# Fluctuation-dissipation relations as efficient tests of equilibration

**Leticia F. Cugliandolo**

Sorbonne Universités, Université Pierre et Marie Curie
Laboratoire de Physique Théorique et Hautes Energies
Institut Universitaire de France
leticia@lpthe.jussieu.fr


**KITP, November 2015.**

# Plan

1. Introduction.
2. Quantum quenches. **L. Foini, LFC & A. Gambassi 11**
3. An 'effective temperature' for *certain* out of equilibrium systems.

   **LFC, J. Kurchan & L. Peliti 97**

   – Measurements and properties.

   – Relation to free-energy densities and entropy.

   – Fluctuation theorems.
4. Conclusions.

# Plan

1. Introduction.
2. Quantum quenches. **L. Foini, LFC & A. Gambassi 11**
3. An ‘effective temperature’ for *certain* out of equilibrium systems.

   **LFC, J. Kurchan & L. Peliti 97**

   – Measurements and properties.
   – Relation to free-energy densities and entropy.
   – Fluctuation theorems.
4. Conclusions.

# Asymptotic limit

**of the dynamics isolated many-body systems**

– Stationary measure reached ?

– In one or several time-regimes ?

– Which one(s) ?

– Thermal *à la* Gibbs-Boltzmann or other ?

All these questions can be posed, and are difficult to answer, in both classical and quantum systems.

# Asymptotic limit

**of the dynamics isolated many-body systems**

– Stationary measure reached ?

– In one or several time-regimes ?

– Which one(s) ?

– Thermal *à la* Gibbs-Boltzmann or other ?

All these questions can be posed, and are difficult to answer, in both classical and quantum systems.

In the following : equilibrium $\equiv$ Gibbs-Boltzmann equilibrium.

# Dynamics in equilibrium

## Conditions on classical systems

Equilibrium is a matter of statics,

instantaneous probability density $\rho(\{\vec{r}_i, \vec{v}_i\}; t_0)$

but also of dynamics,

evolution operators/transition probabilities $U\left(\{\vec{r}_i, \vec{v}_i\}, t_0 \to \{\vec{r}'_i, \vec{v}'_i\}, t\right)$

$\rho \mapsto e^{-\beta H}/Z$ and conditions on $U$ have to be met to ensure that the system reaches the Gibbs-Boltzmann equilibrium at a given time $t_0$.

# Dynamics in equilibrium

## Conditions on quantum systems

Equilibrium is a matter of statics,

instantaneous probability density $\hat{\rho}(t_0)$

but also of dynamics,

evolution operators $\hat{U}(t_0 \to t)$

$\hat{\rho} \mapsto e^{-\beta \hat{H}}/Z$ and $\hat{U} \mapsto e^{-i\hat{H}(t-t_0)/\hbar}$ to ensure that the system reaches Gibbs-Boltzmann equilibrium at a given time $t_0$.

# Aim of this talk

**in a sentence**

Advocate the use of fluctuation-dissipation relations as tests of

Gibbs-Boltzmann equilibration.

# FDRs

The fluctuation-dissipation theorem is a model-dependent relation between the linear response functions and the correlations of the corresponding spontaneous fluctuations.

In equilibrium, the FDT applies to any pair of observables.

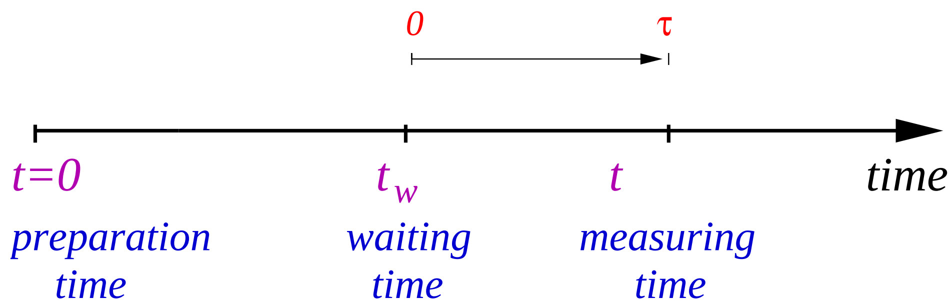
The FDT involves the temperature but no other characteristic of the system.

