Some issues on classical and quantum dynamics

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Plan

- **Energy conserving *vs.* dissipative dynamics : setting and formalism.**
- **Classical dissipative systems**

  Generalized Langevin equations.

  Single particle, biological applications.

  Collective phenomena : critical relaxation.
- **Quantum systems**

  Schwinger-Keldysh & Feynman-Vernon modeling.

  Dissipative quantum dynamics.

  Quantum quenches in closed systems.

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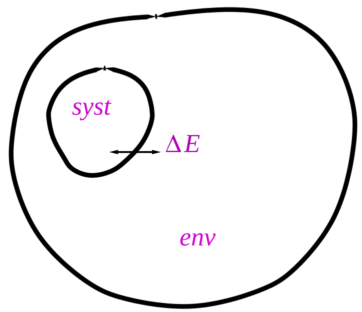
Setting

Aim

Our interest is to describe the **dynamics** of a **classical or quantum system** coupled or not to a **classical or quantum environment**.

The Hamiltonian of the ensemble is

$$\boxed{\mathcal{H} = \mathcal{H}_{syst} + \mathcal{H}_{env} + \mathcal{H}_{int}}$$



The dynamics of all variables are given by Newton or Heisenberg rules, depending on the variables being classical or quantum.

We need to give the initial $\{x_i(0), p_i(0)\}$ or $\hat{\rho}(0)$.

Dissipative case : if $\mathcal{H}_{int} \neq 0$ the total energy is conserved, $E =$ ct, but each contribution is not, in particular $E_{syst} \neq$ ct and we'll take $\boxed{E_{syst} \ll E_{env}}$

Reduced system

Model the environment and the interaction

E.g., an ensemble of harmonic oscillators and a bi-linear coupling :

$$\mathcal{H}_{env} + \mathcal{H}_{int} = \sum_{\alpha=1}^{\mathcal{N}} \left[\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} \left(\frac{c_\alpha}{m_\alpha \omega_\alpha^2} x - q_\alpha \right)^2 \right]$$

Classically (coupled Newton equations) and **quantum mechanically** (easier in a path-integral formalism) one can integrate out the oscillator variables.

Assuming the **environment** is coupled to the sample at the initial time and that its variables are characterized by a **Gibbs-Boltzmann density function** $\rho \propto e^{-\beta(\mathcal{H}_{env}+\mathcal{H}_{int})}$ at inverse temperature β one finds :

a **colored Langevin equation** (classically) or

a **reduced dynamic generating functional** $\mathcal{Z}_{red}$ (quantum mechanically).

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General Langevin equation

The system, $\{r_i^a\}$, with $i = 1, \dots, N$ and $a = 1, \dots, D$, coupled to an **equilibrium environment** evolves according to the **Langevin eq.**

$$\underbrace{m\ddot{r}_i^a(t)}_{} + \underbrace{\int_{t_0}^{t} dt' \, \mathbf{\Gamma}(t-t')\dot{r}_i^a(t')}_{} = \underbrace{-\frac{\delta V(\{\vec{r}_i\})}{\delta r_i^a(t)}}_{} + \underbrace{\xi_i^a(t)}_{} \; .$$

Inertia **friction** **deterministic force** **noise**

Coloured noise with correlation $\langle \xi_i^a(t)\xi_j^b(t') \rangle = k_B T \delta_{ij}\delta^{ab} \, \mathbf{\Gamma}(t-t')$ and zero mean.

T the **temperature** of the equilibrium bath and k_B the Boltzmann constant.

The **friction kernel** is $\mathbf{\Gamma}(t-t')$.

Proof : see, *e.g.*, **Weiss 99**.

Colored noise

Generic : Most of the exact **fluctuation-dissipation relations** in and out of equilibrium remain unaltered for generic Γ, *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 Γ.

The interesting cases are

$$\frac{\mathbf{S}(\omega)}{\omega} = 2\gamma_0 \left(\frac{\omega}{\omega_0}\right)^{\alpha-1} e^{-\omega/\Lambda}$$

with Λ a large-frequency cut-off.

