Non-Markov dissipative classical & quantum dynamics

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Plan

- **Dissipative dynamics : setting and formalism**.
- **Classical systems**

  Generalized Langevin equations.

  Single particle, biological applications.

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

  Schwinger-Keldysh & Feynman-Vernon modeling.

  Quantum Brownian motion and quenches

  Many-body systems ; effect on transitions.

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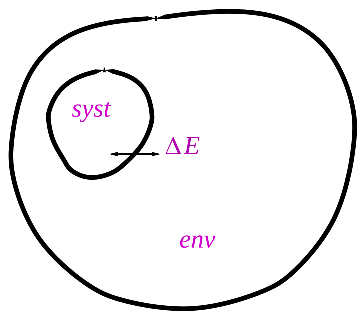
Dissipative systems

Aim

Our interest is to describe the **dynamics** of a **classical or quantum system** coupled 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 $\hat{\rho}(0)$.

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 $i = 1, \ldots, N$ and $a = 1, \ldots, D$, coupled to an **equilibrium environment** evolves according to the **Langevin eq.**

$$\underbrace{M\ddot{r}_i^a(t)}_{\text{Inertia}} + \underbrace{\int_{t_0}^{t} dt'\, \mathbf{\Sigma}_{\mathbf{B}}^{\mathbf{K}}(t-t')\dot{r}_i^a(t')}_{\text{friction}} = \underbrace{-\frac{\delta V(\{\vec{r}_i\})}{r_i^a(t)}}_{\text{deterministic force}} + \underbrace{\xi_i^a(t)}_{\text{noise}} .$$

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

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

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

The **friction kernel** is $\mathbf{\Sigma}_{\mathbf{B}}^{\mathbf{K}}(t-t')$.

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 $\Sigma_{\rm B}^{\rm K}$, 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 $\Sigma_{\rm B}^{\rm K}$.

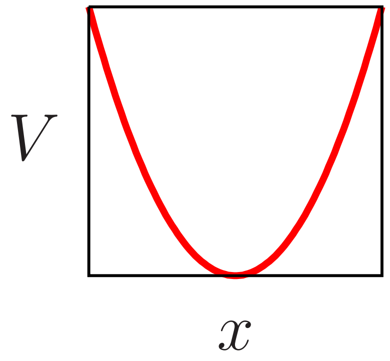
The interesting cases are

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

g the ‘friction coefficient’ and Γ_E the Euler-function.

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

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

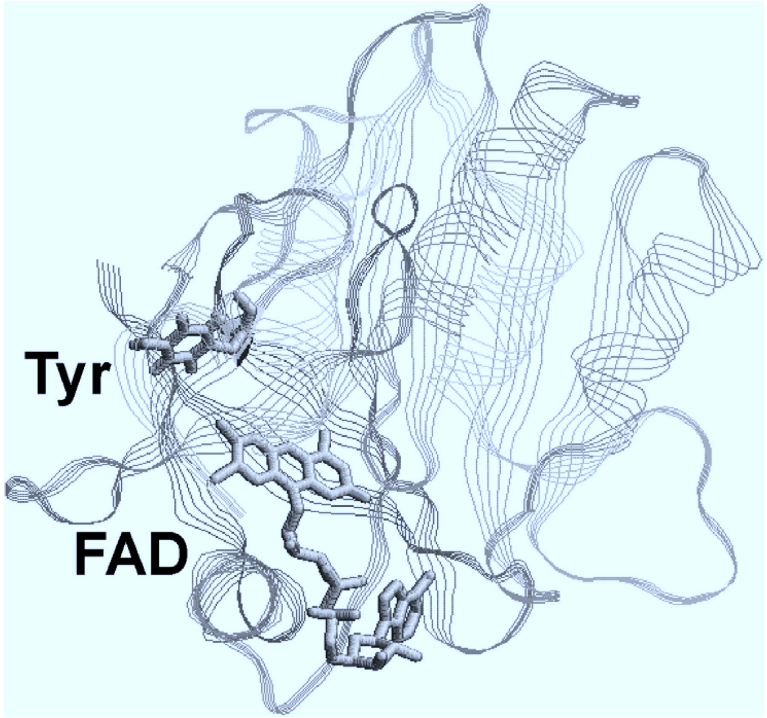
with $E_{\alpha,1} = \sum_{k=0} \frac{z^k}{\Gamma_E(\alpha k+1)}$ the Mittag-Leffler function.