Whenever the FDT does not apply, the system is out of equilibrium.

Why insist upon looking at FDRs ? Because they go beyond the functional form of correlation functions.

# Two-time observables

## Correlations




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

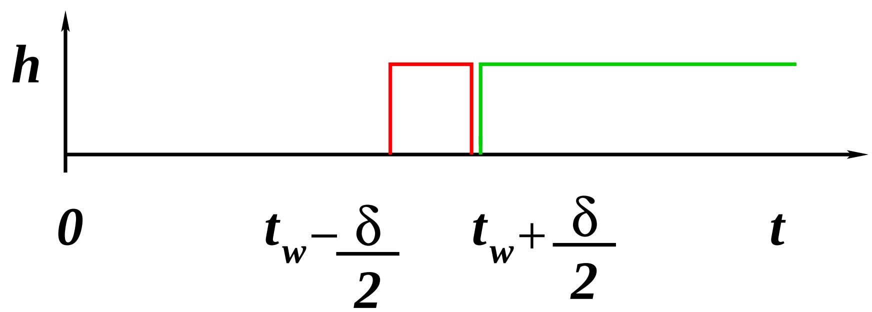
$$C_{AB}(t, t_w) \equiv \langle\, \hat{A}(t)\hat{B}(t_w)\,\rangle$$

expectation value in a quantum system, $\langle \ldots \rangle = \mathrm{Tr} \ldots \hat{\rho}/\mathrm{Tr}\hat{\rho}$

or the average over realizations of the dynamics (initial conditions, random numbers in a MC simulation, thermal noise, etc.) in a classical system.

# Two-time observables

## Linear response




The perturbation couples linearly to the observable $\hat{B}$ at time $t_w$

$$\hat{H} \quad \to \quad \hat{H} - h(t_w)\hat{B}$$

The linear instantaneous response of another observable $\hat{A}(t)$ is

$$R_{AB}(t, t_w) \equiv \left. \frac{\delta \langle \hat{A}(t) \rangle_h}{\delta h(t_w)} \right|_{h=0}$$

Similarly in a classical system

# Linear response

## In an asymptotic steady case

The dynamics are stationary

$$C_{AB} \to C_{AB}(t - t_w) \text{ and } R_{AB} \to R_{AB}(t - t_w)$$

Fourier transforms

$$\tilde{C}_{AB}(\omega) \text{ and } \tilde{R}_{AB}(\omega)$$

Kubo formula, just linear response, to obtain

$$\boxed{-\pi^{-1}\text{Im}\tilde{R}_{AB}(\omega) = \tilde{C}_{AB}(\omega) \mp \tilde{C}_{BA}(-\omega)}$$

Bosons

Fermions

No need to use $\hat{\rho} = Z^{-1}e^{-\beta\hat{H}}$ to prove this relation.

Usual notation : $-\pi^{-1}\text{Im}\chi_{AB}(\omega) = S_{AB}(\omega) \mp S_{BA}(-\omega) = [\hat{A}, \hat{B}]_{\mp}$

# Fluctuation-dissipation theorem

**Gibbs-Boltzmann density operator** $\hat{\rho} = Z^{-1} e^{-\beta \hat{H}}$

$$\tilde{C}_{BA}(-\omega) = e^{\beta\omega} \tilde{C}_{AB}(\omega)$$

and then

$$\boxed{\text{Im}\tilde{R}^{AB}(\omega) = [\hbar^{-1} \tanh(\beta\hbar\omega/2)]^{\pm 1}\, \tilde{C}_{\pm}^{AB}(\omega)}$$

Bosons

Fermions

Classical limit : $\text{Im}\tilde{R}^{AB}(\omega) = \beta\omega\, \tilde{C}^{AB}(\omega)$

# Fluctuation-dissipation relations

**Any evolution**

Just measure

$\text{Im}\tilde{R}^{AB}(\omega)$ and $\tilde{C}_{\pm}^{AB}(\omega)$

take the ratio and extract $\tanh(\beta_{\text{eff}}^{AB}(\omega)\hbar\omega/2)$

In equilibrium all $\beta_{\text{eff}}^{AB}(\omega)$ should be equal to the same constant

# Plan

1. Introduction.
2. Quantum quenches. **L. Foini, LFC & A. Gambassi 11**
3. An ‘effective temperature’ for *certain* out of equilibrium systems.

