



Università degli Studi di Trieste
Dipartimento di Fisica

Quantum Brownian Motion Reconsidered

Frascati FQT 2015

Matteo Carlesso and Rais Angelo Bassi

September 25, 2015

Open Quantum Systems

What is an Open Quantum System?

The typical systems S we consider can be

- A single spin (fermion)
- A chain made of N spins
- A single particle (boson)
- A molecule made of N bosons

The environment E instead can be

- A classical or quantum external field
- A gas in thermodynamical equilibrium
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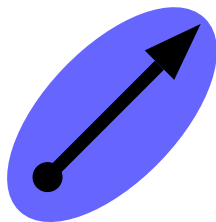
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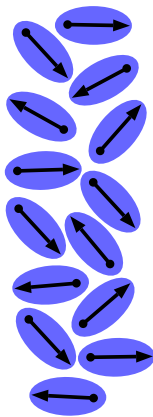
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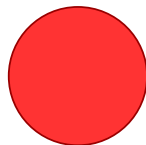


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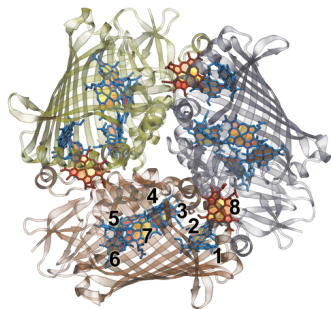
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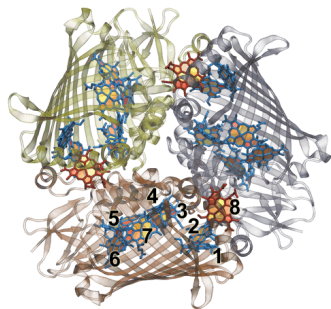
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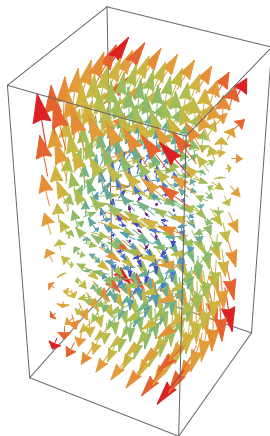
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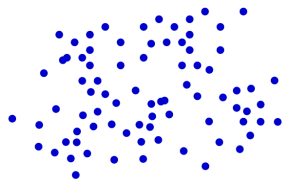


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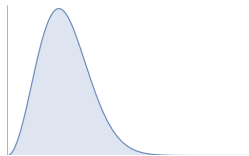
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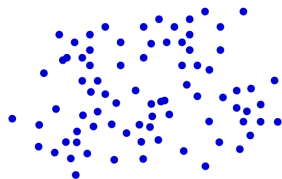


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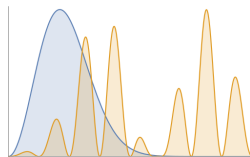
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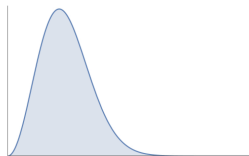
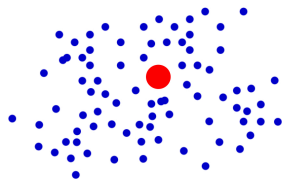
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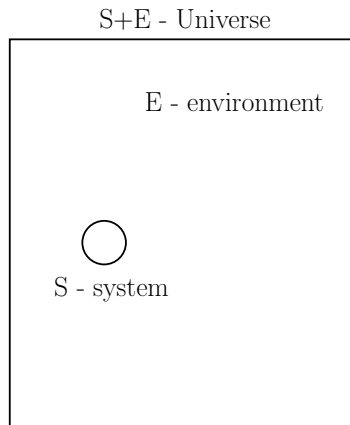
The common way to treat an Open Quantum System S

We consider the system S +
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We average on the degrees of freedom
of the environment