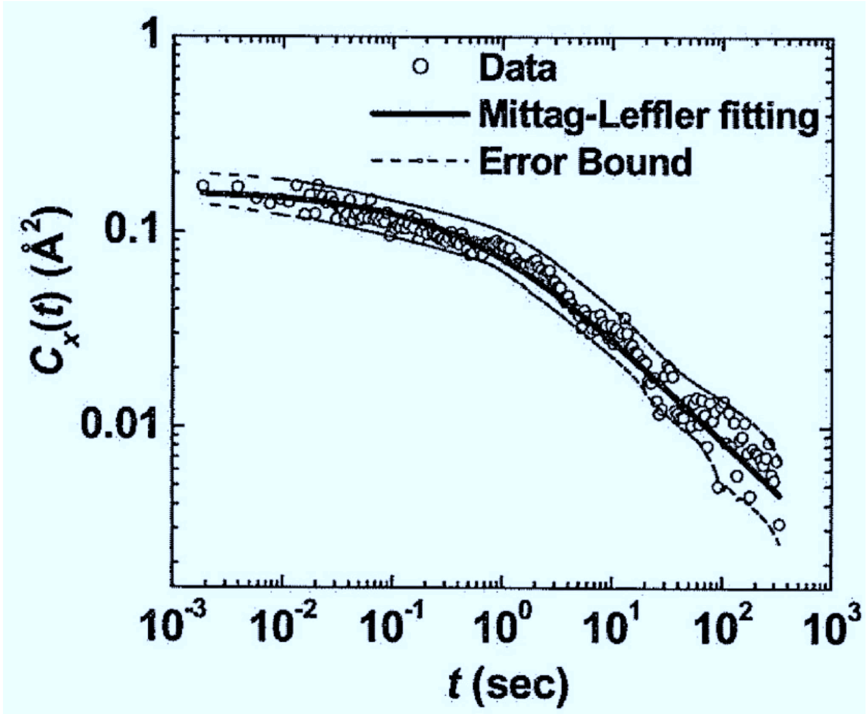
Ohmic bath $\alpha = 1$ $E_{1,1}(z) = e^z$ exponential relaxation.

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 $\qquad \alpha = 0.51 \pm 0.07$

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

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

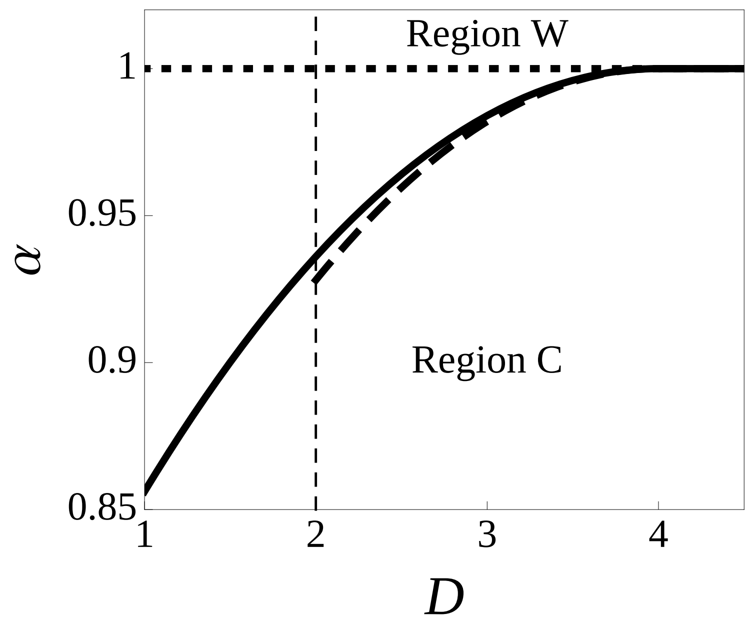
$$\langle \xi_i(\vec{r}, t) \xi_j(\vec{r}\,', t') \rangle = k_B T \delta_{ij} \delta(\vec{r} - \vec{r}\,') \, \mathbf{\Sigma}_B^K (t - t')$$

