Effective temperatures

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Plan

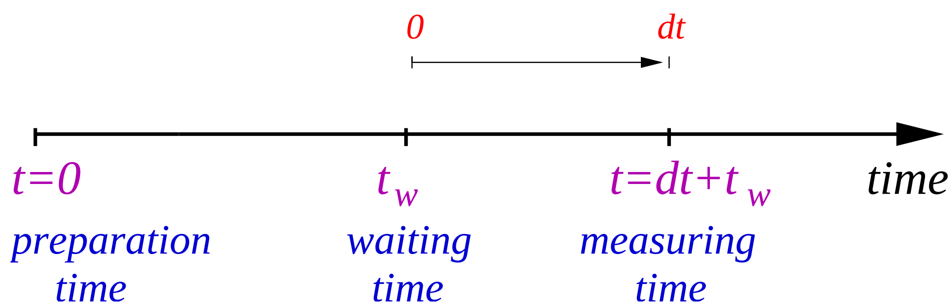
1. Equilibrium *vs.* out of equilibrium.
2. Temperature in equilibrium.
3. An 'effective temperature' for *certain* out of equilibrium systems.
   – Measurement and properties.
   – Relation to entropy : Edwards' measure.
   – Fluctuation theorems.
4. Conclusions.

In and out of equilibrium

Take a mechanical point of view and call $\{\vec{r}_i\}(t)$ the variables

(*e.g.* particles' coordinates $\{x_i(t)\}$ and momenta $\{p_i(t)\}$).

Choose an initial condition $\{\vec{r}_i\}(0)$ and let the system evolve.



- In equilibrium $t_w > t_{eq}$ thermodynamics and statistical mechanics

  apply and temperature is a well-defined concept.

- Out of equilibrium $t_w < t_{eq}$ thermodynamics and statistical mechanics

  do not apply.

In some cases, is there a quantity to be associated to a temperature ?

Temperature in equilibrium

For long temperature was a not well-understood concept in popular wisdom, often confused with heat.

With the development of

- Thermodynamics
- Statistical mechanics

the notion of temperature was clarified.

Thermometers

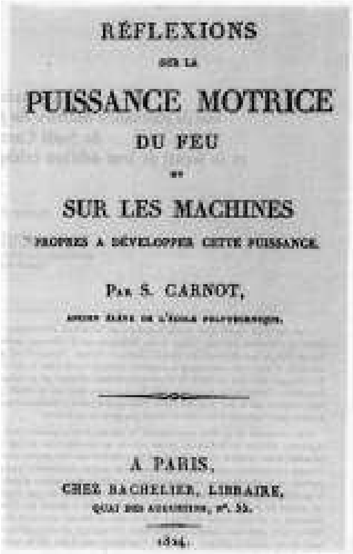
The first thermometer was invented by Santorio Santorii (1561 - 1636)

who improved on Galileo's by adding a **scale**!

Santorio was prof. of Medicine at Univ. di Padova from 1611 to 1629 when moved to Venice where he interacted with Galileo. He initiated the mechanical view of the human body and the use of quantitative measurements in medicine, see *e.g. Ars de statica medicina*, 1614.

Thermodyamics & StatMech

Sadi Carnot (Paris, 1796 - 1832), publication in 1824.



RÉFLEXIONS

PUISSANCE MOTRICE

DU FEU

SUR LES MACHINES

PROPRES A DÉVELOPPER CETTE PUISSANCE.

PAR S. CARNOT,

A PARIS,

CHEZ BACHELIER, LIBRAIRE,

1824.

Ludwig Boltzmann (Vienna, 1844 - Duino, 1906)

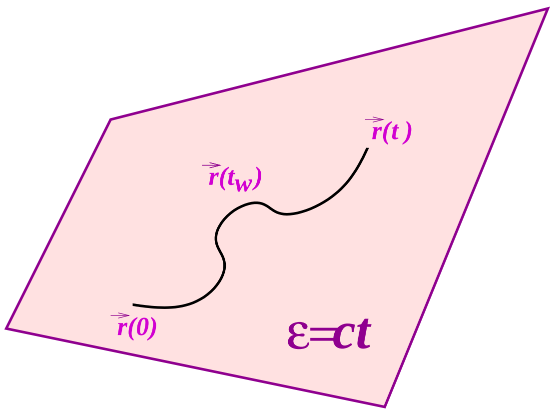
"On the Relation Between the Second Law of the Mechanical Theory of Heat and the Probability Calculus with Respect to the Theorems on Thermal Equilibrium", 1877

$$S = k_B \ln \mathcal{N}$$

$\mathcal{N}$: $\#$ of microstates associated to a macrostate of the system.

Boltzmann committed suicide in Duino, very near ICTP.

