Non-Markovian Gaussian open system dynamics

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Outline

- Open quantum systems: Markovian vs non-Markovian
- Gaussian non-Markovian map
- Gaussian non-Markovian master equation
- Gaussian non-Markovian stochastic unraveling

Open quantum systems

- Interaction between the system and the environment

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_B(0) \qquad \hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I$$

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- Non-Markovian dynamics → solid state (PBG materials) → ultrafast chemical reactions (OLEDs, FMO) → quantum optics

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Hermitian system operators

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- Linear Heisenberg equations of motion for $\hat{A}^j(t)$

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$$= \mathrm{Tr}_B \left[T \exp \left\{ -i \int_0^t d\tau \left(\hat{A}^j_{\tau L} \hat{\phi}_{jL}(\tau) - \hat{A}^j_{\tau R} \hat{\phi}_{jR}(\tau) \right) \right\} \hat{\rho}_S(0) \otimes \hat{\rho}_B(0) \right]$$

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The general Gaussian non-Markovian map reads

$$\mathcal{M}_t = T \exp \left\{ \int_0^t d\tau \int_0^t ds D_{jk}(\tau, s) \left(\hat{A}^k_L(s) \hat{A}^j_R(\tau) - \theta_{\tau s} \hat{A}^j_L(\tau) \hat{A}^k_L(s) - \theta_{s\tau} \hat{A}^k_R(s) \hat{A}^j_R(\tau) \right) \right\}$$

L. Diosi, L. Ferialdi, PRL 113, 200403 (2014).

Gaussian non-Markovian map

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Formal expression ⟶ derive master equation

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$$\Big\downarrow \frac{d}{dt}$$

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Derivation of the master equation

$$\dot{\hat{\rho}}_t = \mathcal{L}_t \hat{\rho}_t \longrightarrow \dot{\mathcal{M}}_t \hat{\rho}_0 = \mathcal{L}_t \circ \mathcal{M}_t \hat{\rho}_0$$

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1. Expand $\mathcal{M}_t$ in Dyson series $\mathcal{M}_t = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} M_t^n$

$$M_t^n = T\left[\prod_{i=1}^{n} \int_0^t dt_i \left[\hat{A}_L^j(t_i) - \hat{A}_R^j(t_i)\right] \int_0^{t_i} ds_i \left[D_{jk}(t_i, s_i)\hat{A}_L^k(s_i) - D_{jk}^*(t_i, s_i)\hat{A}_R^k(s_i)\right]\right]$$

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2. Expand $\dot{\mathcal{M}}_t$ in Dyson series

$$\dot{M}_t^n = n\left[\hat{A}_L^j(t) - \hat{A}_R^j(t)\right] T\left[\int_0^t ds_1 \left[D_{jk}(t, s_1)\hat{A}_L^k(s_1) - D_{jk}^*(t, s_1)\hat{A}_R^k(s_1)\right] \prod_{i=2}^{n} \dots\right]$$

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odd T-product

Derivation of the master equation

3. Exploit Wick's theorem

$$T\left[\left(\int_0^t ds_1 D_{jk}(t,s_1)\hat{A}_L^j(s_1) - D_{jk}^*(t,s_1)\hat{A}_R^j(s_1)\right)\prod_{i=2}^n \ldots\right] =$$

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$$+ \text{ all contractions...}$$

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Linear Heisenberg equations are fundamental to have Wick's contractions that are c-functions

Linear Heisenberg equations

Bosonic system ⟶ Quadratic Hamiltonian

$$\hat{A}^j(s) = \mathcal{C}^j_k(s-t)\hat{A}^k(t) + \tilde{\mathcal{C}}^j_k(s-t)\dot{\hat{A}}^k(t)$$

Wick's contraction: $\overbrace{\hat{A}^k(s)\hat{A}^j(t)} = \left[\hat{A}^j(t), \hat{A}^k(s)\right]\theta(t-s)$

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$$+(n-1)T\left[\left(\int_0^t ds_1 D_{jk(2)}(t,s_1)\hat{A}_L^k(s_1) - D_{jk(2)}^*(t,s_1)\hat{A}_R^k(s_1)\right)\prod_{i=3}^n \ldots\right],$$

