
Measuring effective temperatures in the Generalized Gibbs Ensembles

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Plan

1. Introduction.
2. Fluctuation-dissipation relations.
 - Measurements of effective temperatures and properties.
 - Relation to free-energy densities and entropy.
 - Fluctuation theorems.
3. Quantum quenches.
4. Integrable systems and Generalized Gibbs Ensembles.

LFC, Kurchan & Peliti 97 ; Foini, LFC & Gambassi 11 & 12 ; Foini, Gambassi, Konik & LFC 16 ; de Nardis, Panfil, Gambassi, LFC, Konik & Foini 17

Thanks to the joint autumn programs at KITP 2015

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Introduction

My interests

- Classical and quantum, open and closed, non-equilibrium systems
- Out of equilibrium dynamics typically due to quenches in the environment (open) or the system (closed) parameters.
- Many-body problem in interaction (even quenched randomness)
 - collective phenomena
 - phase transitions
 - emerging thermodynamic behaviour

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Colloidal suspension

Balls in water (bath): easy to visualize

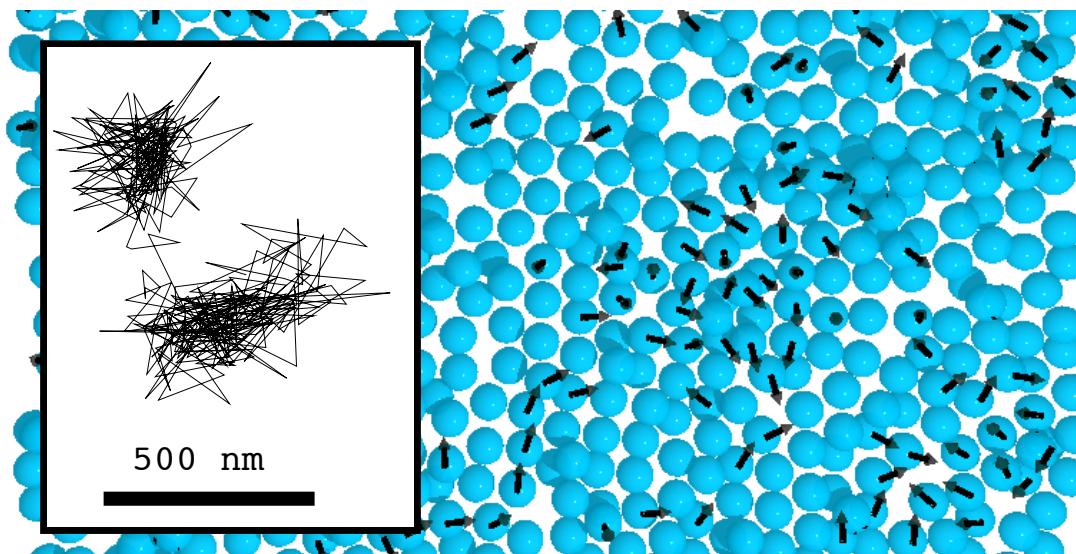


Image from Coutland & Weeks 02

Quench: e.g., a sudden change in temperature or packing fraction.

Colloidal suspension

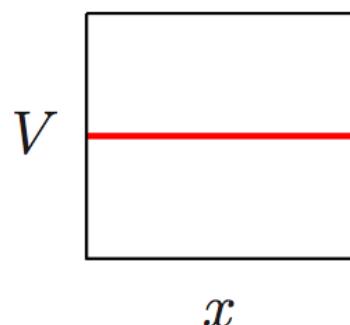
Very dilute limit : Markov normal diffusion

For simplicity, take a one dimensional system, $d = 1$ with $x_0 = v_0 = 0$

The velocity is Gaussian distributed, in equilibrium, equipartition

$$\langle v^2 \rangle = k_B T / m$$

The displacement of the position x crosses over at t_I to diffusive behaviour since $e^{-\beta V}$ is not normalizable.