Definition and properties



- Isolated system $\Rightarrow$ conserved energy $\mathcal{E}$
- Ergodic hypothesis

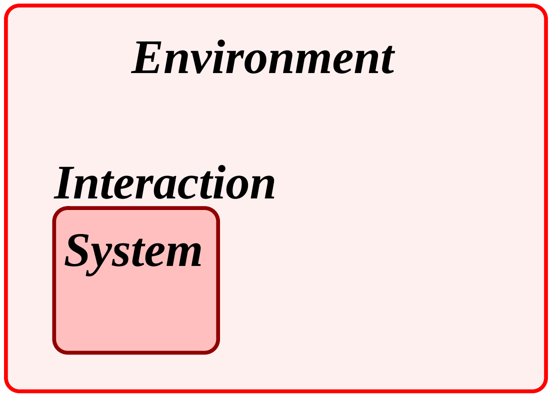
$$S = k_B \ln \mathcal{N} \qquad\qquad \beta \equiv \frac{1}{k_B T} = \left.\frac{\partial S}{\partial \mathcal{E}}\right|_{\mathcal{E}}$$

$$\mathcal{E} = \mathcal{E}_{syst} + \mathcal{E}_{env} + \mathcal{E}_{int}$$

Neglect $\mathcal{E}_{int}$ (short-range int.)

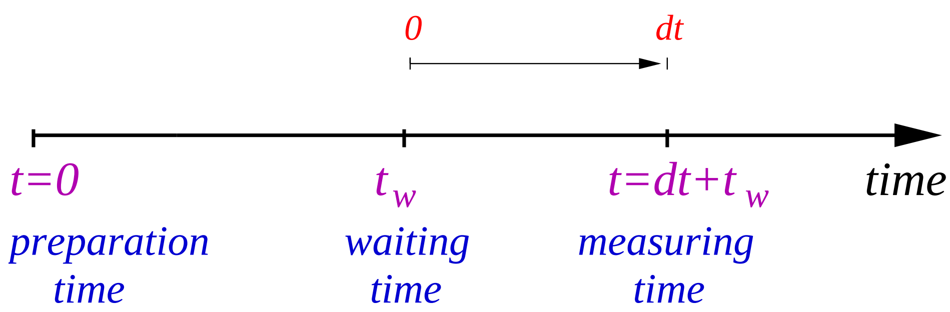
$$\mathcal{E}_{syst} \ll \mathcal{E}_{env}$$

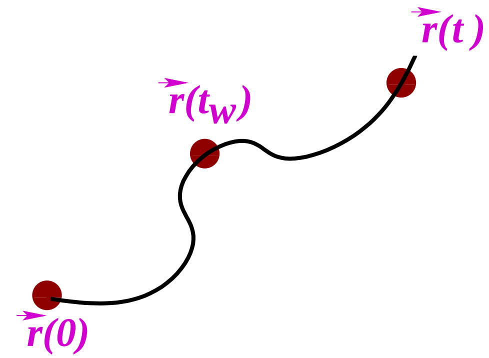
$$p_{ea}(\mathcal{E}_{syst}) = g(\mathcal{E}_{syst}) e^{-\beta \mathcal{E}_{syst}} / Z$$



- Systems in ‘good thermal contact’ : $T_1 = T_2 \Rightarrow$ Thermometers
- ΔQ follows ΔT.

Dynamics





Correlations

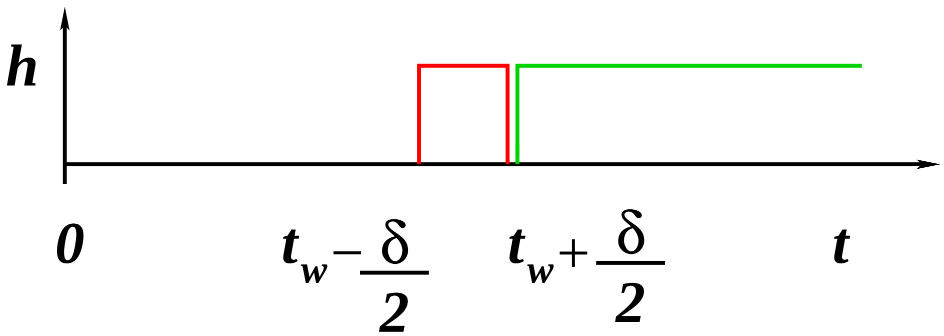
The two-time correlation between $A(\vec{r}(t))$ and $B(\vec{r}(t_w))$ is

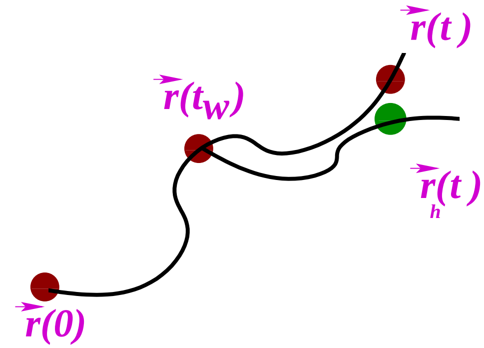
$$C_{AB}(t, t_w) \equiv \langle\, A(\vec{r}(t))B(\vec{r}(t_w))\, \rangle$$

the average is over realizations of the stochastic dynamics (random numbers in a MC simulation, thermal noise in Langevin dynamics, etc.)