Colored noise

Time-dependence and long-time tails

Non-Ohmic cases

$$\Gamma(t-t') \simeq \frac{g}{\Gamma_E(1-\alpha)} \, |t-t'|^{-\alpha-1} \qquad \text{for} \qquad \alpha \neq 1$$

g is the effective 'friction coefficient' (depends on $\alpha, \Lambda, \omega_0$)

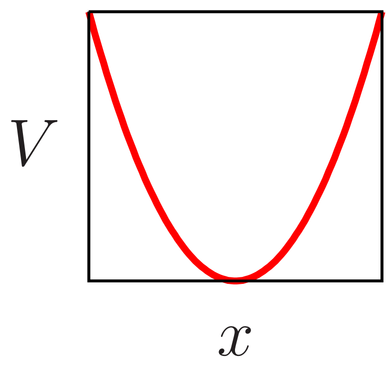
Γ_E is the Euler-function.

Ohmic cases

$$\Gamma(t-t') = 2\gamma_0 \, \frac{\Lambda}{1+(\Lambda t)^2} \to_{\Lambda\to\infty} 2\gamma_0 \delta(t-t') \qquad \text{for} \qquad \alpha = 1$$

Example

a particle in a harmonic potential



$V(x) = \frac{1}{2} m\omega_0^2 x^2$

After a relatively short transient,

independently of the initial condition

equilibrium dynamics

$$C_x(t,t') \equiv \langle x(t)x(t')\rangle \to \frac{1}{m\omega_0^2} E_{\alpha,1}\left(-\frac{m\omega_0^2 |t-t'|^\alpha}{g}\right)$$

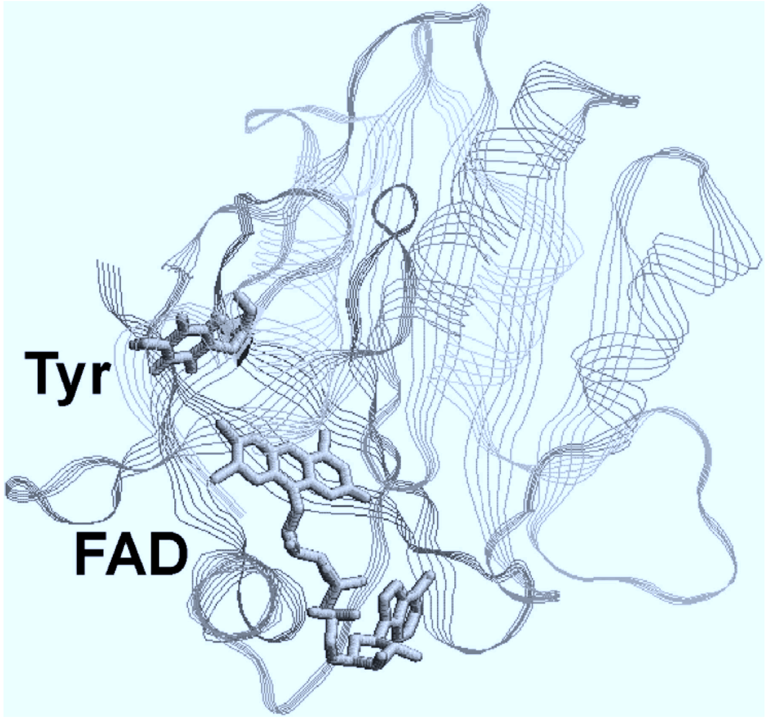
with $E_{\alpha,1} = \sum_{k=0} \frac{z^k}{\Gamma_E(\alpha k+1)}$ the Mittag-Leffler function.