$$\langle x^2(t) \rangle \rightarrow 2D t \quad \text{with}$$

$$D = k_B T / \gamma \quad \text{the diffusion constant.}$$

Coexistence of equilibrium (\vec{v}) and out of equilibrium (\vec{r}) variables

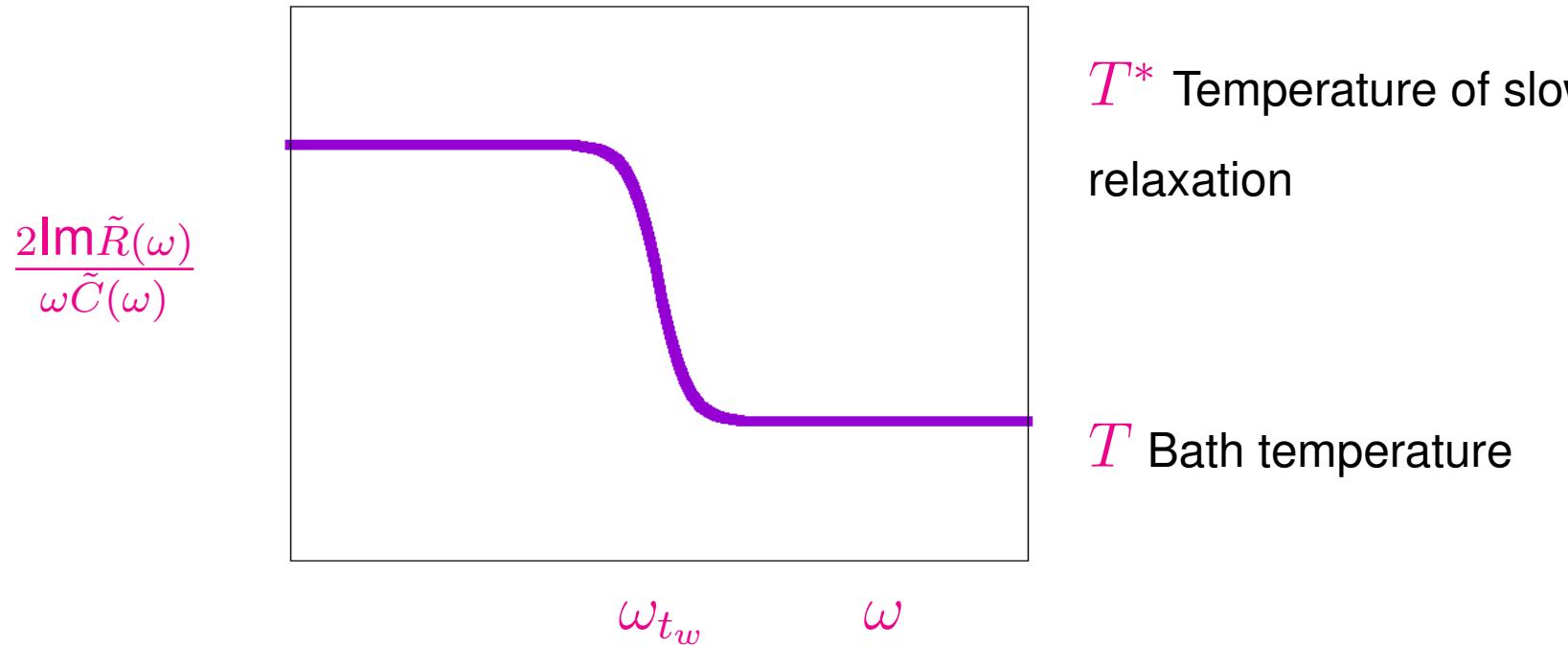
Equilibrium dynamics

Fluctuation-dissipation theorem in the frequency domain



Glassy dynamics

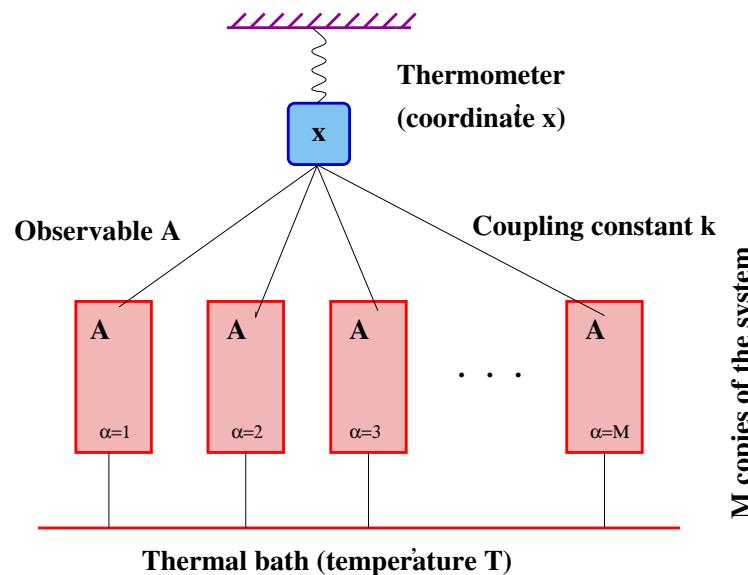
Fluctuation-dissipation relation in the frequency domain



Analytic solution to a mean-field model LFC & J. Kurchan 93

FDR & 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**

Effective temperatures

Glasses, coarsening, driven systems

Different observables can behave differently (e.g. velocity vs. positions).

There is a separation of frequency-scales

with a crossover at, roughly, ωt_w (or controlled by an external drive)

The FDRs take a very special form:

- $\omega t_w \gg 1$ quasi-stationary relation and FDT with bath T
- $\omega t_w \ll 1$ non-stationary relation and FDR with another T^* .

$T_{\text{eff}}(\omega, t_w)$ crosses over from T to T^* that depends upon

- the initial condition before the quench (disordered vs. ordered) ;
- weakly on other parameters of the systems.

Notion of interacting vs. non-interacting concerning partial equilibrations

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Fluctuation-dissipation relations

Quantum setting

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

This is the fluctuation-dissipation theorem (FDT).

If there is a frequency or observable dependence, the system is not in equilibrium

Do these $\beta_{\text{eff}}(\omega)$ play a role in closed systems too ?

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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 $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$ with another Hamiltonian \hat{H} .

Does the system reach some steady state ?

Is it described by a thermal equilibrium density matrix ?

Do at least some observables behave as thermal ones?

Does the evolution occur as in equilibrium ?

Other kinds of density matrices ?

Quantum quenches

Questions

Non-integrable systems expected to eventually thermalise (ETH).

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.

But the functional form of correlation functions can be misleading !

Quantum quenches

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Non-integrable systems expected to thermalise (ETH).

Integrable systems ?

role of initial states ; non critical vs. critical quenches, etc.

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

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

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References & results

4. Integrable systems and Generalized Gibbs Ensembles.

- As a test of non-thermal equilibrium

Foini, LFC & Gambassi 11 & 12

- Effective temp in the GGE for integrable non-interacting systems

Foini, Gambassi, Konik & LFC 16

- Effective temp in the GGE for integrable interacting systems

de Nardis, Panfil, Gambassi, LFC, Konik & Foini 17

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Quantum quench

Quantum 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}_{Γ_0}

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

Evolution with \hat{H}_{Γ} .

Iglói & Rieger 00

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

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

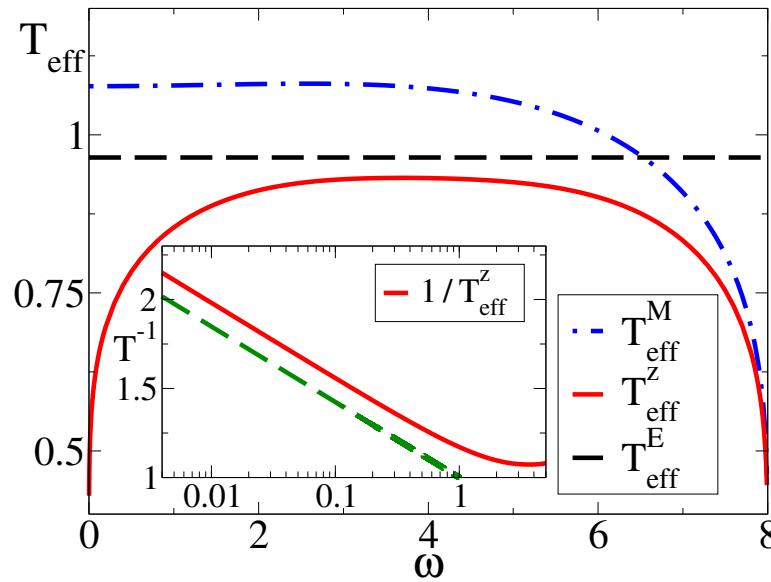
Specially interesting case $\Gamma_c = 1$ the critical point.

Rossini et al. 09

$$\Gamma_0 \rightarrow \Gamma_c = 1$$

T_{eff} from the FDR

$$\hbar \operatorname{Im} \tilde{R}(\omega) = \tanh(\beta_{\text{eff}}(\omega)\omega\hbar/2) \tilde{C}_+(\omega)$$



$$\beta_{\text{eff}}^z(\omega) \neq \beta_{\text{eff}}^M(\omega) \neq \text{ct}$$

Foini, LFC & Gambassi 11 & 12

Similar ideas used in, e.g., Bortolin & Iucci 15 (hard core bosons)

Chiocchetta, Gambassi & Carusotto 15 (photon/polariton condensates), etc.

Summary

Fluctuation-dissipation relations

No Gibbs-Boltzmann equilibrium.

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

Fluctuation-dissipation relations

Can they be used to infer the steady state density operator ?

The Generalised Gibbs Ensemble

Proposal for integrable systems

In an integrable system with N degrees of freedom there are N local conserved charges or integrals of motion \hat{Q}_k , $k = 1, \dots, N$ such that they are mutually commuting $[\hat{Q}_k, \hat{Q}_{k'}]_- = 0$ and they all commute with the Hamiltonian $[\hat{H}, \hat{Q}_k]_- = 0$.

The relevant stationary density operator is expected to be the GGE one

$$\hat{\rho}_{\text{GGE}} = Z^{-1} e^{-\sum_{k=1}^N \lambda_k \hat{Q}_k}$$

in the sense that $\lim_{t \gg t^*} \langle \hat{O}_{\text{loc}} \rangle(t) = \langle \hat{O}_{\text{loc}} \rangle_{\text{GGE}} = \text{Tr } \hat{O}_{\text{loc}} \hat{\rho}_{\text{GGE}}$ for all local \hat{O}_{loc}

The Generalised Gibbs Ensemble

How to fix the λ_k after a quantum quench ?

