Dynamics in complex landscapes

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A tutorial

How does a (large) system reach equilibrium or

what does it do while it evolves out of equilibrium

- **Dynamics in one dimensional energy landscapes**
- **" in the simplest free-energy landscapes**
- **" in complex free-energy landscapes**

In all cases, discussion of time scales, thermalisation, fluctuations

A tutorial

How does a (large) system reach equilibrium or

what does it do while it evolves out of equilibrium

- **Dynamics in one dimensional energy landscapes**

  Conservative dynamics : Newton

  Dissipative dynamics : Langevin

  Equilibrium vs. out of equilibrium

  White (Markov) vs. coloured (memory) noises

  Exponential vs. non-exponential relaxation

  Relaxation, diffusion & activation

- **Dynamics in the simplest free-energy landscapes**

- **Dynamics in complex free-energy landscapes**

In all cases, discussion of time scales, thermalisation, fluctuations

Newton equation

Motion of a particle in one dimension

A particle with mass M and time-dependent position $r(t)$ evolves according to **Newton's eq.**

$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} = \underbrace{F(t)}_{\text{force}}$$

Inertia: mass times acceleration

Force: gradient descent $F(r(t)) = -\left.\frac{dV(r)}{dr}\right|_{r=r(t)}$ in $d=1$

but other options in higher dimensions

or generic $F(t)$

Newton equation

Conservative dynamics in a one dimensional harmonic potential

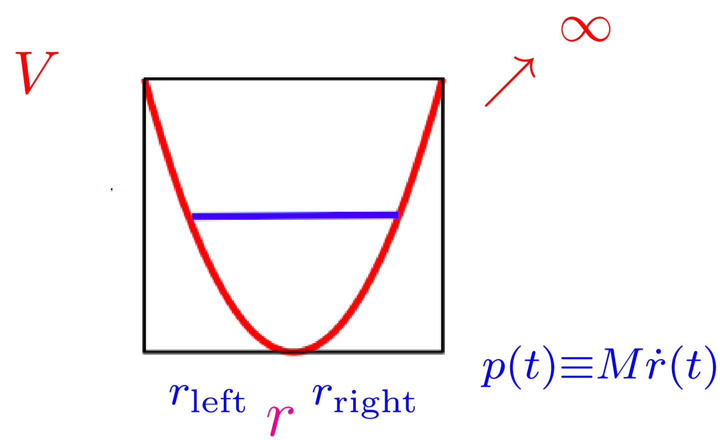
A particle with mass M and time-dependent position $r(t)$ evolves according to **Newton's eq.**

$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} = \underbrace{F(r(t))}_{\text{force}}$$

Force $F(r(t)) = -\left.\frac{dV(r)}{dr}\right|_{r(t)} \Rightarrow$

Constant energy $E = \frac{(p(t))^2}{2M} + V(r(t))$

and confinement $r_{\text{left}} < r < r_{\text{right}}$



Langevin equation

Effects of an environment : dissipation and noise

A particle with mass M and time-dependent position $r(t)$ coupled to a **memory-less equilibrium environment** evolves according to

$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} + \underbrace{\gamma\dot{r}(t)}_{\text{friction}} = \underbrace{F(t)}_{\text{force}} + \underbrace{\xi(t)}_{\text{noise}}$$

Gaussian white noise,

zero mean $\langle\, \xi(t) \,\rangle = 0$ and correlation $\langle\, \xi(t)\xi(t') \,\rangle = 2\gamma k_B T \delta(t - t')$

γ is the friction coefficient, T is the temperature of the equilibrium bath and k_B the Boltzmann constant. $\beta = (k_B T)^{-1}$

The noise is delta-correlated, factor 2γ ensures equilibration of the bath

Langevin equation

Relaxation dynamics in a one dimensional harmonic potential

A particle with mass M and time-dependent position $r(t)$ coupled to a **memory-less equilibrium environment** evolves according to

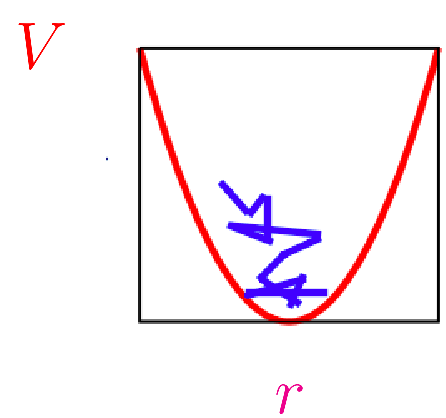
$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} + \underbrace{\gamma\dot{r}(t)}_{\text{friction}} = \underbrace{-M\omega_0^2\, r(t)}_{\text{potential force}} + \underbrace{\xi(t)}_{\text{noise}}$$

Friction/Dissipation $F_d(t) = -\gamma\dot{r}(t) \quad \Rightarrow$

Energy decay $\dfrac{d\langle H(t)\rangle}{dt} = -\gamma\langle\dot{r}^2(t)\rangle$

Relaxation $\langle r(t)\rangle \to r_{\min} + c\, \boxed{e^{-t/\tau}}\, f(\omega t)$

Time-scale $\tau_{\text{over}} = \frac{\gamma}{M\omega_0^2}$ and $\tau_{\text{under}} = \frac{M}{\gamma}$



Langevin equation

Relaxation dynamics in a one dimensional harmonic potential

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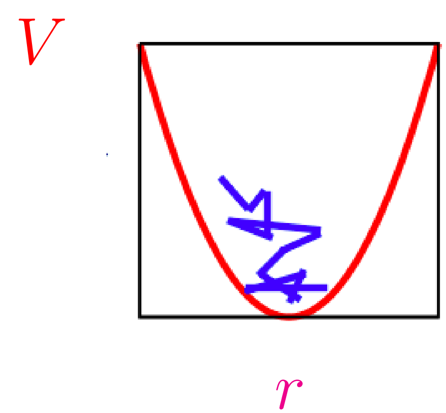
Bath+Potential $\Rightarrow$ Equilibration

$$P(p,r,t) \;\to\; P_{\rm GB}(p,r) = \frac{e^{-\beta H(p,r)}}{Z}$$

$$H(p,r) = \frac{p^2}{2M} + \frac{M\omega_0^2\,(r - r_{\rm min})^2}{2}$$



Newton equation

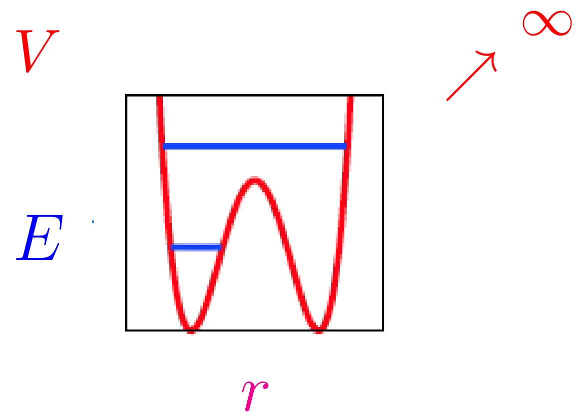
Conservative dynamics in a one dimensional double-well potential

A particle with mass M and time-dependent position $r(t)$ evolves according to **Newton's eq.**

$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} = \underbrace{F(r(t))}_{\text{potential force}}$$

Force $F(t) = -\left.\frac{dV(r)}{dr}\right|_{r(t)} \Rightarrow$

Constant energy $E = \frac{M}{2}\dot{r}^2(t) + V(r(t))$



Langevin equation

Thermal activation over finite barriers

A particle with mass M and time-dependent position $r(t)$ coupled to a **memory-less equilibrium environment** evolves according to

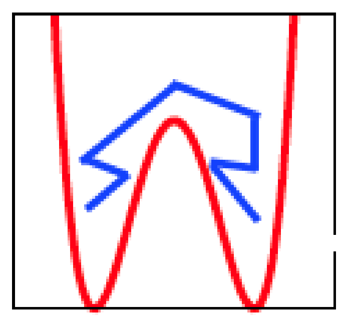
$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} + \underbrace{\gamma\dot{r}(t)}_{\text{friction}} = \underbrace{\mu\, r(t) - g r^3(t)}_{\text{double well force}} + \underbrace{\xi(t)}_{\text{noise}}$$

Friction/Dissipation $F_d(t) = -\gamma\dot{r}(t) \quad \Rightarrow$

$$\frac{d\langle H(t)\rangle}{dt} = -\gamma\langle\dot{r}^2(t)\rangle$$

Activation over the barrier $\boxed{t_A = \tau_0\, e^{\beta\Delta V}}$

V



r

Langevin equation

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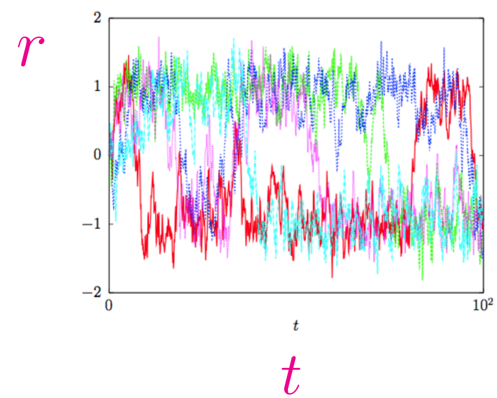
Five independent runs $r(t)$

Bath+Potential $\Rightarrow$ Equilibration

$$P(p,r,t) \;\to\; P_{\rm GB}(p,r) = \frac{e^{-\beta H(p,r)}}{Z}$$



Dynamics in equilibrium

Two properties

- One-time quantities reach their equilibrium values:

$$\boxed{\langle\, A(\{\vec{r}\}_\xi)(t)\,\rangle \;\to\; \langle\, A(\{\vec{r}\})\,\rangle_{\rm GB}}$$

- All time-dependent correlations are stationary **(steady state)**

$$\langle\, A_1(\{\vec{r}\}_\xi)(t_1) A_2(\{\vec{r}\}_\xi)(t_2) \cdots A_n(\{\vec{r}\}_\xi)(t_n)\,\rangle = \langle\, A_1(\{\vec{r}\}_\xi)(t_1+\Delta) A_2(\{\vec{r}\}_\xi)(t_2+\Delta) \cdots A_n(\{\vec{r}\}_\xi)(t_n+\Delta)\,\rangle$$

for any n and Δ. In particular, $\boxed{C(t,t_w) = C(t-t_w)}$

- The fluctuation-dissipation theorem (FDT), a model independent relation between linear responses (susceptibilities) and correlation functions, holds.

In particular, $\boxed{\chi(t,t_w) = (k_B T)^{-1}[C(t,t) - C(t,t_w)]}$ **(thermal)**

Langevin equation

Out of equilibrium diffusion due to flatness of potential

A particle with mass M and time-dependent position $r(t)$ coupled to a **memory-less equilibrium environment** evolves according to

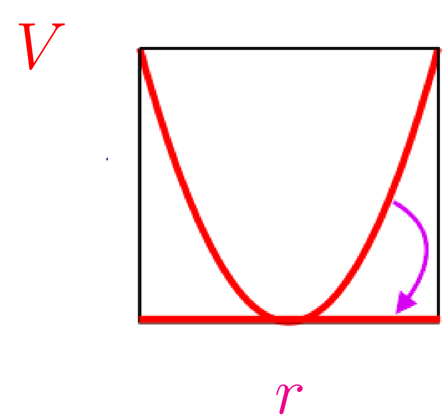
$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} + \underbrace{\gamma\dot{r}(t)}_{\text{friction}} = \underbrace{\cancel{F(r(t))}^{0}}_{\text{flat potential}} + \underbrace{\xi(t)}_{\text{noise}}$$

Friction/Dissipation $F_d(t) = -\gamma\dot{r}(t) \Rightarrow$

$$\langle H(t)\rangle \to \langle p^2\rangle_{\rm GB}/(2M) \qquad \tau_{\rm under} = \frac{M}{\gamma}$$

Normal diffusion

$$\Delta_r(t,t') \equiv \langle (r(t)-r(t'))^2\rangle \to 2\mathcal{D}|t-t'|$$



Langevin equation

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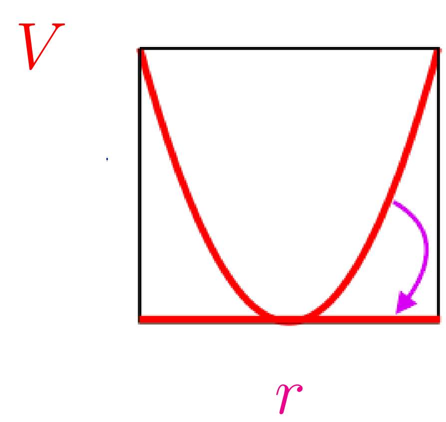
Friction/Dissipation $F_d(t) = -\gamma\dot{r}(t) \;\;\Rightarrow$

$$\langle H(t)\rangle \to \langle p^2\rangle_{\rm GB}/(2M) \qquad \tau_{\rm under} = \frac{M}{\gamma}$$

Self-correlation

$$C_r(t,t') \equiv \langle r(t)r(t')\rangle \to \min(t,t')$$



Langevin equation

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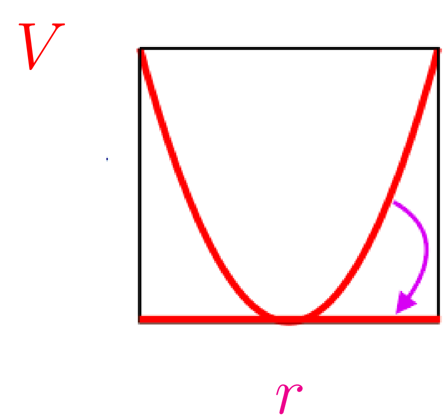
Bath+flat potential

$$P(p,r,t) \to \frac{e^{-\beta\frac{p^2}{2M}}}{Z_p} \times \boxed{\text{unbounded}}$$

momenta equilibrate but coordinates do not



Statements

One dimensional Markov (white noise) Langevin dynamics

Under an environment in equilibrium,

a confining potential $\lim_{r\to\pm\infty} V(r) = \infty$

and finite barriers $\Delta V(r) < \infty$

equilibration of both p and r.

exponential approach to equilibrium $e^{-t/\tau}$ (different τ)

Arrhenius activation over finite barriers $t_A = \tau_0 \, e^{\beta \Delta V}$

Flat potential (or unconfining one)

equilibration of p and out of equilibrium dynamics of r

neither stationarity nor FDT of r observables

General Langevin equation

Non-Markovian dynamics

A particle with mass M and time-dependent position $r(t)$ coupled to an **equilibrium environment with memory** evolves according to

$$\underbrace{M\ddot{r}(t)}_{\text{inertia}} + \underbrace{\int_{t_0}^{t} dt' \, \boldsymbol{\Sigma}_{\mathbf{B}}(t-t')\dot{r}(t')}_{\text{friction}} = \underbrace{F(t)}_{\text{force}} + \underbrace{\xi(t)}_{\text{noise}}$$

Coloured noise with correlation $\langle \, \xi(t)\xi(t') \, \rangle = k_B T \, \boldsymbol{\Sigma}_{\mathbf{B}}(t-t')$ and zero mean.

Equilibrium environment : the same friction kernel and noise correlation $\boldsymbol{\Sigma}_{\mathbf{B}}(t-t')$.

Derivations : see, *e.g.*, **Weiss 99, LFC Les Houches 02**

Coloured noise

Power-law correlations

Generic: Most of the exact **fluctuation-dissipation relations** in and out of equilibrium remain unaltered for generic Σ_{B}, *e.g.* the fluctuation-dissipation theorem, fluctuation theorems, *etc.*

Aron, Biroli & LFC 10

Particular: The **functional form** of the observables depends on the characteristics of the noise, *i.e.* on Σ_{B}.

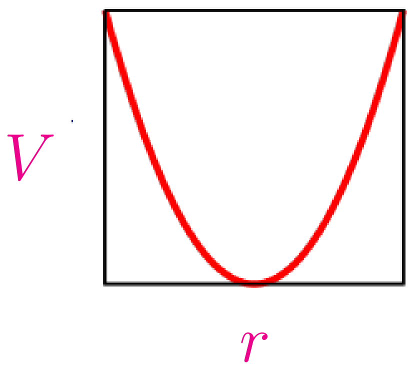
Some interesting cases are

$$\Sigma_{\mathrm{B}}(t-t') = \frac{g}{\Gamma_E(1-\alpha)} \, |t-t'|^{-\alpha} \qquad \text{with} \qquad \alpha > 0$$

g the 'friction coefficient' and Γ_E the Euler-function.