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



Solid line $N = 1$

Dashed line $N = 4$

Dotted horizontal line $N \to \infty$

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

The dynamic exponent

in region W

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

in region C Sub-Ohmic bath

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

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'**,

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

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

Σ^1_B and Σ^2_B are self-consistently determined in terms of correlations and linear responses of the original fields. *cfr.* **DMFT**

How are the collective dynamics determined ?

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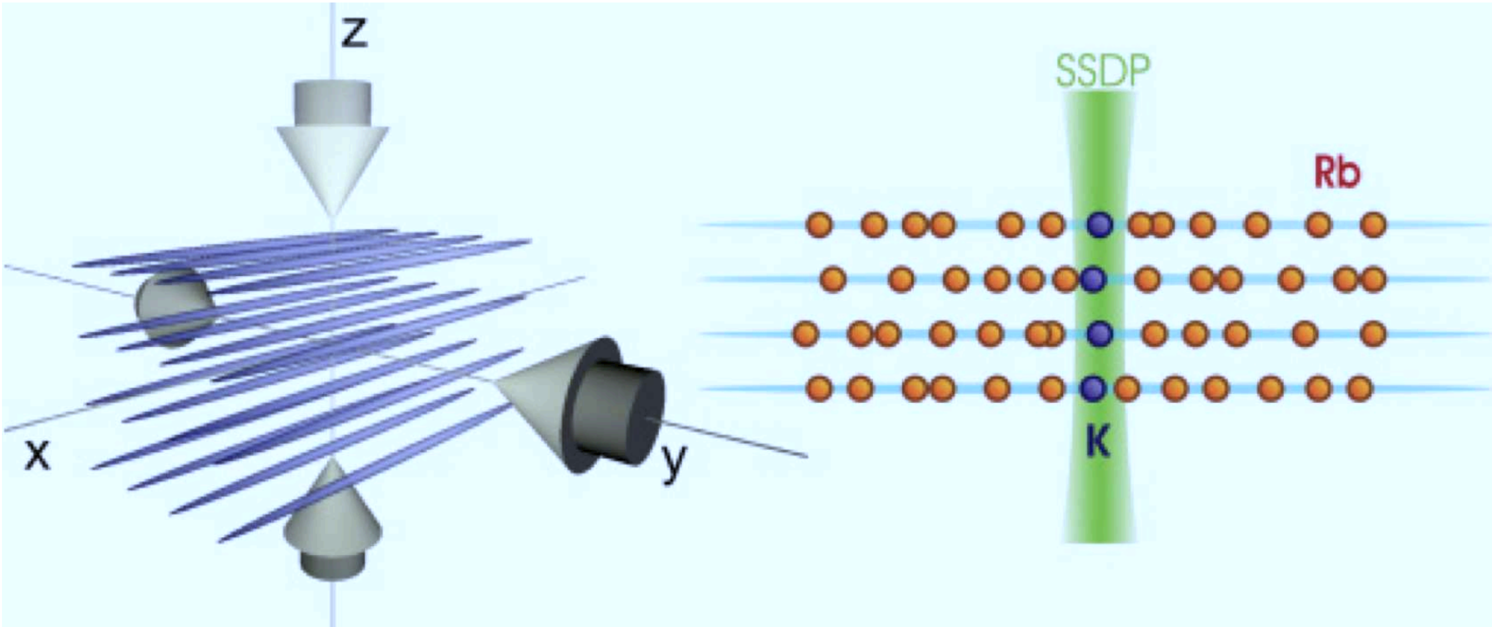
A quantum impurity

