan & Junier, 2004

*Dyre 1987, Bouchaud and Reichman 2003

A dynamics ruled by Entropy

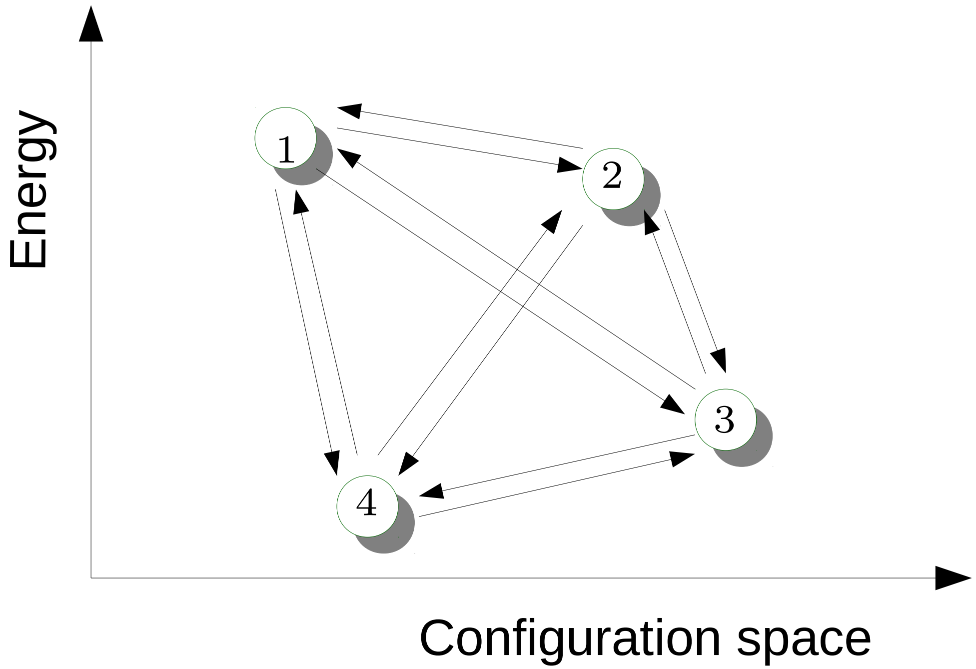




Every configuration dynamically connected with all the others

But let's not introduce artificial barriers!

Step models



Trap model with metropolis dynamics

$$p_{i,j} = \frac{1}{M} min[1, e^{-\beta\,(E_i - E_j)}]$$

Low T:

Barrat, Mézard, Journal de Physique I 5, 941 (1995)

- Aging results do not depend on temperature
- Slowing down entirely due to entropic reasons

Higher T:

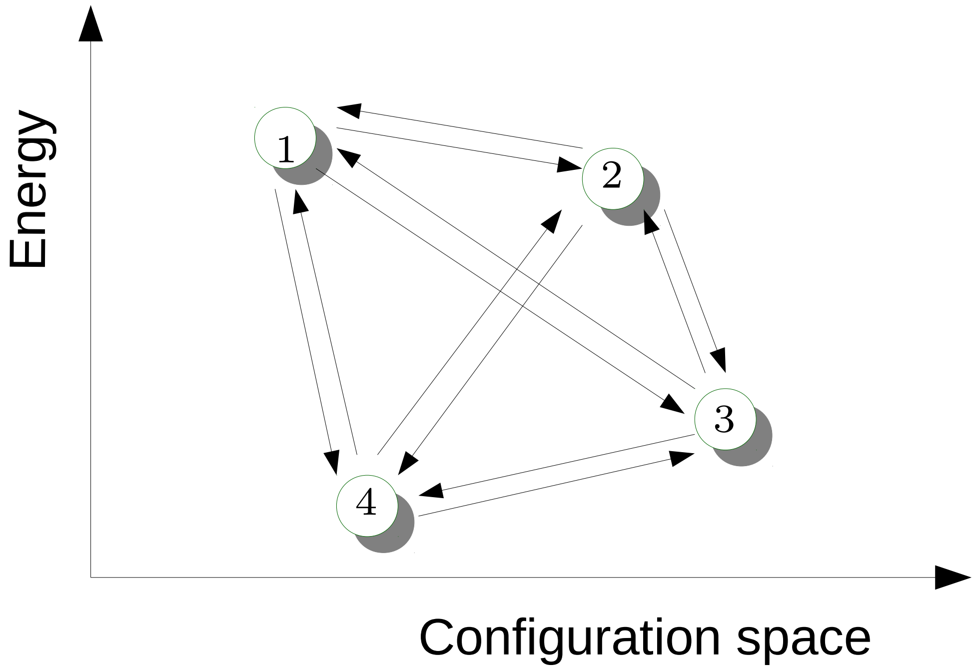
Bertin, J. Phys. A: Math. Gen. 36, 10683 (2003)

