Onset in a finite-size long-range model: the (2+3)-spin spherical model

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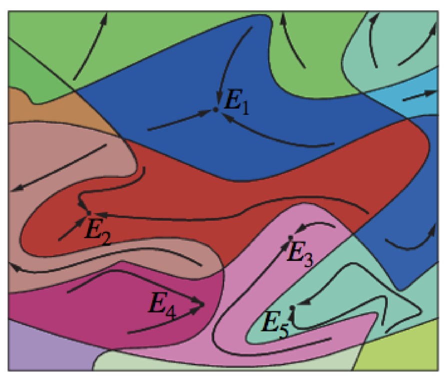
Introduction

We study the gradient descent dynamics and the inherent structures found after a quench from initial conditions well thermalized at temperature T_{in}. In very large systems, the dynamics perfectly agrees with the integration of the mean-field dynamical equations. We analyze finite-size corrections to the thermodynamic limit.

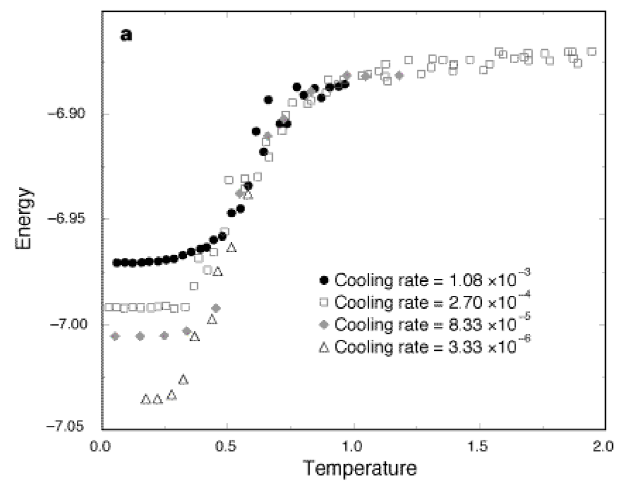
Inherent Structures

Consider the dynamics of a large number of interacting particles in 3-dimension. Initially, they are at equilibrium in the liquid phase, i.e. at a temperature T high enough so they do not form stable structures. Then the system is instantaneously cooled down to a very low temperature. This is equivalent to a gradient descent path in the energy landscape. The final configuration reached this ways is called *Inherent Structure* and it corresponds to a local minimum of the energy landscape.



Simulation of Interacting Particles

$\boldsymbol{T_{onset}}$ is the temperature below which the average energy of *Inherent Structures* strongly depends on the initial temperature.



Mean-field Models of Glass Formers

During the last 25 years, the mean-field (*pure*) p-spin spherical model has become a reference model to understand the out of equilibrium dynamics. However this model has a rather pathological behavior due to the homogeneity of its Hamiltonian. Instead we will consider a natural extension of this model: the mixed p-spin, which presents features more similar to the ones found in the simulation of interacting particles. In particular:

- the dependence of the IS energy on the initial temperature
- the existence of a temperature T_{onset} above which the system forgets its initial condition.

Methods

p-spin Spherical Model

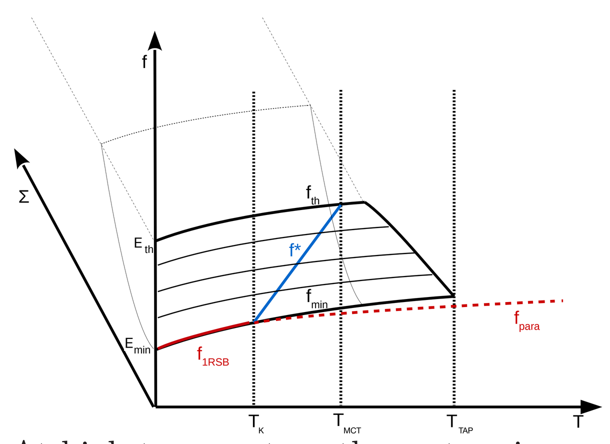
The Hamiltonian of the p-spin spherical model is a random Gaussian function on the N-dimensional sphere ($\sum_i \sigma_i^2 = N$) with covariance:

$$\overline{H[\sigma]H[\tau]} = N f(q_{\sigma\tau}) \qquad q_{\sigma\tau} = \sum_i \sigma_i\tau_i/N$$