in a one dimensional harmonic trap



Catani *et al.* **12**

An impurity

in a one dimensional harmonic trap

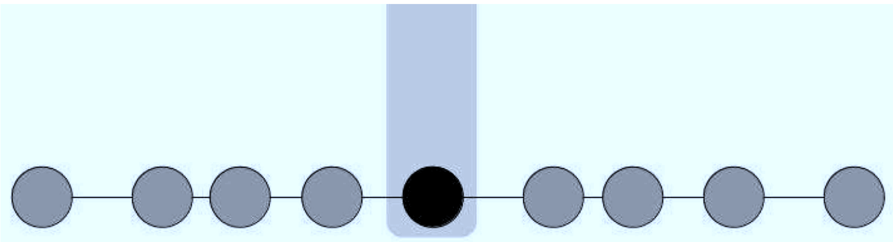
One atom trapped by a laser beam

$$\mathcal{H}^0_{syst} = \frac{1}{2M}\, p^2 + \frac{1}{2} M\omega_0^2\, x^2$$

in contact with a bath made by a different species $\mathcal{H}_{env}$.

Hamiltonian of the coupled system :

$$\mathcal{H}_0 = \mathcal{H}^0_{syst} + \mathcal{H}_{env} + \mathcal{H}_{int}$$



Catani *et al* **12**

All the atoms are within a wide one-dimensional very wide harmonic trap (not shown).

Recall protein problem ; not that different.

Experimental protocol

A quench

Initial equilibrium of the coupled system : $\boxed{\rho(t_0) \propto e^{-\beta \mathcal{H}_0}}$

with
$$\mathcal{H}_0 = \mathcal{H}^0_{syst} + \mathcal{H}_{env} + \mathcal{H}_{int}$$

and
$$\mathcal{H}^0_{syst} = \frac{1}{2M}\, p^2 + \frac{1}{2} M \omega_0^2\, x^2$$

At time $t_0 = 0$ the impurity is released, the laser blade is switched-off and the atom only feels the *wide* confining harmonic potential $\boxed{\omega_0 \to \omega}$ subsequently.

Question : what are the subsequent dynamics of the particle ?

Model the environment

as a Luttinger liquid

Bosons in one dimensional modeled by the density

$$\rho(r) \simeq \rho_0(r) - \frac{1}{\pi}\frac{d\phi(r)}{dr}$$

with the Hamiltonian

$$\mathcal{H}_{env} = \frac{\hbar}{2\pi}\int dr\, \left\{ \frac{uK_L}{\hbar^2}\left[\pi\Pi(r)\right]^2 + \frac{u}{K_L}\left[\frac{d\phi(r)}{dr}\right]^2 \right\}$$

The interaction is

$$\mathcal{H}_{int} = \int dr dr'\, U(|r - r'|)\, \delta(x - r')\, \rho(r)$$

with $\tilde{U}(p) = \hbar v e^{-p/p_c}$ and $p \to p_n = \pi\hbar n/L$

(Quantization of momenta due to the wide harmonic trap ; later $L \to \infty$.)

Path integral formalism

Schwinger-Keldysh generating functional

After a transformation to ladder operators b_p for the bath and defining $Q_p = e^{ipx/\hbar}$ for the impurity, the coupling $\mathcal{H}_{int}$ becomes bilinear with p-dependent coupling constants [depending on $\tilde{U}(p)$].

Real-time path-integral generating functional.

Integration of the bath degrees of freedom (à la Feynman-Vernon) yields :

$$\mathcal{Z}_{red} = \int \mathcal{D}Q_p^+ \mathcal{D}Q_p^- \mathcal{D}Q_p^0 \, e^{\mathcal{S}_{syst}[Q_p^+, Q_p^-, Q_p^0]} \, \Phi[Q_p^+, Q_p^-, Q_p^0]$$

with the influence functional

$$\Phi[Q_p^+, Q_p^-, Q_p^0] = \sum_{p \in \{p_n\}} \Phi_p[Q_p^+, Q_p^-, Q_p^0]$$

Path integral formalism

Schwinger-Keldysh generating functional

Low-energy expansion : $Q_p = e^{ipx/\hbar}$ to quadratic order implies that

Each mode is effectively coupled to a bath ‘harmonic oscillator’.