In an integrable system with N degrees of freedom there are N local conserved charges or integrals of motion \hat{Q}_k , $k = 1, \dots, N$

The GGE density operator

$$\hat{\rho}_{\text{GGE}} = Z^{-1} e^{-\sum_{k=1}^N \lambda_k \hat{Q}_k}$$

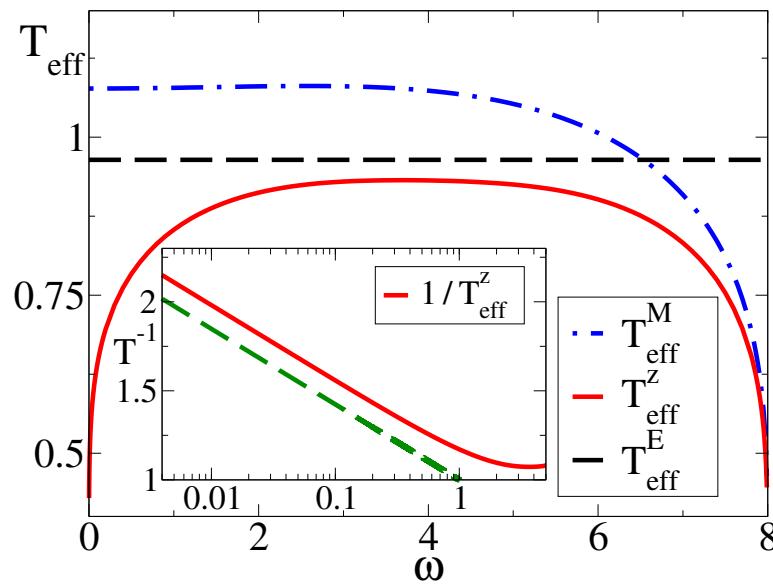
depends on N Lagrange multipliers (related to effective inverse temperatures) that are fixed by imposing

$$\langle \psi_0 | \hat{Q}_k | \psi_0 \rangle = \langle \hat{Q}_k \rangle_{\text{GGE}} = \text{Tr } \hat{Q}_k \hat{\rho}_{\text{GGE}}$$

Quantum quench

Quantum Ising chain : FDR and GGE for $\hat{M} = L^{-1} \sum_{i=1}^L \hat{\sigma}_i^z$

$$\hbar \operatorname{Im} \tilde{R}_M(\omega) = \tanh(\beta_{\text{eff}}^M(\omega) \omega \hbar / 2) \tilde{C}_{M+}(\omega)$$



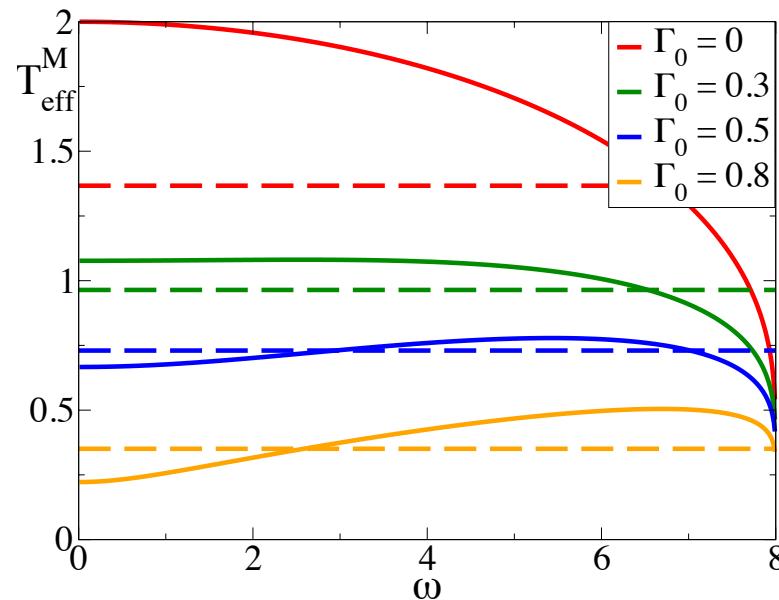
$$T_{\text{eff}}^M(\omega = 2\epsilon_k(\Gamma, \Gamma_0)) = T_k^{\text{GGE}}(\Gamma, \Gamma_0)$$

For finite L , $\operatorname{Im} \tilde{R}_M(\omega)$ and $\tilde{C}_{M+}(\omega)$ are non-zero only at $\omega = 2\epsilon_k$ with ϵ_k the energy of the quasi-particles (free-fermions that diagonalise the Hamiltonian).

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From the FDR to the GGE

Lehman representation

The correlation and linear response are

$$C_+(t_2, t_1) = \frac{1}{2} \langle [\hat{A}(t_2), \hat{A}^\dagger(t_1)]_+ \rangle$$

$$R(t_2, t_1) = i \langle [\hat{A}(t_2), \hat{A}^\dagger(t_1)]_- \rangle \theta(t_2 - t_1)$$

The expectation value $\langle \dots \rangle$ is calculated over a generic density matrix $\hat{\rho}$

(units henceforth such that $\hbar=1$ and $[\hat{X}, \hat{Y}]_\pm \equiv \hat{X}\hat{Y} \pm \hat{Y}\hat{X}$)

Taking a Fourier transform wrt to $t_2 - t_1$

$$\tilde{C}_+(\omega) = \pi \sum_{m,n \geq 0} \delta(\omega + E_n - E_m) |A_{nm}|^2 (\rho_{nn} + \rho_{mm})$$

$$\text{Im } \tilde{R}(\omega) = \pi \sum_{m,n \geq 0} \delta(\omega + E_n - E_m) |A_{nm}|^2 (\rho_{nn} - \rho_{mm})$$

where the sums run over a complete basis of eigenstates $\{|n\rangle\}_{n \geq 0}$ of the Hamiltonian \hat{H} with increasing eigenvalues E_n , and $X_{mn} = \langle m|\hat{X}|n\rangle$.

From the FDR to the GGE

Lehman representation

Note that $\tilde{C}_+(\omega)$ and $\text{Im } \tilde{R}(\omega)$ are non-zero only if ω takes values within the discrete set $\{E_m - E_n\}_{m,n \geq 0}$ (due to the delta functions) and $A_{nm} \neq 0$.

In Gibbs-Boltzmann equilibrium $\rho_{nn} \propto \exp(-\beta E_n)$ since there is a single charge, $\hat{Q}_1 = \hat{H}$, and for any bosonic \hat{A} , the FDT holds $\forall \omega$

$$\hbar \text{Im } \tilde{R}(\omega) = \tanh(\beta \hbar \omega / 2) \tilde{C}_+(\omega)$$

In contrast, for the GGE, $\rho_{nn} \propto \exp(-\sum_k \lambda_k Q_{kn})$ with $Q_{kn} \equiv \langle n | \hat{Q}_k | n \rangle$ and the sums include many terms. However, one can cut these sums by

properly choosing \hat{A} and extracting the λ_k 's from the corresponding FDR

Quantum quench

Hard-core bosons in one dimension

Consider the Lieb-Liniger model with density ϱ

$$\hat{H}_c = \int dx \left[\partial_x \hat{\phi}^\dagger(x) \partial_x \hat{\phi}(x) + c \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\phi}(x) \right]$$

initialized in the ground state of $\hat{H}_{c=0}$ and evolved with $\hat{H}_{c \rightarrow \infty}$

a non interacting problem

Mapping to hard-core bosons, that after a Jordan-Wigner transformation become free fermions,

$$\hat{H}_{c \rightarrow \infty} = \sum_k \epsilon_k \hat{f}_k^\dagger \hat{f}_k \text{ with } \epsilon_k = k^2$$