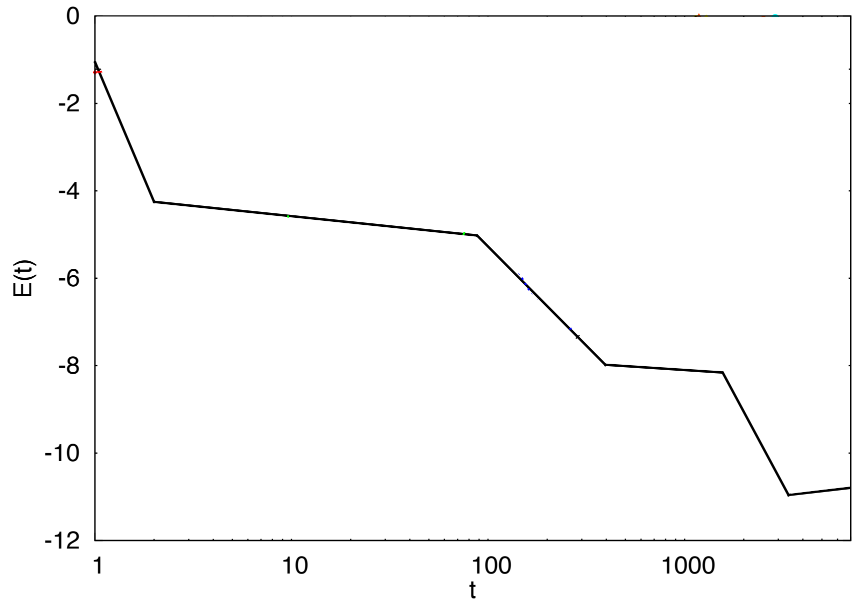
- Aging results do depend on temperature
- Slowing down due to entropy-energy competition
- Though escaping times still non-Arrhenius

C.C. and E. Marinari PRE 92, 010301 (2015)

- and it is impossible to recover the trap aging behaviour

Energy/Entropy-ruled path selection





- Low T, energy typically decreases
- High T, energy regularly bounces back, without apparent need
- Effective Threshold Energy
- Dynamical Basins can be defined

C.C. and E. Marinari PRE 92, 010301 (2015)

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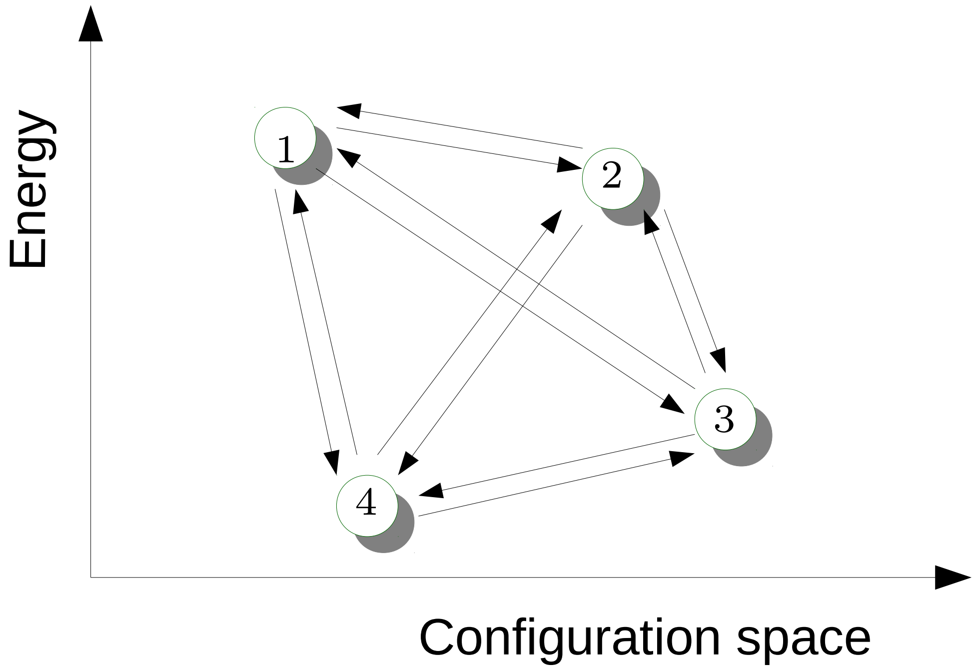