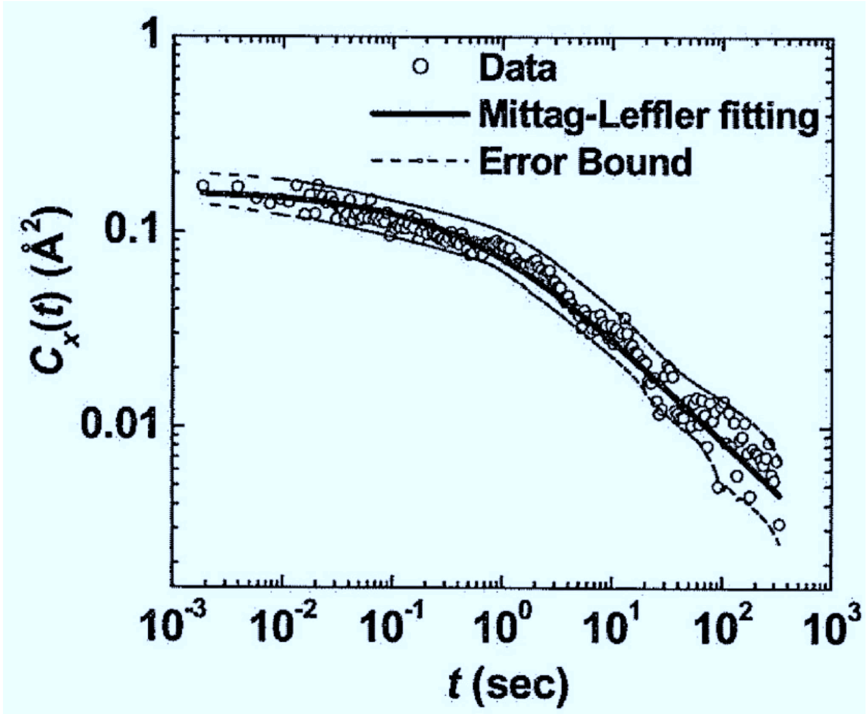
Only for an Ohmic bath $\alpha \to 1$ **the relaxation is exponential** $E_{1,1}(z) = e^z$

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

Protein dynamics

Questions : what are the potential and the bath ?





$x(t)$ distance between Tyr and FAD $\alpha = 0.51 \pm 0.07$

Yang *et al* 03 ; Min, Luo, Cherayil, Kou & Xie 05

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 :

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

Overdamped relaxation dynamics

$$\int_{t_0}^{t} dt' \, \mathbf{\Gamma}(t - t') \frac{\partial}{\partial t'} \vec{\phi}(\vec{r}, t') = - \frac{\delta \mathcal{H}}{\delta \vec{\phi}(\vec{r}, t)} + \vec{\xi}(\vec{r}, t)$$

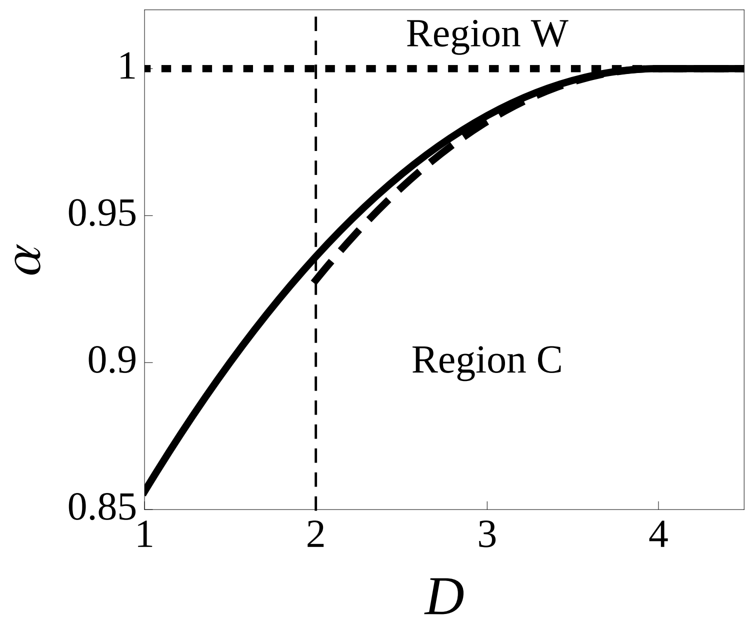
$$\langle \xi_i(\vec{r}, t) \xi_j(\vec{r}', t') \rangle = k_B T \delta_{ij} \delta(\vec{r} - \vec{r}') \, \mathbf{\Gamma}(t - t')$$

Equilibrium initial condition $\qquad P[\vec{\phi}(\vec{r}, t_0)] \propto e^{-\beta \mathcal{H}[\phi(\vec{r}, t_0)]}$

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

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

in region C Sub-Ohmic bath

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

Solid line $N = 1$

Dashed line $N = 4$

Dotted horizontal line $N \to \infty$

Bonart, LFC & Gambassi 11

Interest ?

In classical interacting systems (*e.g.* glasses, active matter, powders) sometimes one selects some variables and treats the rest in some self-consistent way.