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4. Iterate Wick's theorem

Non-Markovian master equation

$$\dot{\hat{\rho}}_t = -\left(\hat{A}^i_L(t) - \hat{A}^i_R(t)\right)\left[\int_0^t ds \mathbb{D}_{ij}(t,s)\hat{A}^j_L(s) - \mathbb{D}^*_{ij}(t,s)\hat{A}^j_R(s)\right]\hat{\rho}_t$$

$$\mathbb{D}_{ij}(t,s) = \sum_{n=1}^{\infty}(-1)^{n-1}D_{ij(n)}(t,s)$$

→ Bath correlation function

→ Wick's contractions

↓ Recursive definition

Master equation for bosonic systems

We exploit the solution of Heisenberg equations:

$$\hat{A}^j(s) = \mathcal{C}^j_k(s-t)\hat{A}^k(t) + \tilde{\mathcal{C}}^j_k(s-t)\dot{\hat{A}}^k(t)$$

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$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H},\hat{\rho}\right] + \Gamma_{jk}(t)\left[\hat{A}^j,\left[\hat{A}^k,\hat{\rho}\right]\right] + \Theta_{jk}(t)\left[\hat{A}^j,\left[\dot{\hat{A}}^k,\hat{\rho}\right]\right]$$

$$+i\Xi_{jk}(t)\left[\hat{A}^j,\left\{\hat{A}^k,\hat{\rho}\right\}\right] + i\Upsilon_{jk}(t)\left[\hat{A}^j,\left\{\dot{\hat{A}}^k,\hat{\rho}\right\}\right]$$

$$\Gamma_{jk}(t) = -\int_0^t ds\,\mathbb{D}^{Re}_{jl}(t,s)\mathcal{C}^l_k(t-s)$$

L. Ferialdi, PRL 116, 120402 (2016).

Hu-Paz-Zhang Master Equation

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$$\downarrow$$

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Stochastic unraveling

A stochastic Schroedinger equation with solution $|\psi_t\rangle$ is the "stochastic unraveling" of $\mathcal{M}_t$ if

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Interaction with a complex stochastic processes: $H_I(t) = \hat{A}^j(t)\phi_j(t)$

Gaussian processes: $D_{jk}(\tau, s) = \mathbb{E}\left[\phi_j^*(\tau)\phi_k(s)\right]$ $S_{jk}(\tau, s) = \mathbb{E}\left[\phi_j(\tau)\phi_k(s)\right]$

Stochastic unraveling

Most general Gaussian, non-Markovian stochastic unraveling

$$\frac{d|\psi_t\rangle}{dt} = -i\hat{A}^j(t)\left(\phi_j(t) + \int_0^t ds[D_{jk}(t,s) - S_{jk}(t,s)]\frac{\delta}{\delta\phi_k(s)}\right)|\psi_t\rangle$$

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L. Diosi, L.F., PRL 113, 200403 (2014).

Non-Markovian dissipative QMUPL

$$\frac{d|\psi_t\rangle}{dt} = \left[-i\left(H_0 + \frac{\lambda\mu}{2}\{\hat{q},\hat{p}\}\right) + \sqrt{\lambda}\left(\hat{q} + i\mu\hat{p}\right)\phi(t) - 2\sqrt{\lambda}\hat{q}\int_0^t dsD(t,s)\frac{\delta}{\delta\phi(s)}\right]|\psi_t\rangle$$

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$$\frac{d|\psi_t\rangle}{dt} = -i\hat{A}^j(t)\left(\phi_j(t) + \int_0^t ds[D_{jk}(t,s) - S_{jk}(t,s)]\frac{\delta}{\delta\phi_k(s)}\right)|\psi_t\rangle$$

$$\downarrow$$

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H},\hat{\rho}\right] + \Gamma_{jk}(t)\left[\hat{A}^j,\left[\hat{A}^k,\hat{\rho}\right]\right] + \Theta_{jk}(t)\left[\hat{A}^j,\left[\dot{\hat{A}}^k,\hat{\rho}\right]\right]$$

$$+\Xi_{jk}(t)\left[\hat{A}^j,\left\{\hat{A}^k,\hat{\rho}\right\}\right] + \Upsilon_{jk}(t)\left[\hat{A}^j,\left\{\dot{\hat{A}}^k,\hat{\rho}\right\}\right]$$

Non-Markovian dissipative QMUPL

$$\frac{d|\psi_t\rangle}{dt} = \left[-i\left(H_0 + \frac{\lambda\mu}{2}\{\hat{q},\hat{p}\}\right) + \sqrt{\lambda}\left(\hat{q} + i\mu\hat{p}\right)\phi(t) - 2\sqrt{\lambda}\hat{q}\int_0^t dsD(t,s)\frac{\delta}{\delta\phi(s)}\right]|\psi_t\rangle$$

$$\frac{d|\psi_t\rangle}{dt} = -i\hat{A}^j(t)\left(\phi_j(t) + \int_0^t ds[D_{jk}(t,s) - S_{jk}(t,s)]\frac{\delta}{\delta\phi_k(s)}\right)|\psi_t\rangle$$

$$\downarrow$$

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}(t),\hat{\rho}] + i\Xi_\mu(t)[\hat{q}^2,\hat{\rho}] + i\Upsilon_\mu(t)[\hat{q},\{\hat{p},\hat{\rho}\}]$$

$$+\Gamma_\mu(t)[\hat{q},[\hat{q},\hat{\rho}]] + \Theta_\mu(t)[\hat{q},[\hat{p},\hat{\rho}]] + \gamma_\mu(t)[\hat{p},[\hat{p},\hat{\rho}]]$$