Example

a particle in a harmonic potential



$V(r) = \frac{1}{2} M\omega_0^2 \, r^2$

After a relatively short transient,

independently of the initial condition

equilibrium dynamics

$$C_r(t,t') \equiv \langle r(t) r(t') \rangle \to \frac{1}{M\omega_0^2} E_{\alpha,1}\left(-\frac{M\omega_0^2 \, |t-t'|^\alpha}{\gamma} \right)$$

with $E_{\alpha,1} = \sum_{k=0} \frac{z^k}{\Gamma_E(\alpha k+1)}$ the Mittag-Leffler function.

Only for an Ohmic bath $\alpha = 1$ **the relaxation is exponential** $E_{1,1}(z) = e^z$

non-Ohmic bath $\alpha \neq 1$ $E_{\alpha,1}(z) \to z^{-1}$ for $z \to -\infty$ **power-law relaxation.**

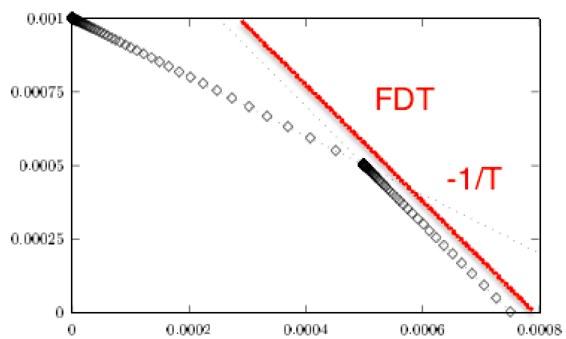
Example

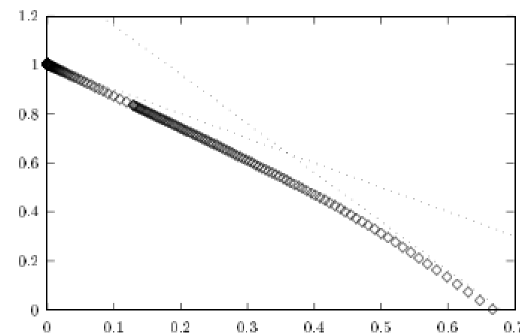
Time-scales & FDT violations in the simple oscillator

Coupling to one bath at temperature T *vs.*

Coupling to several baths with different time-scales and temperatures

$$\chi(t, t_w) = \chi(t - t_w)$$





$$C(t, t_w) = C(t - t_w)$$

Two scales Not well-separated scales

LFC & Kurchan 99

Statements

One dimensional Markov Langevin dynamics

Even the long-term dynamics may depend on the microscopic dynamics, in this case as induced by the bath.

The approach to equilibration can be non-exponential

in this example, it is dictated by the noise correlation

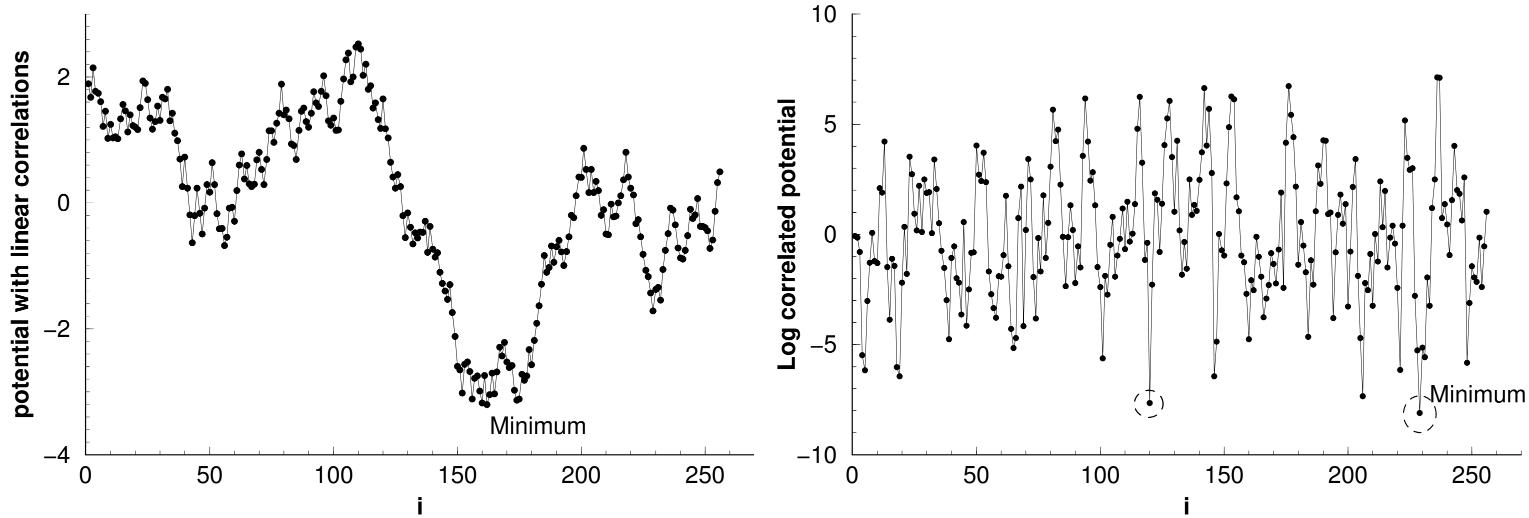
It is hard to conclude on thermal equilibration from the functional form of the observables or stationary correlation functions

The comparison between correlation functions and linear response functions gives more detailed information in this respect

Langevin equation

Diffusion in random quenched potentials

V



Figs. from **Carpentier & Le Doussal 00**

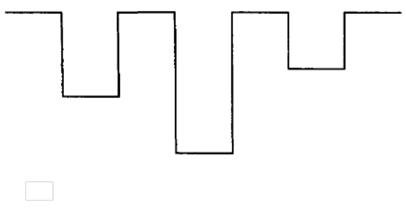
MSD $$\boxed{\Delta_r(t,t') \equiv \langle (r(t) - r(t'))^2 \rangle \to 2\mathcal{D}|t-t'|^a}$$

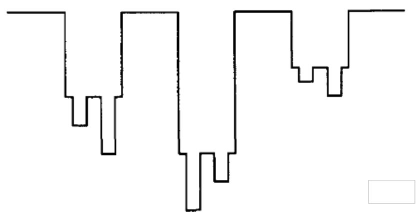
Interest in anomalous diffusion a, renormalisation of diffusion constant $\mathcal{D}$, etc.

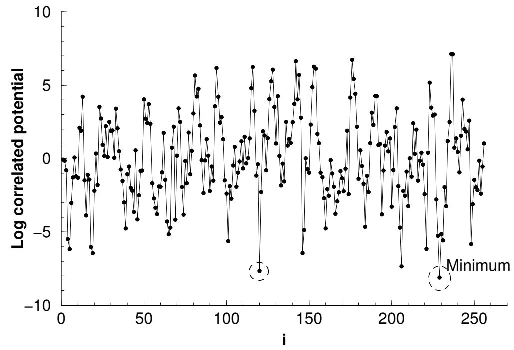
Reviews **Bouchaud & Georges 90, Metzler & Klafter 00, Havlin & ben-Avraham 02**

Trap models

For dynamics in real but also phase space







Bouchaud 92 Bouchaud & Dean 95 **Carpentier & Le Doussal 00**

Variations on the connectivity of the traps, the trapping time distributions, the nesting of traps within traps, etc.

Many studies including

Ben Arous, Bovier, Gayrard, Jerny 02-08, Baity-Jesi, Biroli, Cammarota 17-18

More on the relation with disordered systems' dynamics later

A tutorial

How does a (large) system reach equilibrium or

what does it do while it evolves out of equilibrium

- **One dimensional energy landscapes**
- **The simplest free-energy landscape : many variables - large dimensions**

  Time-dependent Ginzburg-Landau equation

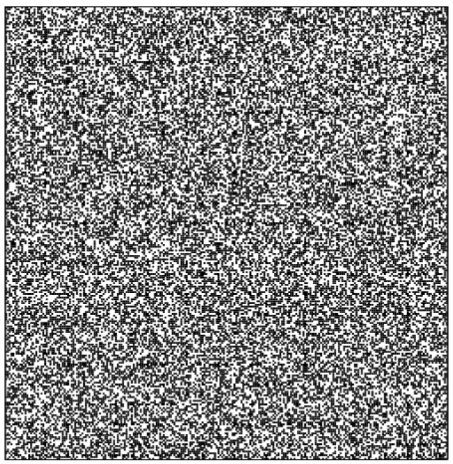
    Collective effects

    Critical relaxation

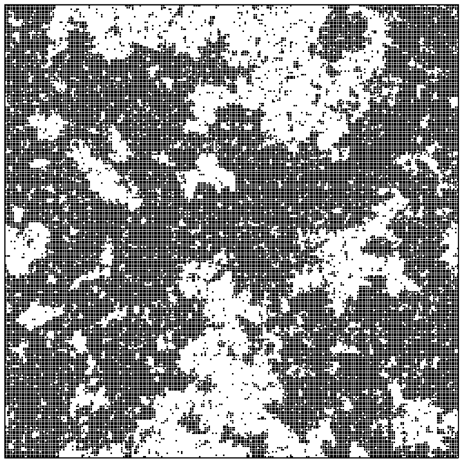
- **Complex free-energy landscapes**
- **Time scales, thermalisation**

Ferromagnetism

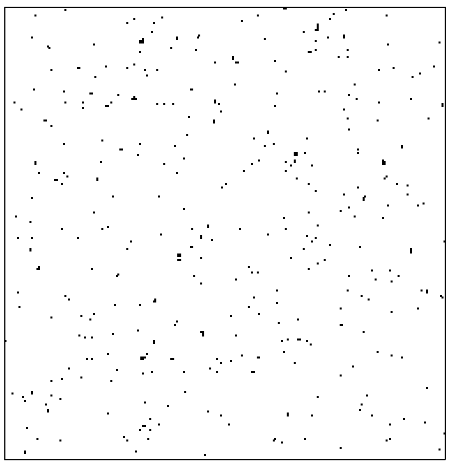
Equilibrium configurations - up & down spins in a $2d$ Ising model



$T \to \infty$



$T = T_c$

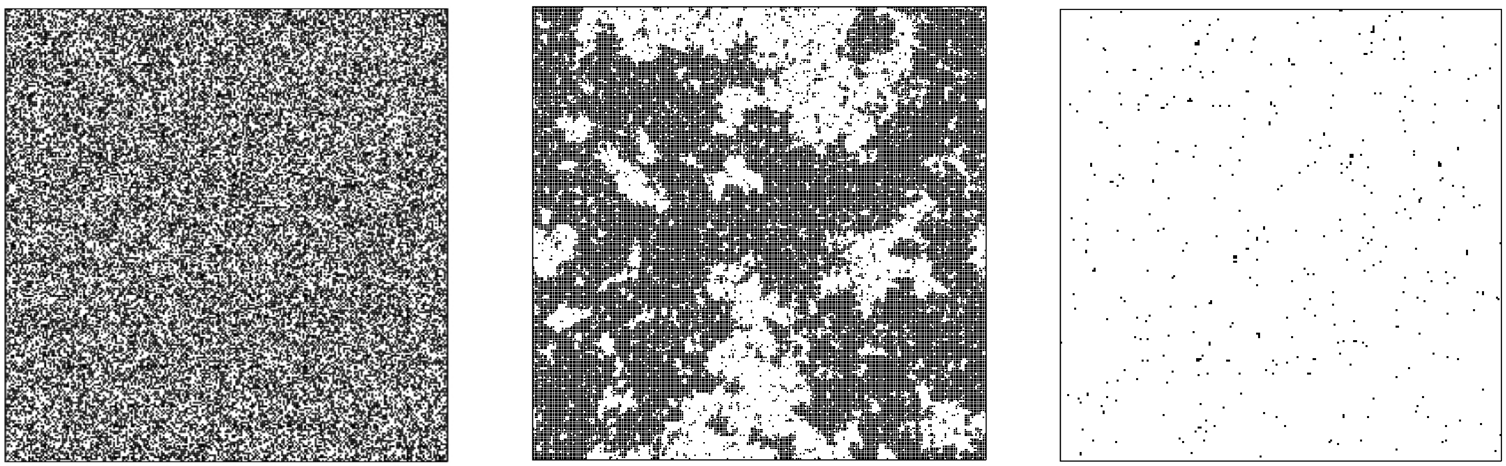


$T < T_c$

Simplest physical problem with a phase transition : Disordered high temperature phase, 2nd order phase transition, spontaneous symmetry breaking below T_c, two ordered low temperature phases related by symmetry (all up or all down decorated with thermal fluctuations).

Ferromagnetism

Equilibrium configurations - up & down spins in a $2d$ Ising model



$T \to \infty$ $\qquad$ $T = T_c$ $\qquad$ $T < T_c$

Static questions: coarse-grained local order parameter, effective “weight” functional *i.e.* free-energy functional $\Rightarrow$ Ginzburg-Landau approach

Models

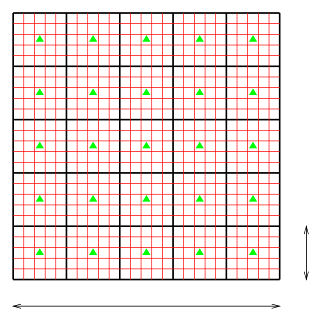
Discrete *vs.* continuous

Ising spin models

$$H = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$$

Field theory for the order parameter

$$\mathcal{F}[\phi] = \int d^D r \left[\frac{1}{2}(\nabla\phi)^2 + \frac{\mu}{2}\phi^2 + \frac{g}{4}\phi^4) \right]$$



$$\phi(\vec{r}) = \mathcal{V}_{\vec{r}}^{-1} \sum_{i \in V_{\vec{r}}} s_i$$

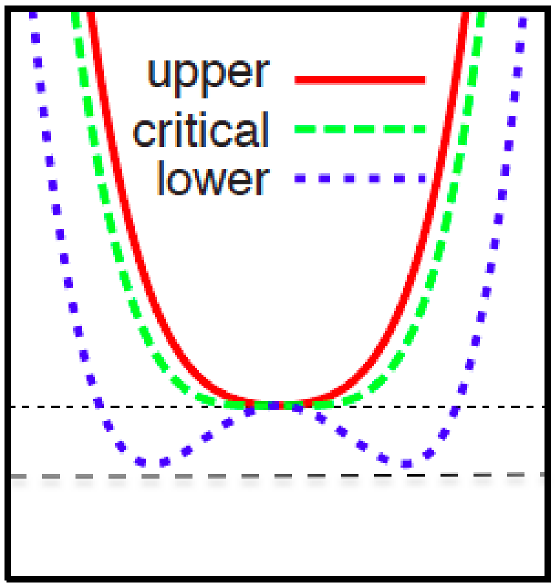
$\mathcal{F}[\phi] \propto L^d$ while $\mathcal{V}_{\vec{r}} = \delta^d \ll \ell^d \ll L^d$

Generalisations to vector models. **Quenched disorder** can be introduced by taking the J_{ij} or the parameters in the field theory to be random distributed.