Results in an effective Langevin equation with a **self-consistent 'bath'**,

$$M\ddot{\phi}(t) + \int_{t_0}^{t} dt' \, \mathbf{\Gamma^1}(t,t')\dot{\phi}(t') = -\frac{\delta V(\{\phi\})}{\delta\phi(t)} + \xi(t) \ .$$

Coloured noise with correlation $\langle \, \xi(t)\xi(t') \, \rangle \propto \mathbf{\Gamma^2}(t,t')$

$\mathbf{\Gamma}^1$ and $\mathbf{\Gamma}^2$ are self-consistently determined in terms of correlations and linear responses of the original fields. *cfr.* **MCT, DMFT**

How are the collective dynamics determined ?

Message

- The equilibrium relaxation of even the simplest system in contact with a colored bath is **non-exponential**.

- The **dynamic critical exponent** can be modified by a sufficiently ‘slow’ colored bath.

It is hard to conclude on thermal equilibration from the functional form of the observables

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Many-body

Interacting rotors under a bias

The system's Hamiltonian is

$$\mathcal{H}_{syst} = \frac{\Gamma}{2\mathcal{M}} \sum_{i=1}^{N} \vec{L}_i^2 - \frac{\mathcal{M}}{2\sqrt{N}} \sum_{i<j} J_{ij} \vec{n}_i \vec{n}_j$$

with usual commutation rules between L_i^a and n_j^b.

Each variable is coupled to two 'leads' or electron reservoirs at equal temperature T but with different chemical potential, $\mu_R - \mu_L = eV$.

We set the system in contact with the reservoir at time t_0.

Decoupled density matrix $\varrho(t_0) = \varrho_{syst}(t_0) \otimes \varrho_{env}(t_0)$ and

random initial condition for the rotors.

Many-body

Interacting rotors under a bias

The interaction with the two leads leads to

$$\mathcal{S}_{int} = -\frac{1}{2} \sum_{rs=\pm} \int dt dt' \, \Sigma_B^{rs}(t,t') \, \sum_i \vec{n}_i^r(t) \vec{n}_i^s(t')$$

with the bath induced kernels

$$\Sigma_B^{rs}(t,t') = -irs\hbar\omega_c^2 \left[G_{rs}^R(t,t') G_{sr}^L(t',t) + L \leftrightarrow R \right]$$

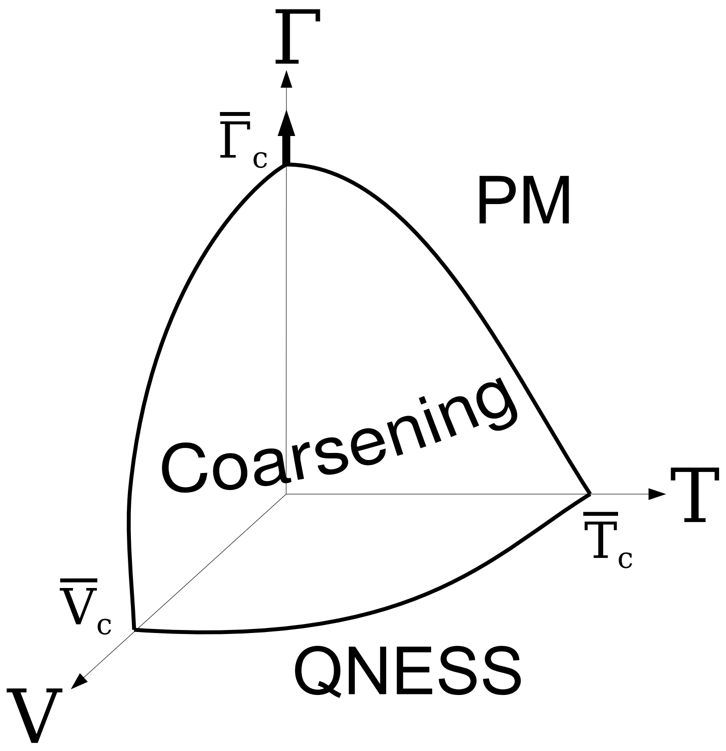
and $G_{rs}(t,t') \equiv -i\langle \mathcal{T} \psi_r(t) \psi_s^\dagger(t') \rangle$