Conclusions

- We have derived the moste general Gaussian, completely positive, trace preserving, non-Markovian master equation.

- Stochastic unraveling allows to investigate the non-Markovian QMUPL model

Momentum coupling

$$\hat{H}_I(t) = \hat{A}^j(t)\hat{\phi}_j(t) \longrightarrow \left[\hat{q}(t) + \mu\hat{p}(t)\right]\hat{\phi}(t)$$

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$$+\Gamma_\mu(t)[\hat{q},[\hat{q},\hat{\rho}]]+\Theta_\mu(t)[\hat{q},[\hat{p},\hat{\rho}]]+\gamma_\mu(t)[\hat{p},[\hat{p},\hat{\rho}]]$$

Momentum coupling

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}(t) - \hbar\Xi_\mu(t)\hat{q}^2 - \hbar\Upsilon_\mu(t)\{\hat{q},\hat{p}\},\hat{\rho}]$$

$$+\sum_{i,j} a_{ij}(t)\left(\hat{F}_i\hat{\rho}\hat{F}_j - \frac{1}{2}\left\{\hat{F}_j\hat{F}_i,\hat{\rho}\right\}\right)$$

$$\hat{F}_1 = \hat{q} \qquad \hat{F}_2 = \hat{p}$$

$$a(t) = \begin{pmatrix} -2\Gamma_\mu(t) & -\Theta_\mu(t) + i\Upsilon_\mu(t) \\ -\Theta_\mu(t) - i\Upsilon_\mu(t) & -2\gamma_\mu(t) \end{pmatrix}$$

Non-Markovianity

$\det[a(t)] > 0 \longrightarrow$ Markovian dynamics

$\det[a(t)] < 0 \longrightarrow$ Non-Markovian dynamics

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$$\det[a(t)] = 4\Gamma_\mu(t)\gamma_\mu(t) - \left(\Theta_\mu(t)^2 + \Upsilon_\mu(t)^2\right)$$

Non-Markovianity

$\det[a(t)] > 0$ $\longrightarrow$ Markovian dynamics

$\det[a(t)] < 0$ $\longrightarrow$ Non-Markovian dynamics

$$\det[a(t)] = 4\Gamma_\mu(t)\gamma_\mu(t) - \left(\Theta_\mu(t)^2 + \Upsilon_\mu(t)^2\right)$$

$$= -\left[(\Theta_\mu(t) + \mu\Gamma_\mu(t))^2 + \Upsilon_\mu(t)^2\right] < 0$$

Non-Markovian for any (non-singular) bath correlation function

Caldeira-Leggett master equation

Interaction Hamiltonian: $\hat{H}_I(t) = \hat{A}^j(t)\hat{\phi}_j(t) \longrightarrow \hat{q}(t)\hat{\phi}(t)$

$$\mathcal{D}[\hat{\rho}] = D_{jk}(t)\left(\hat{A}^j\hat{\rho}\hat{A}^k - \frac{1}{2}\left\{\hat{A}^k\hat{A}^j, \hat{\rho}\right\}\right) \longrightarrow -\frac{D(t)}{2}\left[\hat{q}, \left[\hat{q}, \hat{\rho}\right]\right]$$

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$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}, \hat{\rho}\right] + \gamma T\left[\hat{q}, [\hat{q}, \hat{\rho}]\right] + \Xi\left[\hat{q}, \{\hat{q}, \hat{\rho}\}\right] + \Upsilon\left[\hat{q}, \{\hat{p}, \hat{\rho}\}\right]$$

divergent

Caldeira-Leggett master equation

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divergent

$$D^{\mathrm{Re}}(t,s) = \hbar\int_0^\infty d\omega J(\omega)\coth\left(\frac{\hbar\omega}{2k_B T}\right)\cos\omega(t-s) \longrightarrow \text{divergent}$$

$$D^{\mathrm{Im}}(t,s) = \hbar\int_0^\infty d\omega J(\omega)\sin\omega(t-s)$$