Dynamics

Linear response





The perturbation couples linearly to the observable $B(\{\vec{r}_i\})$

$$E \quad \rightarrow \quad E - hB(\{\vec{r}_i\})$$

The linear instantaneous response of another observable $A(\{\vec{r}_i\})$ is

$$\mathbf{R_{AB}(t,t_w)} \equiv \left\langle \left. \frac{\delta A(\{\vec{r}_i\})(t)}{\delta h(t_w)} \right|_{h=0} \right\rangle$$

The linear integrated response or dc susceptibility is

$$\chi_{\mathbf{AB}}(\mathbf{t},\mathbf{t_w}) \equiv \int_{t_w}^{t} dt'\, R_{AB}(t,t')$$

Rue de Fossés St. Jacques et rue St. Jacques

Paris 5ème Arrondissement.

LFC

Fluctuation-dissipation th.

Equilibrium spontaneous (C) and induced (R) fluctuations

If $p(\{\vec{r}\}), t_w) = p_{eq}(\{\vec{r}\})$

- The dynamics is stationary, $C \to C(t - t_w)$ and $R \to R(t - t_w)$.
- The fluctuation-dissipation th. $R(t - t_w) = -\frac{1}{k_B T} \frac{\partial C(t-t_w)}{\partial t} \; \theta(t - t_w)$

holds and implies

$$\chi(t - t_w) \equiv \int_{t_w}^{t} dt' \, R(t, t') = \frac{1}{k_B T}[1 - C(t - t_w)] \; .$$

In glassy systems below T_g : breakdown of stationarity & FDT.

$$\chi(t, \mathbf{t_w}) \equiv \int_{\mathbf{t_w}}^{t} dt' \, R(t, t') \qquad \text{and} \qquad C(t, \mathbf{t_w})$$

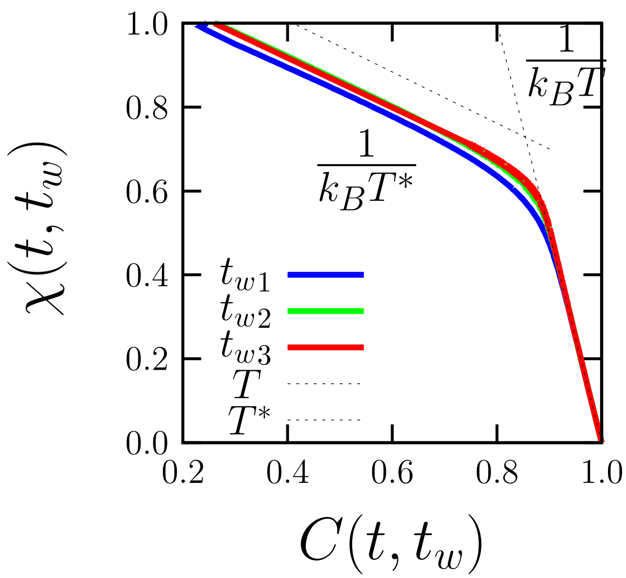
not obviously related.

Fluctuation-dissipation

Solvable cases : p spin-models

- Stochastic dynamics of a particle in an infinite dimensional space under the effect of a quenched random potential.

- A fully-connected (Curie approximation) spin model with as many ferromagnetic as antiferromagnetic couplings.



Parametric construction

t_w fixed

$t : t_w \to \infty$ or

$dt : 0 \to \infty$.

LFC & Kurchan 93

Fluctuation-dissipation

Proposal

For non-equilibrium systems, relaxing slowly towards an **asymptotic** limit (*cfr.* threshold in p spin models) such that one-time quantities [*e.g.* $\mathcal{E}(t)$] approach a finite value

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

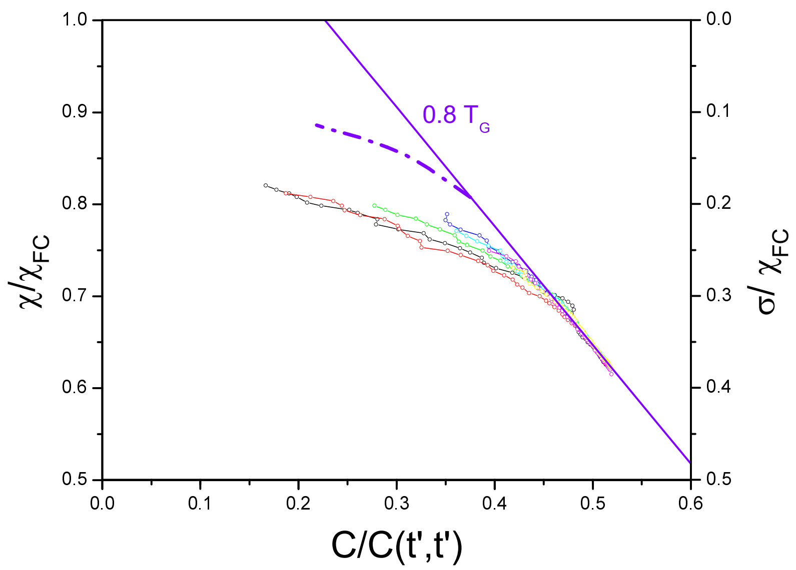
For weakly forced non-equilibrium systems in the limit of **small work**