Ferromagnetism

Bi-valued equilibrium states related by symmetry

$v[\phi] = \frac{\mu}{2}\phi^2(\vec{r}) + \frac{g}{4}\phi^4(\vec{r})$



Potential density

$\Delta v[\phi] = \mathcal{O}(1)$

$\phi(\vec{r})$

Ginzburg-Landau free-energy

Scalar order parameter

Disordered phase (high T, $\mu > 0$)

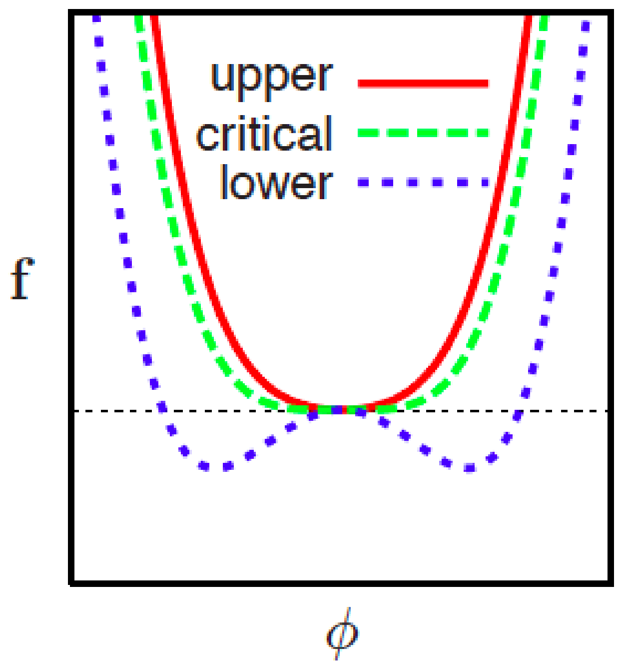
Ordered phases (low T, $\mu < 0$)

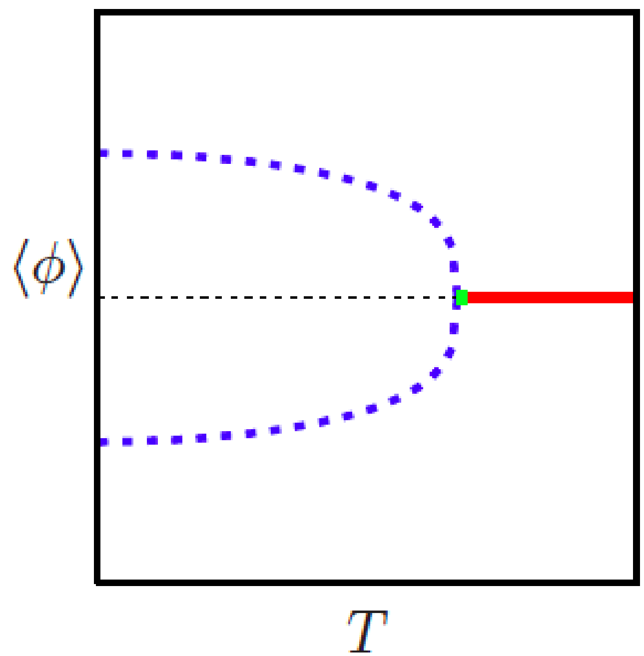
Critical point (T_c, $\mu = 0$)

Ferromagnetism

Free-energy density for the global order parameter

$\int d^D r \, (\nabla\phi)^2 \Rightarrow \phi(\vec{r}) = \phi$ and $f = L^{-d} \int d^D r \, v[\phi(\vec{r})] = v(\phi)$



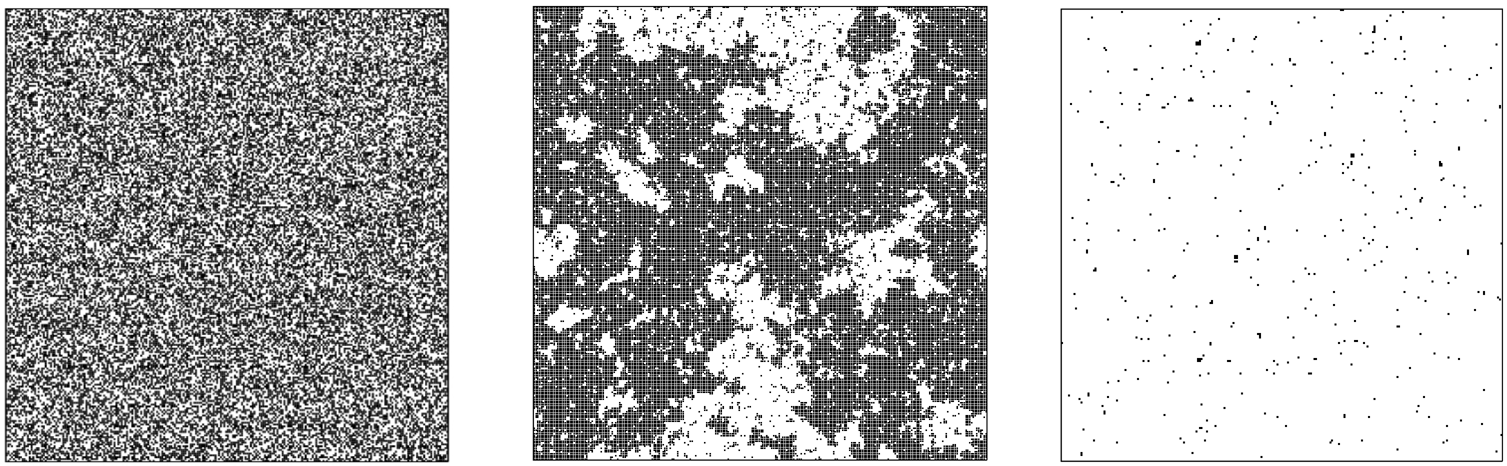


$\langle\phi\rangle = \phi_{\mathrm{saddle-point}} = \phi_{\min} \equiv \phi$ s. t. $v'[\phi] = 0$ & $v''[\phi] > 0$

The barrier is $\Delta f = \mathcal{O}(1)$ but $\boxed{\Delta\mathcal{F}}$ diverges with L

Ferromagnetism

Equilibrium configurations - up & down spins in a $2d$ Ising model



$T \to \infty$ $T = T_c$ $T < T_c$

Dynamic question: starting from equilibrium at $T_0 \to \infty$ how is equilibrium at $T = T_c$ or $T < T_c$ approached and attained ?

Models

Dynamics for discrete and continuous

Ising spin models

$$H = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$$

NCOP [$\uparrow\downarrow \mapsto \uparrow\uparrow$]

COP [$\uparrow\downarrow \mapsto \downarrow\uparrow$]

Field theory for the order parameter

$$\mathcal{F}[\phi] = \int d^D r \left[\tfrac{1}{2}(\nabla\phi)^2 - \tfrac{\mu}{2}\phi^2 + \tfrac{g}{4}\phi^4) \right]$$

$$\partial_t \phi(\vec{r}, t) = -\delta_{\phi(\vec{r},t)} \mathcal{F}[\phi] + \xi(\vec{r}, t)$$

$$\partial_t \phi(\vec{r}, t) = -\nabla^2 \delta_{\phi(\vec{r},t)} \mathcal{F}[\phi] + \xi(\vec{r}, t)$$

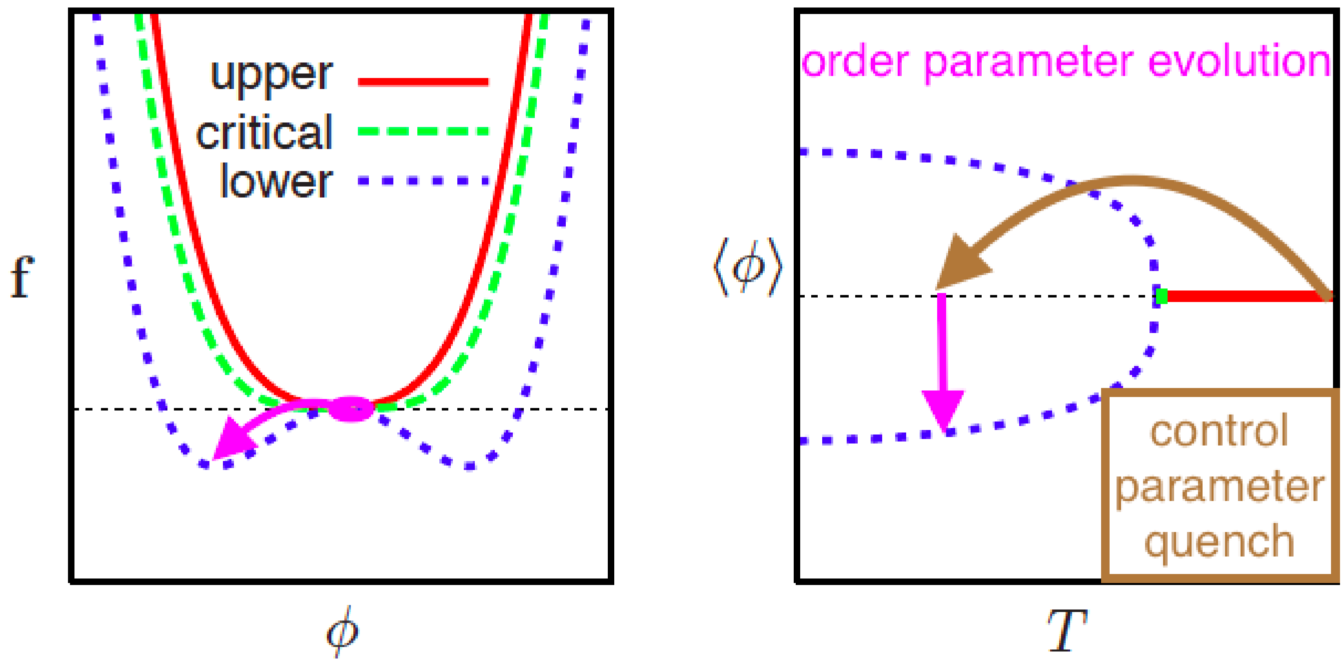
Overdamped limit and white noise commonly accepted

In the COP case $\langle \xi(\vec{x}, t) \xi(\vec{y}, t') \rangle = 2 k_B T \nabla^2 \delta(\vec{x} - \vec{y}) \delta(t - t')$

Generalisations for vector cases. **Quenched disorder** can be introduced by taking the J_{ij} or the parameters in the field theory to be random distributed.

Ferromagnetism

Naively expected spontaneous symmetry breaking



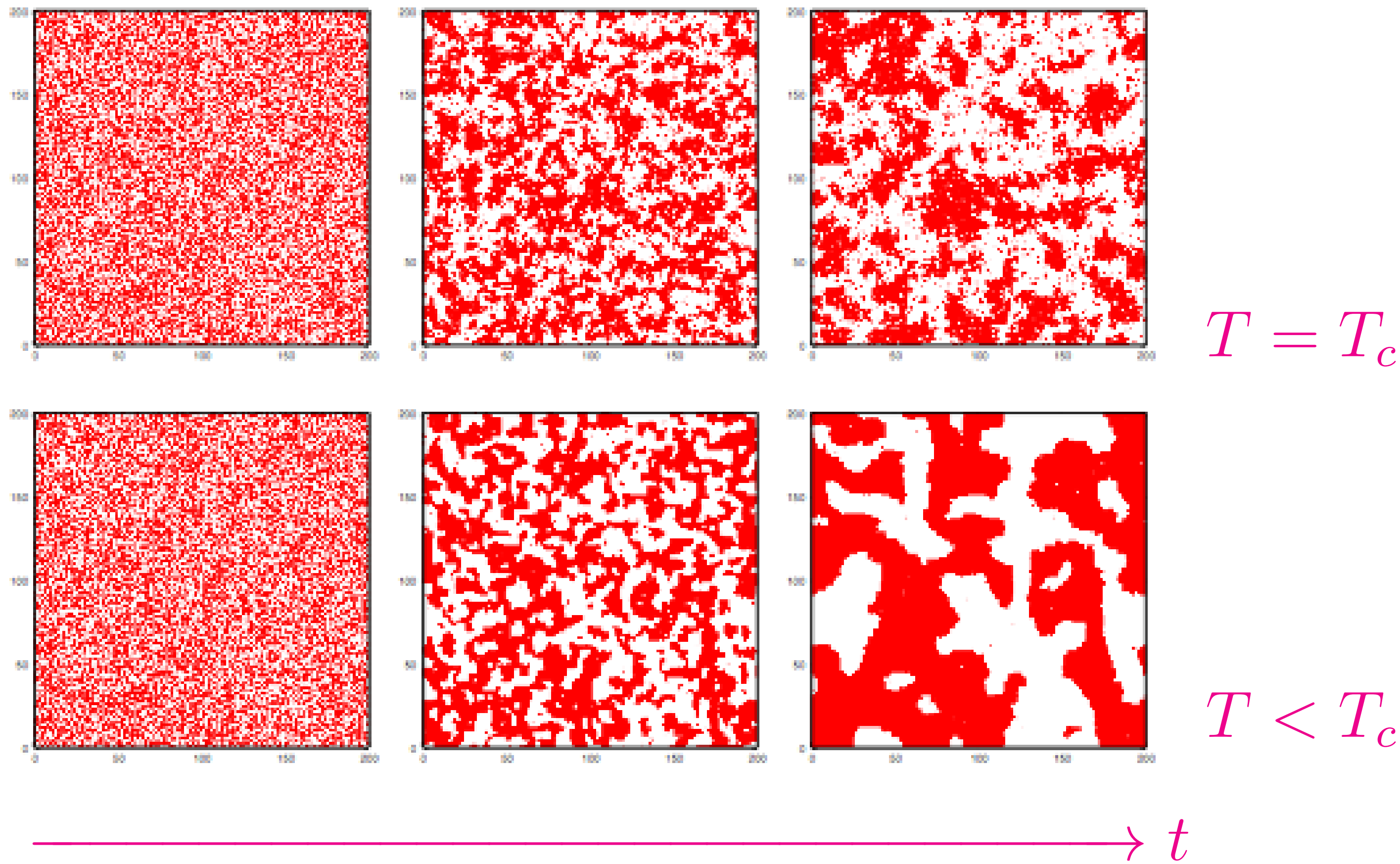
The magenta arrows are naively expected

but diverging times with the system size $t = \mathcal{O}(L^{z_d})$ are needed to reach this regime

and even longer times $t_A = \mathcal{O}(e^{\Delta\mathcal{F}/(k_B T)})$ are needed to restore the symmetry

Ferromagnetism

Snapshots after an instantaneous quench from $T_0 \to \infty$ to T at $t = 0$



At $T = T_c$ **critical dynamics**

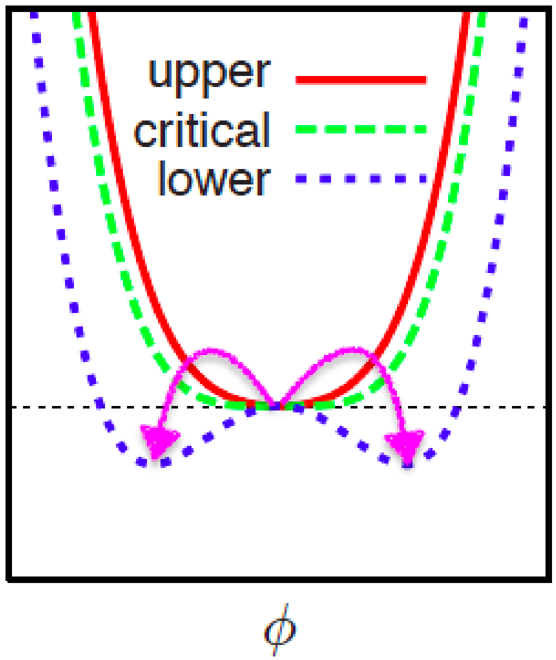
At $T < T_c$ **coarsening**

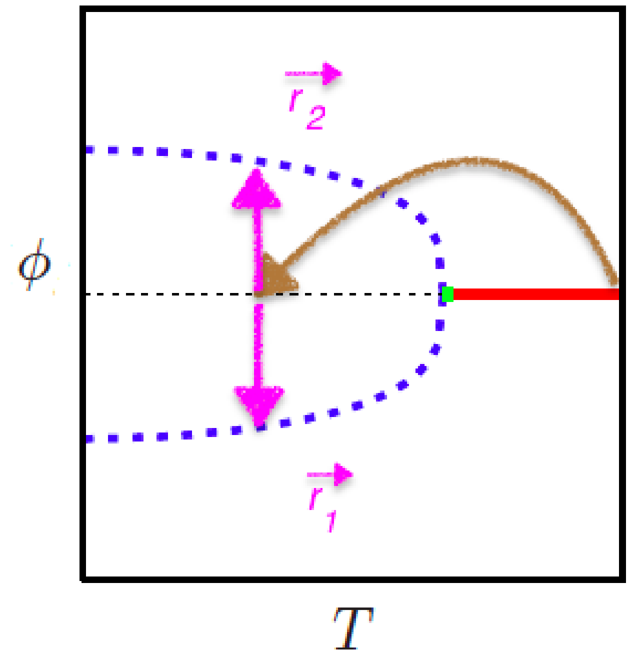
A certain number of interfaces or domain walls in the last snapshots.