- *pure* 3-spin model
  $f(q) = \frac{1}{2}q^3 \longrightarrow H[\sigma] = J^{ijk}\sigma_i\sigma_j\sigma_k$
- *mixed* (3+4)-spin model
  $f(q) = \frac{1}{2}(q^3+q^4) \longrightarrow H[\sigma] = J^{ijk}\sigma_i\sigma_j\sigma_k + J^{ijkl}\sigma_i\sigma_j\sigma_k\sigma_l$

with Js i.i.d. Gaussian couplings.

Random First Order Transition in temperature:



	3-spin	(3+4)-spin
T_K	0.5861	0.7621
T_{MCT}	0.6124	0.8052
E_{th}	−1.1547	−1.6905
E_{min}	−1.17167	−1.73307

At high temperature the system is paramagnetic.
At T_{MCT} the paramagnetic state starts to partition in a large number of states.
At T_K only the lowest states contribute to thermodynamic quantities.

Pathological Homogeneity of *Pure* models

$\mu = \sum_i \sigma_i \partial_{\sigma_i} H[\sigma]$ is the radial reaction (Lagrange multiplier)
in *pure* models: $\mu = pH[\sigma]$

'Inherent Structure protocol' for the dynamics:

$$\begin{cases} \partial_t\sigma_i(t) = -\frac{\partial H}{\partial\sigma_i}(t) - \mu(t)\sigma_i(t) \\ P[\sigma(0)] = e^{-\beta' H[\sigma(0)]}/Z(\beta') \end{cases}$$

from which a closed set of integro-differential equations for correlation and response:

$$C(t,t') \equiv \langle\sigma_i(t)\sigma_i(t')\rangle \qquad R(t,t') \equiv \frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i(t')}$$

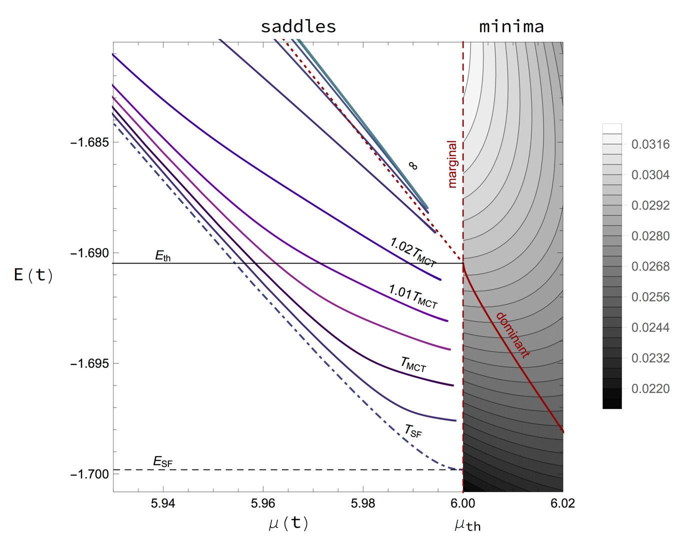
Which are the asymptotic states reached by this dynamics?

Asymptotic Dynamics
numerical integration
of dynamical equations

VS

Energy Landscape
analytical study
of stationary points of $H[\sigma]$

Many marginal energies!



- *pure* models:
  $\mu(t) = pE(t)$
- *mixed* models:
  $E(t) \not\propto \mu(t)$
  the dynamics can reach points in a whole region of the (E,μ) plane.

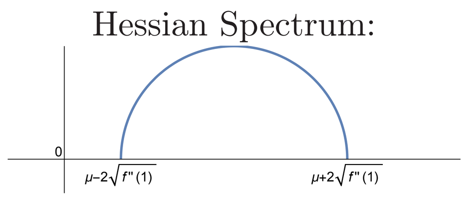
Both systems relax towards marginal minima.