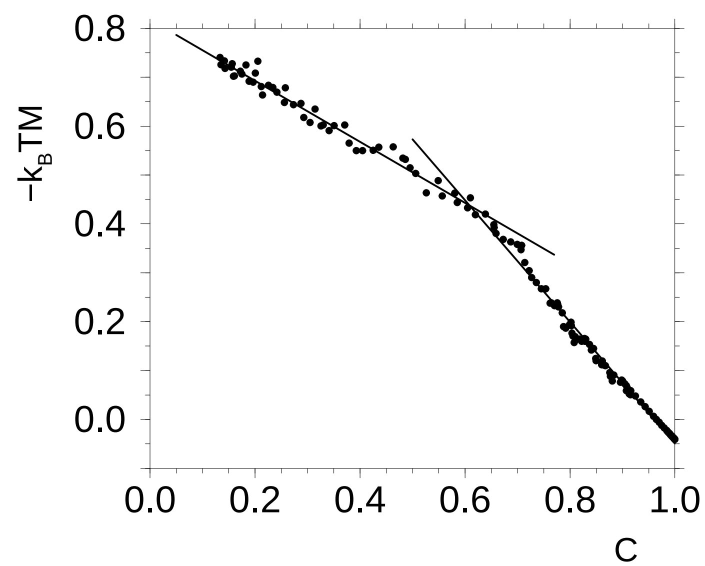
$$\lim_{\substack{\epsilon\to\mathbf{0} \\ C(t,t_w)=C}} \chi(t,t_w) = f_\chi(C)$$

LFC & Kurchan 94

FDT in relaxing glasses

Experiments and simulations





Spin-glass (thiospinel)

Hérisson & Ocio 01

Lennard-Jones binary mixture

J-L Barrat & Kob 01

also in glycerol (**Grigera & Israeloff 99**), colloidal suspensions & polymer glasses (exps.), silica, vortex glasses (**Bustingorry, Kolton, Domínguez** *et al*), dipolar glasses (**Cannas, Gleiser & Tamarit**) (sim.), *etc.*

Phenomenology

Scales

In all these systems the dynamics occur

- In quasi-equilibrium [$\chi = \frac{1}{k_B T}(1 - C)$] when

$$t \gtrsim t_w \qquad \text{or} \qquad q_{ea} \leq C \leq 1.$$

- Clearly out of equilibrium when

$$t > t_w \qquad \text{or} \qquad C \leq q_{ea}.$$

In structural glassy systems one finds

$$\chi = \frac{1}{k_B T^*} \left(q_{ea} - C\right) + \frac{1}{k_B T} \left(1 - q_{ea}\right)$$

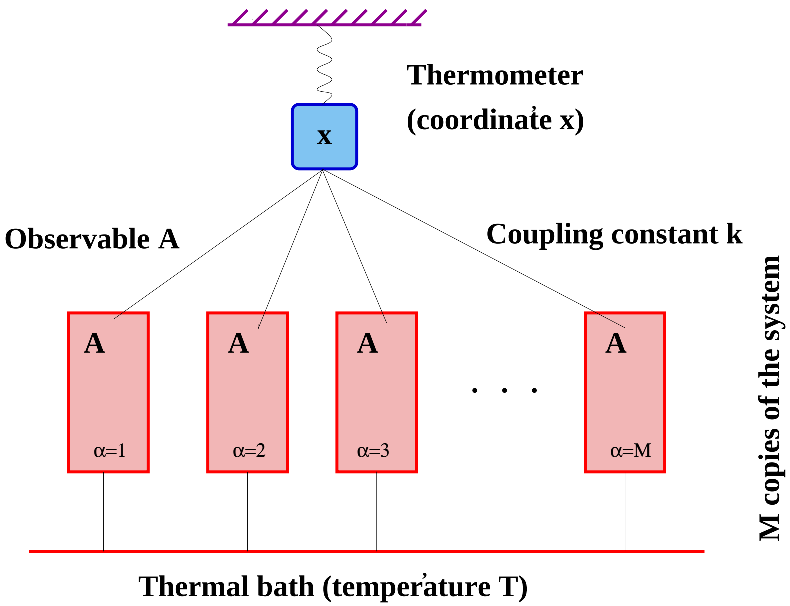
Interpretation

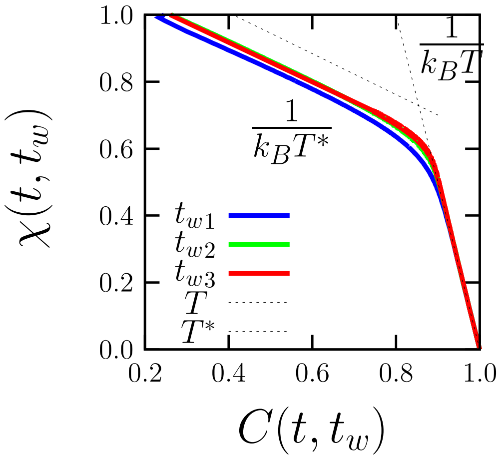
- In particle systems, rattling within cages *vs.* structural relaxation.