   **LFC, J. Kurchan & L. Peliti 97**

   – Measurements and properties.
   – Relation to free-energy densities and entropy.
   – Fluctuation theorems.
4. Conclusions.

# Plan

1. Introduction.

2. Quantum quenches. **L. Foini, LFC & A. Gambassi 11**

3. An ‘effective temperature’ for *certain* out of equilibrium systems.

   **LFC, J. Kurchan & L. Peliti 97**

   – Measurements and properties.

   – Relation to free-energy densities and entropy.

   – Fluctuation theorems.

4. Conclusions.

# Isolated quantum systems

## Quantum quenches

- Take an isolated quantum system with Hamiltonian $\hat{H}_0$
- Initialize it in, say, $|\psi_0\rangle$ the ground-state of $\hat{H}_0$ (or any $\hat{\rho}(t_0)$)
- Unitary time-evolution with $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$ with a Hamiltonian $\hat{H}$.

**Does the system reach some steady state ?**

**Are at least some observables described by thermal ones?**

**When, how, which?**

# Quantum quenches

## Questions

**Does the system reach a thermal equilibrium density matrix ?**

**Does its dynamics satisfy the equilibrium rules ?**

different cases of interest : non-integrable *vs.* integrable systems ; role of initial states ; non critical *vs.* critical quenches, *etc.*

- Definition of $T_e$ from $\langle\psi_0|\hat{H}|\psi_0\rangle = \langle\hat{H}\rangle_{T_e} = Z_{\beta_e}^{-1}$ Tr $\hat{H}e^{-\beta_e\hat{H}}$

Just one number, it can always be done

- Comparison of dynamic and thermal correlation functions, *e. g.*

$C(r,t) \equiv \langle\psi_0|\hat{\phi}(\vec{x},t)\hat{\phi}(\vec{y},t)|\psi_0\rangle$ *vs.* $C(r) \equiv \langle\hat{\phi}(\vec{x})\hat{\phi}(\vec{y})\rangle_{T_e}$.

**Calabrese & Cardy ; Rigol et al ; Cazalilla & Iucci ; Silva et al, etc.**

But the functional form of correlation functions can be misleading !

# Quantum quenches

## Questions

Does the system reach a thermal equilibrium density matrix ?

Does its dynamics satisfy the equilibrium rules ?

different cases of interest : non-integrable *vs.* integrable systems ; role of initial states ; non critical *vs.* critical quenches, *etc.*

- Definition of $T_e$ from $\langle \psi_0 | \hat{H} | \psi_0 \rangle = \langle \hat{H} \rangle_{T_e} = Z_{\beta_e}^{-1} \text{Tr} \, \hat{H} e^{-\beta_e \hat{H}}$

Just one number, it can always be done

- Comparison of dynamic and thermal correlation functions, *e. g.*

$$C(r,t) \equiv \langle \psi_0 | \hat{\phi}(\vec{x},t) \hat{\phi}(\vec{y},t) | \psi_0 \rangle \text{ vs. } C(r) \equiv \langle \hat{\phi}(\vec{x}) \hat{\phi}(\vec{y}) \rangle_{T_e} .$$

**Calabrese & Cardy ; Rigol et al ; Cazalilla & Iucci ; Silva et al, etc.**

Proposal : put qFDT to the test to check whether $T_{\rm eff} = T_e$ exists

# Fluctuation-dissipation relations

## Quantum SU(2) Ising chain

The initial Hamiltonian $$\hat{H}_{\Gamma_0} = -\sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \Gamma_0 \sum_i \hat{\sigma}_i^z$$

The initial state $|\psi_0\rangle$ ground state of $\hat{H}_{\Gamma_0}$

Instantaneous quench in the transverse field $\Gamma_0 \to \Gamma$

Evolution with $\hat{H}_{\Gamma}$.