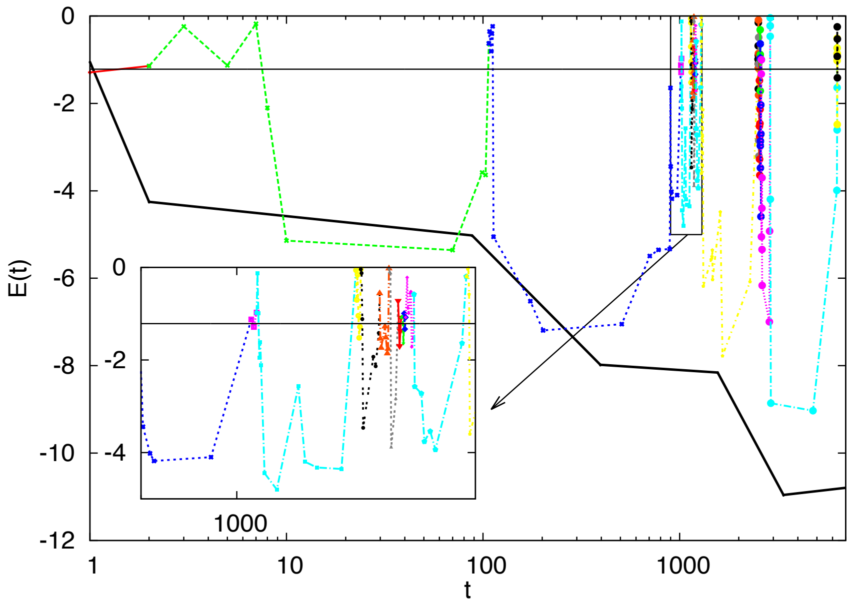

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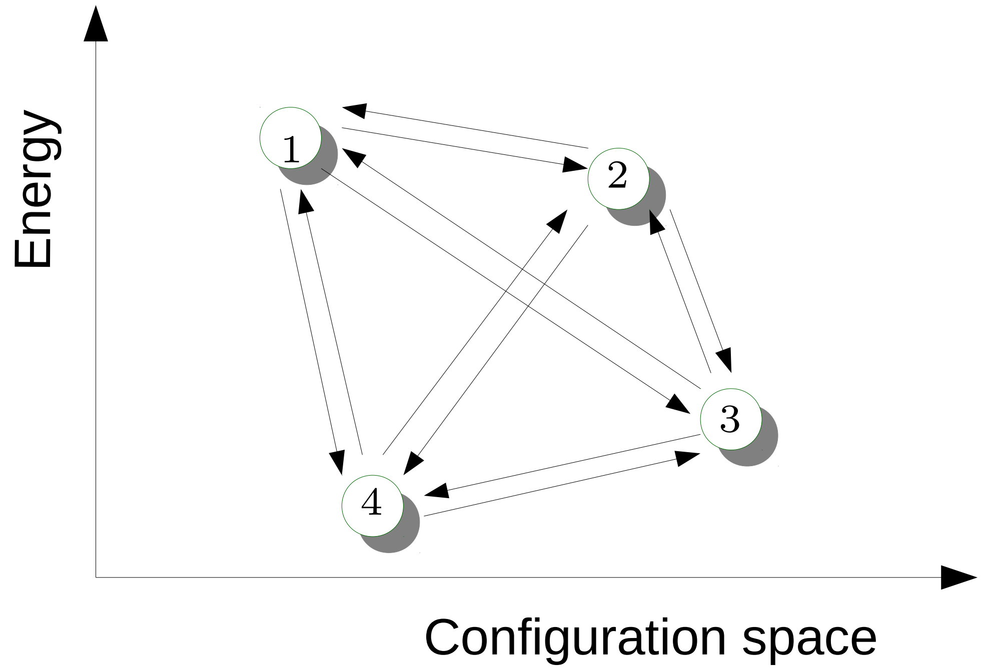

