Toward an effective description of non-Markovian dynamics

Luca Ferialdi
Mathematisches Institut
LMU München

Outline

- Open systems and non-Markovian dynamics
- Indipendent oscillators model
- Chain representation & effective description
- Results & future work

Open quantum systems

- Interaction between the system and the environment

$$\rho = \rho_{\mathrm{S}} \otimes \rho_{\mathrm{E}} \qquad\qquad H = H_{\mathrm{S}} + H_{\mathrm{E}} + H_{\mathrm{INT}}$$

- General evolution has a complicated form

$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = -i\,\mathrm{tr}_{\mathrm{E}}[H, \rho(t)] \longrightarrow$$ it is necessary to introduce some approximation

Markovian vs non-Markovian dynamics

- Markovian dynamics: the evolution has no memory terms

$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = -i[H, \rho_{\mathrm{S}}(t)] + \mathcal{D}[\rho_{\mathrm{S}}(t)] \qquad \mathcal{D}[\rho_{\mathrm{S}}(t)] = \sum_k \gamma_k \left(A_k \rho A_k^\dagger - \frac{1}{2}\left\{ A_k^\dagger A_k, \rho \right\} \right)$$

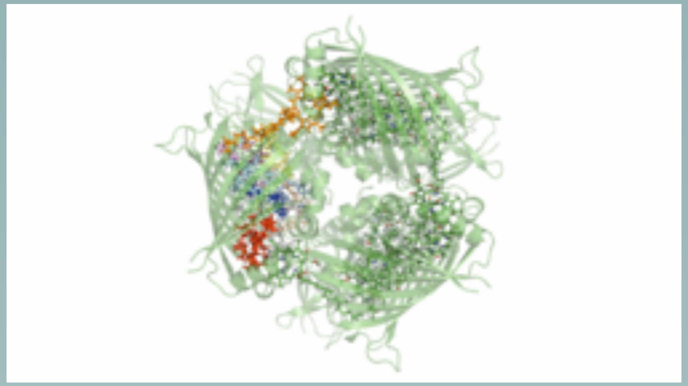
- Physics: the bath timescale is much faster than the system

- Non-Markovian dynamics $\longrightarrow$ memory terms

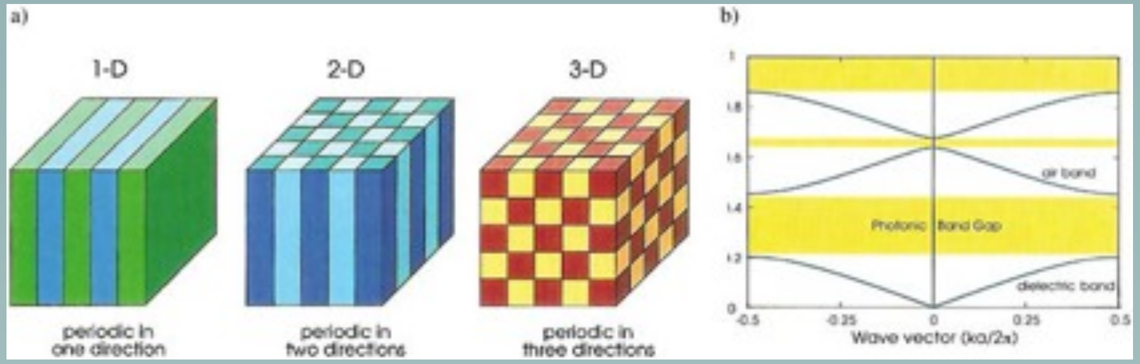
$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = \int_{t_0}^{t} ds K(t,s)\rho_{\mathrm{S}}(s)$$

Why non-Markovian dynamics?

ultrafast chemical reactions (OLEDs, FMO)



solid state
(PBG materials)



quantum optics

statistical mechanics

collapse models

Non-Markovian dynamics

- "Non-Markovian" is all what goes beyond the Markov approximation, no characterization is implied

↓

one needs to introduce a characterization, e.g. a particular model

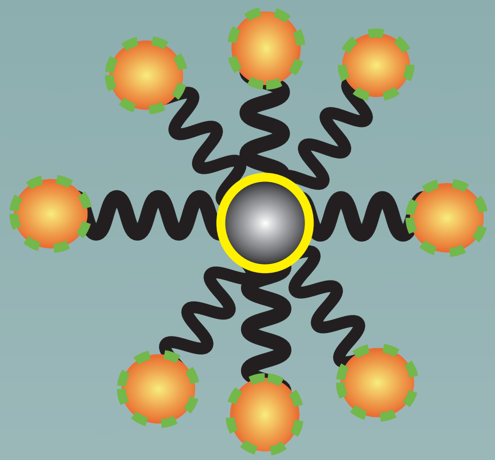
- All models proposed so far are phenomenological

↓

lack of description emerging from first principles

The independent oscillators model

- System bilinearly coupled to N independent harmonic oscillators



- Hamiltonian

$$H = \frac{p^2}{2M} + V(x) + x \sum_{k=1}^{N} c_k q_k + \sum_{k=1}^{N} \frac{1}{2}\left(p_k^2 + \omega_k^2 q_k^2\right)$$

- Environmental coupling is determined by the spectral density

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{c_k^2}{\omega_k} \delta(\omega - \omega_k)$$

The independent oscillators model

- Generalized Langevin equation (GLE)

$$M\ddot{x}(t) + M\int_0^t ds\,\eta(t-s)\dot{x}(s) + V_x(t) = f(t)$$

where $\eta(t-s),\ f(t)$ are functions of $J(\omega)\,,\ \{q_k(0), \dot{q}_k(0)\}$

- Well known model:
  - → Quantum Brownian Motion
  - → Fluctuation dissipation relation
  - → Suitable to understand thermal and stochastic effects

What do we learn about NM?