We look on the dynamics
of the system S alone

→ We obtain the reduced dynamics of
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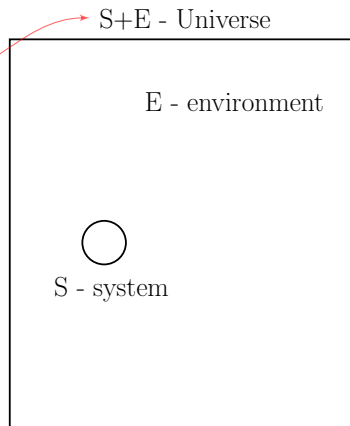
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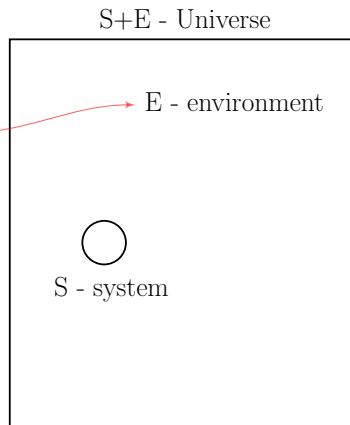
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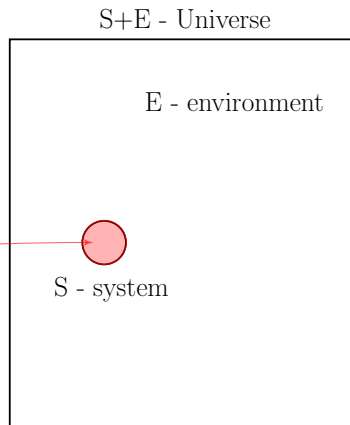
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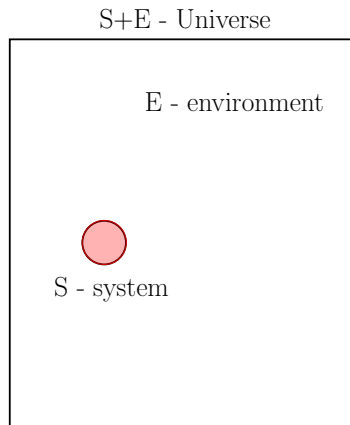
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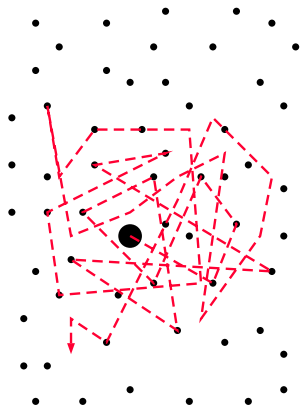
Brownian Motion

The Brownian Motion is considered as the paradigm of an open system in the classical and in the quantum case.

Modeled as a boson immersed in a gas of particles at thermal equilibrium

Discovered by Brown (1828) as the motion of pollen on the water surface

Its random motion is due to the interaction with the water molecules
Einstein (1905) and Langevin (1908)



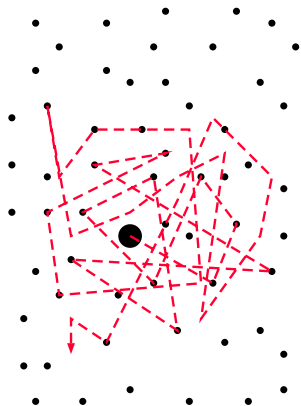
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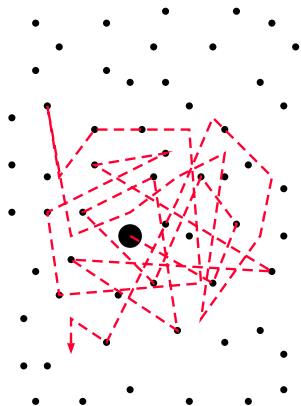
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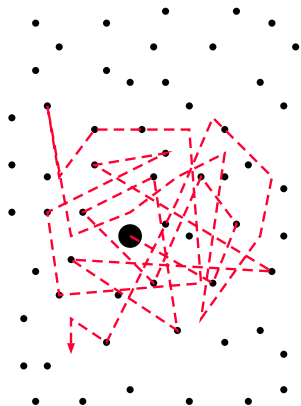
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Classical Brownian Motion

The classical effective description is given by the well known Langevin equation

$$M\ddot{x}(t) + \partial_x V(x) + \eta\dot{x}(t) = F(t)$$

The **acceleration** depends on the **external potential**, **viscous Stokes term** and the **stochastic force** $F(t)$ is governed by

$$\begin{aligned}\langle F(t) \rangle &= 0 \\ \langle F(t)F(s) \rangle &= 2\eta K_B T \delta(t-s)\end{aligned}$$