with $\psi_r(t), \psi_r^\dagger(t)$ the fermionic fields

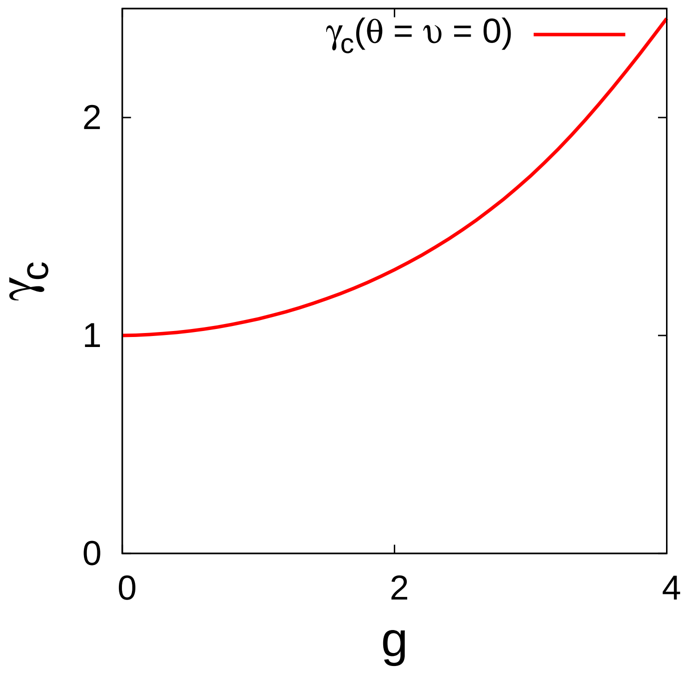
and $\mathcal{T}$ the time-ordering operator on the closed contour.

Many-body

Interacting rotors under a bias



Potential (V) – Temp. (T)
– Quantum fluct. (Γ)
phase diagram



Dependence of

$$\gamma_c \equiv (4\hbar/3\pi)^2 \overline{\Gamma}_c / J = 1 + 9/2\ g^2$$

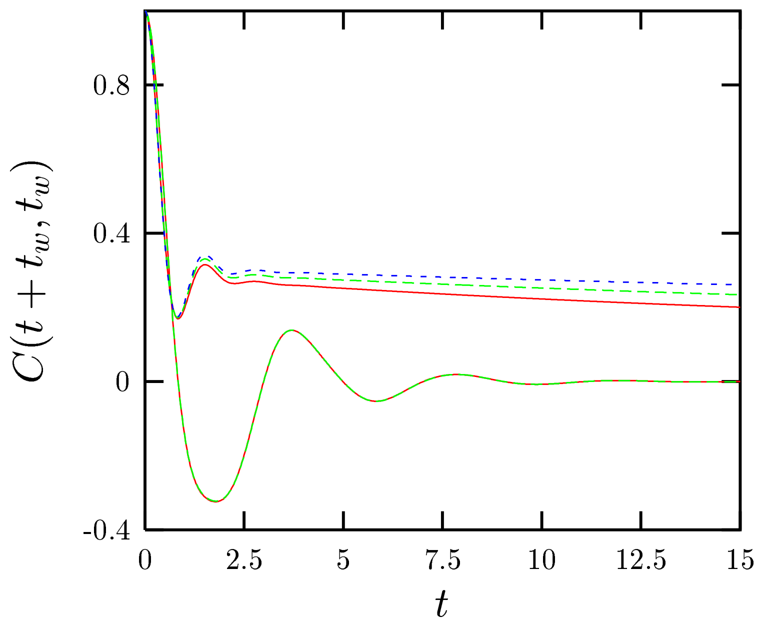
on the strength of the bath ($g = \hbar\omega_c/\epsilon_F$).