The conserved charges are $\langle \hat{Q}_k \rangle = \langle \hat{f}_k^\dagger \hat{f}_k \rangle = 4\varrho^2 / (\epsilon_k^2 + 4\varrho^2)$

and the Lagrange multipliers $\lambda_k = \ln[\epsilon_k^2 / (4\varrho^2)]$

Quantum quench

Hard-core bosons in one dimension

Consider again the $c = 0$ to $c \rightarrow \infty$ quench of the Lieb-Liniger model

In the stationary limit, the density operator $\hat{\rho}(q, t)$ (for $q \neq 0, \pi$)

$$C_+(q, t) = \sum_k e^{-i(\epsilon_k - \epsilon_{k-q})|t|} \left(\frac{n_{k-q} + n_k}{2} - n_{k-q} n_k \right)$$
$$R(q, t) = i\theta(t) \sum_k e^{-i(\epsilon_k - \epsilon_{k-q})t} (n_{k-q} - n_k)$$

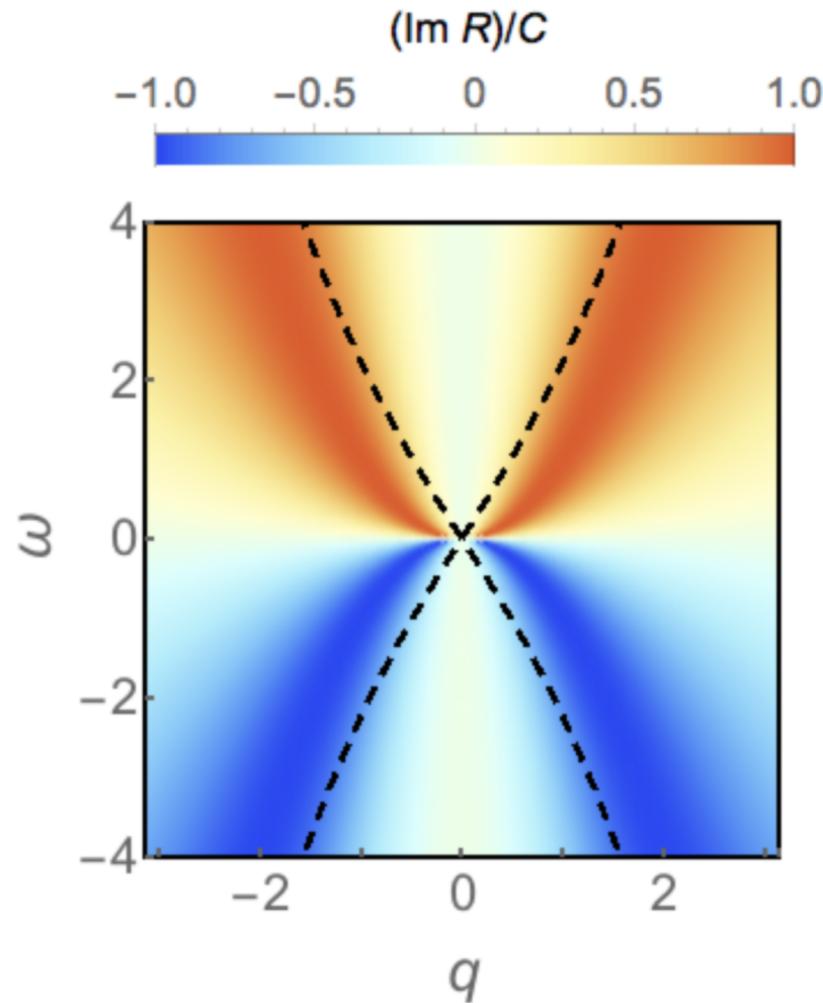
The Fourier transform picks $\omega = \epsilon_k - \epsilon_{k-q}$ with two solutions $k_{1,2}(q, \omega)$

Measuring at frequency ω and wave-vector q related by $\omega = 2\epsilon_{(q+\pi)/2}$,
a single mode is selected, $k_1 = k_2 = (q + \pi)/2$, and the FDR becomes

$$\boxed{\text{Im } R(q, \omega_q) / C_+(q, \omega_q) = \tanh \lambda_q \quad \text{with} \quad \lambda_q = \ln[\epsilon_q^2 / (4\varrho^2)]}$$

Quantum quench

Hard-core bosons in one dimension



Quantum quench

The one dimensional Bose gas

Consider the Lieb-Liniger model with density ϱ

$$\hat{H}_c = \int dx \left[\partial_x \hat{\phi}^\dagger(x) \partial_x \hat{\phi}(x) + c \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\phi}(x) \right]$$

initialized in the ground state of $\hat{H}_{c=0}$ and evolved with $\hat{H}_{c<+\infty}$, now

an interacting problem

Bethe Ansatz solution:

$$\lim_{t \rightarrow \infty} \langle \hat{O} \rangle = \langle \vartheta_{\text{GGE}} | \hat{O} | \vartheta_{\text{GGE}} \rangle$$

with the eigenstate $|\vartheta_{\text{GGE}}\rangle$ characterised by a “mode occupation” $\vartheta_{\text{GGE}}(\lambda)$ computed, for this problem, in

Quantum quench

The one dimensional Bose gas

Let us parametrize $\vartheta_{\text{GGE}}(\lambda)$ as

$$\vartheta_{\text{GGE}}(\lambda) = \frac{1}{1+e^{\epsilon(\lambda)}}$$

and $\epsilon(\lambda_F)=0$.

One particle-hole kinematics at low momentum $k \ll k_F = \pi\varrho$

The FDR of the density-density correlation and linear response is

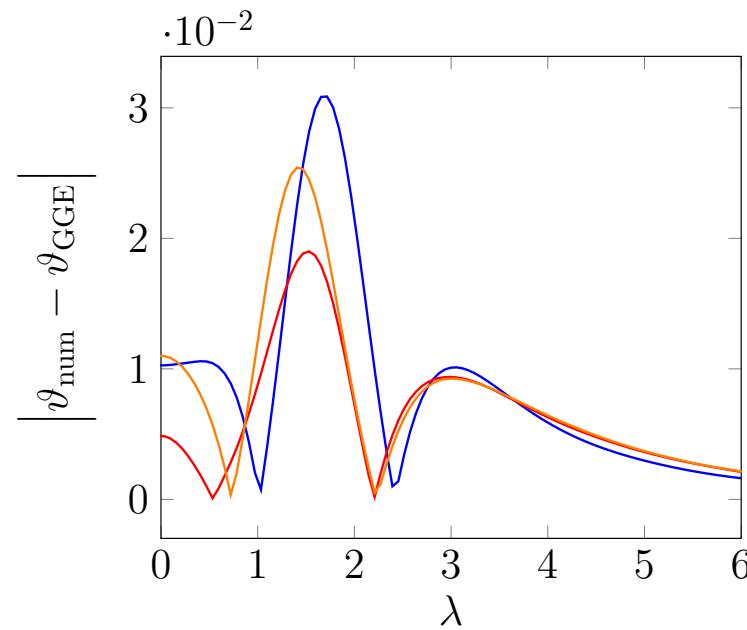
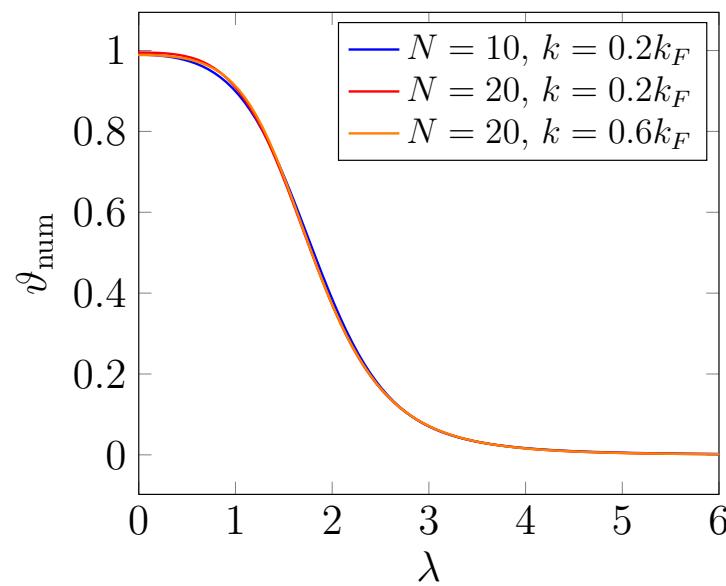
$$\boxed{\text{Im } \tilde{R}(k, \omega)/\tilde{C}_+(k, \omega) = \tanh(k\partial_\lambda\epsilon(\lambda)/(2\pi\rho_t(\lambda)))|_{\lambda(k, \omega)}}$$