**Iglói & Rieger 00**

Reviews : **Karevski 06 ; Polkovnikov et al. 10 ; Dziarmaga 10**

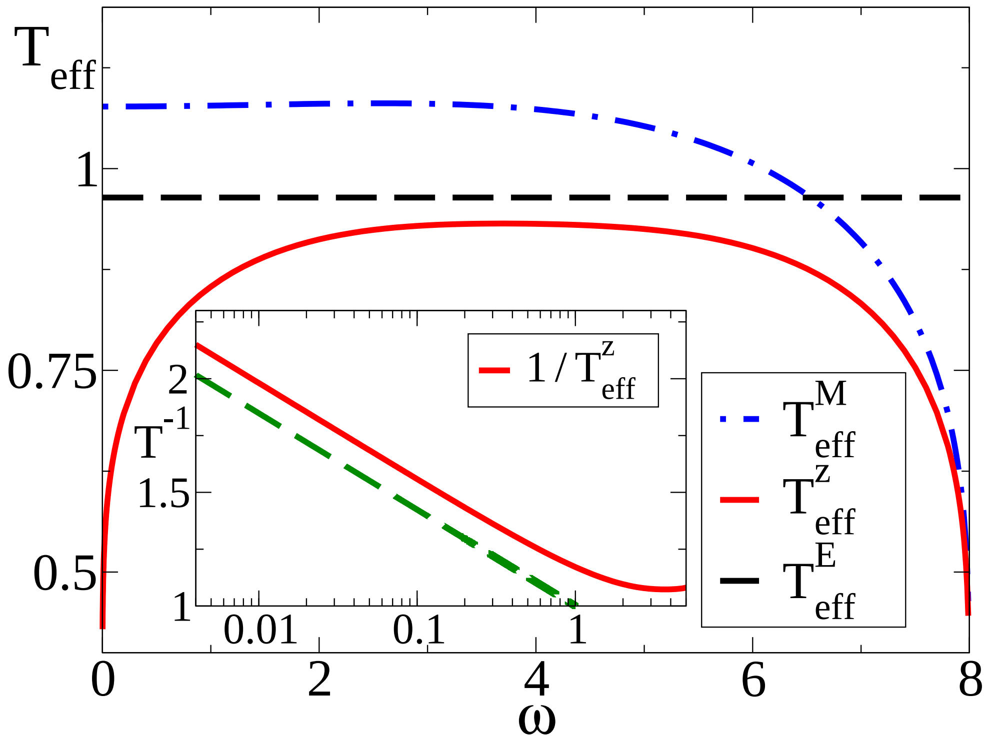
Observables : correlation and linear response of local longitudinal and transverse spin, etc.

Specially interesting case $\Gamma_c = 1$ the critical point. **Rossini et al. 09**