Properties of Stationary Points

- *pure* models: one threshold energy E_{th} at which dominant minima become saddles
- *mixed* models: whole line of energies at which minima becomes saddles

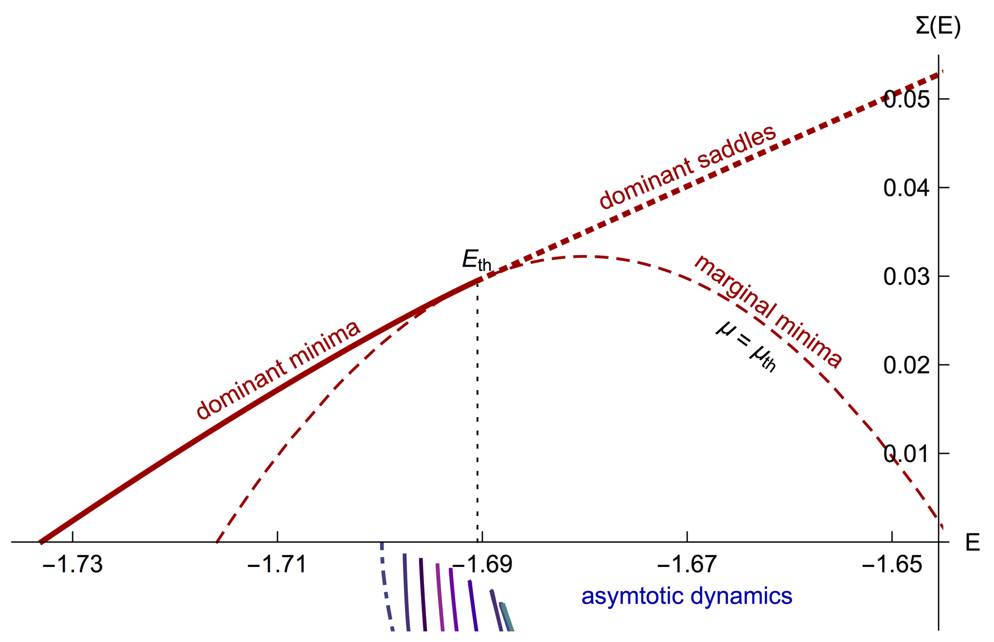
Hessian matrix: $H''_{ij} + \mu\delta_{ij}$
shifted GOE matrix
$\mathrm{Var}[H''_{ij}] = \frac{1}{N}f''(1)$.

Hessian Spectrum:



Does the dynamics go towards the most numerous marginal minima?

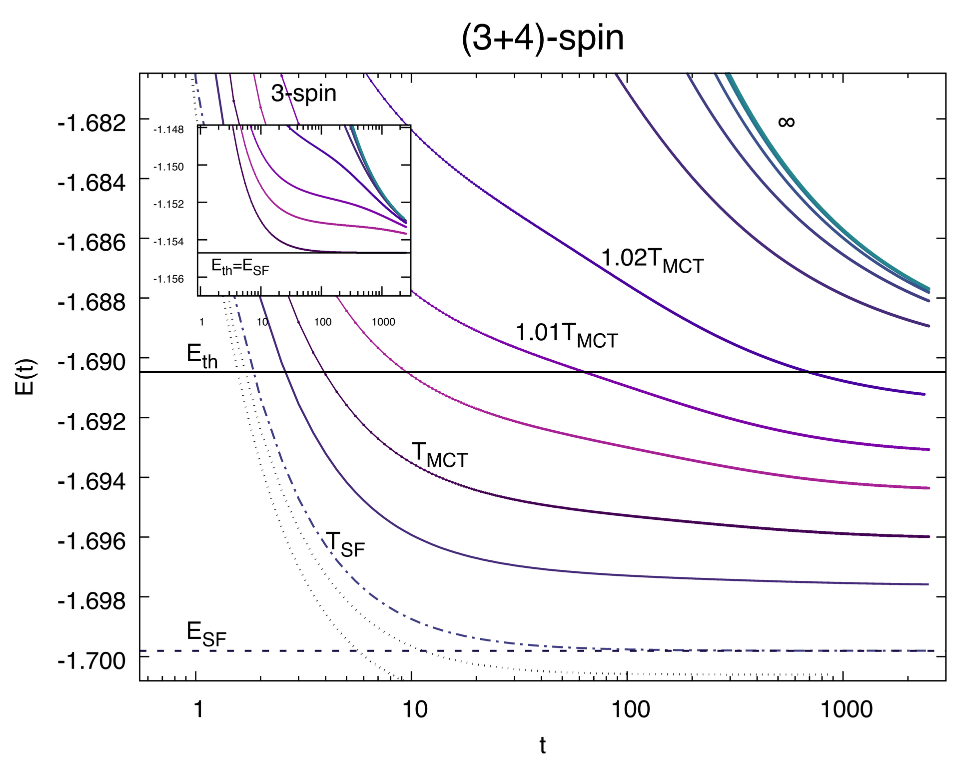
$$\boldsymbol{\Sigma(E,\mu)} = \log\left(\#\text{ of stationary points with fixed } \boldsymbol{E} \text{ and } \boldsymbol{\mu}\right)$$