The effective action has delayed quadratic interactions mediated by

$$\Sigma_B^K(t-t') = \frac{2}{M}\int_0^\infty d\nu\, \frac{S(\nu)}{\nu}\, \cos[\nu(t-t')]$$

(high T limit) with the spectral density

$$S(\nu) = \frac{\pi}{2L}\sum_{p_n}\frac{K_L}{2\pi\hbar^3}\frac{|p_n|^3}{\hbar^2}|\tilde{U}(p_n)|^2\,\delta(\nu - u|p_n|/\hbar)$$

$$\to g\left(\frac{\nu}{\omega_c}\right)^3 e^{-\nu/\omega_c} \qquad \text{for} \qquad L\to\infty\ .$$

$g = K_L v^2\omega_c^3/u^4$ with $\omega_c = up_c/\hbar$ **Super-Ohmic diss.** $\boxed{\alpha = 3}$

Path integral formalism

Schwinger-Keldysh generating functional

The action is quadratic in all remaining variables (that have to do with the position of the impurity).

The generating functional of all expectation values and correlation functions can be computed by the stationary phase method (exact in this case) as done in

Grabert & Ingold's review

with some differences : rôle of initial condition, quench in harmonic trap, spectral density.

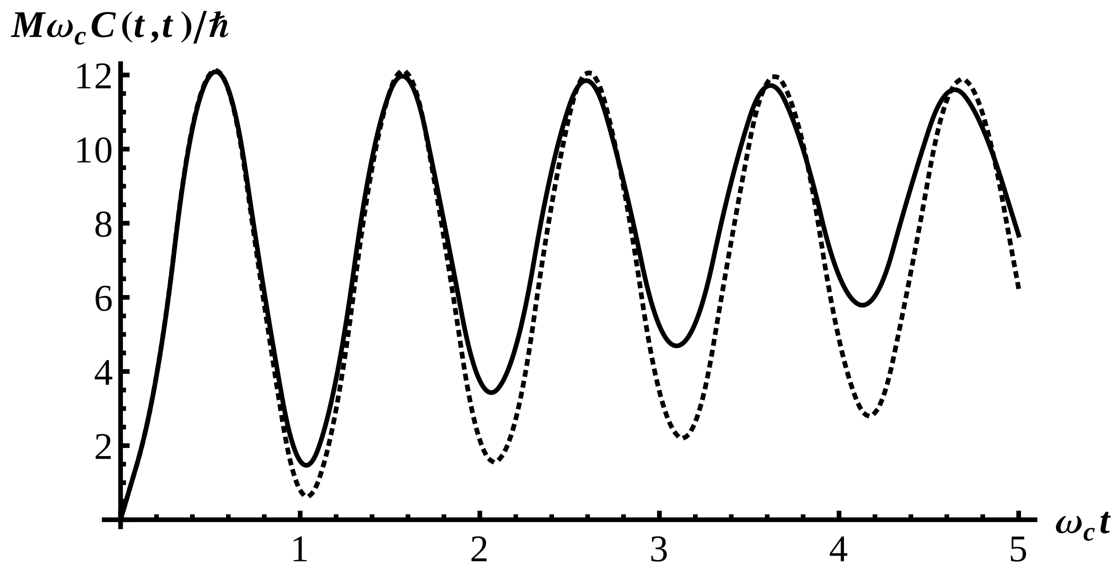
In particular, the equal-times correlation function $C_x(t,t) = \langle x(t)x(t)\rangle = \langle x^2(t)\rangle$.