Without entering the technical details, $\epsilon(\lambda)$, $\rho_t(\lambda)$ and $\lambda(k, \omega)$ depend on $\vartheta_{\text{GGE}}(\lambda)$.

Computing the left-hand-side one can reconstruct $\vartheta_{\text{GGE}}(\lambda)$ and compare it to the exact form derived by **de Nardis et al 14**

Quantum quench

Hard-core bosons in one dimension



v_{num} from FDR & v_{GGE} from direct calculation.

Error due to the low k expansion present in both evaluations.

Summary

Fluctuation-dissipation relations

The FDRs of carefully chosen, but quite natural, observables “contain” the GGE effective temperatures.

They can be used to measure them or, even more generally, to construct the steady state density matrix.

Advantages:

One does not have to know the conserved charges.

Just one observable needs to be used. The sweeping is made in frequency and wave-vector.

References

4. Integrable systems and Generalized Gibbs Ensembles.

- As a test of non-thermal equilibrium

Foini, LFC & Gambassi 11 & 12

- **Integrable non-interacting systems**

Foini, Gambassi, Konik & LFC 16

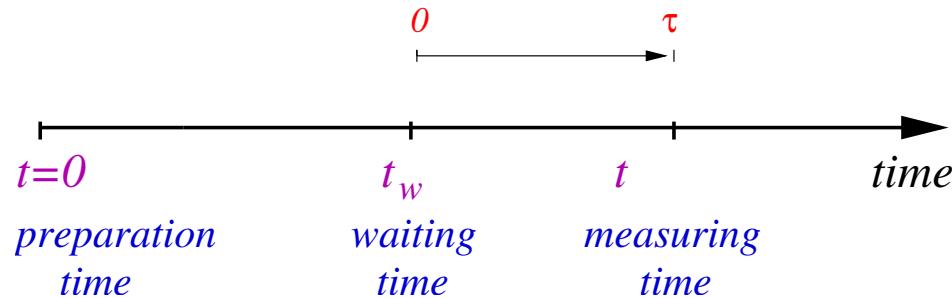
- **Integrable interacting systems**

de Nardis, Panfil, Gambassi, LFC, Konik & Foini 17

Thanks to the joint autumn programs at KITP 2015

Two-time observables

Correlations



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

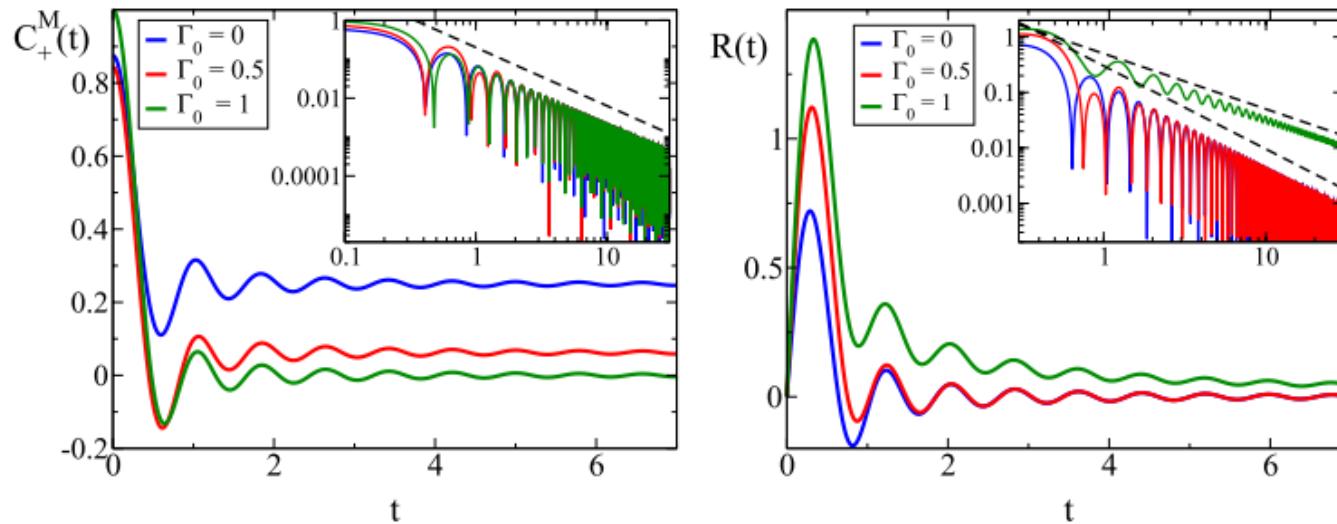
$$C_{AB}(t, t_w) \equiv \langle \hat{A}(t) \hat{B}(t_w) \rangle$$

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

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

The observable M

Correlation & linear response



The two-time correlation & linear response between two observables $\hat{A}(t)$ and $\hat{B}(t_w)$ are

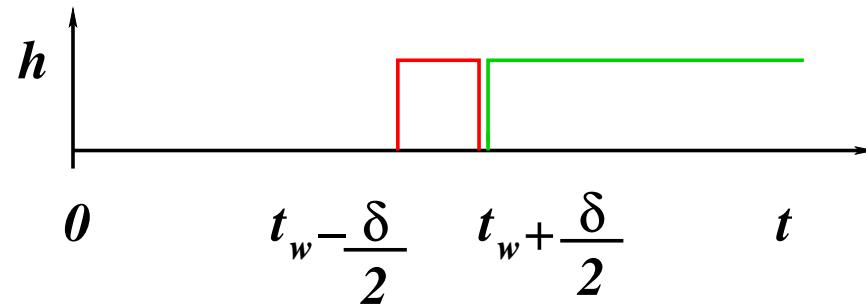
$$C_{AB}^\pm(t, t_w) \equiv \langle [\hat{A}(t), \hat{B}(t_w)]_\pm \rangle$$

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

or the average over realizations of the dynamics (initial conditions, random num-