- We do learn:
  - → new non-Markovian (or memory) effects
  - → how they affect the system's dynamics

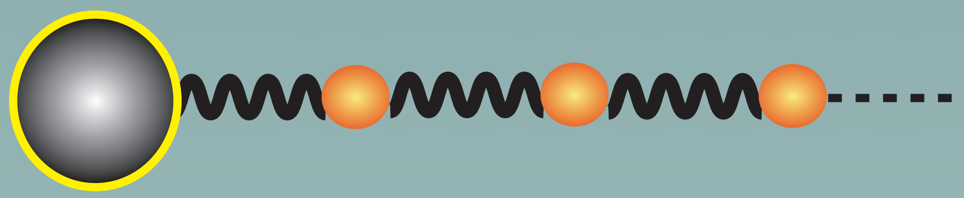
- We do not learn: how they arise from the microscopic motion

↓

aim of the project is to understand how non-Markovian effects emerge from microscopic motion

The chain model

- System coupled to a chain of N harmonic oscillators



- Hamiltonian

$$H = \frac{p^2}{2M} + V(x) + DxX_1 + \sum_{k=2}^{N} D_{k-1}X_{k-1}X_k + \sum_{k=1}^{N} \frac{1}{2}\left(P_k^2 + \Omega_k^2 X_k^2\right)$$

- It gives a more physical idea of propagation

↓

more suitable to study short time effects

The chain representation

- Idea: chain representation of the independent oscillators bath

Independent

$$\begin{pmatrix} \ddot{q}_1(t) \\ \ddot{q}_2(t) \\ \ddot{q}_3(t) \\ \vdots \end{pmatrix} = - \begin{pmatrix} \omega_1^2 & 0 & 0 & \dots \\ 0 & \omega_2^2 & 0 & \dots \\ 0 & 0 & \omega_3^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \end{pmatrix}$$

Chain

$$\begin{pmatrix} \ddot{X}_1(t) \\ \ddot{X}_2(t) \\ \ddot{X}_3(t) \\ \vdots \end{pmatrix} = - \begin{pmatrix} \Omega_1^2 & -D_1 & 0 & \dots \\ -D_1 & \Omega_2^2 & -D_2 & \dots \\ 0 & -D_2 & \Omega_3^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} X_1(t) \\ X_2(t) \\ X_3(t) \\ \vdots \end{pmatrix}$$

- Find orthogonal Q such that

$$Q \begin{pmatrix} \omega_1^2 & 0 & 0 & \dots \\ 0 & \omega_2^2 & 0 & \dots \\ 0 & 0 & \omega_3^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} Q^T = \begin{pmatrix} \Omega_1^2 & -D_1 & 0 & \dots \\ -D_1 & \Omega_2^2 & -D_2 & \dots \\ 0 & -D_2 & \Omega_3^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \rightarrow$$

inverse eigenvalue problem

- Collective motion:

$$X_k = \sum_j Q_{kj} q_j$$

The chain representation

- Iteratively substitute equations of motion

- General evolution for the chain model

$$x(t) = F_N(t) + \frac{D^2}{\mu_1\mu_2(\mu_2^2 - \mu_1^2)} \int_0^t (\mu_2 \sin[\mu_1(t-s)] - \mu_1 \sin[\mu_2(t-s)]) F_N(s) ds$$

$$F_N(t) = \tilde{f}_N(t) + \sum_{i=2}^{N} \left(\prod_{l=0}^{i} \frac{D_l}{\Omega_l} \right) \frac{D_{i-1}}{D_i} \int_0^t K_i(t-s) X_{i-1}(s) ds$$

$x(0),\ \dot{x}(0)$ (deterministic) — $\{X_i(0),\ \dot{X}_i(0)\}$ (stochastic)

- Suitable to understand the propagation of NM effects

Effective description

- Short times → truncated chain

- First proposed by chemical physicists
  - ↗ looking for faster simulations
  - → complicated transformation through hierarchical baths
  - ↘ fitting parameters with observed dynamics

- Approximation for the kernel of the GLE:

$$\eta(t) \simeq \eta^{(n)}(t) + o(t^{4n})$$

Where do we stand?

- Final goal: Prove that $$\forall\, n, \exists\, T : \tilde{x}^{(\mathrm{n})}_{\mathrm{TC}}(t) \simeq x_{\mathrm{IO}}(t), \forall\, t \leq T$$

- Good hint ➞ the kerneks $K_i(t-s)$ have a nested structure

- Future perspective: application of the chain model to condensed matter (NRG techniques)