Main Result

Under-threshold Dynamics!

Contrary to pure models, in mixed models the dynamics started in the ergodic phase reaches states that are below the threshold energy E_{th}.



While in pure models T_{MCT} marks the division between in-state fast relaxation and intra-states aging relaxation, in mixed models there are two key temperatures:

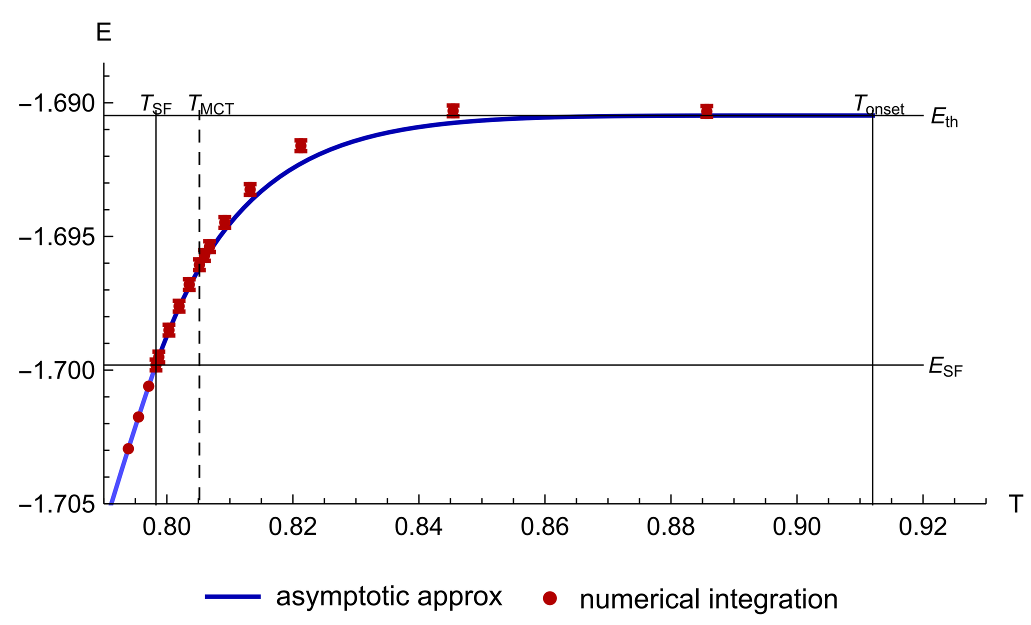
$$T_{SF} = 0.7983 < T_{MCT} \quad \longleftrightarrow \quad E_{SF} = -1.6998$$
$$T_{onset} \approx 0.91 > T_{MCT} \quad \longleftrightarrow \quad E_{th} - 1.6905$$