# Quantum quench

## $T_{\rm eff}$ from the transverse spin FDR

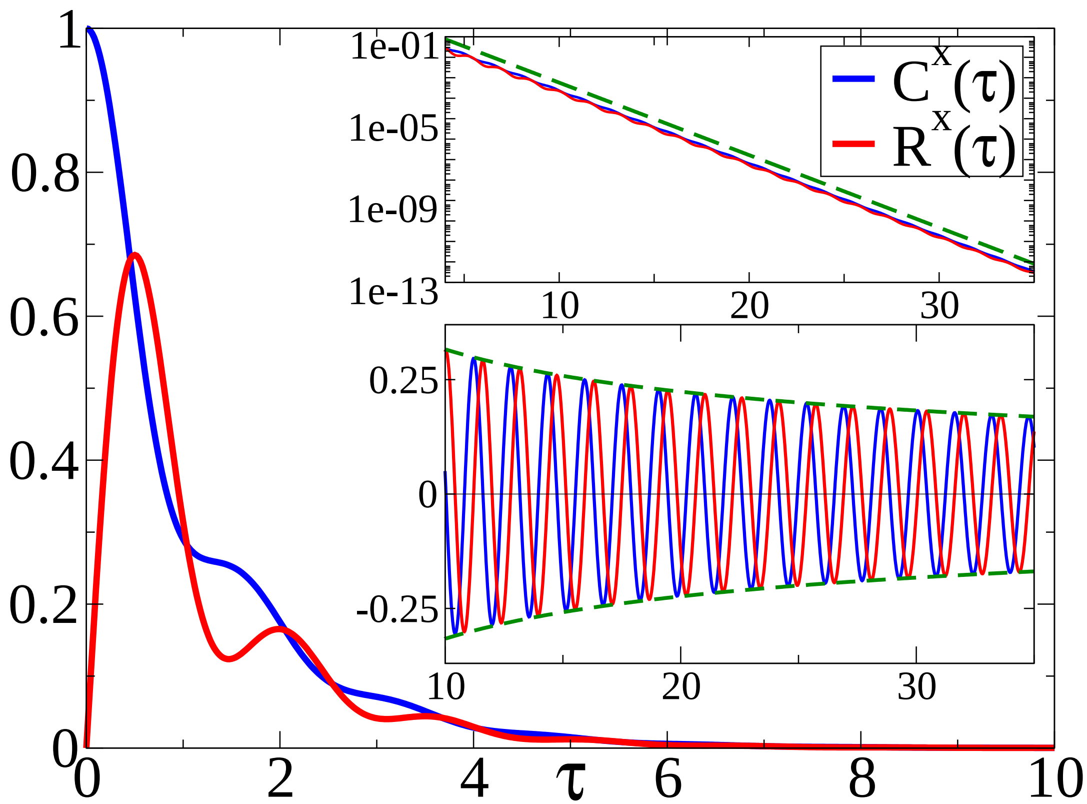
$$\hbar \, \mathrm{Im} R^z(\omega) = \tanh\left(\frac{\beta^z_{\rm eff}(\omega)\omega\hbar}{2}\right) C^z_+(\omega)$$




But $\beta^z_{\rm eff}(\omega)$ and $\beta^M_{\rm eff}(\omega) \neq$ ct

# Quantum quench

## $T_{\rm eff}$ from the longitudinal spin FDR




Insets

$e^{-\tau/\tau_{\rm c}}$

$\tau^{-2}\sin(4\tau+\phi)$

$$C^x(\tau) \simeq A_{\rm c} e^{-\tau/\tau_{\rm c}}[1 - a_{\rm c}\tau^{-2}\sin(4\tau+\phi_{\rm c})]$$

$$R^x(\tau) \simeq A_R e^{-\tau/\tau_{\rm c}}[1 - a_R\tau^{-2}\sin(4\tau+\phi_R)]$$

**Foini, LFC & Gambassi 11**

# Quantum quench

**$T_{\rm eff}$ from FDT ?**

For sufficiently long-times such that one drops the power-law correction

$$-\beta^x_{\rm eff} \simeq \frac{R^x(\tau)}{d_\tau C^x_+(\tau)} \simeq -\frac{\tau_{\rm c} A_R}{A_{\rm c}}$$

A constant consistent with a classical limit but

$$T^x_{\rm eff}(\Gamma_0) \neq T_e(\Gamma_0)$$

Morever, a complete study in the full time and frequency domains confirms that $T^x_{\rm eff}(\Gamma_0, \omega) \neq T^z_{\rm eff}(\Gamma_0, \omega) \neq T_e(\Gamma_0)$ (though the values are close).