Two-time observables

Linear response



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

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

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

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

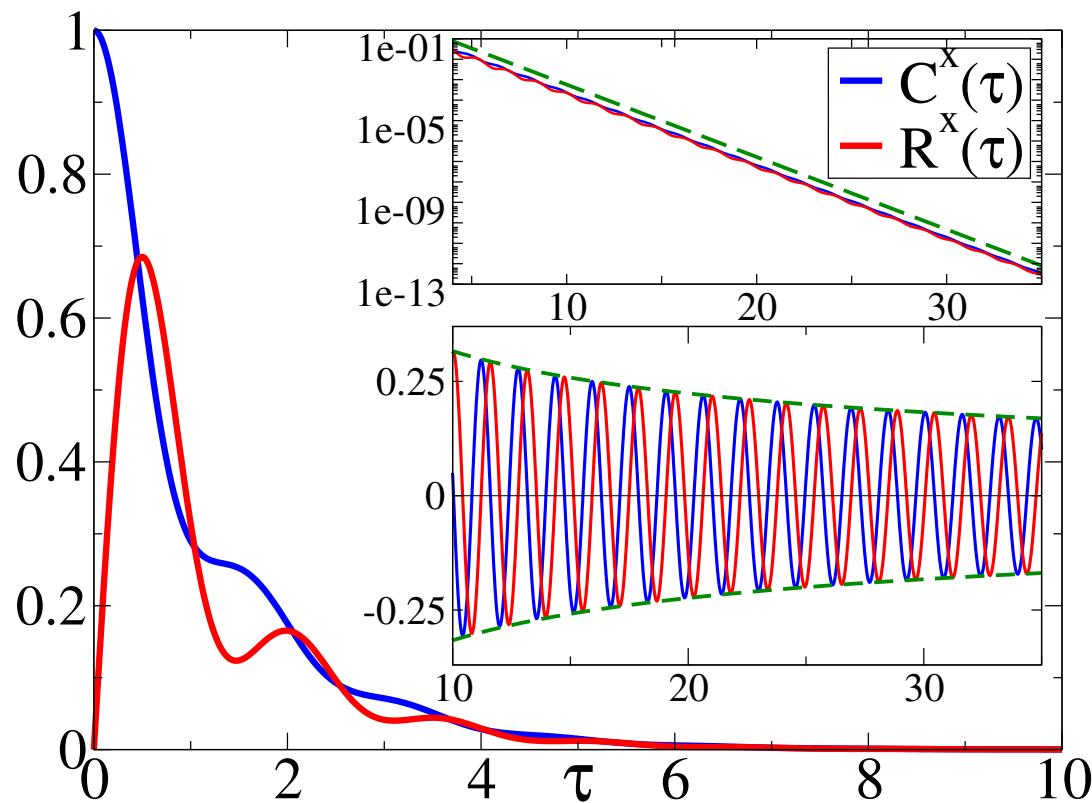
$$\text{Im} \tilde{R}^{AB}(\omega) = [\hbar^{-1} \tanh(\beta \hbar \omega / 2)]^{\pm 1} \tilde{C}_{\pm}^{AB}(\omega)$$

Bosons
Fermions

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

Quantum quench

T_{eff} from the longitudinal spin FDR



Insets

$$e^{-\tau/\tau_c}$$

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

$$C^x(\tau) \simeq A_c e^{-\tau/\tau_c} [1 - a_c \tau^{-2} \sin(4\tau + \phi_c)]$$

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

Quantum quench

T_{eff} from FDT ?

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

$$-\beta_{\text{eff}}^x \simeq \frac{R^x(\tau)}{d_\tau C_+^x(\tau)} \simeq -\frac{\tau_c A_R}{A_c}$$

A constant consistent with a classical limit but

$$T_{\text{eff}}^x(\Gamma_0) \neq T_e(\Gamma_0)$$

Moreover, a complete study in the full time and frequency domains confirms that $T_{\text{eff}}^x(\Gamma_0, \omega) \neq T_{\text{eff}}^z(\Gamma_0, \omega) \neq T_e(\Gamma_0)$ (though the values are close).

Fluctuation-dissipation relations as a probe to test thermal equilibration

No equilibration for generic Γ_0 in the quantum Ising chain

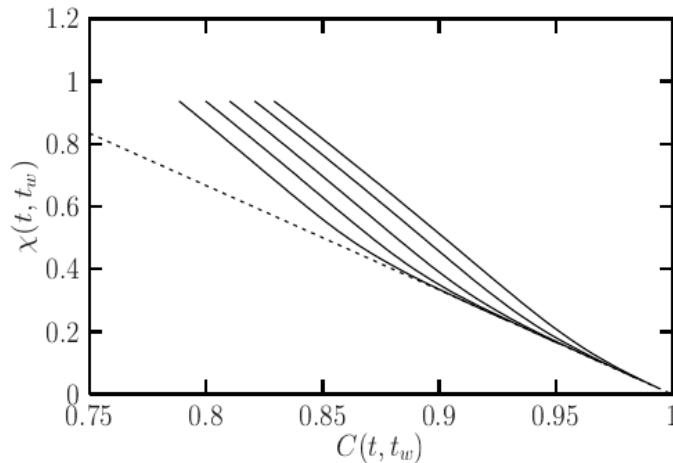
FDT & effective temperatures

Role of initial conditions

$T^* > T$ found for quenches from the disordered into the glassy phase

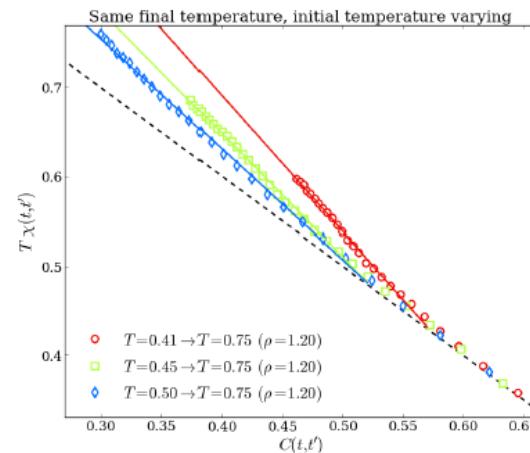
(Inverse) quench from an ordered initial state,