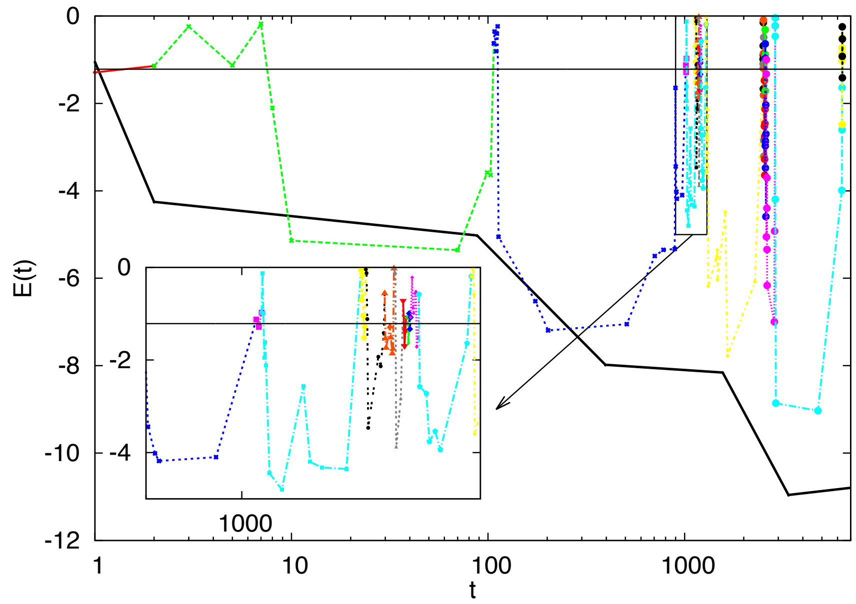

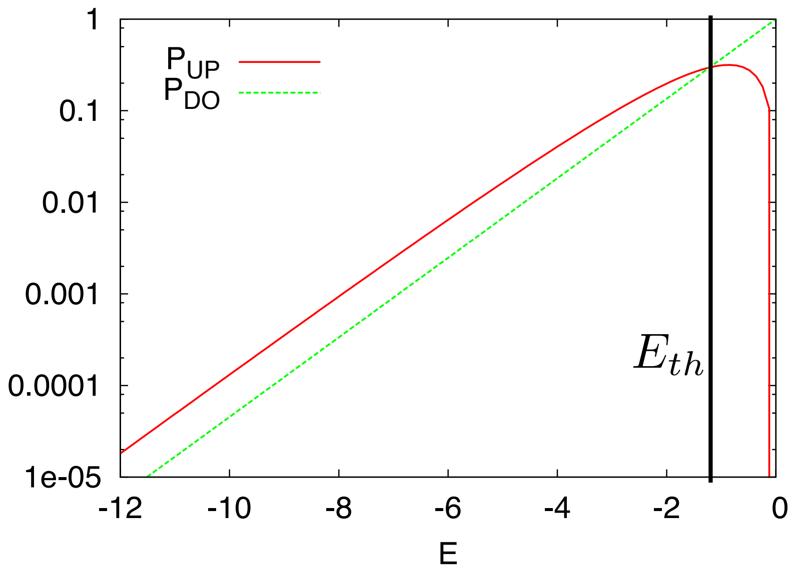

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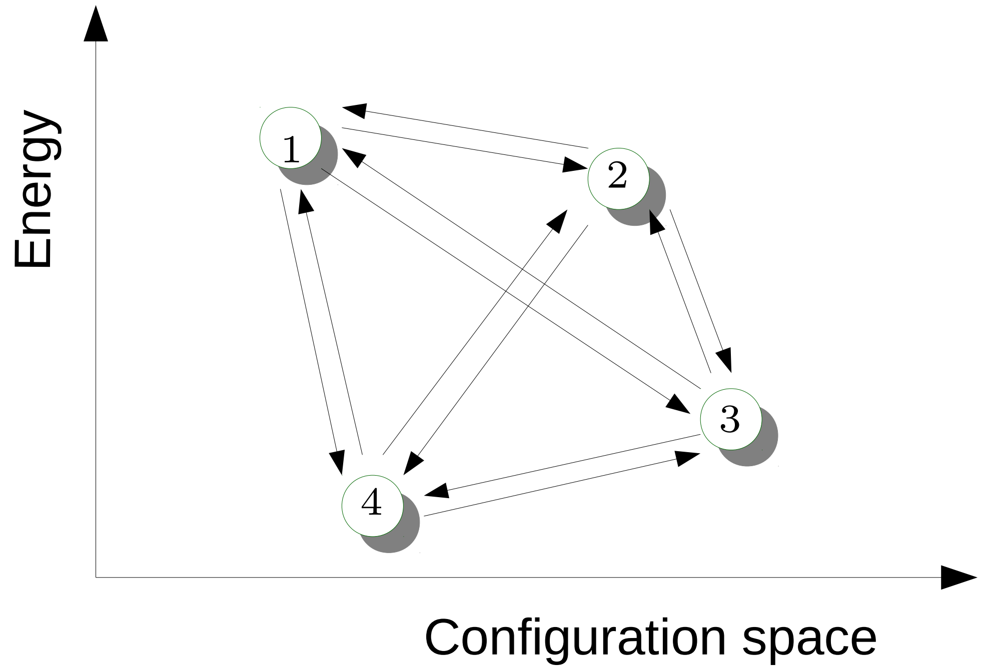