Ferromagnetism

Coarsening - domain growth - dynamic scaling

$v[\phi(\vec{r})]$

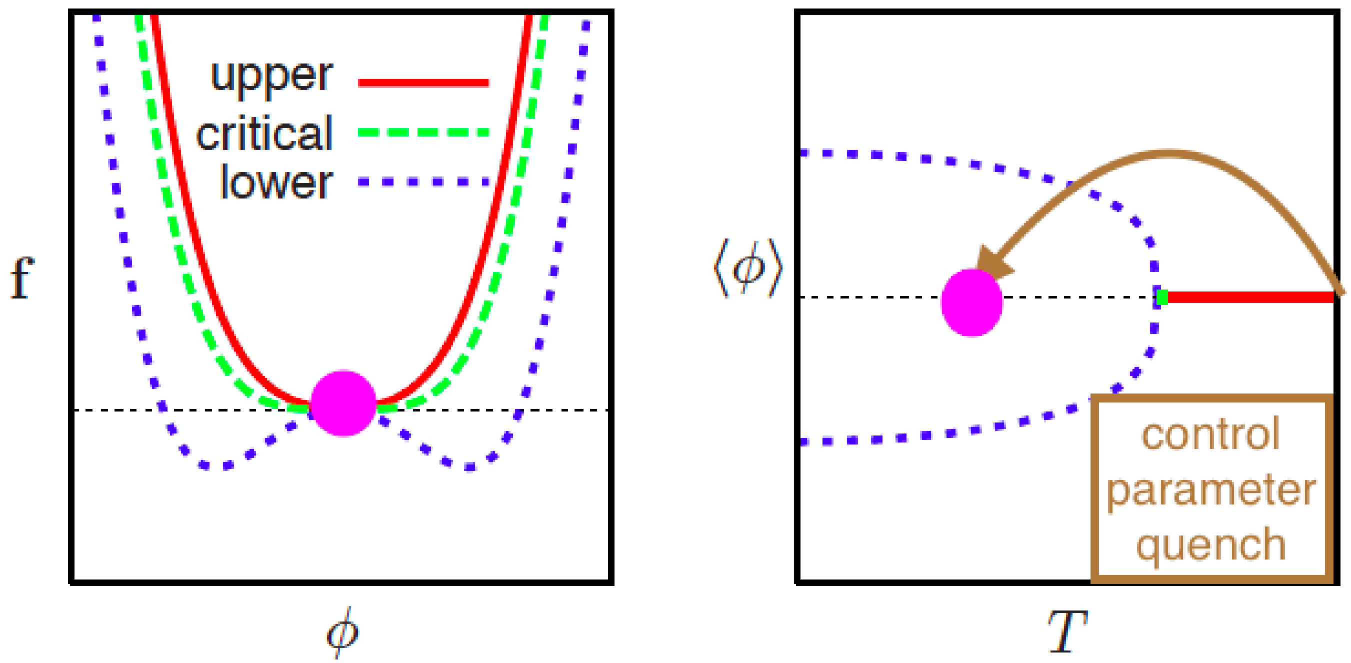




Locally the system chooses one or the other equilibrium state order with equal probability

Ferromagnetism

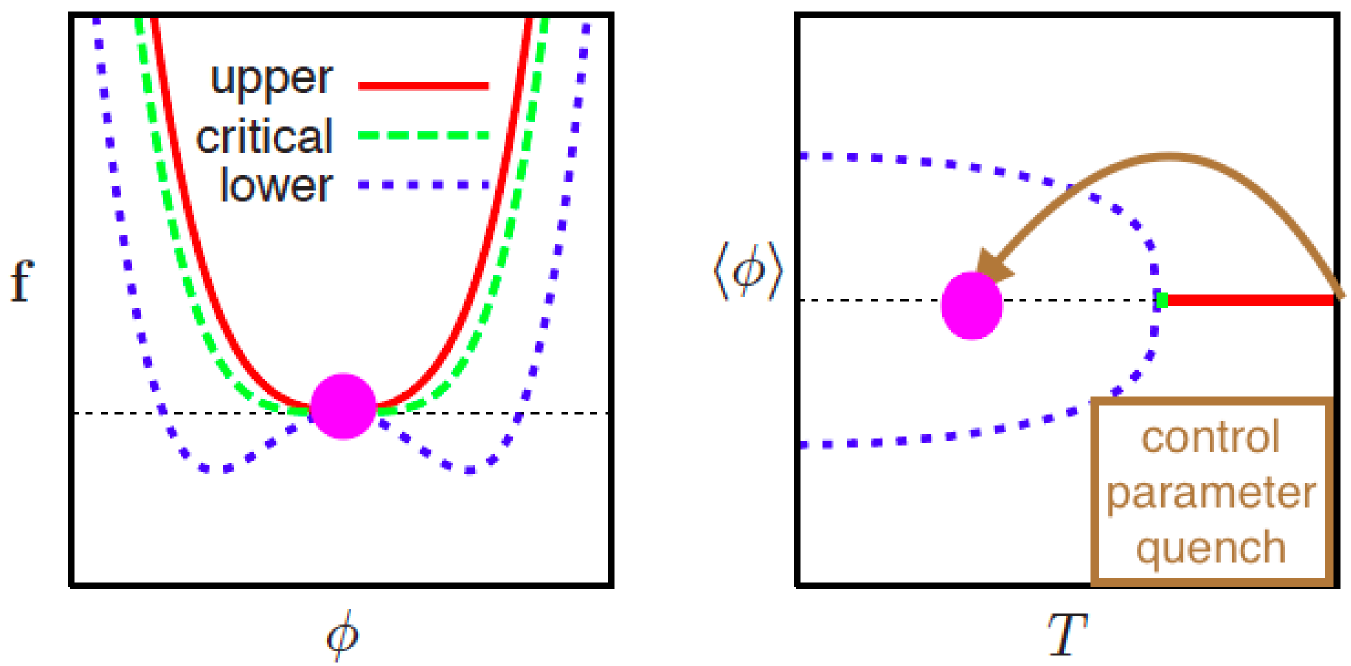
Coarsening - domain growth - dynamic scaling



In the $L \to \infty$ limit, for finite times with respect to L, the global or averaged order parameter vanishes, $\langle\phi\rangle = 0$, and the representative point remains at the top of the barrier

Ferromagnetism

Coarsening - domain growth - dynamic scaling



Note that in this representation there is only one independent variable, the global ϕ. The remaining $L^d - 1$ "longitudinal" (flat) directions orthogonal to this one are not shown

Scales

Times and system size

Thermodynamic limit taken first

$$\lim_{t\to\infty}\lim_{L\to\infty}$$

just coarsening is observed, dynamics far from equilibrium

Diverging times with system size, different regimes, depending on how one scales t and L :

- $t = \mathcal{O}(L^{z_d})$ approach to order, spontaneous symmetry breaking
- $t = \mathcal{O}(e^{\Delta \mathcal{F}})$ jump over barrier global reversals

Scales

Times and system size

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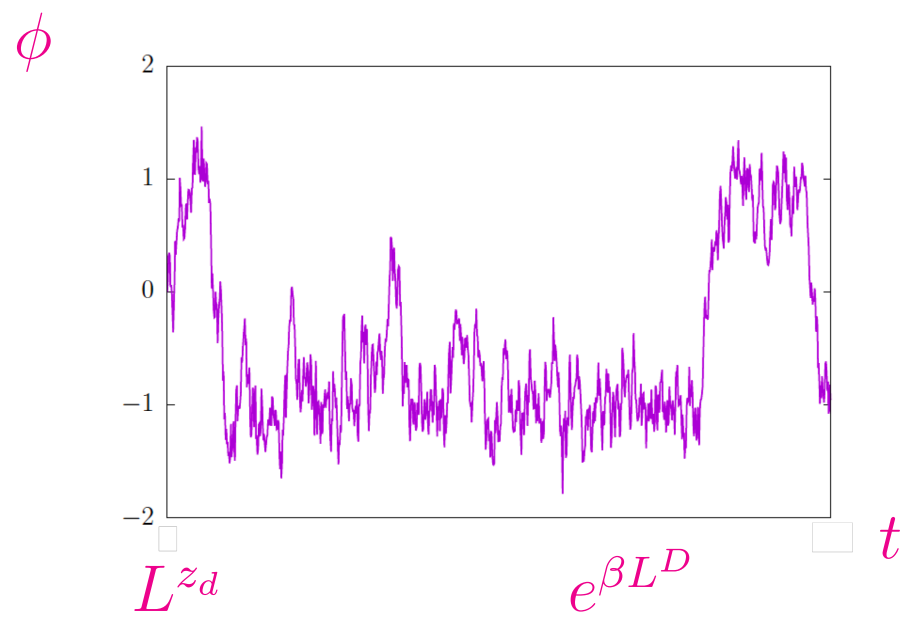


(Sketch)

Scales

Times and system size

Diverging times with system size, different regimes, depending on how one scales t and L :

- $t = \mathcal{O}(L^{z_d})$ approach to order, spontaneous symmetry breaking
- $t = \mathcal{O}(e^{L^D})$ jump over barrier global reversals

In this case, it is easy to beat the slow dynamics :

apply a pinning field that selects one equilibrium state

$H \mapsto H - h \sum_{i=1}^{N} s_i$ implying $\mathcal{F}[\phi] \mapsto \mathcal{F}[\phi] - h \int d^D r \, \phi(\vec{r})$

More on flat directions in this context **Kurchan & Laloux 96**

Collective phenomena

Critical relaxation in the classical O(N) model

N-component field $\vec{\phi} = (\phi_1, \ldots, \phi_N)$ in a D-dim. space $\vec{r} = (r_1, \ldots, r_D)$.

Ginzburg-Landau type free-energy :

$$\mathcal{F}[\vec{\phi}] = \int d^D r \left\{ \frac{1}{2} [\nabla \vec{\phi}(\vec{r})]^2 - \frac{\mu}{2} \phi^2(\vec{r}) + \frac{\lambda}{4} \phi^4(\vec{r}) \right\}$$

Over-damped relaxation dynamics

$$\int_{t_0}^{t} dt' \, \mathbf{\Sigma}_B(t-t') \frac{\partial}{\partial t'} \phi_i(\vec{r}, t') = -\frac{\delta \mathcal{F}[\vec{\phi}]}{\delta \phi_i(\vec{r}, t)} + \xi_i(\vec{r}, t)$$

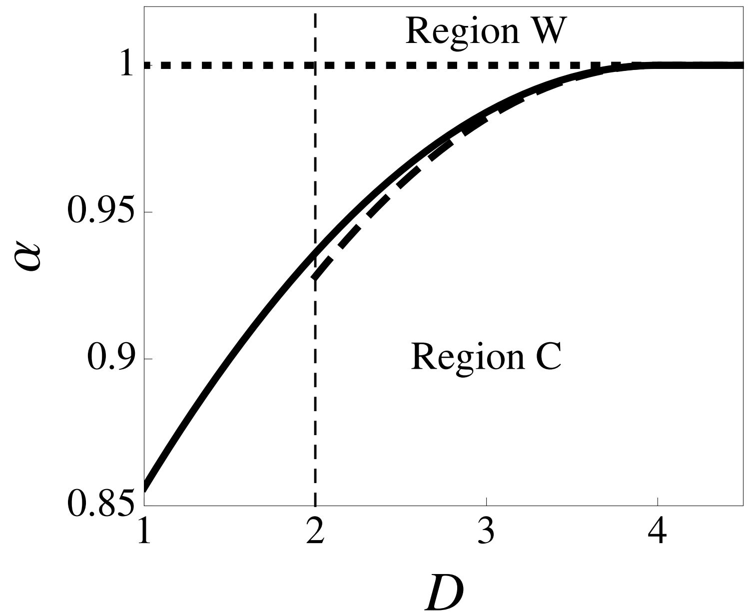
$$\langle \xi_i(\vec{r}, t) \xi_j(\vec{r}\,', t') \rangle = k_B T \delta_{ij} \delta(\vec{r} - \vec{r}\,') \, \mathbf{\Sigma}_B(t-t')$$

$$\mathbf{\Sigma}_\mathbf{B}(t-t') = \frac{g}{\Gamma_E(1-\alpha)} \, |t-t'|^{-\alpha} \qquad \text{with} \qquad \alpha > 0$$

High-temperature initial conditions $\qquad P[\vec{\phi}(\vec{r}, t_0)] \propto e^{-\phi^2(\vec{r}, t_0)/(2\Delta^2)}$

Critical relaxation

$\epsilon = 4 - D$–expansion in the classical $O(N)$ model



$D_c(\alpha) = 4 \qquad T_c(\alpha) = T_c$

The dynamic exponent

in region W

$$z_d = 2 + \frac{N+2}{(N+8)^2}\left[3\ln\frac{4}{3} - \frac{1}{2}\right]\epsilon^2$$

in region C Sub-Ohmic bath

$$z_d = \frac{2}{\alpha}\left[1 - \frac{N+2}{4(N+8)^2}\epsilon^2\right]$$

Solid line $N = 1$

Dashed line $N = 4$

Dotted horizontal line $N \to \infty$

sub-Ohmic bath : slower relaxation

Bonart, LFC & Gambassi 11

Gagel, Orth & Schmalian 15

Statements

Non-frustrated collective relaxation

Slow (non exponential) relaxation

Non-trivial collective effects and competition

From the point of view of landscapes:

importance of flat directions along hidden/longitudinal directions)

Effect of bath correlations (memory) on critical relaxation

More on effective Langevin equations with memory and coloured noise later

A tutorial

How does a (large) system reach equilibrium or

what does it do while it evolves out of equilibrium

- **One dimensional energy landscapes**
- **The simplest free-energy landscape : many variables - large dimensions**
- **Complex free-energy landscapes**

  Models

  Schwinger-Dyson equations & single variable equation

  Pure p-spin and SK-like models

  Ricci-Tersenghi's talk for mixtures of p spins

  Separation of time scales, aging, FDT, effective temperatures

  Dynamics from the landscape point of view

  Non-potential forces

Models

If focus on glasses realistic *vs.* approximate

Particles in interaction

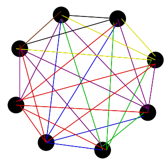
Pair potential $V = \frac{a}{r_{ij}^6} - \frac{b}{r_{ij}^{12}}$

Spins in interaction

RKKY $V = \frac{\sin(2\pi k_F r_{ij})}{r_{ij}^3} s_i s_j$

Fully connected disordered models

$$V = \sum_{i_1 \dots i_p} J_{i_1 \dots i_p} s_{i_1} \dots s_{i_p}$$



e.g., $p = 2$

They are frustrated.

The p-spin disordered models have quenched disordered interactions : $J_{i_1 \dots i_p}$ drawn from a probability distribution $P(J_{i_1 \dots i_p})$, typically Gaussian.

Mean-field models : defined on a complete or dilute graph.

Langevin dynamics

System coupled to a memory-less equilibrium bath

Overdamped limit
$$\underbrace{\gamma \dot{s}_i(t)}_{\text{friction}} = \underbrace{F_i(t)}_{\text{force}} + \underbrace{\xi_i(t)}_{\text{white noise}}$$

Potential/conservative force
$$F_i[\{s_k\}] = -\frac{\delta V[\{s_k\}]}{\delta s_i(t)}$$
with, *e.g.*

$V = \sum_{i_1 \ldots i_p} J_{i_1 \ldots i_p} s_{i_1} \ldots s_{i_p}$ and $J_{i_1 \ldots i_p}$ fully symmetric w/r to $i_l \leftrightarrow i_m$

Non-potential force
$$F_i[\{s_k\}] = -p \sum_{i_2 \ldots i_p} J_{i i_2 \ldots i_p} s_{i_2} \ldots s_{i_p}$$

with $J_{i_1 \ldots i_p}$ fully symmetric w/r to $i_l \leftrightarrow i_m$ for $l, m = 2, \ldots, p$ but asymmetric w/r to $i_1 \leftrightarrow i_m$ for $m = 2, \ldots p$

Rheology, neural nets, etc.