Aron, Biroli & LFC 09 & 10

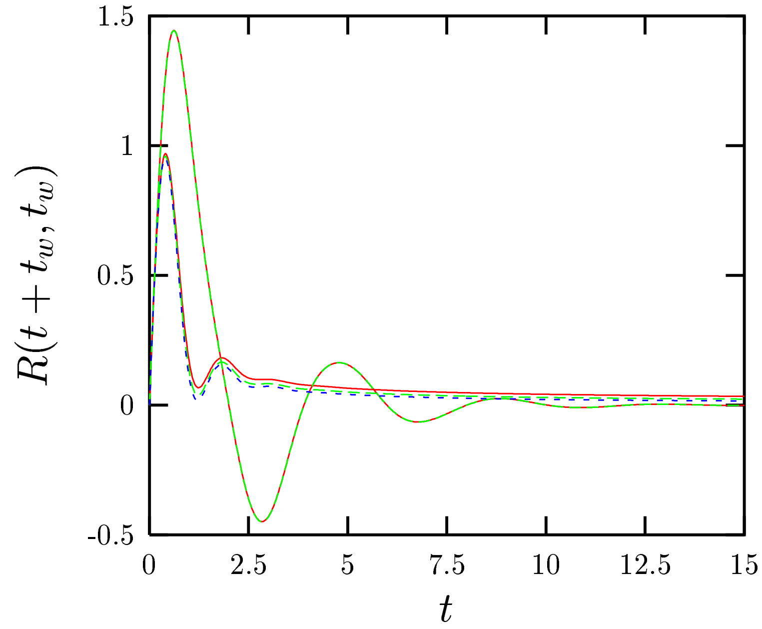
Real-time dynamics

Dissipative spherical p-spin model

Symmetric correlation



Linear response



Comparison between $g = 0.2$ (PM) and $g = 1$ (SG)

PRB 66, 014444 (02).

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Quantum quench

Setting

- Take a quantum closed system and suddenly change a parameter.
- *E.g.*, the quantum Ising chain

$$H_{\Gamma_0} = -\sum \sigma_i^x \sigma_{i+1}^x + \Gamma_0 \sum \sigma_i^z$$

  Transverse field $\Gamma_0 \to \Gamma$

Rieger & Iglói 90s

- **Questions :**

  Does the system reach a thermal equilibrium measure ?

  Under which conditions ?

  (*e.g.*, integrable vs. non-integrable systems ; sub *vs.* critical quenches)

Calabrese & Cardy ; Rossini et al., etc.

Is there some kind of emerging effective bath ?

Quantum quench

Previous studies

- Definition of T_e from time-independent observables :

$$\langle H_\Gamma \rangle_{\Gamma_0} = \langle H_\Gamma \rangle_{T_e}$$

$\langle M^x_\Gamma \rangle_{\Gamma_0} = \langle M^x_\Gamma \rangle_{T_e}$, *etc.*

(We know these can be very misleading in glassy systems.)

- Definition of T_e from the functional form of correlation functions :

$C(r) \equiv \langle \sigma_i^x(t)\sigma_j^x(t)\rangle_{\Gamma_0}$ *vs.* $C_{eq}(r) \equiv \langle \sigma_i^x(t)\sigma_j^x(t)\rangle_{T_e}$, *etc.*

(Recall what was discussed in the classical part of the talk.)

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

Fluctuation-dissipation theorem

Classical dynamics in 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 equilibrium

The quantum FDT reads

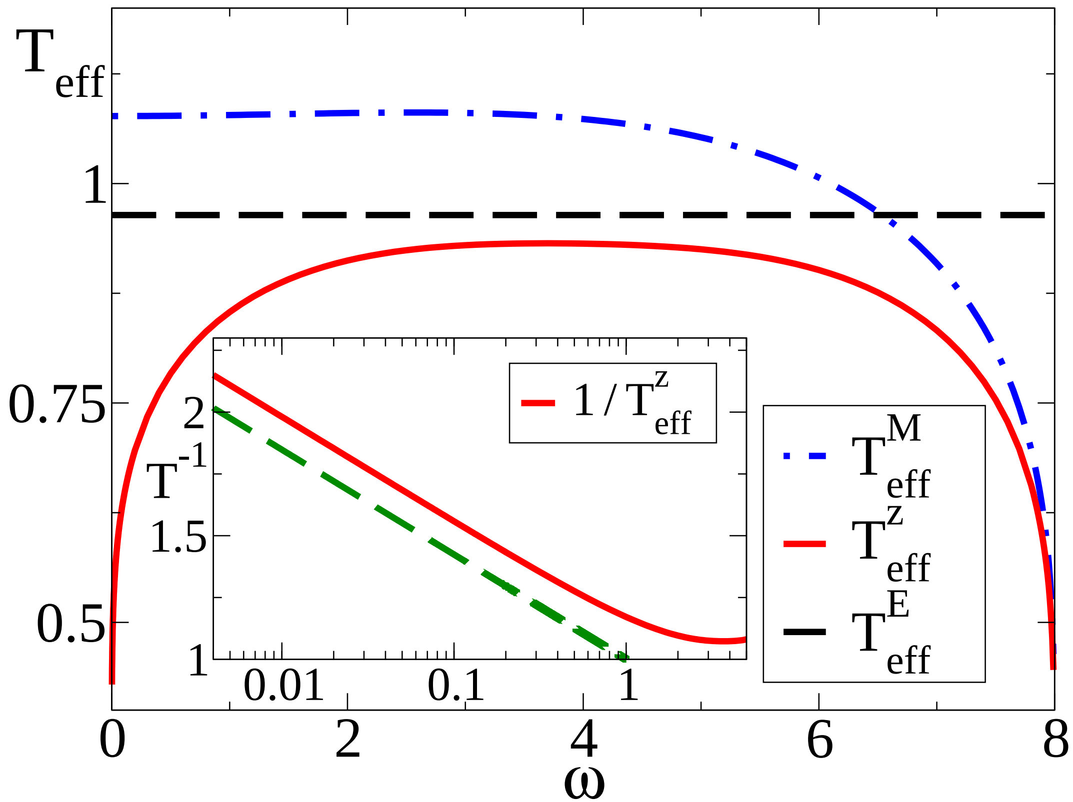
$$\chi(\tau) = \int_0^\tau d\tau' \; R(\tau') = \int_0^\tau d\tau' \int_{-\infty}^{\infty} \frac{i d\omega}{\pi\hbar} \; e^{-i\omega\tau'} \; \tanh\left(\frac{\beta\hbar\omega}{2}\right) C(\omega)$$