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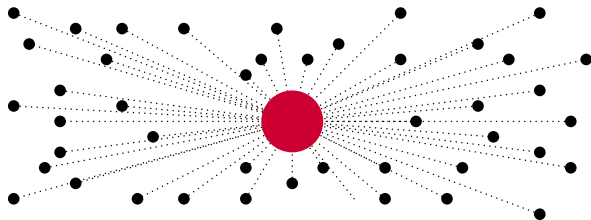
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Classical Brownian Motion

To obtain the Langevin equation from an Hamiltonian approach we can consider the Ullersma Hamiltonian (1966)

$$H \equiv \frac{p^2}{2M} + V(x) + \sum_k \frac{P_k^2}{2m} + \sum_k \frac{1}{2} m \omega_k^2 \left(R_k - \frac{C_k}{m \omega_k^2} x \right)^2$$

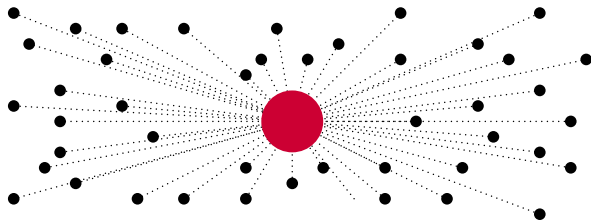


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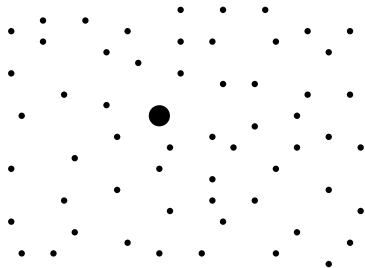
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$$\hat{H} \equiv \left(\frac{\hat{p}^2}{2M} + \frac{M}{2} \omega_R^2 \hat{x}^2 \right) + \hat{x} \sum_k C_k \hat{R}_k + \left(\sum_k \frac{\hat{P}_k^2}{2m} + \frac{m}{2} \omega_k^2 \hat{R}_k^2 \right)$$

System S - Brownian particle

Particles of the environment

Interaction between system S
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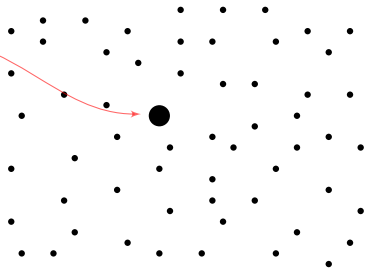
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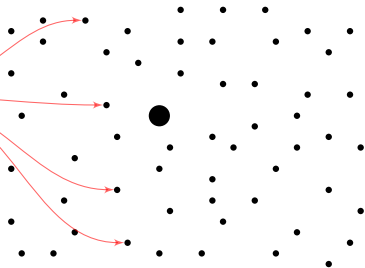
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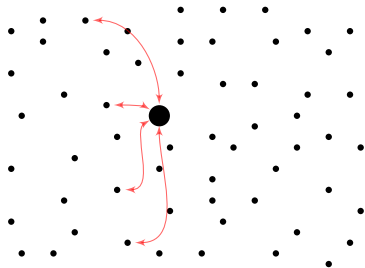
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Model for the interaction

The interaction Hamiltonian contains the coupling constants C_k

$$\hat{H}_I \equiv \hat{x} \sum_k C_k \hat{R}_k$$

In order to characterize the interaction we introduce the spectral density $J(\omega)$

$$J(\omega) \equiv \sum_k \frac{C_k^2}{2m\omega_k} \delta(\omega - \omega_k)$$

$J(\omega)$ describes how strong is the coupling constant C_k respect to the correspondent environment frequency ω_k