Langevin dynamics

System coupled to a memory-less equilibrium bath

Overdamped limit $$\underbrace{\gamma \dot{s}_i(t)}_{\text{friction}} = \underbrace{F_i(t)}_{\text{force}} + \underbrace{\xi_i(t)}_{\text{white noise}}$$

Initial conditions

- Rapid quench from very high temperature mimicked by random initial conditions $s_i(0)$, taken, e.g. from a Gaussian pdf $\Rightarrow$ uncorrelated with the quenched randomness $J_{i_1 \dots i_p}$.
- Correlated with $J^{\rm symm}_{i_1 \dots i_p}$, e.g. $P_{\rm GB}(\beta_{\rm in})$ for some initial inverse temp. $\beta_{\rm in}$

General : random potential correlation

$$[V(\{s_k\})V(\{s'_l\})] = N f(N^{-1} \textstyle\sum_{k=1}^N s_k s'_k) = N f(C)$$

Time-dependent order parameters

In the limit $N \to \infty$ the evolution of the fully-connected models is completely captured/described by the two-time correlation and linear response (thermal and disorder averaged)

$$C(t,t_w) \equiv \frac{1}{N}\sum_i [\langle s_i(t)s_i(t_w)\rangle] \; ,$$
$$\chi(t,t_w) \equiv \frac{1}{N}\sum_i \int_{t_w}^{t} dt' \; R(t,t') = \frac{1}{N}\sum_i \int_{t_w}^{t} dt' \; [\left.\frac{\delta\langle s_i(t)\rangle_h}{\delta h_i(t')}\right|_{h=0}] \, .$$

and the correlation with the initial condition

$$C_0(t,0) \equiv \frac{1}{N}\sum_i [\langle s_i(t)s_i(0)\rangle]$$

in cases in which this is correlated with the quenched randomness.

Dynamic equations

Integro-differential eqs. on the correlation and linear response

In the $N \to \infty$ limit exact causal Schwinger-Dyson equations

$$(\partial_t - z_t)C(t,t_w) = \int dt' \, \left[\Sigma(t,t')C(t',t_w) + D(t,t')R(t_w,t')\right]$$
$$+2TR(t_w,t) \ ,$$
$$(\partial_t - z_t)R(t,t_w) = \int dt' \, \Sigma(t,t')R(t',t_w) + \delta(t-t_w) \ ,$$

where the self-energy and vertex depend on C and R. For the potential models

$$D(t,t_w) = f'(C(t,t_w)) \ , \quad \Sigma(t,t_w) = f''(C(t,t_w))R(t,t_w)$$

The Lagrange multiplier z_t is fixed by $C(t,t) = 1$. Random initial conditions.

See **LFC & Kurchan 93, Ben Arous, Dembo & Guionnet 06**, also **Dembo's** talk

Dynamic equations

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$$(\partial_t - z_t)R(t,t_w) = \int dt' \, \Sigma(t,t')R(t',t_w) + \delta(t-t_w) \; ,$$

where the self-energy and vertex depend on C and R. For the potential p-spin model

$$\boxed{D(C) = f'(C) = \tfrac{p}{2}C^{p-1} \; , \;\; \Sigma(C,R) = D'(C)\,R = f''(C)R}$$

The Lagrange multiplier z_t is fixed by $C(t,t) = 1$. Random initial conditions.

see **LFC & Kurchan 93, Ben Arous, Dembo & Guionnet 06**, also **Dembo's** talk

Dynamic equations

Integro-differential eqs. on the correlation and linear response

In the $N \to \infty$ limit exact causal Schwinger-Dyson equations

$$(\partial_t - z_t) C(t, t_w) = \int dt' \, \left[\Sigma(t, t') C(t', t_w) + D(t, t') R(t_w, t') \right]$$
$$+ 2T R(t_w, t) \; ,$$
$$(\partial_t - z_t) R(t, t_w) = \int dt' \, \Sigma(t, t') R(t', t_w) + \delta(t - t_w) \; ,$$

where the self-energy and vertex depend on C and R. For the non-potential models

$$\boxed{D(C) \qquad \Sigma(C, R) \neq D'(C) \, R}$$

explicit violation of FDT

see **Crisanti & Sompolinsky 87, LFC, Kurchan, Le Doussal & Peliti 97, etc.**

Dynamic equations

Equilibrium initial conditions

In the $N \to \infty$ limit exact causal Schwinger-Dyson equations

$$(\gamma\partial_t - z_t)R(t,t_w) = \int dt' \; \Sigma(t,t')R(t',t_w) + \delta(t-t_w)$$

$$(\gamma\partial_t - z_t)C(t,t_w) = \int dt' \; [\Sigma(t,t')C(t',t_w) + D(t,t')R(t_w,t')]$$

$$\boxed{+\beta_{\rm in} \sum_{a=1}^{n} D_a(t,0)C_a(t_w,0)} + 2TR(t_w,t)$$

$$\boxed{(\gamma\partial_t - z_t)C_a(t,0) = \int dt' \, \Sigma(t,t')C_a(t',0) + \beta_{\rm in} \sum_{a=1}^{n} D_b(t,0)Q_{ab}}$$

$a = 1, \ldots, n \to 0$, replica method to deal with $e^{-\beta_{\rm in} H}$ and fix Q_{ab}

Houghton, Jain & Young 86, Franz & Parisi 95, Barrat, Burioni & Mézard 96

Dynamic equations

Single variable self-consistent over-damped Langevin equation

$$\underbrace{\gamma \dot{s}_i(t)}_{\text{friction}} + \underbrace{\int_0^t dt' \; \Sigma(t,t') s_i(t')}_{\text{self-generated friction}} - \underbrace{z(t) s_i(t)}_{\text{sph constraint}} =$$

$$= \underbrace{\xi_i(t)}_{\text{white noise}} + \underbrace{\eta_i(t)}_{\text{self-consist noise}}$$

$$\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} D(t,t')$$

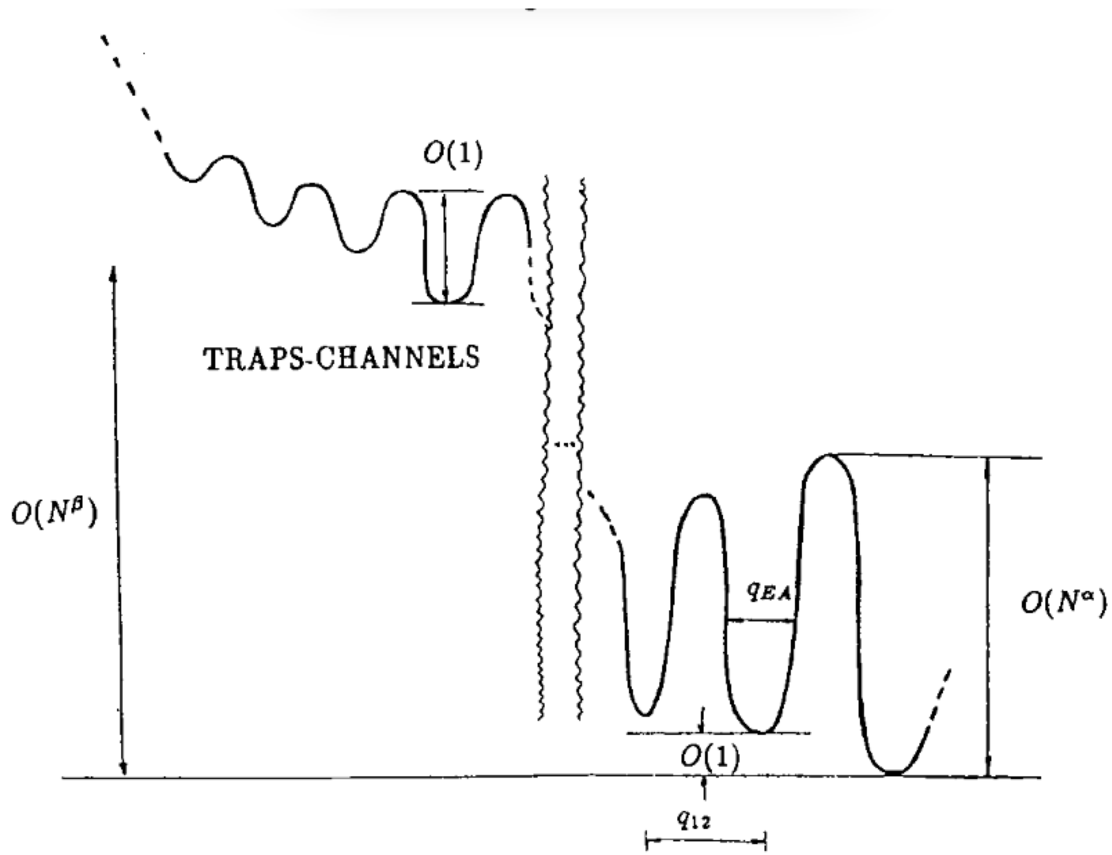
Σ and D are self-consistently determined in terms of correlations and linear responses of the original fields.

cfr. **Mode Coupling Th (Götze et al), Dynamic Mean-Field Th (Georges & Kotliar)**

see **Sompolinsky 81, LFC & Kurchan 00**

Free-energy landscapes

Two representative fully-connected disordered spin models



p-spin model

$\alpha = 1$

$\beta = 1$

$T < T_d$

SK-like models

$\alpha < 1$

$\beta < 1$

$T < T_s = T_d$

Image from **LFC & Kurchan 95**

Rieger 91, Kurchan, Parisi & Virasoro 93, Cavagna, Giardina & Parisi 98-02,

Crisanti, Leuzzi, Montanari, Ricci-Tersenghi & Rizzo 00s

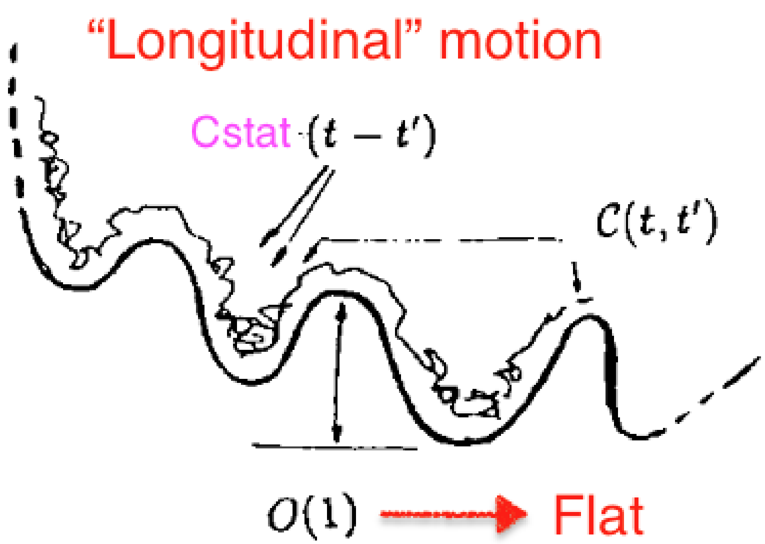
Quench from $T_0 > T_d$ to $T < T_d$

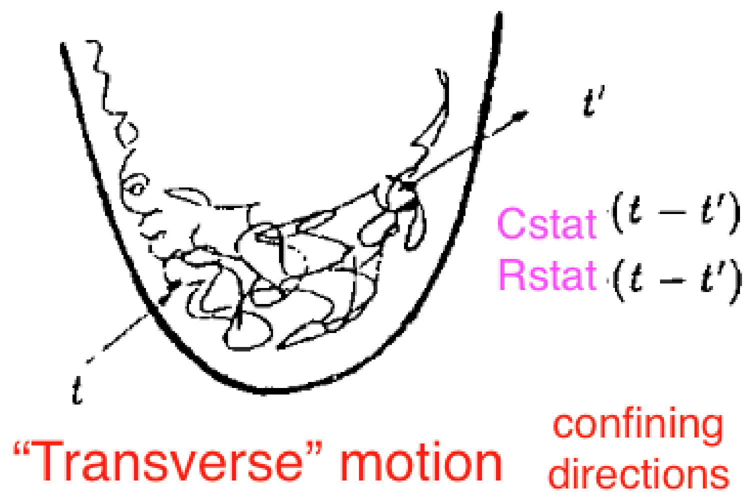
Long t_w after $N \to \infty$: separation of time-scales

$$C(t,t') = \mathcal{C}(t,t') + C_{\rm stat}(t-t')$$

Slow motion

Fast motion





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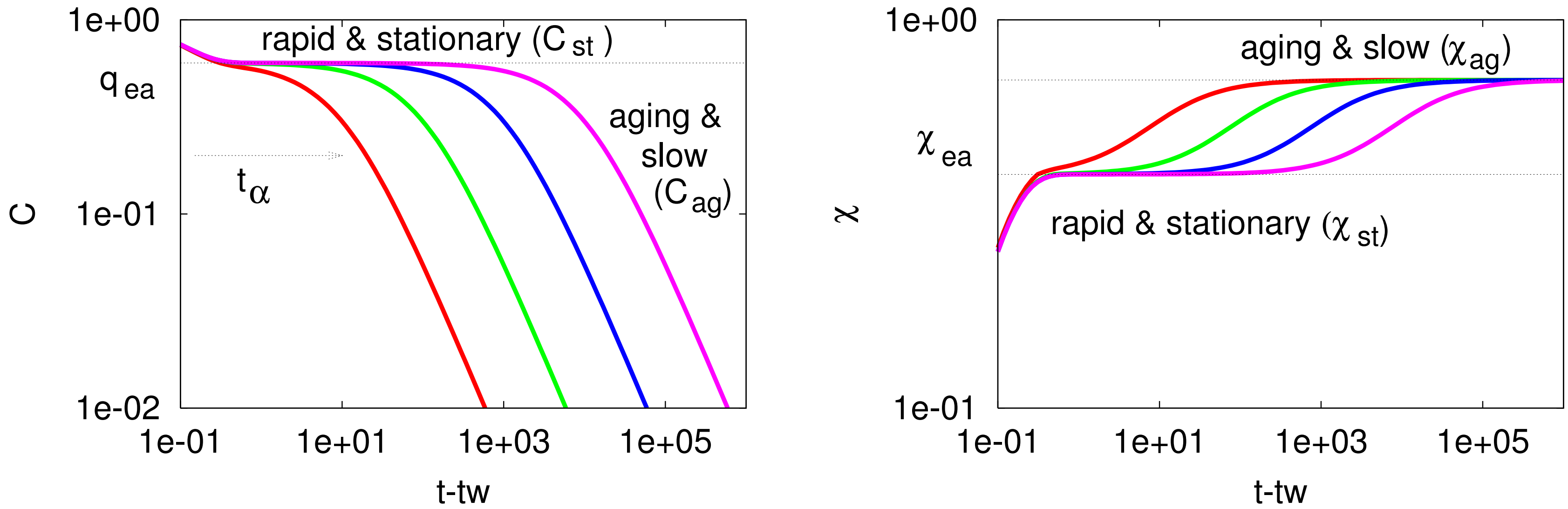
Quench from $T_0 > T_d$ to $T < T_d$

Long t_w after $N \to \infty$: separation of time-scales



Sketch of the **separation of time-scales** in the out of equilibrium relaxation

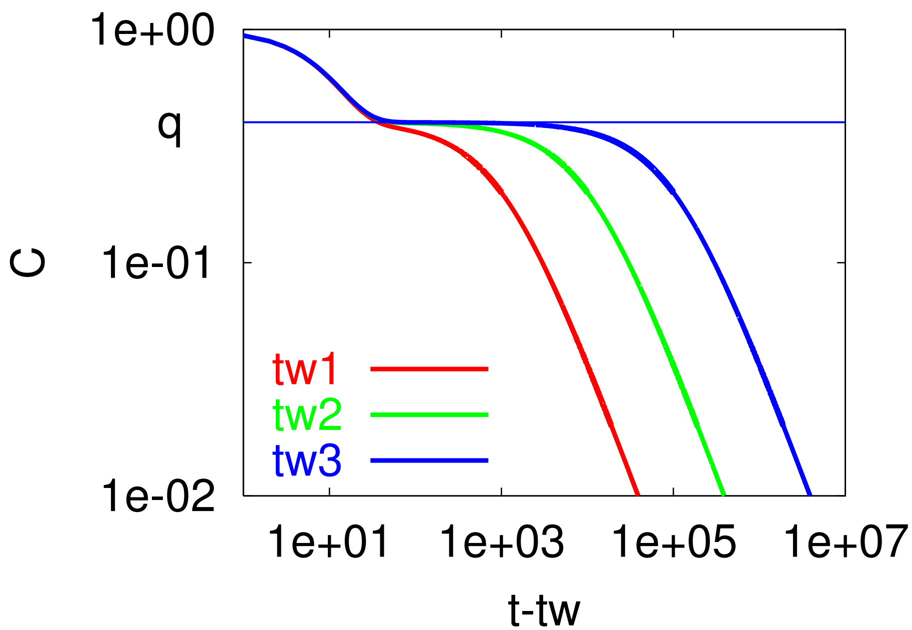
The actual form of the aging relaxation is different in the two families of models

