Collective motion and chain representation of non-Markovian dynamics

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Outline

- Opens systems and non-Markovian dynamics
- Indipendent oscillators model
- Collective motion and chain representation
- Future work

Open quantum systems

- Interaction between the system and the environment

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

- General evoltion 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 ⟶ 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?

- Experimental: → ultrafast chemical reactions (OLEDs, FMO) → solid state (PBG materials) → quantum optics

- Theoretical: → inflation models / semiclassical gravity → statistical mechanics → collapse models

Non-Markovian dynamics

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

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

- All models proposed so far are phenomenological

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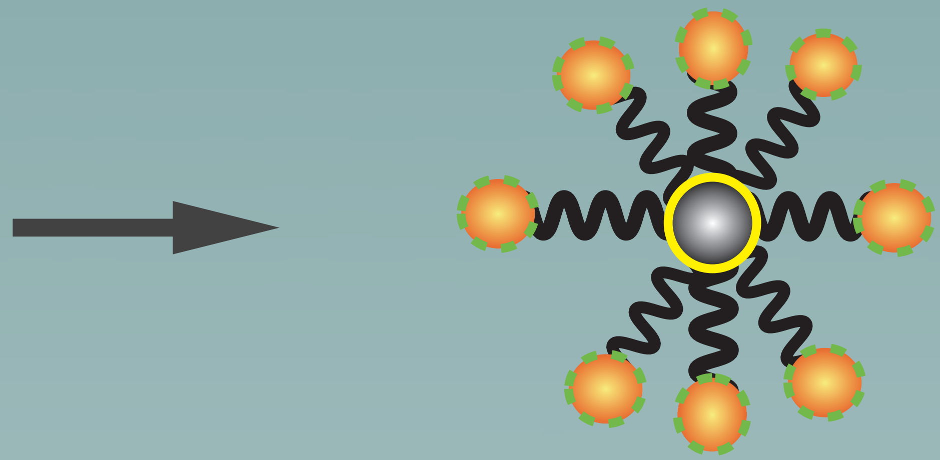
lack of description emerging from first principles

The independent oscillators model

- System bilinearly coupled to N **independent** harmonic oscillators



- Hamiltonian

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

- 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)

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

where $K(t-s)$, $f(t)$ are functions of $J(\omega)$, $\{x_k(0), \dot{x}_k(0)\}$

- Well known model: → Quantum Brownian Motion → Master equation → Fluctuation dissipation relation → ...

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

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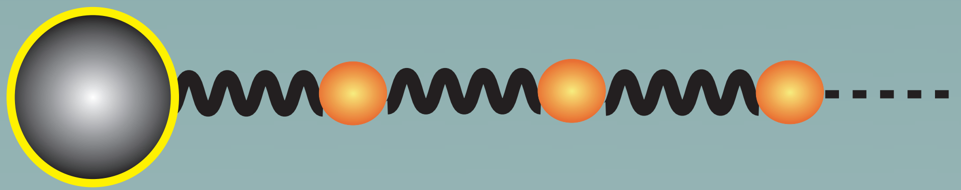
aim of the project is to understand how non-Markovian effects emerge from microscopic motion

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

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more suitable to study short time effects

The chain representation

- Idea: chain representation of the independent oscillators bath

Independent

$$\begin{pmatrix} \ddot{x}_1(t) \\ \ddot{x}_2(t) \\ \ddot{x}_3(t) \\ \vdots \end{pmatrix} = -\begin{pmatrix} \omega_1^2 & 0 & 0 & \dots \\ 0 & \omega_2^2 & 0 & \dots \\ 0 & 0 & \omega_3^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ \vdots \end{pmatrix}$$

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

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

inverse eigenvalue problem

- Collective motion:

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

The chain representation

- 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:

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

Where do we stand?

- The inverse eigenvalue problem has unique solution

- General evolution for the chain model has a complicated form

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no more a GLE but nested integrals

- Final goal:
Prove that

$$\forall\, n, \exists\, T : \tilde{x}^{(\mathrm{n})}_{\mathrm{TC}}(t) = x_{\mathrm{IO}}(t), \forall\, t \leq T$$