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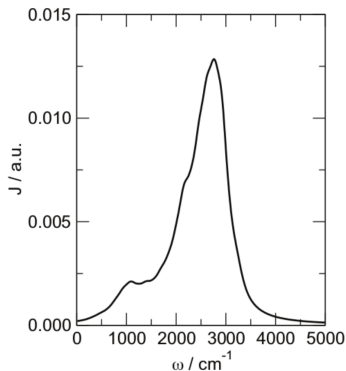
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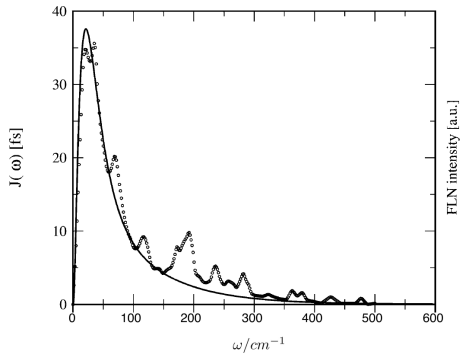
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Martinazzo, Hughes, Martelli, Burghardt
J. Chem. Phys., 377, 2010



Adolphs and Renger
Biophys. J., 91(8), 2006

Caldeira-Leggett model

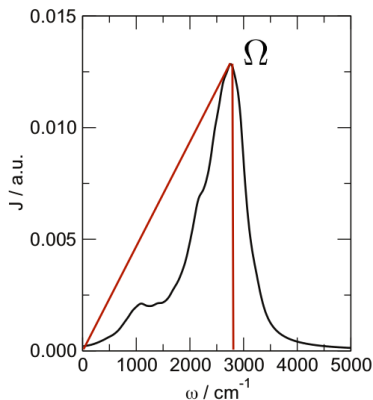
Caldeira and Leggett (1983) choose a pure ohmic spectral density

$$J(\omega) = \frac{2M\gamma}{\pi} \omega \Theta(\Omega - \omega)$$

They obtain the Quantum Langevin equation in limit of $\Omega \rightarrow +\infty$

$$\ddot{\hat{x}}(t) + \omega_R^2 \hat{x}(t) + 2\gamma \dot{\hat{x}}(t) = \frac{\hat{B}(t)}{M}$$

where $\hat{B}(t)$ is described by $\langle \hat{B}(t) \rangle$ and $\langle \hat{B}(t) \hat{B}(s) \rangle$



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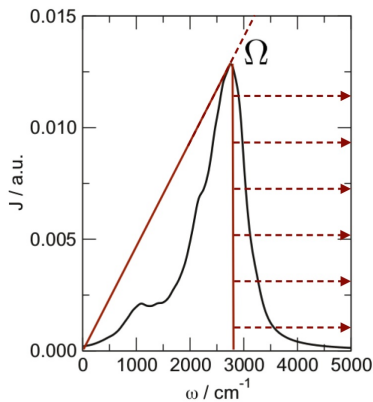
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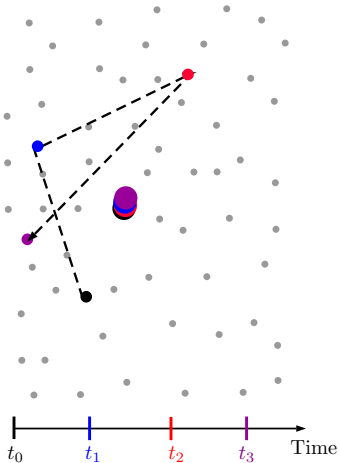
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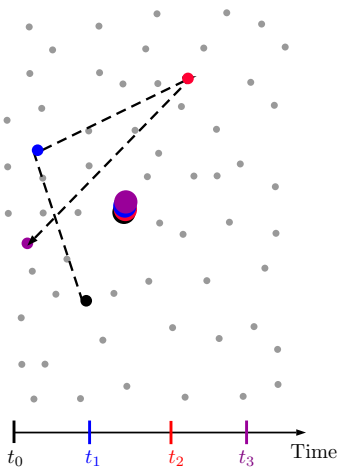
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Caldeira-Leggett master equation

For this spectral density ($\Omega \rightarrow +\infty$) we have

$$\langle \hat{B}(t) \rangle = 0$$

$$\langle \hat{B}(t) \hat{B}(s) \rangle \text{ diverges!}$$

The high temperature limit $\beta \rightarrow 0$ removes the divergence and it results the Caldeira-Leggett master equation (1983)

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}_S(t)] - \frac{i\gamma}{\hbar} [\hat{x}, \{\hat{p}, \hat{\rho}_S(t)\}] - \frac{2M\gamma}{\hbar^2\beta} [\hat{x}, [\hat{x}, \hat{\rho}_S(t)]]$$

However this master equation is NOT POSITIVE.