$$T^* < T$$



2d XY model or O(2) field theory

Berthier, Holdsworth & Sellitto 01

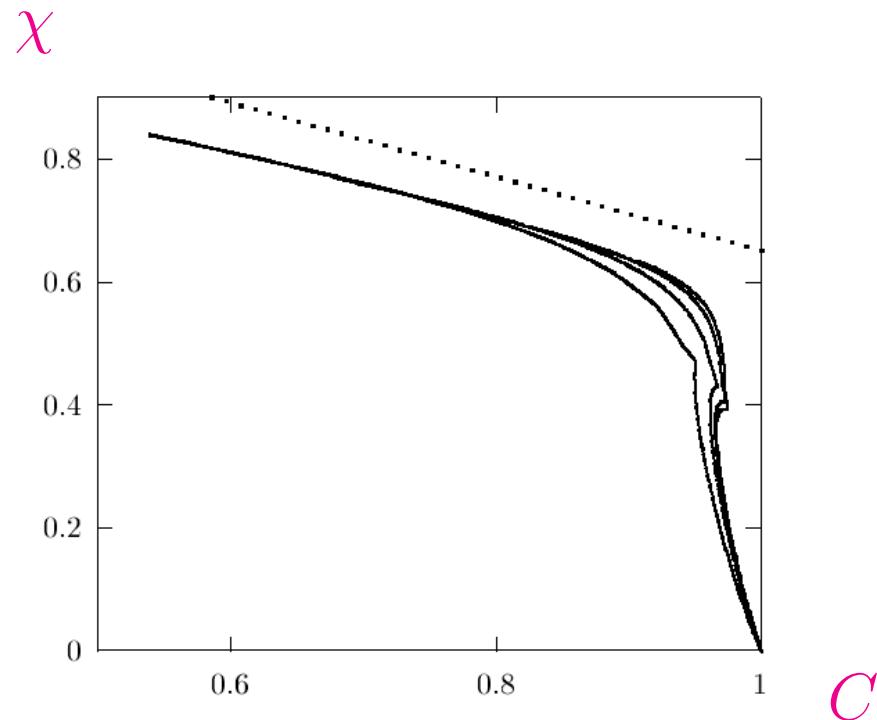
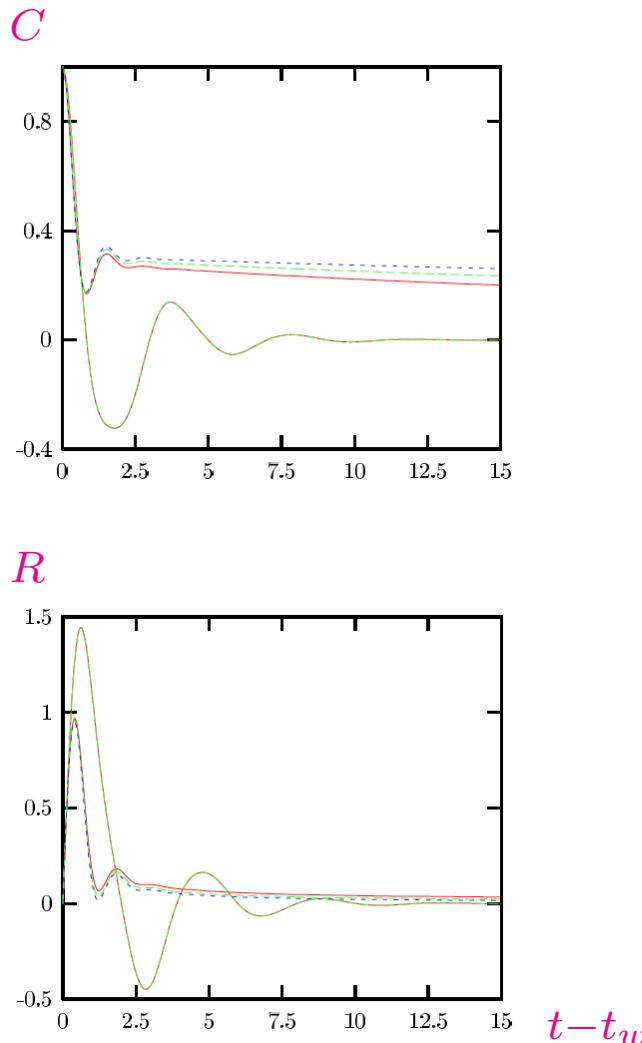


Binary Lennard-Jones mixture

Gnan, Maggi, Parisi & Sciortino 13

Dissipative quantum glasses

Quantum p -spin model coupled to a bath of oscillators

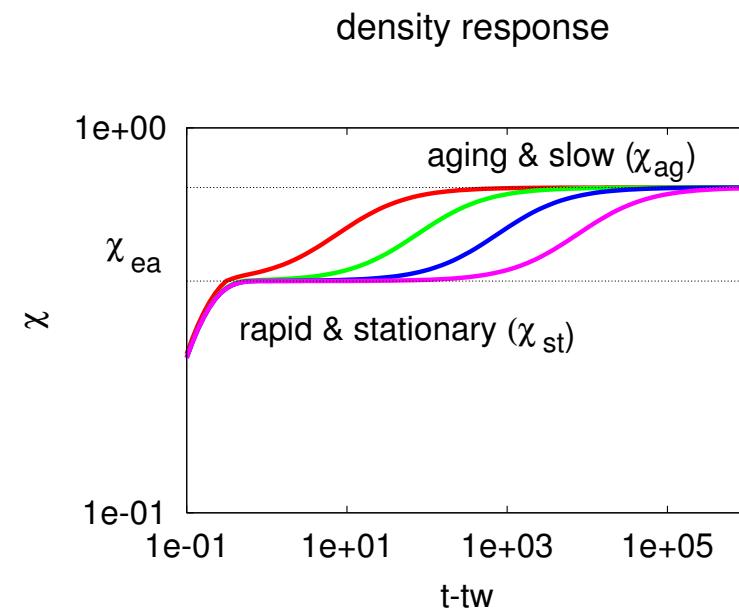
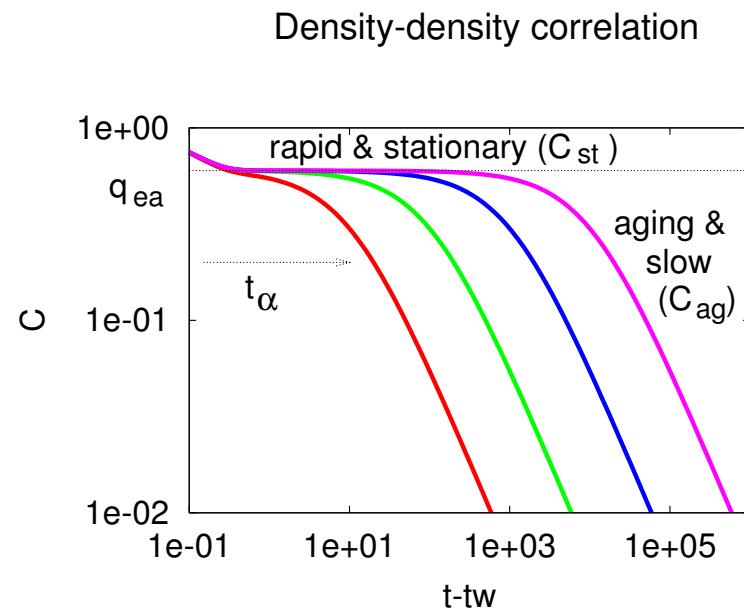