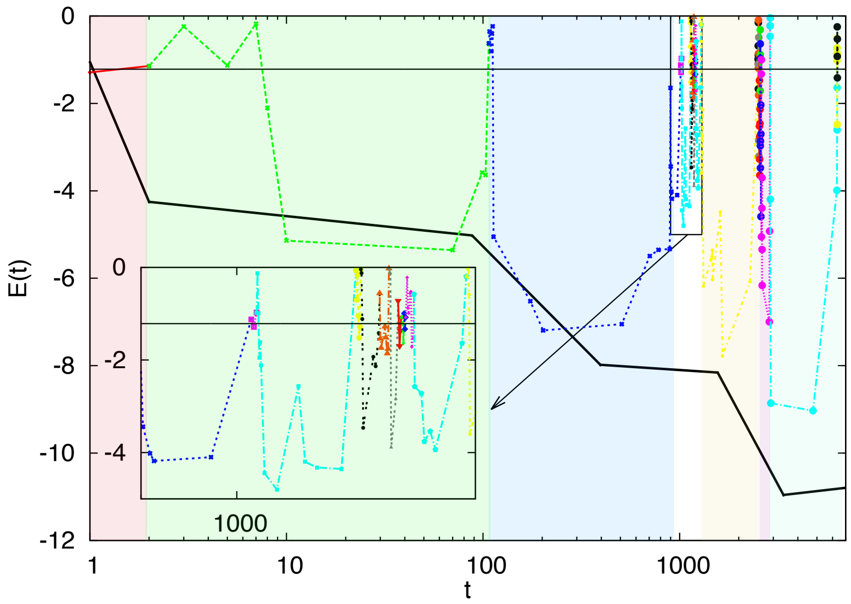

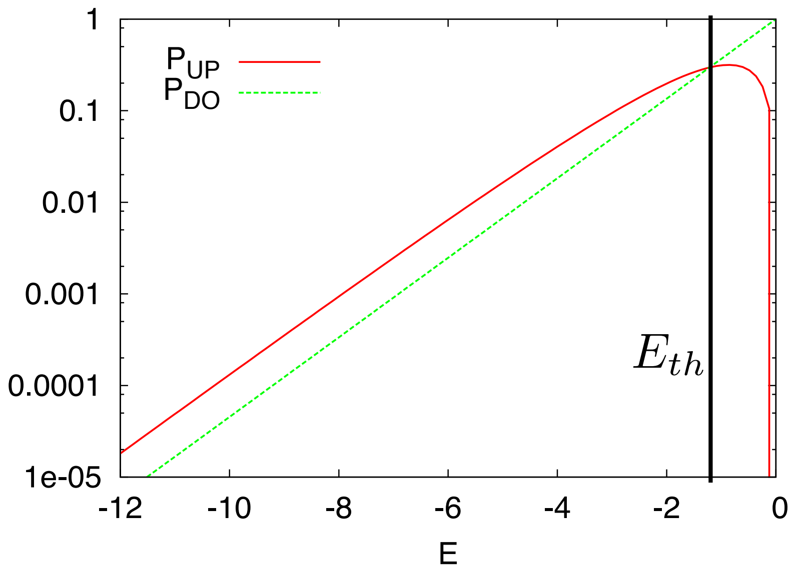

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