Equal–time correlation function

Theory

$$C_x(t,t) \equiv \langle x^2(t) \rangle$$

Damped oscillations



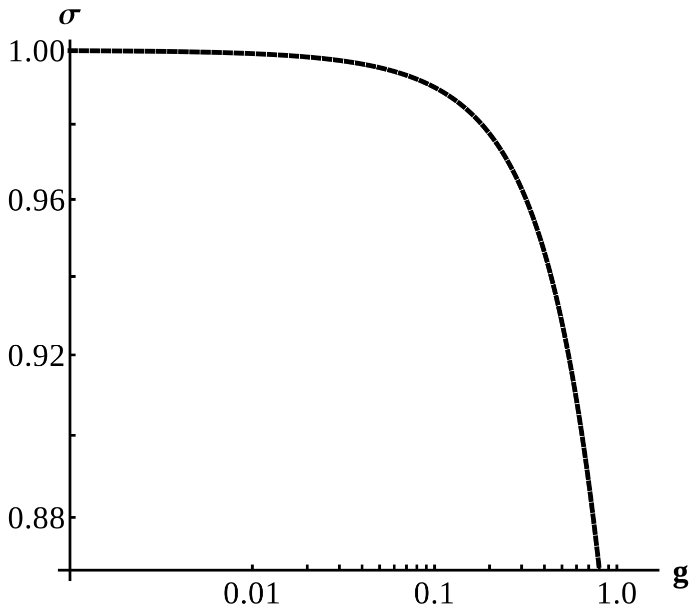
For two values of the coupling to the bath (to be made precise below).

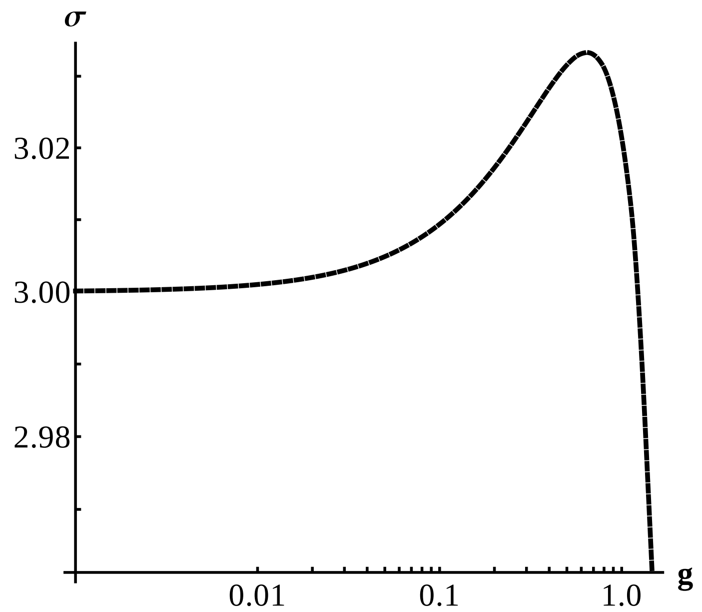
Bonart & LFC 12

Oscillating frequency

Dependence on the coupling to the bath (g) and the trap (ω/ω_c)

σ/ω_c





g

$\omega/\omega_c = 1$

$\omega/\omega_c = 3$

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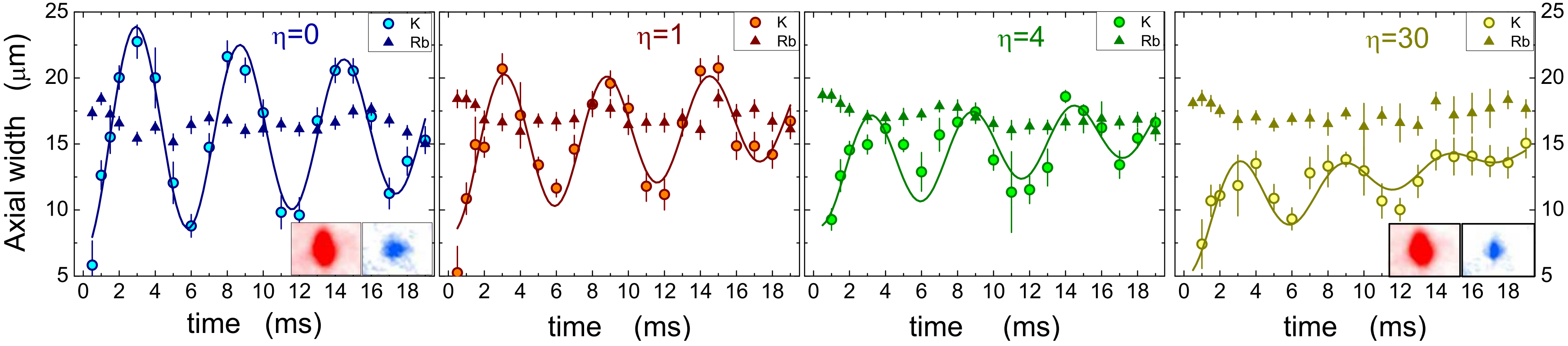
Equal–time correlation function