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Hu, Paz and Zhang (1992) provide instead a well defined master equation for any physical spectral density $J(\omega)$.

The Hu-Paz-Zhang master equation is

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It is a time dependent, exact, analytic and general solution.

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It is a time dependent, exact, analytic and general solution.

Heisenberg picture

$$\frac{d}{dt} \langle \hat{O}_S \rangle_t = \begin{cases} \text{Tr} \left[\frac{\hat{\rho}_S(t)}{dt} \hat{O}_S \right] & \text{Schrödinger picture} \\ \text{Tr} \left[\hat{\rho}_S \frac{d\hat{O}_S(t)}{dt} \right] & \text{Heisenberg picture} \end{cases}$$

Heisenberg picture

The equation we look for is the adjoint master equation

$$\frac{d}{dt}\hat{O}_S(t) = \mathbb{L}_t \left[\hat{O}_S(t) \right]$$

where the operator $\hat{O}_S(t)$ is obtained as

$$\hat{O}_S(t) = \text{Tr}^{(B)} \left[\hat{\rho}_B \left(\hat{U}_t^\dagger \hat{O}_S \hat{U}_t \right) \right] = \Phi_t \left[\hat{O}_S \right]$$

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Heisenberg picture

The von Neumann representation of the operators

$$\hat{O}_S = \int d\lambda d\mu \mathcal{O}(\lambda, \mu) \hat{\chi}_S(\lambda, \mu)$$

We describe the operator \hat{O}_S in terms of a kernel $\mathcal{O}(\lambda, \mu)$ and the structure of the algebra $\hat{\chi}_S(\lambda, \mu) = \exp(i\lambda\hat{x} + i\mu\hat{p})$

The dynamical map Φ_t acts only on $\hat{\chi}_S$

$$\Phi_t [\hat{O}_S] = \int d\lambda d\mu \mathcal{O}(\lambda, \mu) \Phi_t [\hat{\chi}_S(\lambda, \mu)]$$

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Heisenberg picture

We consider the evolution of $\hat{\chi}_S(t)$ obtained as

$$\hat{\chi}_S(t) = \text{Tr}^{(B)} \left[\hat{\rho}_B \left(\hat{\mathcal{U}}_t^\dagger \hat{\chi}_S \hat{\mathcal{U}}_t \right) \right]$$

The time derivative is

$$\begin{aligned} \frac{d\hat{\chi}_S(t)}{dt} = & \frac{i}{\hbar} \left[\hat{H}_{eff}(t), \hat{\chi}_S(t) \right] - \frac{1}{2} K_{11}(t) [[\hat{\chi}_S(t), \hat{x}], \hat{x}] + \\ & - iK_{12}^{\mathbf{I}}(t) \{[\hat{\chi}_S(t), \hat{p}], \hat{x}\} - K_{12}^{\mathbf{R}}(t) [[\hat{\chi}_S(t), \hat{x}], \hat{p}] \end{aligned}$$

Therefore we have the

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Heisenberg picture

The evolution of the characteristic operator $\hat{\chi}_S(t)$ is described by

$$\frac{d\hat{\chi}_S(t)}{dt} = \mathbb{L}_t [\hat{\chi}_S(t)]$$

\mathbb{L}_t is a linear functional of \hat{x} , \hat{p} e $\hat{\chi}_S(t)$, **independent** from λ e μ

Therefore by linearity we obtain the adjoint master equation

$$\frac{d\hat{O}_S(t)}{dt} = \int d\lambda d\mu \mathcal{O}(\lambda, \mu) \mathbb{L}_t [\hat{\chi}_S(t)] = \mathbb{L}_t [\hat{O}_S(t)]$$

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Heisenberg picture

From the adjoint master equation we want to obtain the master equation for the states:

$$\frac{d\hat{O}_S(t)}{dt} = \mathbb{L}_t [\hat{O}_S(t)] \rightarrow \frac{d\hat{\rho}_S(t)}{dt} = \tilde{\mathbb{L}}_t^* [\hat{\rho}_S(t)]$$

We were able to obtain explicitly the form of $\tilde{\mathbb{L}}_t$ directly from

$$\tilde{\mathbb{L}}_t = \Phi_t^{-1} \circ \mathbb{L}_t \circ \Phi_t$$

Results

Our master equation is equivalent to the one of Hu, Paz and Zhang (1992)

In weak coupling regime (analytic verification)
and beyond (numerical verification)

We provide a simpler form of the coefficients of master equation.