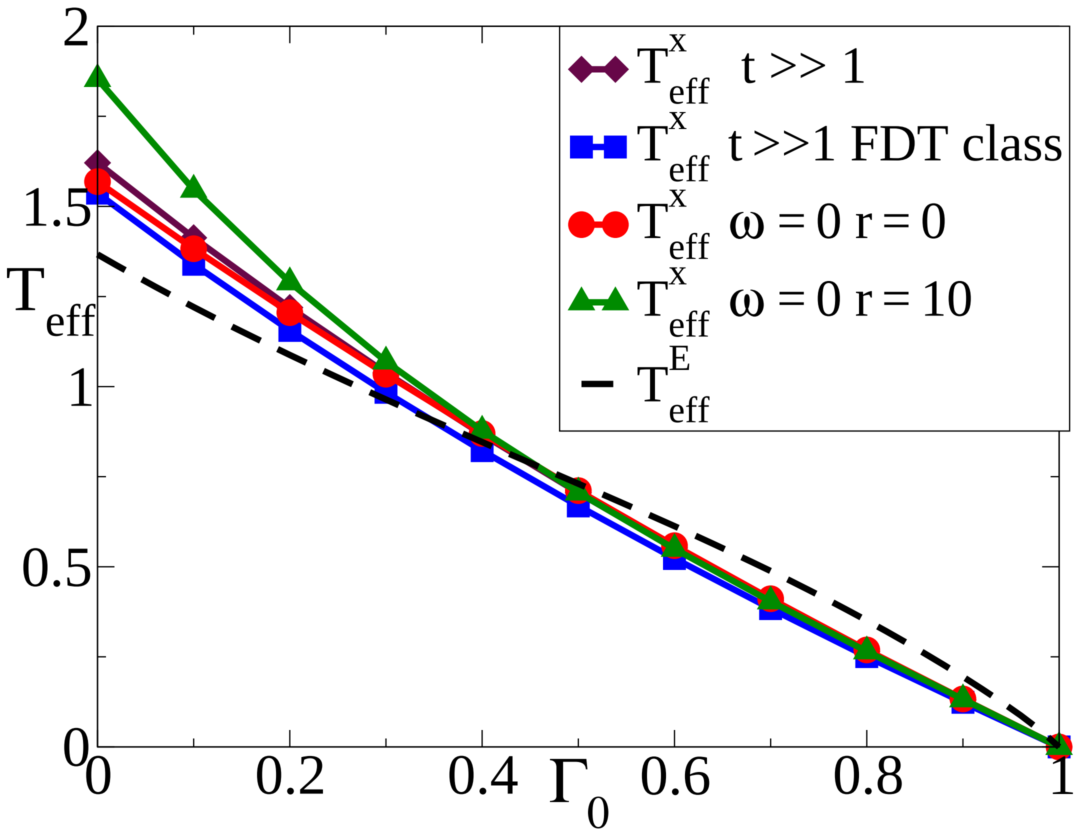
**Fluctuation-dissipation relations as a probe to test thermal equilibration**

**No equilibration for generic $\Gamma_0$ in the quantum Ising chain**

# Quantum quench

**No $T_{\text{eff}}$ from FDT**

A quantum quench $\Gamma_0 \to \Gamma_c = 1$ of the **isolated Ising chain**




**Foini, LFC & Gambassi 11**

# Another example

**$1d$ hard-core bosons in a super-lattice potential**

Fermionic representation :

$$\hat{H}_0(\Delta) = -\sum_i \hat{f}_i^\dagger \hat{f}_{i+1} + \text{h.c.} + \Delta \sum_i (-1)^i f_i^\dagger f_i$$

Quench from the ground state of $\hat{H}_0(\Delta)$ to $\hat{H} = \hat{H}_0(\Delta = 0)$.