Experiment

$$C_x(t,t) \equiv \langle x^2(t) \rangle$$

Damped oscillations

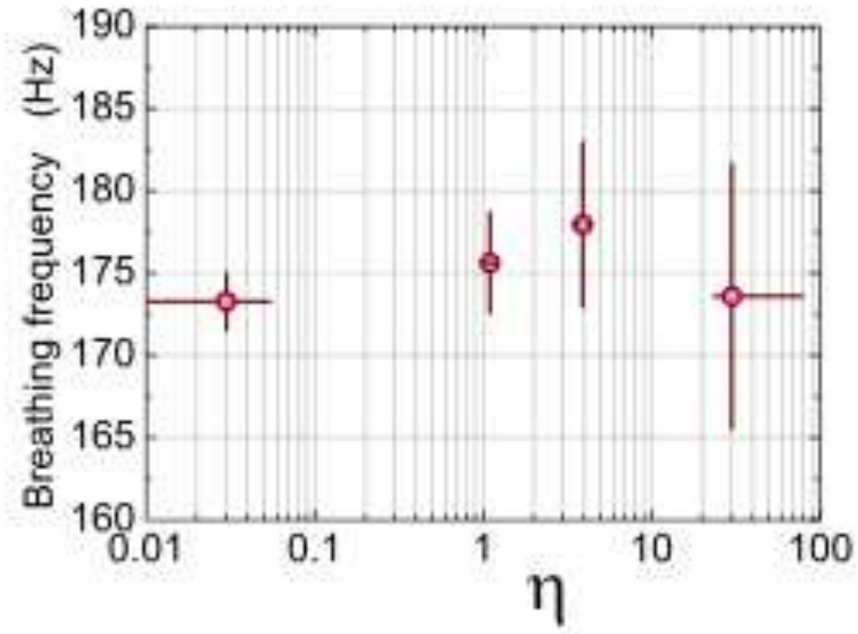


For four values of the coupling to the bath.

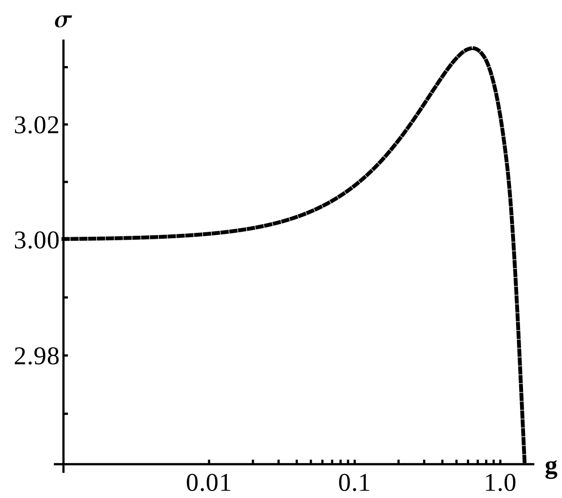
Catani *et al.* **12**

Oscillating frequency

Theory vs experience



σ/ω_c for $\omega/\omega_c = 3$



σ increases with the coupling to the bath for sufficiently narrow (large ω/ω_c) harmonic traps.

The height of the peak depends on ω/ω_c. with ω_c the cut-off of bath spectral function. Order of magnitude similar to the one measured.