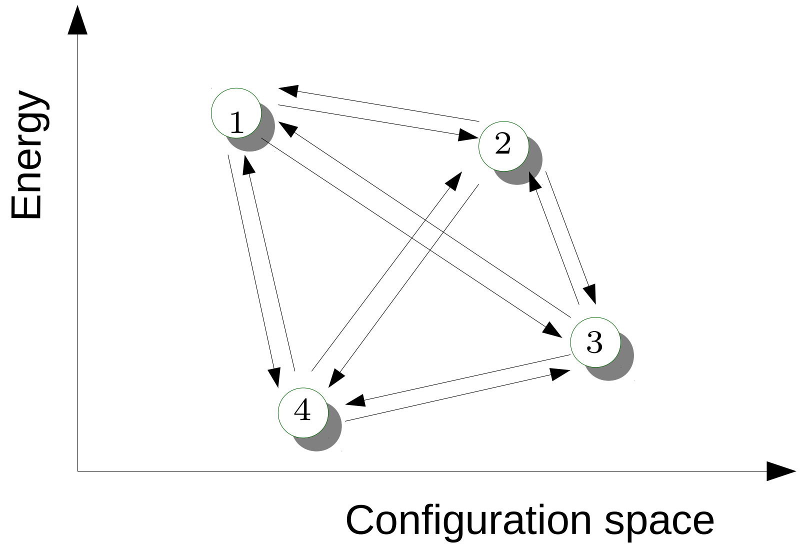
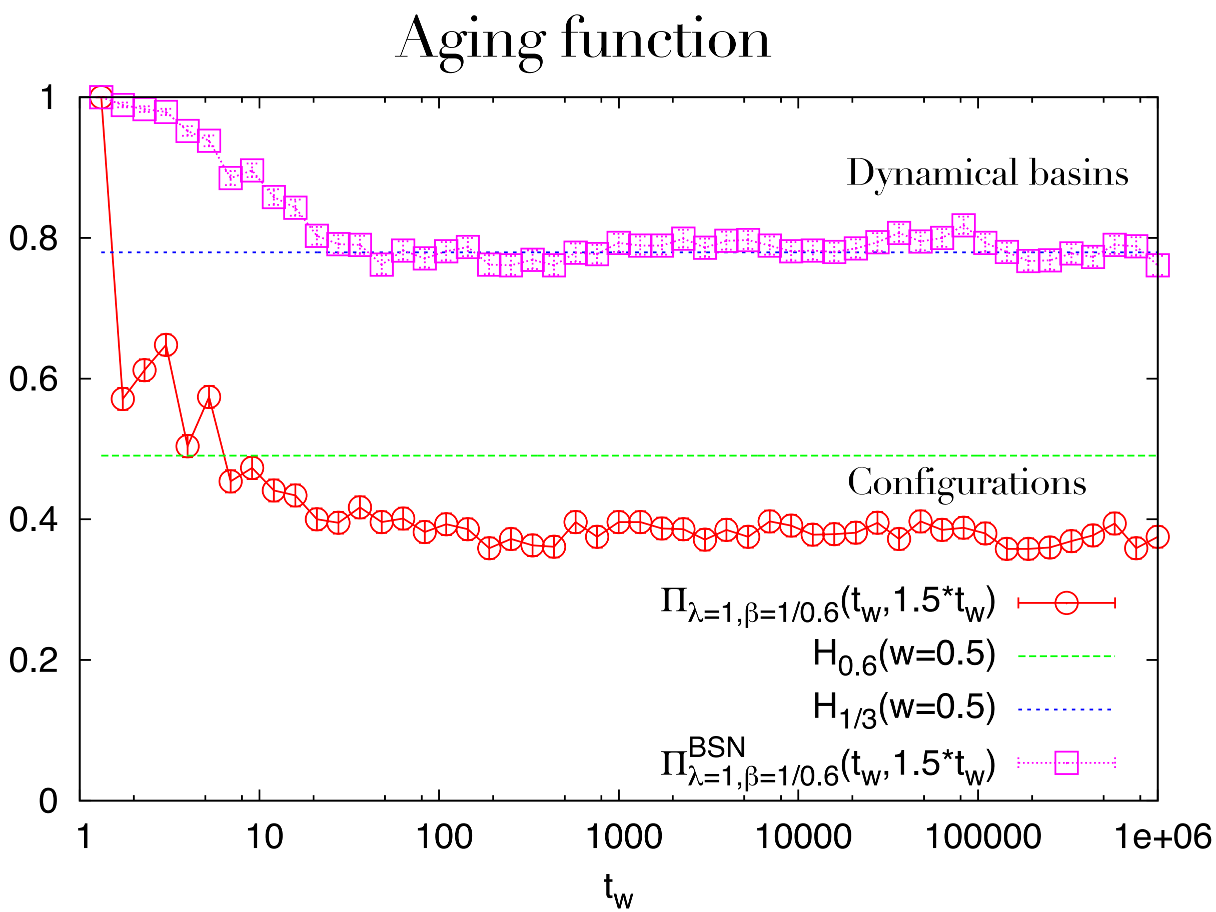
Effective Trap dynamics