Plugging such an *Ansatz* in the coupled integro-diff eqs. allows one to solve them

Quench from $T_0 > T_d$ to $T < T_d$

Long t_w after $N \to \infty$: separation of time-scales

Fast $\quad C(t,t_w) \approx f_{st}\left(\frac{L_{\rm st}(t)}{L_{\rm st}(t_w)}\right)$ with $L_{\rm st}(t) = e^{t/\tau}$



Slow

$$C_{\rm ag}(t,t_w) \approx f_c\left(\frac{L(t)}{L(t_w)}\right)$$

$$\partial_t C_{\rm ag}(t,t_w) \ll C_{\rm ag}(t,t_w)$$

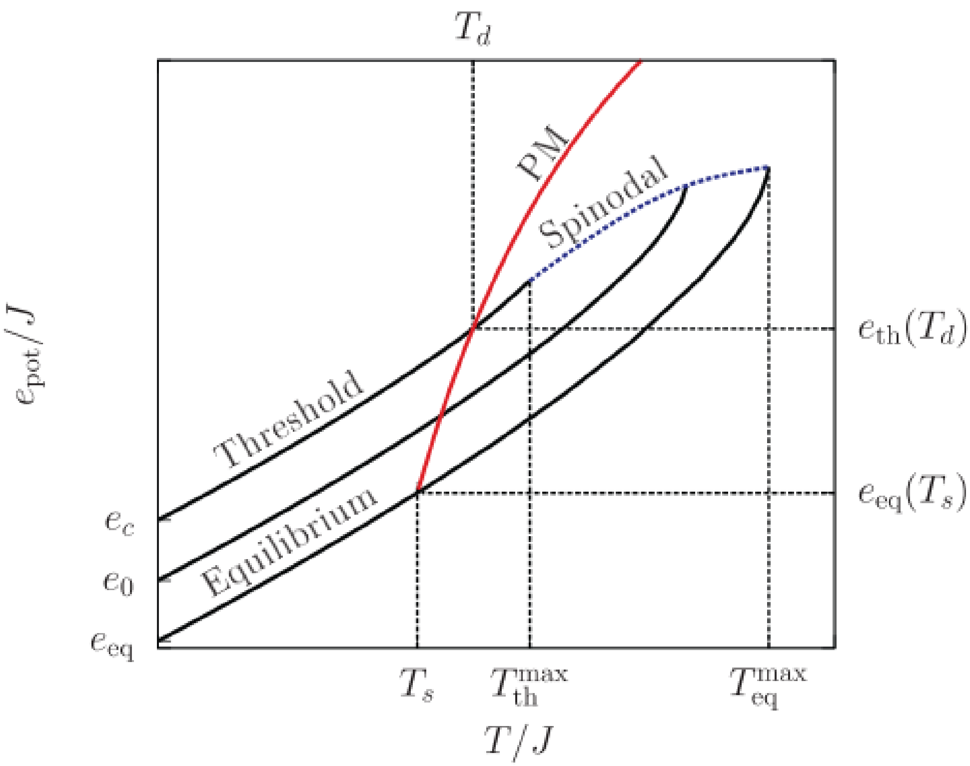
log-log scale !

Eqs. for the slow relaxation $C_{\rm ag} \equiv C < q$:

Approx. asymptotic time-reparametization invariance $\qquad t \to h(t)$

(Free-)energy density

Pure $p \geq 3$ spin-models



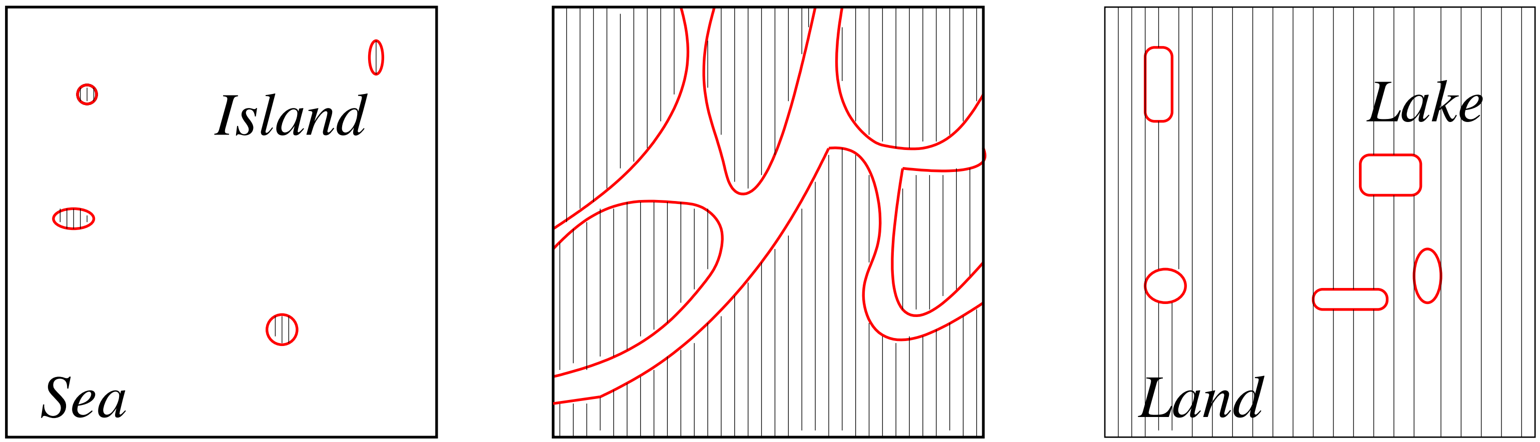
At $T < T_d$: $\lim_{t\to\infty} e(t) = e_{\rm th} > e_{\rm eq}$ **LFC & Kurchan 93**

The threshold level is flat (Hessian analysis).

Confirmation from the dynamic TAP approach in **Biroli 00**

View from above the landscape

Level determined by asymptotic (free-)energy density



Above threshold | At threshold | Below threshold

The system is like a ship :

freely navigating the sea above the threshold $T > T_d$

following "narrow" channels at the threshold $T < T_d$

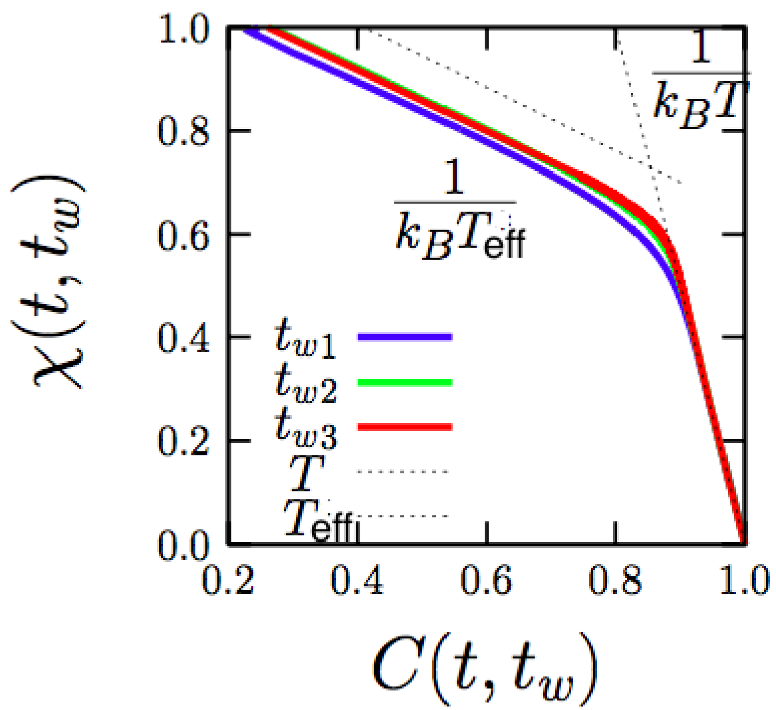
confined to lakes below the threshold $T_{\rm in} < T_d$ and $T < T_{\rm spinodal}$

Figs. from **LFC Les Houches 02**

Fluctuation-dissipation

Pure $p \geq 3$ spin-models

A quench from $T_0 \to \infty$ to $T < T_d$



Parametric construction

t_w fixed

$t_{w_1} < t_{w_2} < t_{w_3}$

t : $t_w \to \infty$ or

$\tau \equiv t - t_w$: $0 \to \infty$

used as a parameter

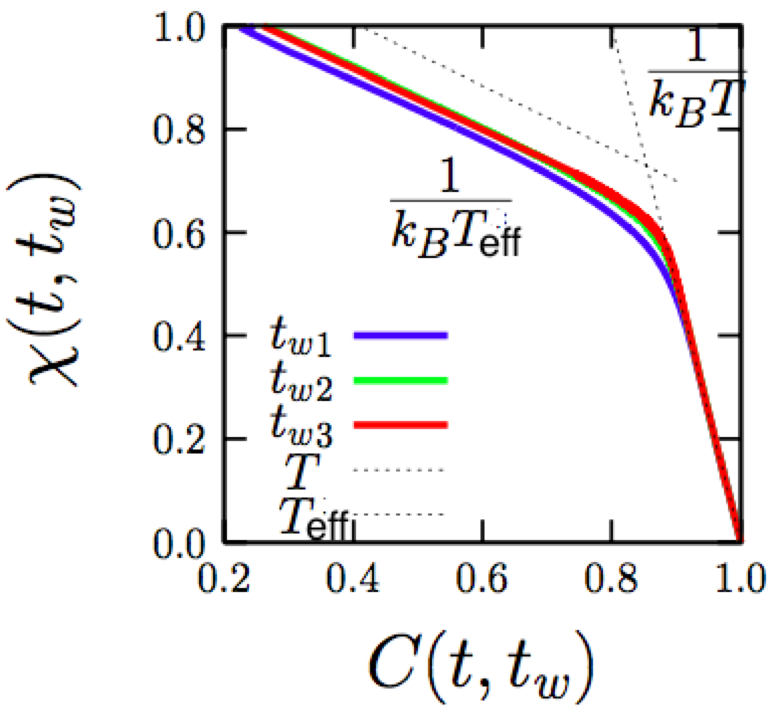
Note that $T_{\text{eff}} > T$

LFC & Kurchan 93 Effective temperature interpretation **LFC, Kurchan & Peliti 97**

Fluctuation-dissipation

Pure $p \geq 3$ spin-models

A quench from $T_0 \to \infty$ to $T < T_d$



Parametric construction

t_w fixed

$t_{w_1} < t_{w_2} < t_{w_3}$

t : $t_w \to \infty$ or

$\tau \equiv t - t_w : 0 \to \infty$

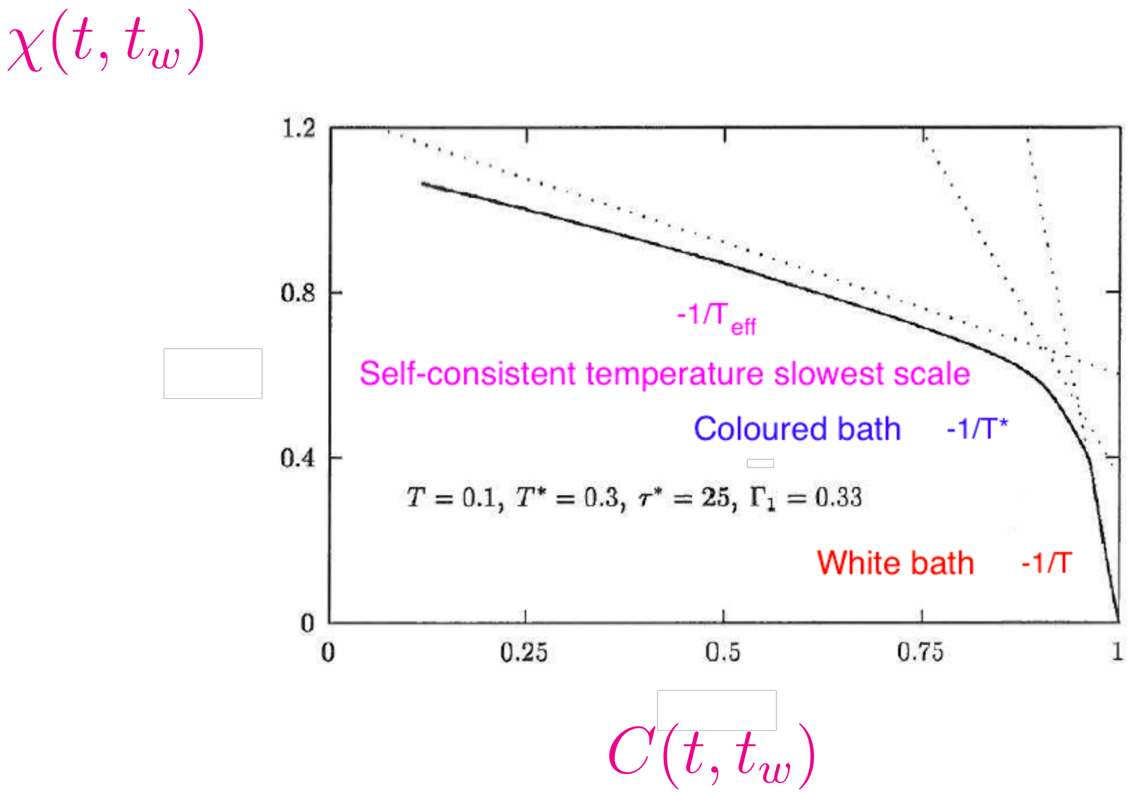
used as a parameter

Note that $T_{\text{eff}} > T$

Physical picture : each scale evolves with its own "clock" $L(t)$ and its own temperature (T, the temperature of the bath, or T_{eff} in this case)

Effective temperature

Pure p spin coupled to multiple baths

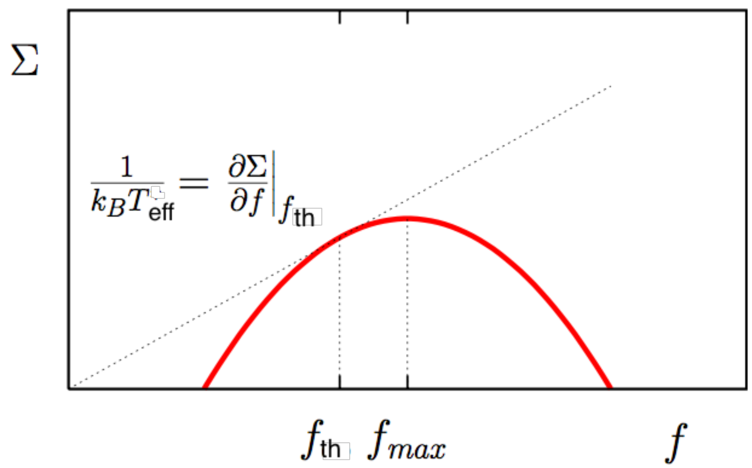


The two baths induce their scales and temperatures and the last one is self-consistently determined by the system itself.

Is $T_{\rm eff}$ related to an entropy ?

Yes, configurational entropy

$$\Sigma(f) = k_B \ln \mathcal{N}(f) \qquad \Rightarrow \qquad \boxed{\frac{1}{k_B T_{\rm eff}} = \left.\frac{\partial \Sigma(f)}{\partial f}\right|_{f_{\rm th}}}$$



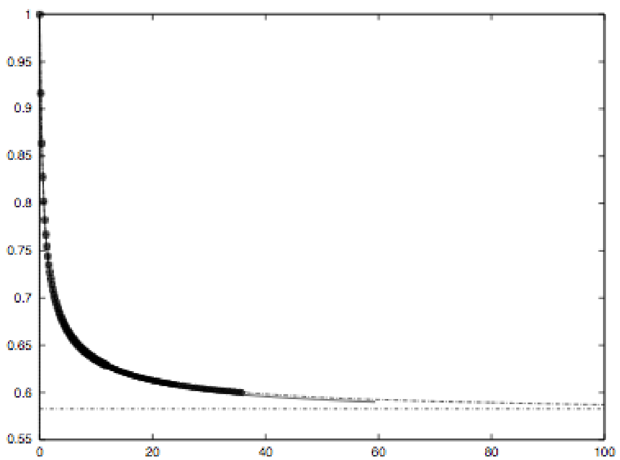
NB $f_{max} \neq f_{\rm th} \Rightarrow$ failure of 'maximum entropy principles'.