- In magnetic coarsening, thermal fluctuations within domains *vs.* domain wall motion.

FDT & effective temperatures

Can one interpret the slope as a temperature ?





(1) Measurement with a **thermometer** with

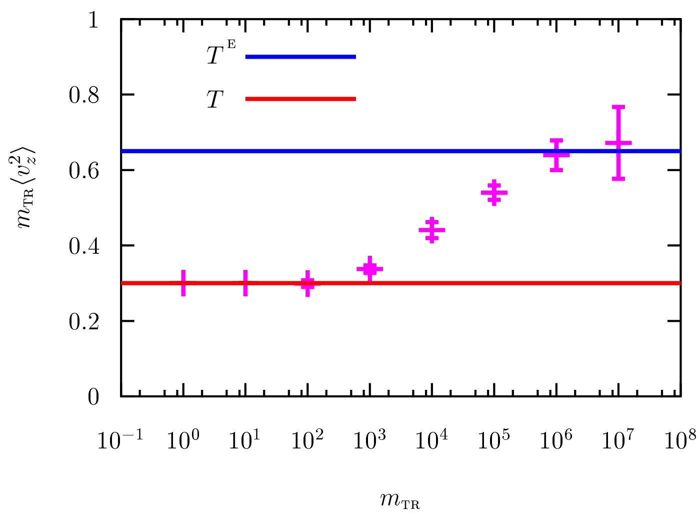
- Short internal time scale τ_0, fast dynamics is tested and T is recorded.
- Long internal time scale τ_0, slow dynamics is tested and T^* is recorded.

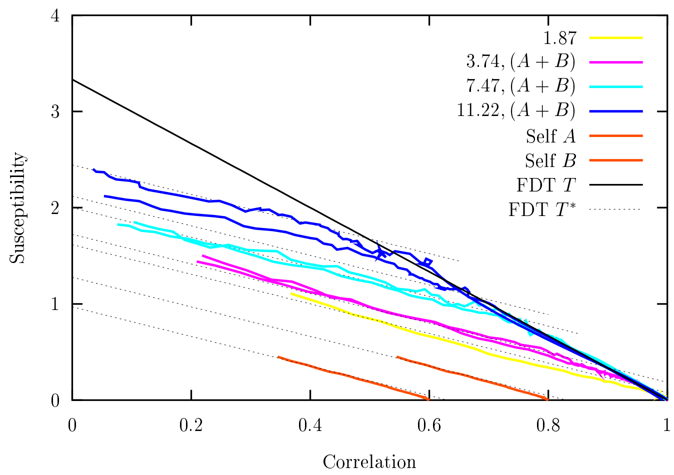
(2) **Partial equilibration** (3) **Direction of heat-flow**

LFC, Kurchan & Peliti, 97

FDT & effective temperatures

Sheared binary Lennard-Jones mixture





Left : The kinetic energy of a tracer particle (the thermometer) as a function of its mass ($\tau_0 \propto \sqrt{m_{tr}}$) $\frac{1}{2} m_{tr} \langle v_z^2 \rangle = \frac{1}{2} k_B T_{eff}$.

Right : $\chi_k(C_k)$ plot for different wave-vectors k : partial equilibrations.