Although $\hat{\rho} \mapsto \hat{\rho}_{\rm GGE} \approx \hat{\rho}_{\rm GB}$ for $\Delta \gg |\omega_k| = \mathcal{O}(1)$

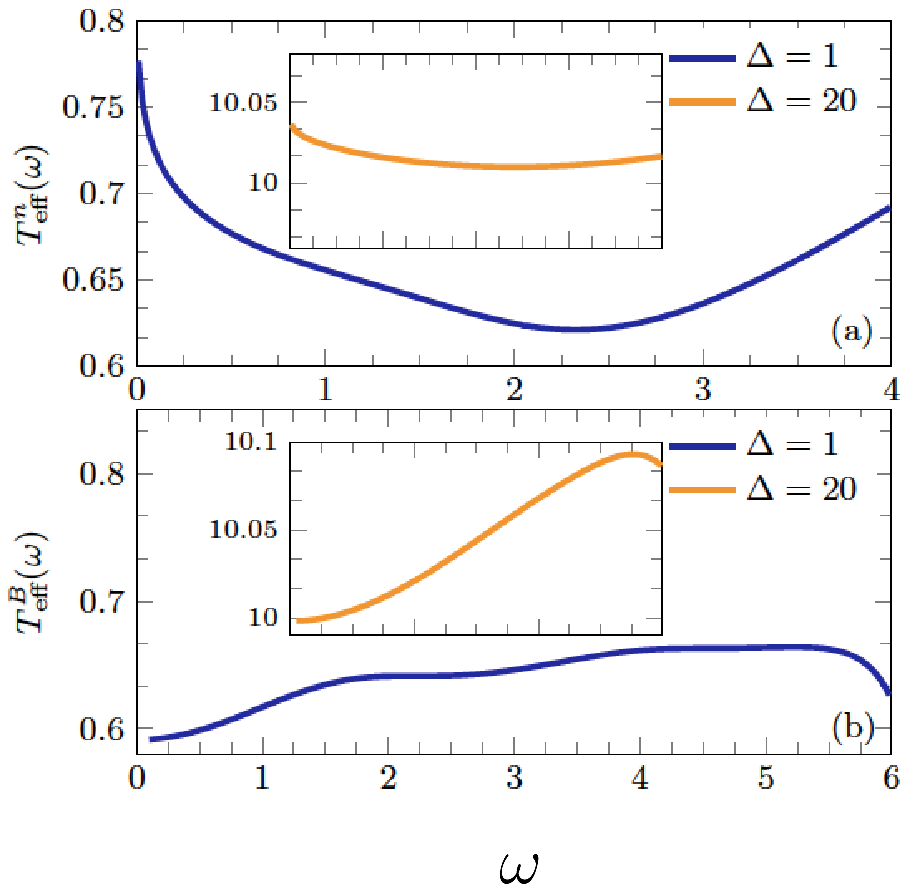
**Chung, Iucci & Cazalilla 12**

the FDT is not satisfied in this same limit, and different FDRs yield different $T_{\rm eff}$s.

**Bortolin & Iucci 15**

# Another example

**$1d$ hard-core bosons in a super-lattice potential**




(local) density operator

$\hat{A} = \hat{B} = \hat{n}_i \hat{n}_i$

(non-local) boson operator

$\hat{A} = \hat{B} = \hat{b}_i^\dagger \hat{b}_i$

**Bortolin & Iucci 15**

Similar ideas in models of photon/polariton condensates,

**Chiocchetta, Gambassi, Carusotto 15**

# Summary

## Fluctuation-dissipation relations

- Use of **fluctuation-dissipation relations** in the dynamics of closed quantum systems to check for Gibbs-Boltzmann equilibrium.

# Effective temperatures

## What happens in glasses ?

Glasses are out of equilibrium.

There is a separation of time-scales in their relaxation,

with a crossover at, roughly, $\omega t_w$

The FDRs take a very special form :

$\omega t_w \ll 1$ quasi-stationary relation and FDT OK.

$\omega t_w \gg 1$ non-stationary relation and a single constant $T_{\rm eff}$.