For some examples we have an explicit form of the master equation.

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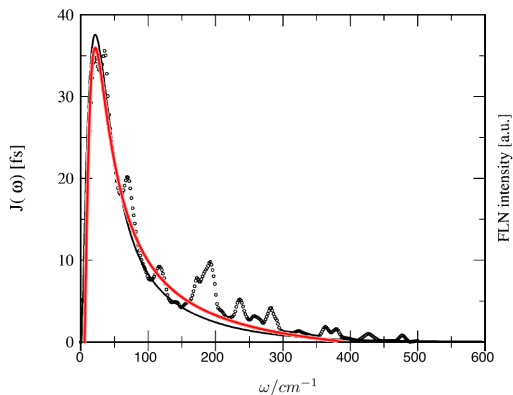
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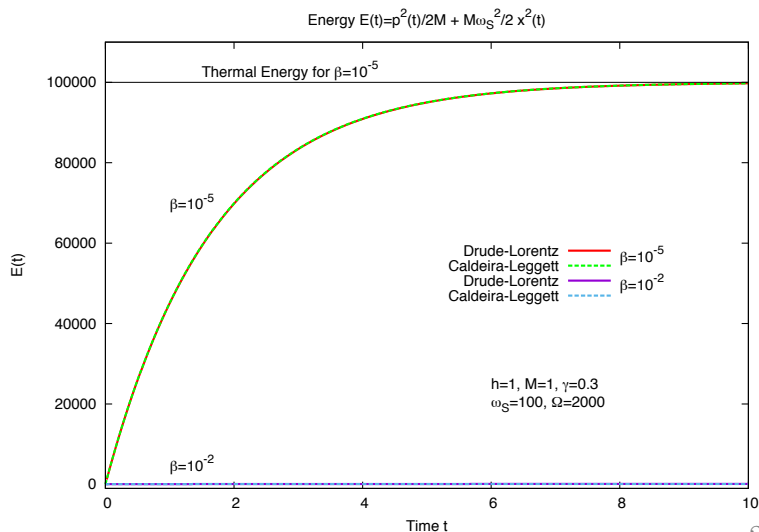
Example

For the Drude-Lorentz spectral density

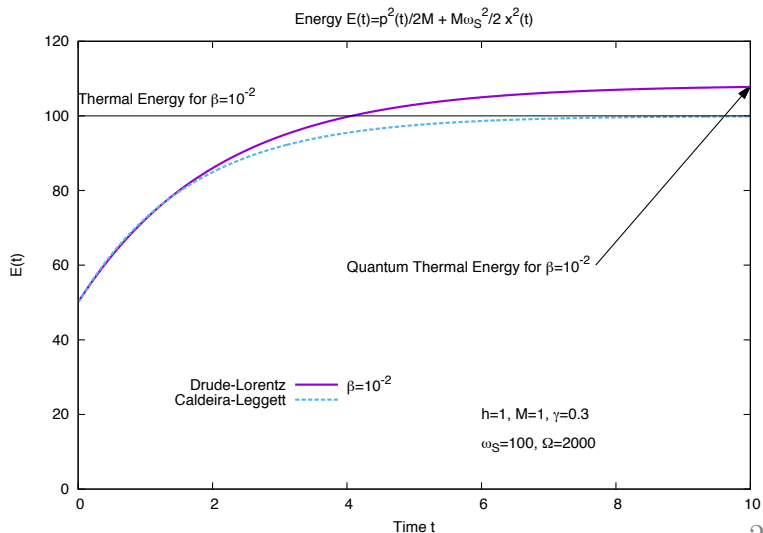
$$J(\omega) = \frac{2M\gamma}{\pi} \omega \frac{\Omega^2}{\omega^2 + \Omega^2}$$