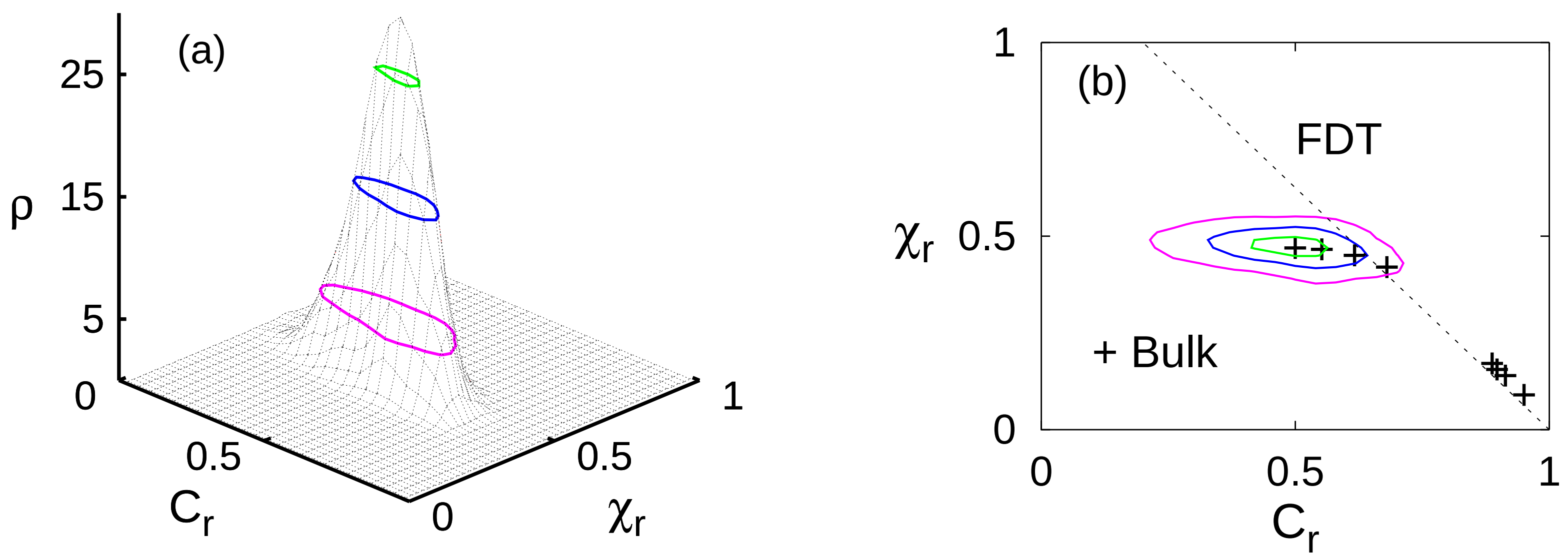
J-L Barrat & Berthier 00

Fluctuations in FDT

All subregions in space tend to have the temperature

in the same time-scale, *e.g.* $C_r < q_{ea}$

Simulations



$3d$ Edwards-Anderson spin-glass

Castillo, Chamon, LFC, Iguain & Kennett 02

Expected behaviour

Loosely

- The system 'remembers' the structure it had initially.

  When cooled down through T_c the structural degrees of freedom are **hotter** than expected in equilibrium at the working temperature.

  Tool 40s

  When heated up from equilibrium at $T = 0$ the structural degrees of freedom are **colder** than expected at the working temperature.

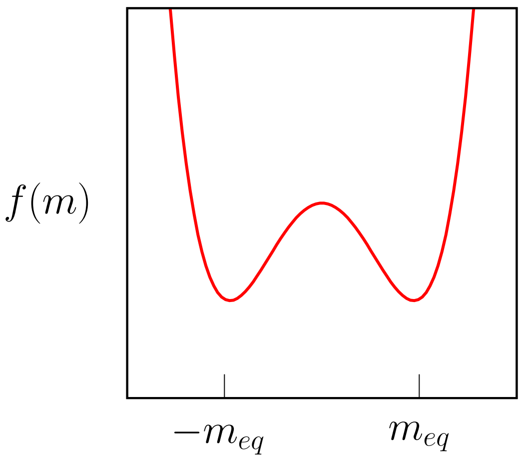
  see *e.g. interface dynamics* **Bustingorry, LFC & Iguain 07**

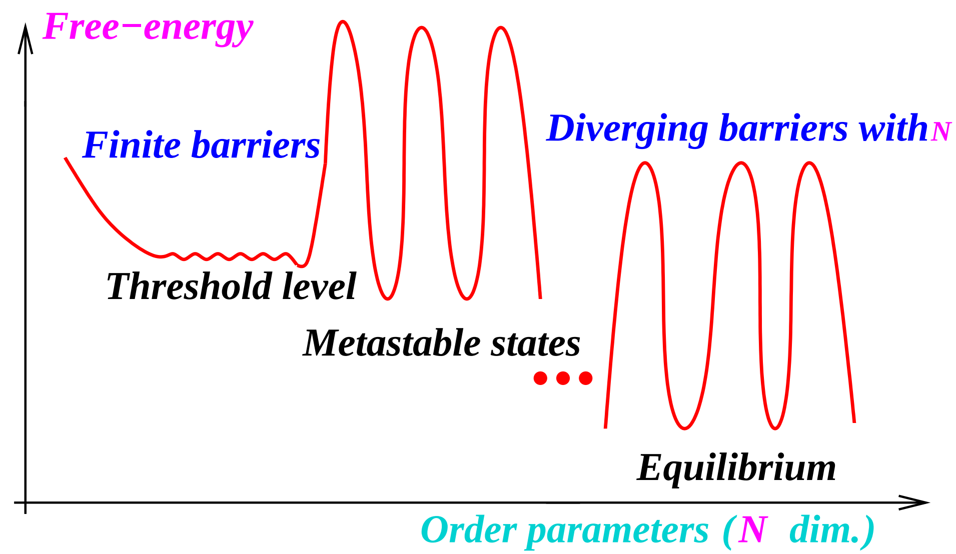
T_{eff} *can be computed analytically in concrete albeit simplified models ; it can be measured directly numerically and experimentally.*

Is T_{eff} related to an entropy ?