Bonart & LFC 12

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

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

with the bath induced kernels

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

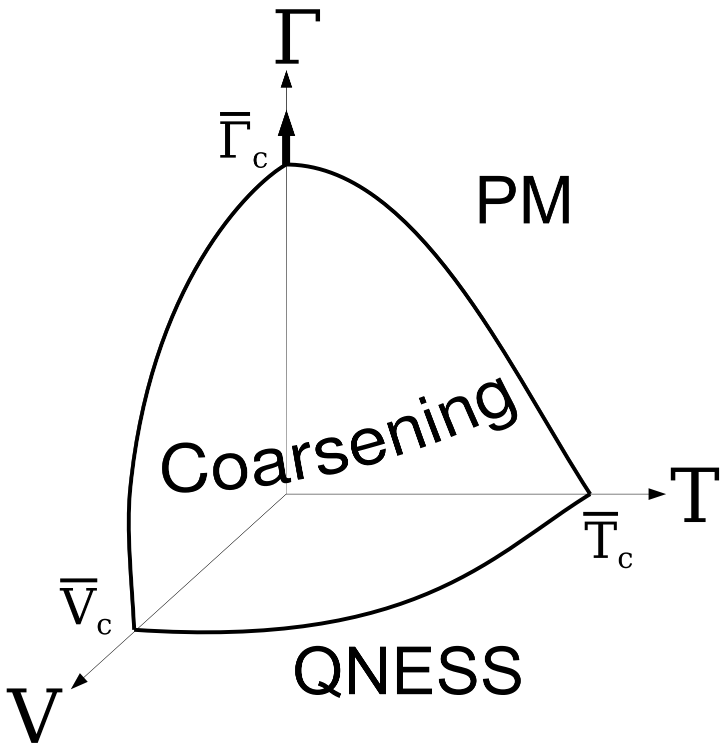
and $G_{rs}(t,t') \equiv -i\langle \mathcal{T} \psi_r(t) \psi_s^\dagger(t') \rangle$

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

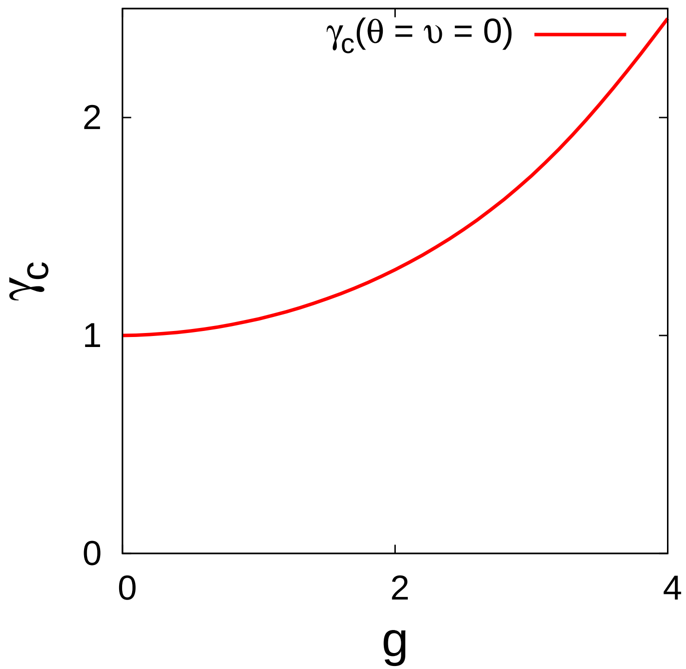
and $\mathcal{T}$ the time-ordering operator on the closed contour.

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

Summary

- **Classical and quantum dissipative dynamics :**

  very similar once in path-integral formalism.

- **Classical systems**

  Single particle : one of many discussions of non-Markovian environments in bio-physics.

  Collective phenomena : just the first (?) non-trivial calculation for the effect on the critical slowing down in second-order phase transitions.

  Focus on the dependence on the kernel tails $\boxed{\alpha}$

  No no-trivial effects produced by the bath strength $\boxed{g}$

  (apart, of course, of dependence of equilibration time).

Summary

- **Quantum systems**

  Quantum Brownian motion and quenches : a rather simple problem with non-trivial consequences of the bath strength $\boxed{g}$

  Many-body systems ; effect on transitions and collective dynamics.

- **Some issues in progress**

  Quantum critical dynamics at second-order phase transitions [*e.g.* in the quantum O(N) model]

  Bonart, LFC & Gambassi

  Phase ordering in a spin chain coupled to semi-infinite spin chains acting as baths.

  Bonart, Foini & LFC