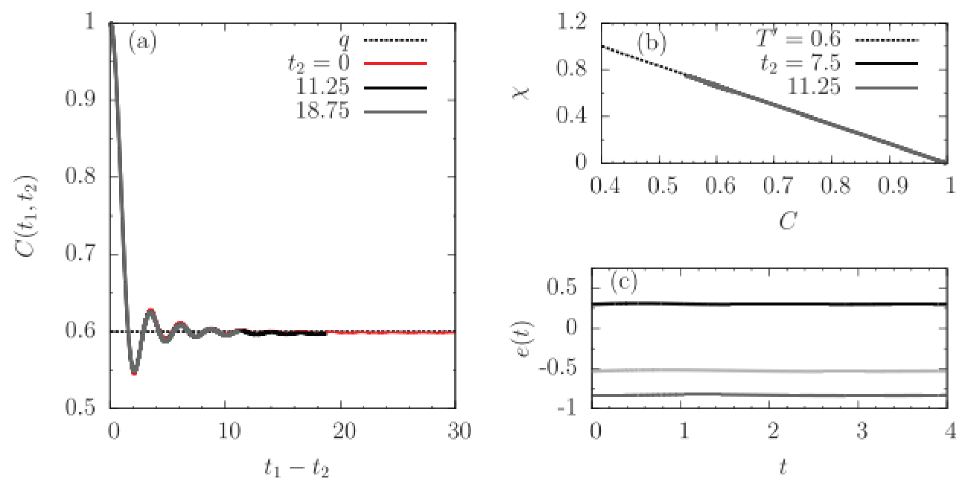
Edwards & Oakshott 89, Monasson 95, Nieuwenhuizen 98

Sketchy view : many amorphous solid configurations ($\Sigma \Leftrightarrow T_{\rm eff}$) and vibrations around them ($f \Leftrightarrow T$).

Following TAP states

Long t_w after $N \to \infty$: trapping



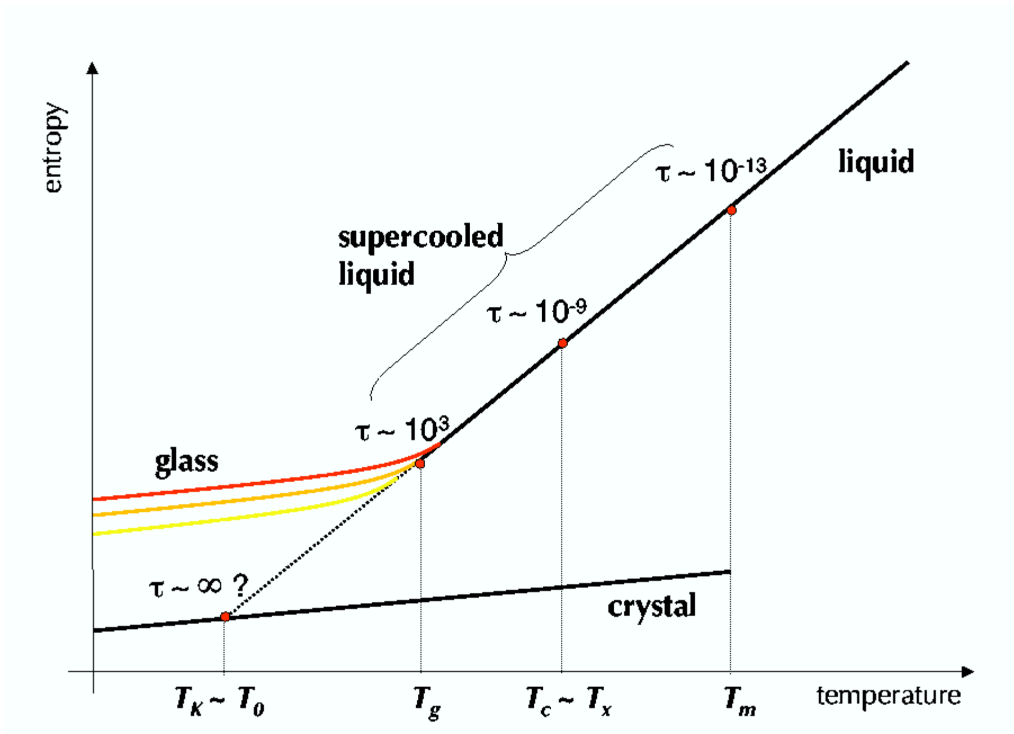


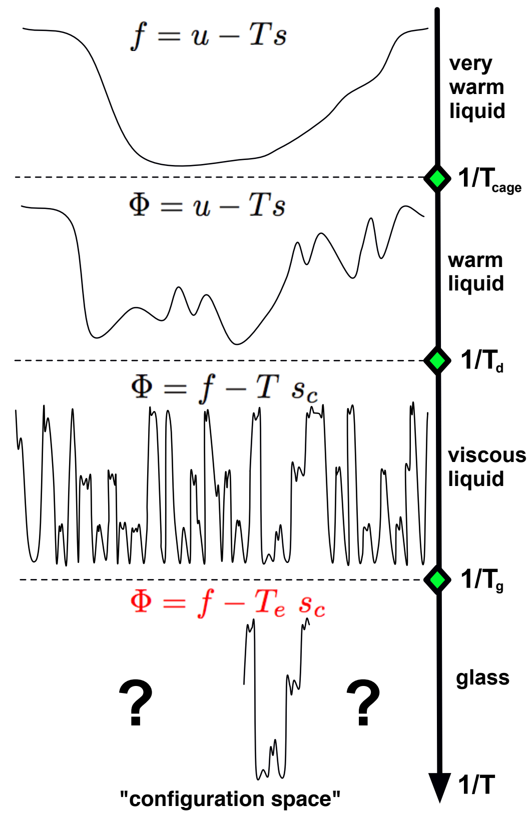
$$C_0(t,0) \to c \neq 0$$

Barrat, Burioni & Mézard 96 — Langevin dynamics

LFC, Lozano & Nessi 17 — Newton dynamics isolated system

Structural glasses





The ruggedness of the free-energy landscape increases upon decreasing temperature until a configurational entropy crisis arises (at **Kauzmann** T_K).

Numerical simulations : one cannot access $\mathbf{f}$ but one can explore $\mathbf{e}$, potential energy landscape.

reviews **Wales 03, Heuer 08**

Statements

Pure p-spin model

The pure p spin model

Relaxation dynamics after a quench

separation of time-scales, stationary & aging

FDT and its violation

Partial thermal equilibration interpretation

Approach to the threshold flat level where marginal states are, $\mathcal{O}(1)$ above the equilibrium energy density

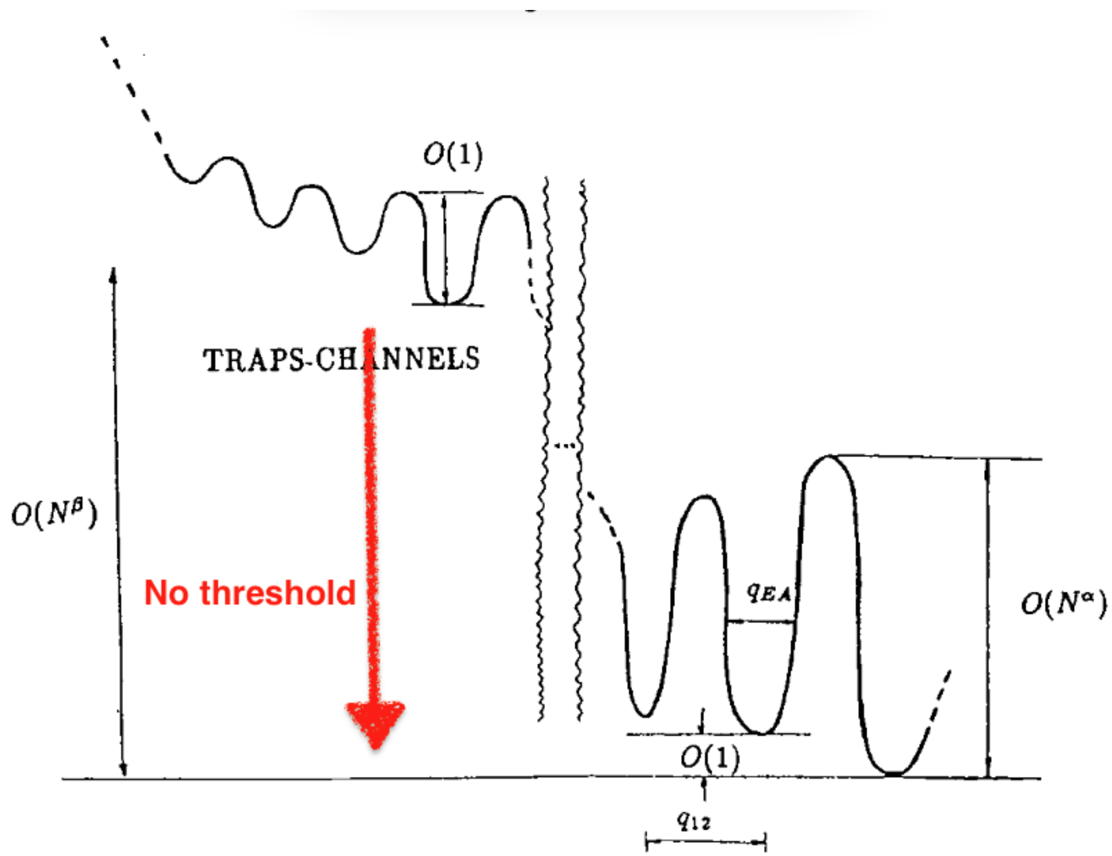
Dynamic TAP equations

Following TAP states

No chaos in temperature, smooth

Free-energy landscapes

Two representative fully-connected disordered spin models



p-spin model

$\alpha = 1$

$\beta = 1$

$T < T_d$

SK-like models

$\alpha < 1$

$\beta < 1$

$T < T_s = T_d$

Image from **LFC & Kurchan 95**

Fluctuation-dissipation

Proposal

For non-equilibrium systems, relaxing slowly towards a situation such that **one-time quantities** [*e.g.* the energy-density $\mathcal{E}(t)$] **approach a finite value**

$$\lim_{\substack{\mathbf{t_w}\to\infty \\ C(t,t_w)=C}} \chi(t,t_w) = f_\chi(C)$$

Also or weakly forced non-equilibrium systems in the limit of small work

The effective temperature is
$$-\frac{1}{T_{\rm eff}(C)} \equiv \frac{\partial\chi(C)}{\partial C}$$

LFC & Kurchan 94, Franz & Mézard 94

Time ultrametricity

Proposal

For non-equilibrium systems, relaxing slowly towards a situation such that **one-time quantities** [*e.g.* the energy-density $\mathcal{E}(t)$] **approach a finite value**, any three correlations

$$\boxed{C(t_1, t_2), \;\; C(t_2, t_3), \;\; C(t_1, t_3)}$$

for $t_3 < t_2, < t_1$ behave such that

$$\boxed{C(t_1, t_3) = \min[C(t_1, t_2), C(t_2, t_3)]}$$

Ultrametricity in time.

Also or weakly forced non-equilibrium systems in the limit of small work

LFC & Kurchan 94, Franz & Mézard 94

Statements

SK-like models

Relaxation dynamics after a quench

separation of time-scales, stationary & time-ultrametricity

FDT and its violation $x(C) = \frac{T}{T_{\rm eff}(C)} = \frac{f'''(C)}{f''(C)} \sqrt{\frac{f''(q)}{f''(C)}}$

An increasing $x(C)$ implies $\eta(C) \equiv \frac{f'''(C)}{(f''(C))^{3/2}} < \eta(q)$

Partial thermal equilibration interpretation

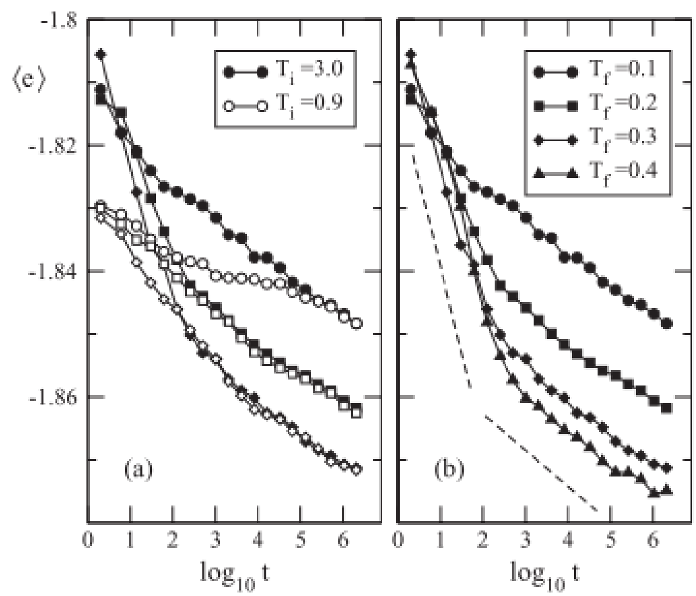
Approach to the equilibrium level (where marginal states are)

$$x(C) = \frac{T}{T_{\rm eff}(C)} = x_{\rm Parisi}(C) \Leftrightarrow P(C) = P_{\rm Parisi}(C)$$

LFC & Kurchan 94, Baldassarri et al. 95, Franz, Mézard, Parisi & Peliti 99

Beyond $N \to \infty$

The random orthogonal model



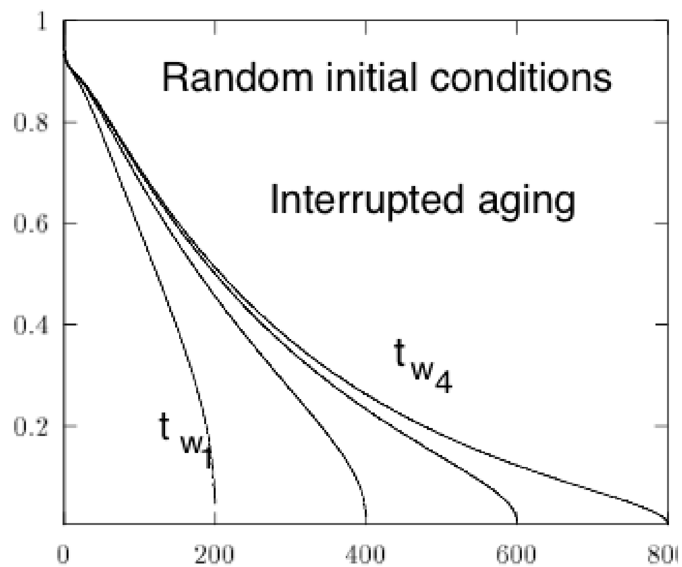
from algebraic at $t \ll N$ to logarithmic at $t(N)$ energy relaxation
from an approach to the threshold to activation below it

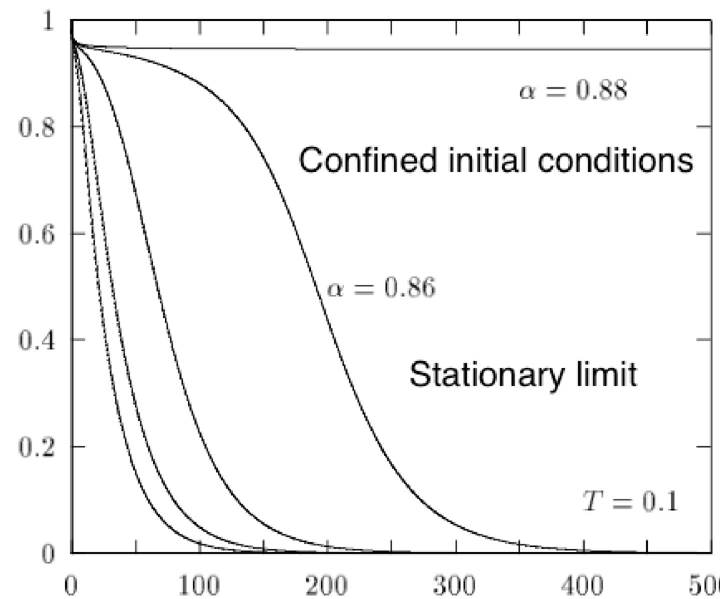
Crisanti & Ritort 00

Can one see the TAP states ?