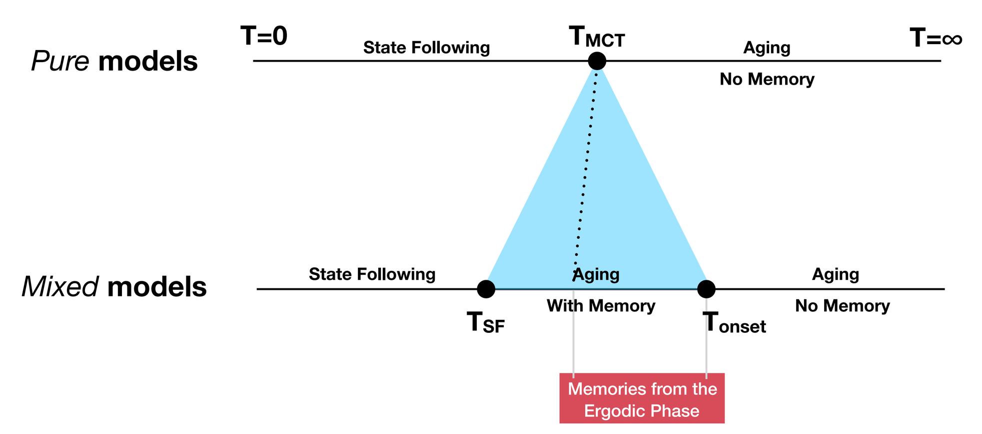
T_{onset} is obtained from asymptotic approximation.

A new phase emerges!!!

Mixed p-spin models presents 3 phases of relaxation:

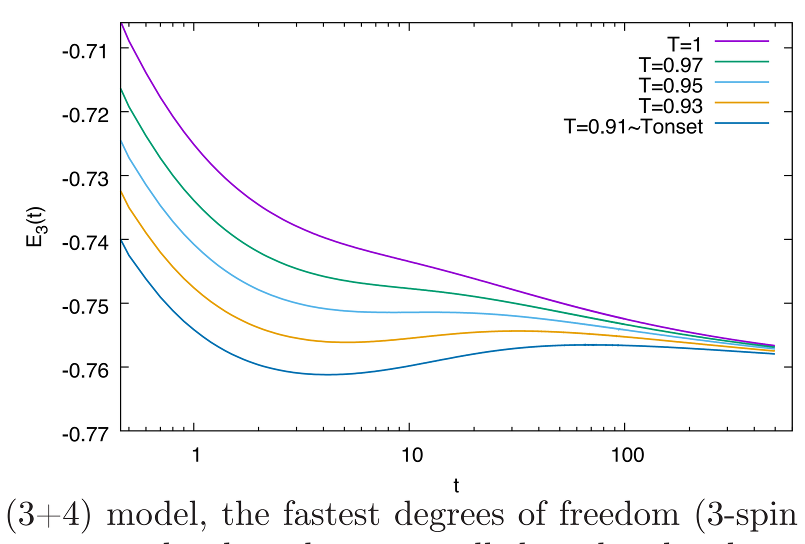
- $\boldsymbol{T > T_{onset}}$:
  loss of memory of the initial condition ($\lim_{t\to\infty} C(t,0) = 0$)
  'aging' relaxation towards threshold states ($E = E_{th}$)
- $\boldsymbol{T_{SF} < T < T_{onset}}$:
  memory of the initial condition ($\lim_{t\to\infty} C(t,0) \neq 0$)
  'aging' relaxation towards under-threshold states ($E_{SF} < E < E_{th}$)
- $\boldsymbol{T < T_{SF}}$:
  exponential relaxation inside modified state (State Following)





It is remarkable that T_{MCT}, which is the temperature that defines the equilibrium ergodicity breaking, does not appear to have any special role in the out-of-equilibrium dynamics.

Short Time Signature of T_{onset}?



In the (3+4) model, the fastest degrees of freedom (3-spin interactions) start to relax but then are pulled up by the slowest 4-spin interactions. The energy of 3-spin $E_3(t)$ develop a flex in the relaxation around T_{onset}. Is this the mechanism for under-threshold dynamics?

Perspectives

The mixed p-spin mean-field model presents an out-of-equilibrium dynamics that is even richer than initially expected. More remarkably, between T_{SF} and T_{onset}, a new phase emerges. The coupling of marginality with memory of the initial condition needs to be better understood. At the mean-field level, we need to understand how broad this behavior is, and to search for universal quantities that characterize this new phase. We also need to examine the relevance of this new phase in finite-dimensional models, both in simulations and in experiments.

References

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