Complicated relation between χ and C

Quantum quench

$T_{\rm eff}$ **from transverse spin** σ_i^z **and** $M = N^{-1}\sum_i \sigma_i^z$ **qFDTs ?**

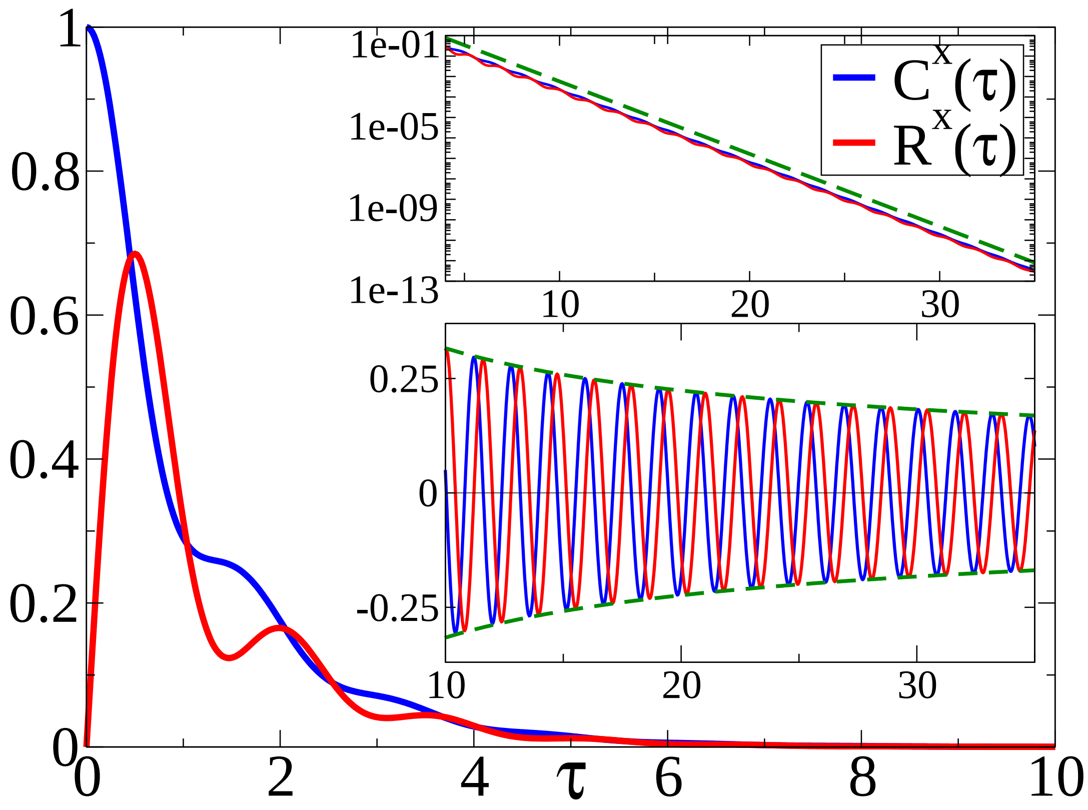
$$\text{Im}R^z(\omega) = \tanh\left(\frac{\beta^z_{\rm eff}(\omega)\omega\hbar}{2}\right) C^z_+(\omega)$$



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

Quantum quench

T_{eff} from longitudinal spin σ_i^x qFDT ?



$$C_+^x(\tau) \simeq A_C e^{-\tau/\tau_C}[1 - a_C \tau^{-2} \sin(4\tau + \phi_C)]$$

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

Quantum quench

$T_{\rm eff}$ from longitudinal spin σ_i^x qFDT ?