Non-potential force

Driven $p = 3$ spherical model, $N \to \infty$





Waiting-time dependence (α fixed) and α dependence in steady state

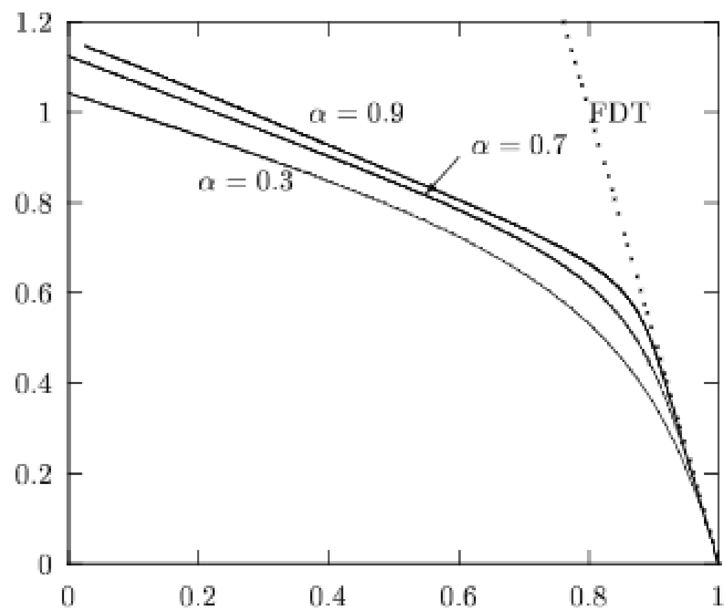
$$J_{ii_2i_3\ldots i_p} = J^{\text{symm}}_{ii_2i_3\ldots i_p} + \alpha J^{\text{asymm}}_{ii_2i_3\ldots i_p} \quad \Rightarrow \quad \Sigma \neq D'R$$

LFC, Kurchan, Le Doussal & Peliti 97

Non-potential force

Driven $p = 3$ Ising spin model with $N \to \infty$

$\chi(t, t_w)$



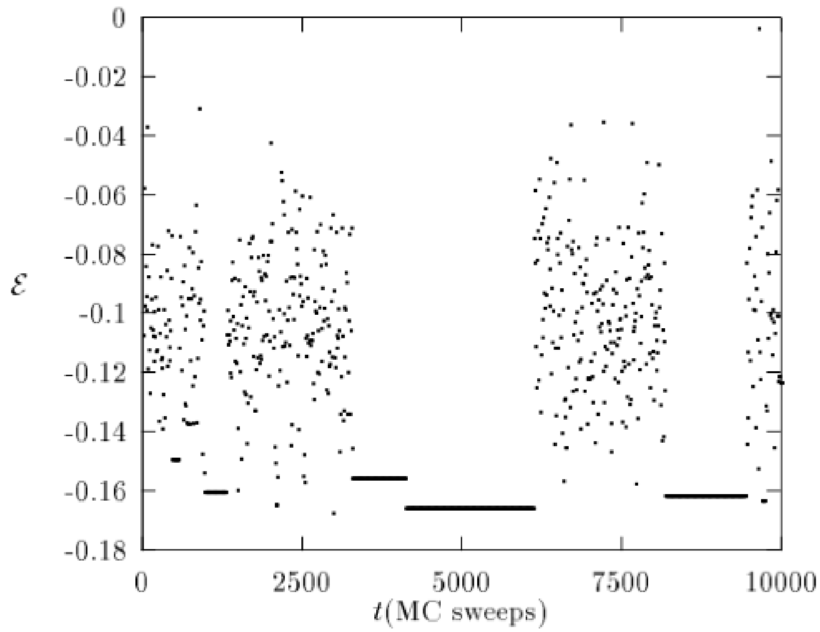
$C(t, t_w)$

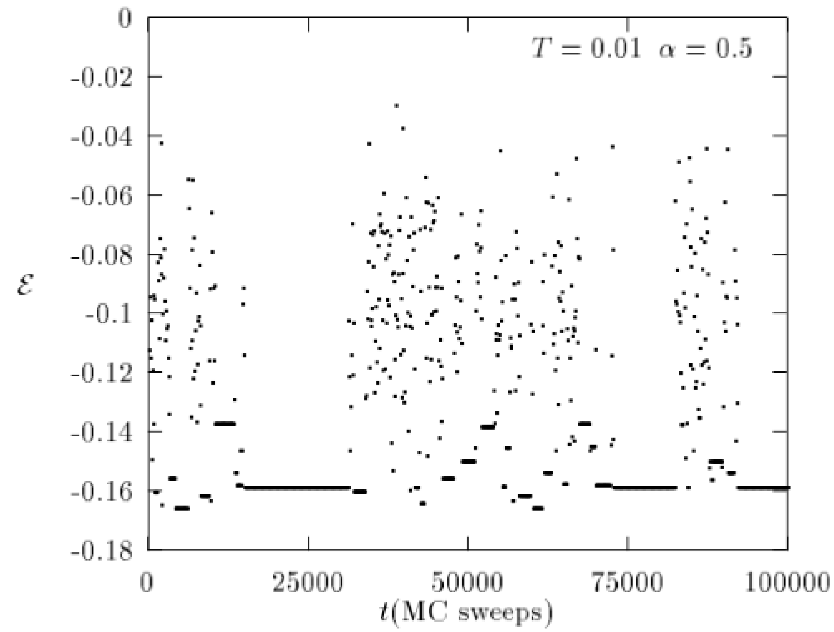
$T_{\rm eff}$ admits the good limit for $\alpha \to 1$

More on this from a rheological viewpoint **Barrat, Berthier, Kurchan 00**

Non-potential force

Trapping in the driven $p = 3$ spherical model, $N = 50$





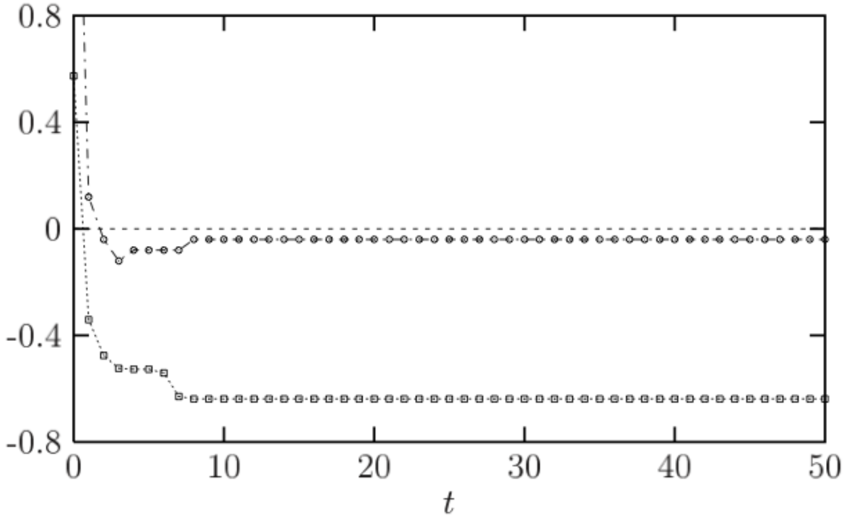
Time dependent energy density

$$J_{ii_2i_3\ldots i_p} = J^{\text{symm}}_{ii_2i_3\ldots i_p} + \alpha J^{\text{asymm}}_{ii_2i_3\ldots i_p} \quad \Rightarrow \quad \Sigma \neq D'R$$

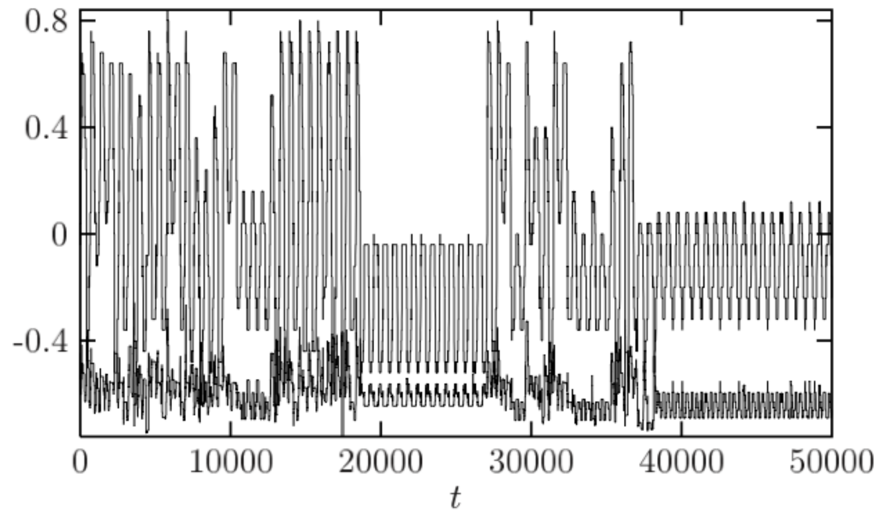
LFC, Kurchan, Le Doussal & Peliti 97

Time-dependent force

Driven $p = 3$ Ising spin model with $N = 50$



$h = 0$

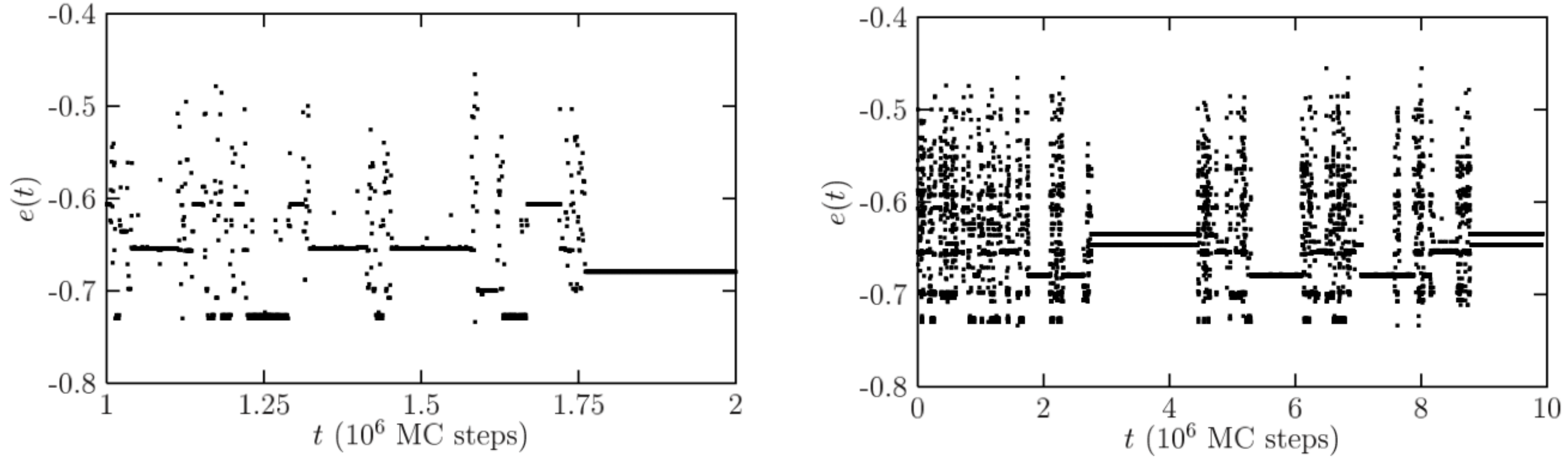


$$h(\omega, t) = h \cos(\omega t)$$

Time dependent magnetisation and energy density

Time-dependent force

Driven $p = 3$ Ising spin model with $N = 50$



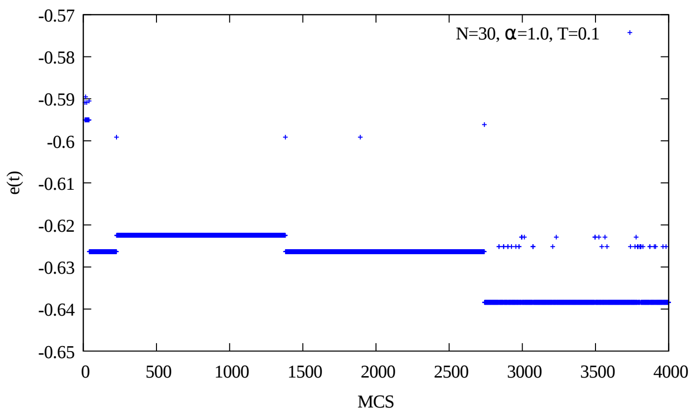
$h(\omega, t) = h\cos(\omega t)$ with $h = 2,\ \omega = 0.01$

Stroboscopic-time dependent magnetisation and energy density

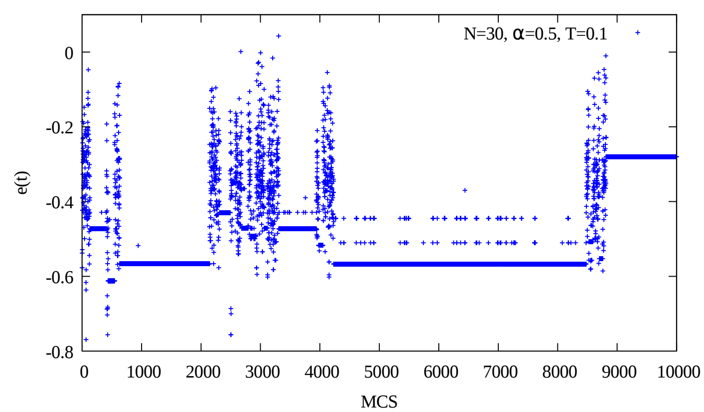
Simulations

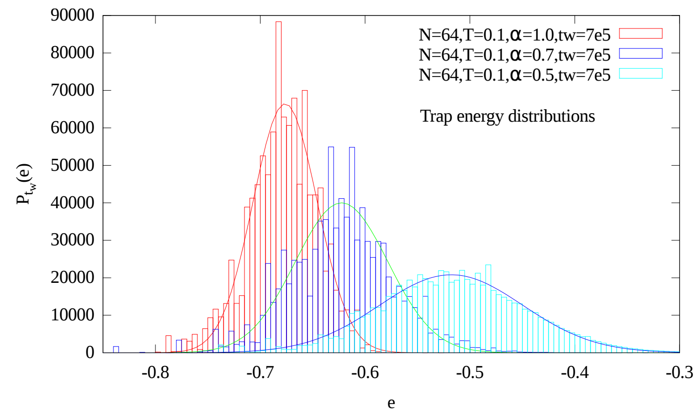
Ising fully-connected p spin models with $N = 30$

Symmetric couplings



Asymmetric couplings





Stariolo & LFC in progress

Statements

Finite N and non-potential forces

Evidence for trapping below threshold

Possibility to test trapping ideas

Better characterisation of trapping times, also barriers ?

Chaotic periods, what is the system actually doing ?

Links to math-phys results on dynamics **Ben Arous et al**

After 2000

Lines of research, out of equil. dynamics of these models

Rheology

Barrat, Berthier & Kurchan 00-04

Fluctuations

Castillo, Chamon, Charbonneau, Corberi, LFC, Kennett, Reichman, Sellitto & Yoshino 02-12

Glassy aspects of active matter

Berthier, Kurchan, Dasgupta, Gov, Szamel, etc. 13-19

Quantum dissipative

Aron, Baldwin, LFC, Biroli, Giamarchi, Grempel, Laumann, Le Doussal, Lozano, Schehr, Schiró, Busiello, Scardicchio, Saburova, Sushkova, etc. 99 -19

Quenches in isolation : integrability vs. thermalisation

LFC, Lozano, Nessi, Picco, Tartaglia 17-18

Ecology, neural nets, etc.

Agoritsas, Biroli, Burin, Fyodorov, Zamponi, Zdebodorová's talk, Fisher's talk

$$x = \frac{T}{T_{\rm eff}} = \frac{1-q}{q}\left[\frac{qf''(q)-f'(q)}{f'(q)}\right]$$ for 1RSB-like

$$x(C) = \frac{T}{T_{\rm eff}(C)} = \frac{q}{4}\frac{f'''(C)}{f''(C)}\sqrt{\frac{f''(q)}{f''(C)}}$$ for full RSB

$$\eta(C) \equiv \frac{f'''(C)}{[f''(C)]^{3/2}} < \eta(q)$$ to be full RSB