Classical FDT beyond the shoulder

Out of equilibrium decoherence

Glassy dynamics

Non stationary relaxation & separation of time-scales



$$C(t, t_w)$$

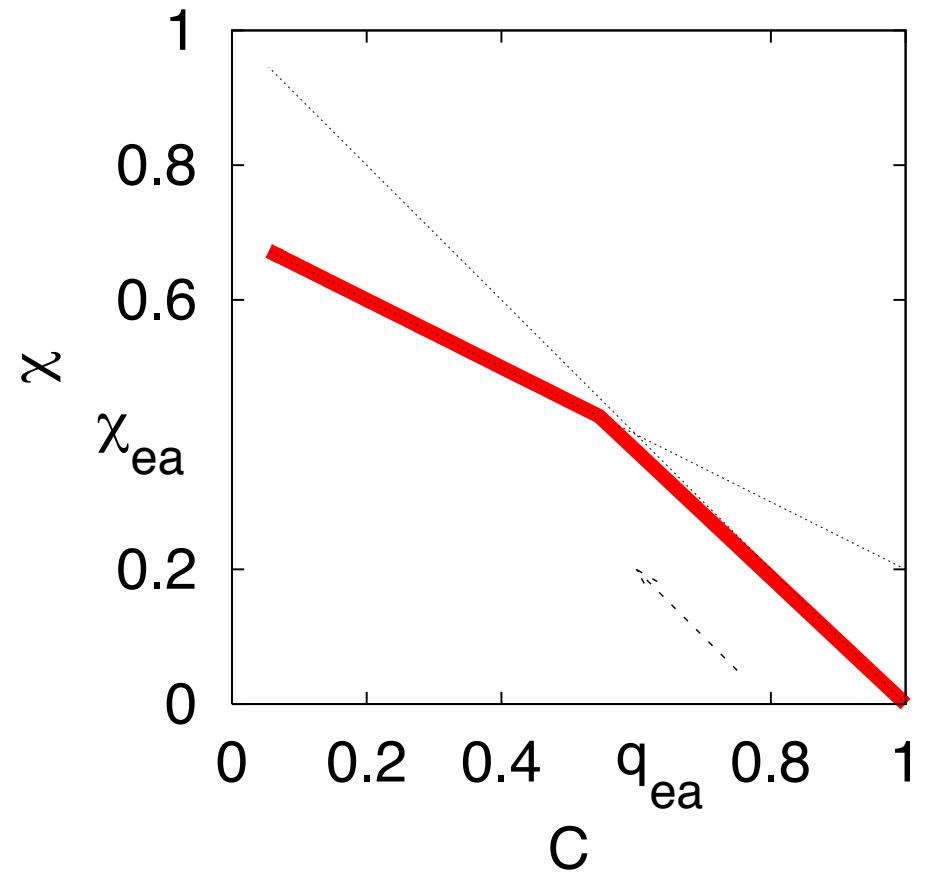
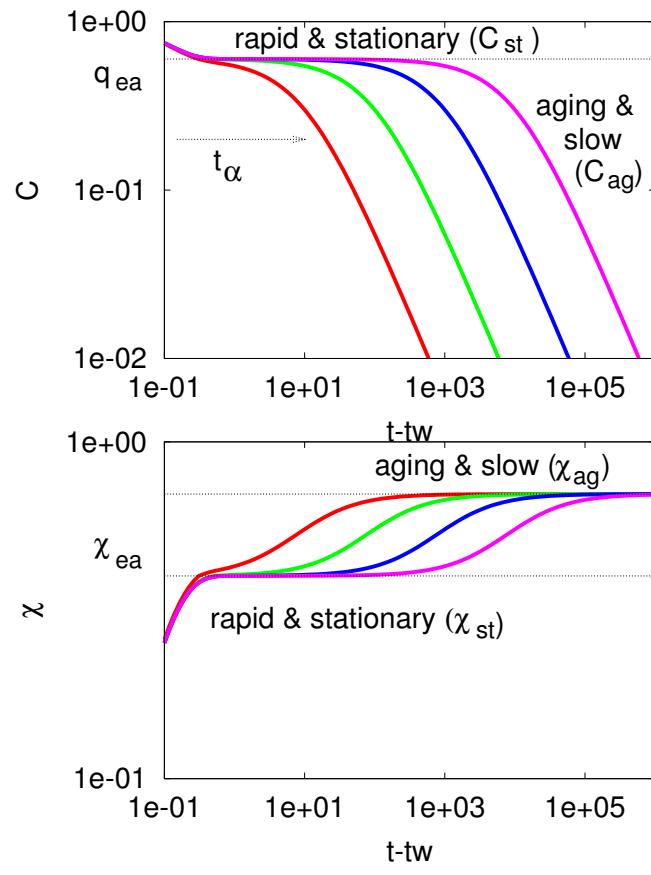
Correlation

$$\chi(t, t_w) = \int_{t_w}^t dt' R(t, t')$$

Time-integrated linear response

Glassy dynamics

Fluctuation-dissipation relation: parametric plot



Another example

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

Fermionic representation :

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

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

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

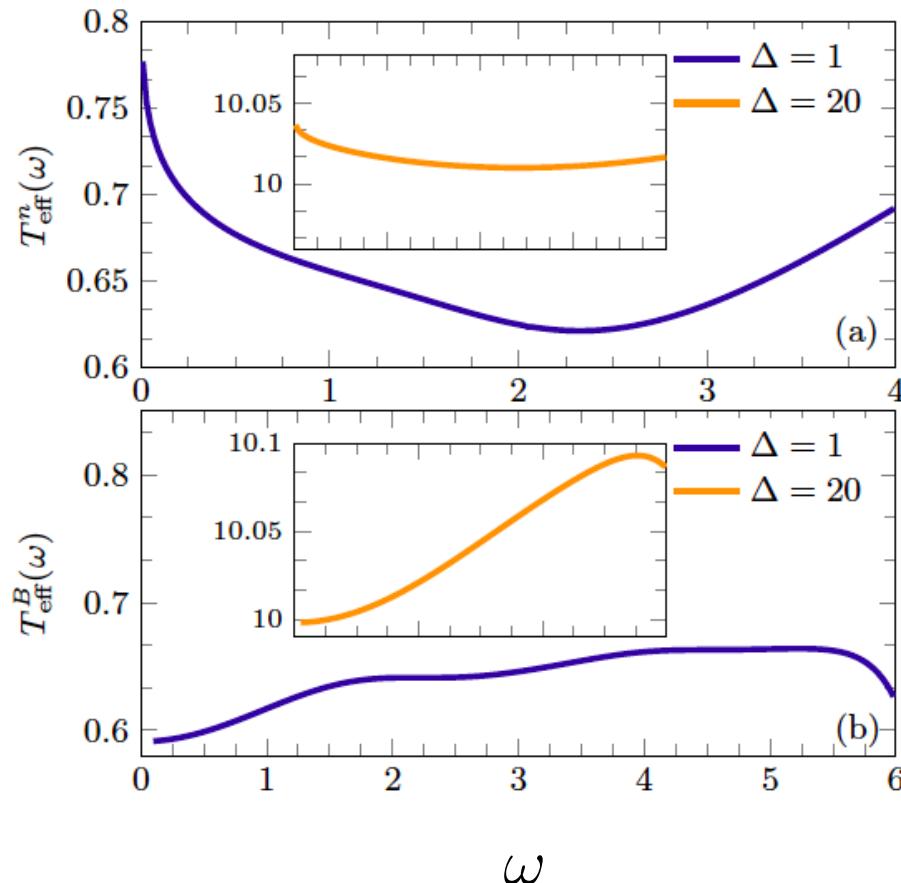
Chung, Iucci & Cazalilla 12

the FDT is not satisfied in this same limit, and different FDRs yield different T_{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

Fluctuation-dissipation theorem

Classical dynamics in Gibbs-Boltzmann equilibrium

The classical FDT for a stationary system with $\tau \equiv t - t_w$ reads

$$\chi(\tau) = \int_0^\tau dt' R(t') = -\beta[C(\tau) - C(0)] = \beta[1 - C(\tau)]$$

choosing $C(0) = 1$.

Linear relation between χ and C

Quantum dynamics in Gibbs-Boltzmann equilibrium

The quantum FDT reads

$$\chi(\tau) = \int_0^\tau d\tau' R(\tau') = \int_0^\tau d\tau' \int_{-\infty}^{\infty} \frac{id\omega}{\pi\hbar} e^{-i\omega\tau'} \tanh\left(\frac{\beta\hbar\omega}{2}\right) C(\omega)$$

Complicated relation between χ and C