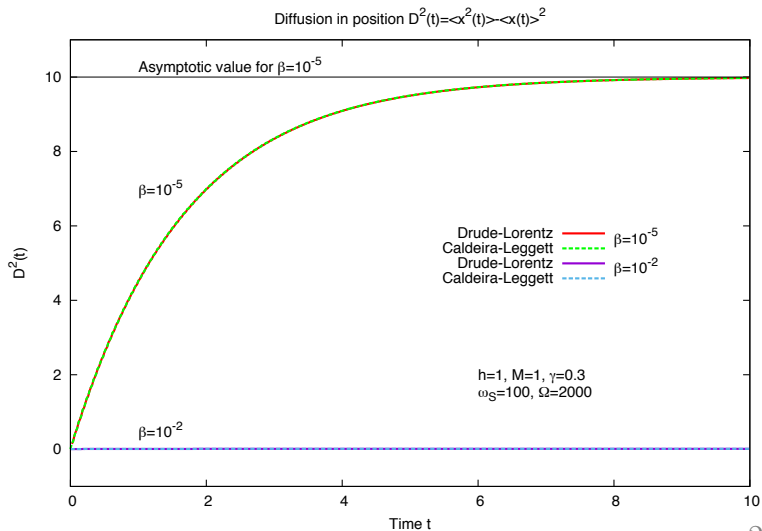
Energy of the system



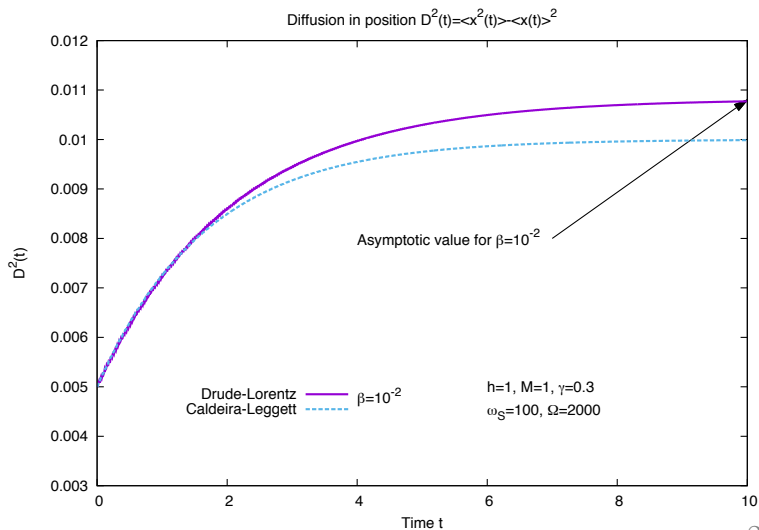
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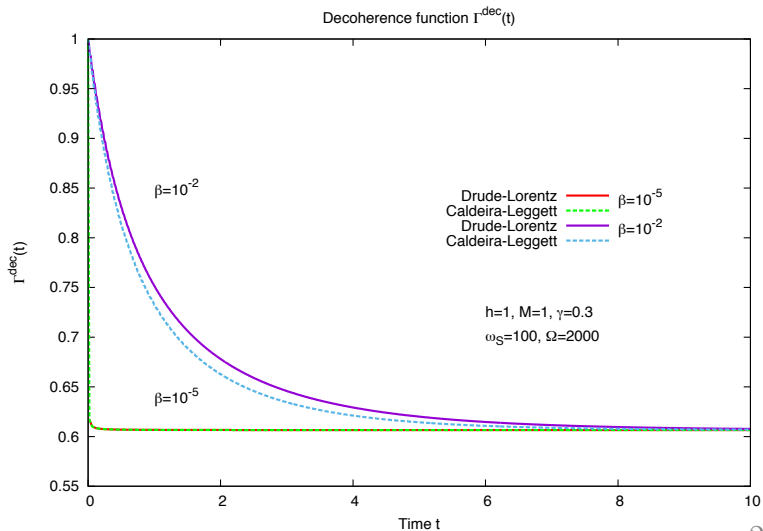
Diffusion of the system



Diffusion of the system



Decoherence function



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Quantum Brownian Motion Reconsidered

Open Quantum System

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Hu-Paz-Zhang master equation

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