Configurational entropy

An exponentially large number of metastable states is reached dynamically





Curie-Weiss (ferro)

Sketch of free-energy landscape

Threshold level is reached asymptotically

e.g. $\lim_{t_w \to \infty} \mathcal{E}(t) = \mathcal{E}_\infty > \mathcal{E}_{eq}$.

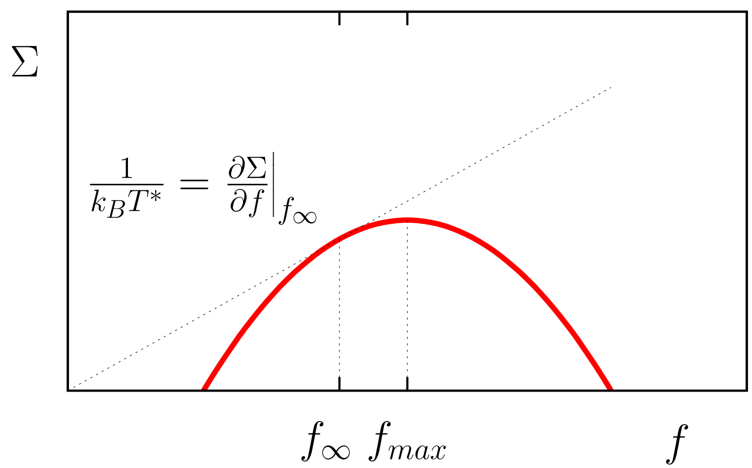
Well-understood in mean-field models with the

Thouless-Anderson-Palmer technique

Is T_{eff} related to an entropy ?

Configurational entropy

$$\Sigma(f) = k_B \ln \mathcal{N}(f) \qquad \Rightarrow \qquad \frac{1}{k_B T^*} = \left.\frac{\partial \Sigma(f)}{\partial f}\right|_{f_\infty}$$



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

Numerical tests in kinetically facilitated models **A. Barrat, Kurchan, Sellitto & Loreto**, a model of granular matter **Makse & Kurchan**, simple spin models **J. J. Brey** *et al*, **Dean & Lefèvre**, *etc.*

Early 00s

Is T_{eff} related to an entropy ?

Proposal to describe granular matter

- Static granular matter : blocked states $mgd \gg k_B T$
- Hypotheses to describe weakly driven granular matter :

– walk from blocked state to blocked state

– blocked states are visited with equal probability working at

fixed V (and $\mathcal{E}$) : $P(\{\vec{r}_i\}_{\text{blocked}}) = \text{constant}$.

– From the entropy of blocked states

$$S(V,\mathcal{E}) = k_B \ln \# \text{ blocked states}(V,\mathcal{E})$$

define the temperature $T_{Edw}^{-1} = \frac{\partial S(V,\mathcal{E})}{\partial \mathcal{E}}$

and the compactivity $X_{Edw}^{-1} = \frac{\partial S(V,\mathcal{E})}{\partial V}$

Edwards & Oakeshott 89

Fluctuation theorems

Take a system *in equilibrium* and drive into a

non-equilibrium steady state

with a perturbing force. The fluctuations of 'entropy production rate'

$$p \equiv (\tau\sigma_+)^{-1} \int_{-\tau/2}^{\tau/2} dt\, W(S_t)/T$$

where S_t is the trajectory of the system in phase space,

T is the temperature of the equilibrated unperturbed system,

$W(S_t)$ is the work done by the external forces, and

$T\sigma_+ \equiv \int dx P_{st}(x) W(x) \sim \lim_{\tau\to\infty} \frac{1}{\tau} \int_{-\tau/s}^{\tau/s} dt\, W(t)$ is an

average over the steady state distribution, **satisfy**

$$\xi(p) - \xi(-p) = p\sigma_+ \qquad \text{with} \qquad \xi(p) \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \ln \pi_\tau(p)$$

and π_τ the probability density of p.

Cohen, Morriss & Evans 90 ; Gallavoti & Cohen 93

Fluctuation theorems

Take a glass *out of equilibrium* and take it into a

driven steady glassy state

with a perturbing force.

For which entropy production rate does a fluctuation theorem hold ?