Effective threshold energy

induces

Effective Trap Dynamics



Further results

REM used as a first proxy for p-spin (i.e. first steps to dynamics of spiked tensor)

- but REM neglects correlations of neighbouring conf.-> Correlated REM

  MBJ Achard Biroli 2018

- the p-spin challenge:

  simulations (well hidden effective threshold and dynamical basins)

  Ravasio, Billoire, Biroli, CC

  analytic study of barriers -> evidence for a minimal barrier

  Ros, Biroli, CC, arXiv:1809.05448 (2018)

  Rocchi, Franz

- supercooled liquids, the ultimate challenge:

  simulations (barriers, metabasins, localisation)

  MBJ, Biroli, Reichman

Conclusion

Goal: understand finite d and sparse networks dynamics

- Study Mean Field models at $t \sim \exp(N)$
- Effective description (Trap-like) of dynamics in rough landscapes
- Effective description (Trap-like) of dynamics even without barriers

-> effective barriers can be energetic or entropic

Glassy landscapes: competition of both factors

- Will effective trap descriptions be useful to predict glass dynamics?

- Will effective trap dynamics find application elsewhere?

Thank you!

MBJ, Achard & Biroli, 2018

Connecting REM and *p*-spin

- *p*-spin ≡ *p*-body interactions
- For activated dynamics need finite N, so $p \leq N$
- Energy correlations in the *p*-spin:

$$\overline{E_a E_b} = N q_{ab}^p$$

q_{ab}: overlap b/ a and b

- *E.g. correlation between neighbors*

REM	p-spin
$\overline{E_a E_b} = 0$	$\overline{E_a E_b} = e^{-2\alpha} > 0 \quad , \quad \alpha = \frac{p}{N} < 1$

- For any $N < \infty$ there is always a positive correlation, so **the p-spin cannot tend to the REM**

Correlated REM (CREM)

- Construct a REM
- Impose correlations of the *p*-spin without constraint $p \leq N$

$$\overline{E_a E_b} = N q_{ab}^{\alpha N}$$

Smooth interp. between models:

α ~ 1/N: p-spin regime

α ~ 1: weak correlations

α ≥ log(N): REM behavior

Barriers in p-spin

Ros, Biroli, CC, arXiv:1809.05448 (2018)

x = entropy of stationary points