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

$$-\beta_{\rm eff}^x \simeq \frac{R^x(\tau)}{d_\tau C_+^x(\tau)} \simeq -\frac{\tau_C A_R}{A_C}$$

A constant consistent with a classical limit but

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

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

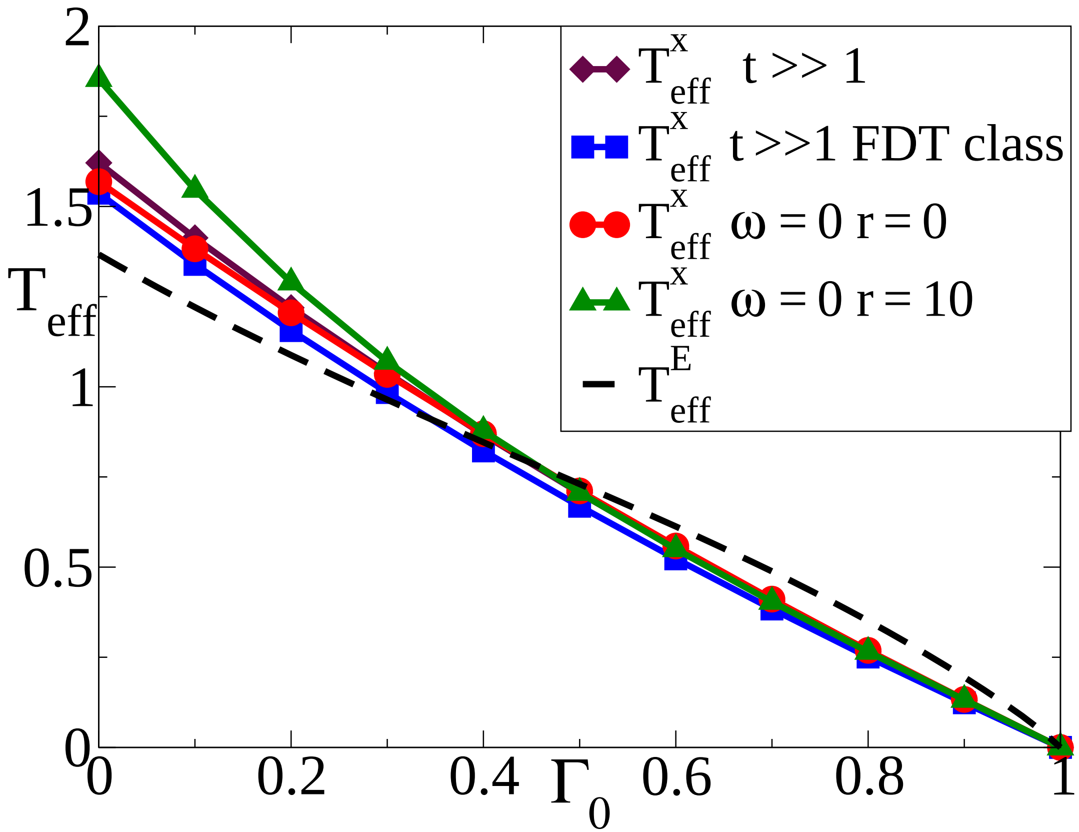
Fluctuation-dissipation relations as a probe to test thermal equilibration

No equilibration for generic Γ_0

Quantum quench

No $T_{\rm eff}$ from FDT

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



Foini, LFC & Gambassi 11

Conclusions

- The same 'Field-theoretic methods' are used in classical and quantum dynamic problems.

- Exotic environments can have non-trivial effects on classical and quantum systems.
  - They change time-scaling in classical systems.
  - They may even change the nature and location of phase transitions in quantum systems.

- Questions on thermalization after quantum quenches.
  - Difficult to answer both classically and quantum mechanically.
  - Idea : use fluctuation-dissipation relations as tests of equilibration.