Since there is no meaning to T but there is to T_{eff} the proposal is to

replace

$$\int_{-\tau/2}^{\tau/2} dt \; \frac{W(t)}{T} \quad \rightarrow \quad \int_{-\tau/2}^{\tau/2} dt \; \frac{W(t)}{T_{eff}(t)}$$

with $T_{eff}(t)$ the effective temperature as measured from

the fluctuation-dissipation relation of the *unperturbed* relaxing system

with its two values T and T^*

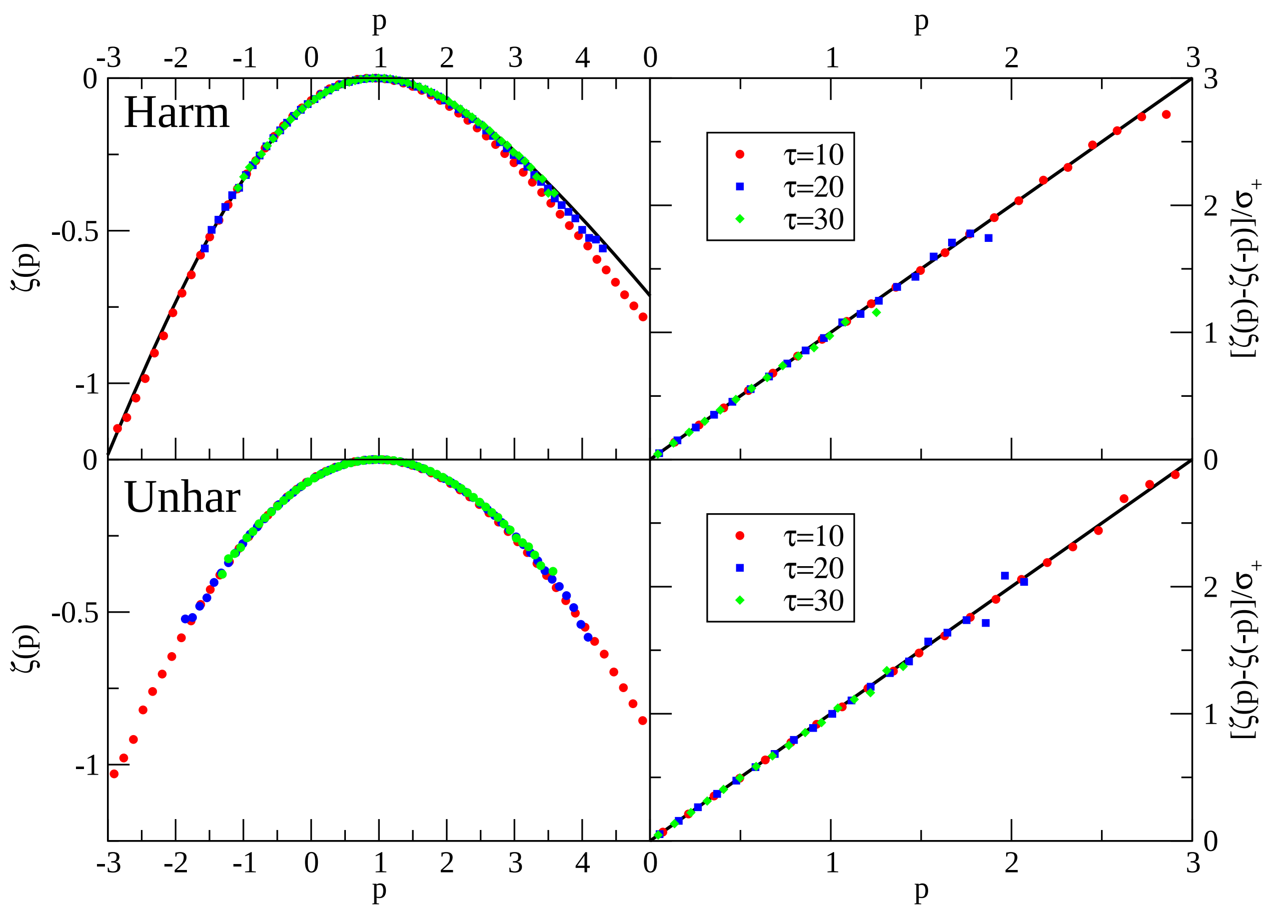
Zamponi, Bonetto, LFC & Kurchan 05

Fluctuation theorems

Driving glassy systems

A harmonic and an unharmonic oscillator driven out of equilibrium

by two baths with different time-scales and temperatures.



Zamponi, Bonetto, LFC & Kurchan 05

Summary

• Everything I presented is rigurously true in **mean-field disordered models** – large N, large d or, in other words, within the mode-coupling approach to glassy systems.

• Good **numerical evidence** in glassy models : Lennard-Jones (**Grigera** *et al*), vortex glasses (**Bustingorry, Kolton, Domínguez, LFC**), granular matter (**Makse & Kurchan**), thin magnetic films (**Cannas, Gleiser & Tamarit**), *etc.*

• Extended Arrhenius law for activation (**Ilg & J-L Barrat**).

• **Experimental results** are less clear. **Grigera & Israeloff** in **glycerol** but...

cfr. **Jabbari-Bonn (Amsterdam)** *vs* **Abou-Gallet (Paris)** *vs* **Ciliberto** *et al* **(Lyon)** *vs* **Bartlett** *et al* **(Bristol)** using **laponite**.

• Quantum extensions (**LFC & Lozano**).

How far do these ideas extend ?

Small entropy production needed