$T_{\rm eff}$ depends upon

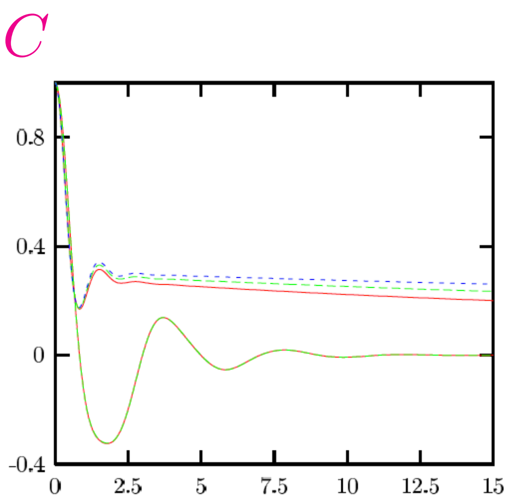
the initial condition before the quench (disordered vs. ordered) ;

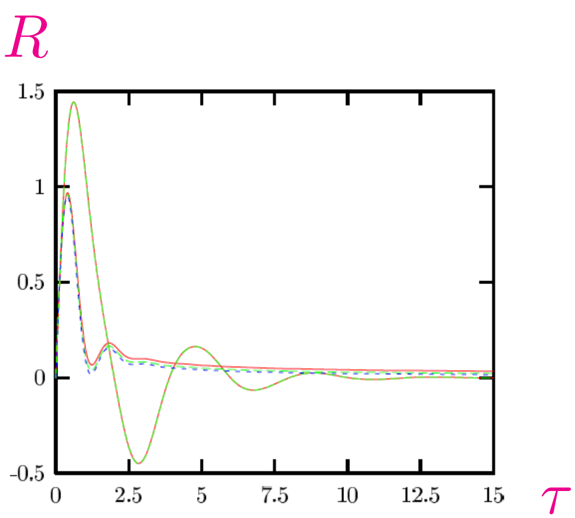
weakly on other parameters of the systems.

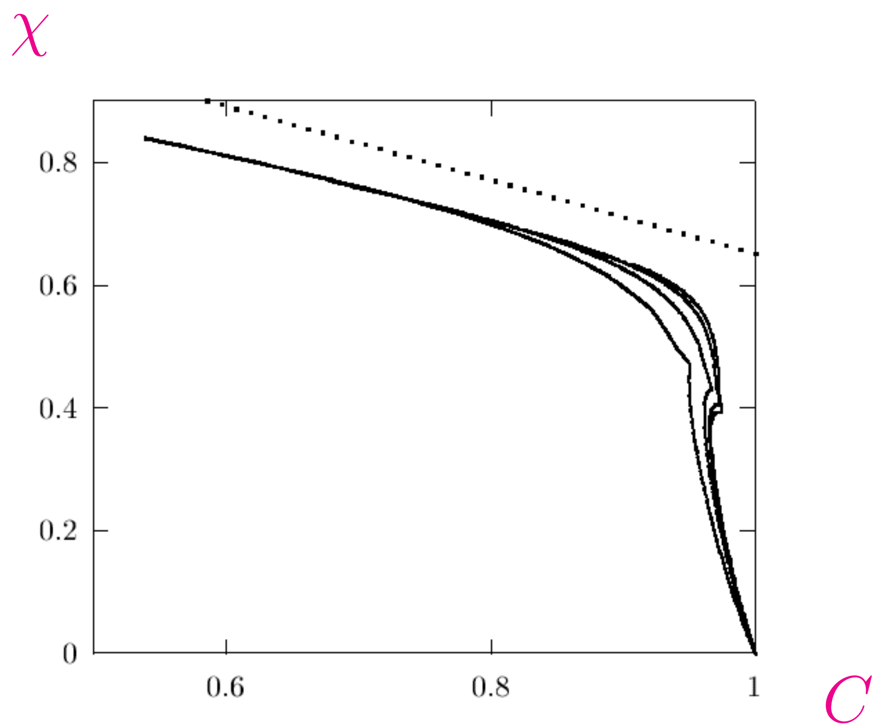
**LFC 11**, review

# Dissipative quantum glasses

## Quantum $p$-spin coupled to a bath of harmonic oscillators




**Out of equilibrium decoherence**

**LFC & Lozano 98**