



# 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

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$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I$$

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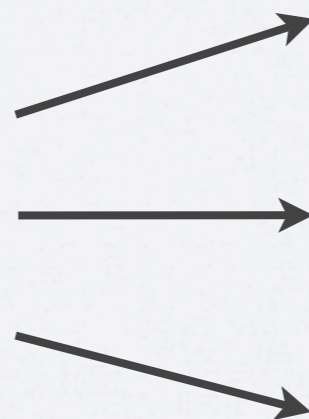
$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}_S, \hat{\rho}] + D_{jk}(t) \left( \hat{A}^j \hat{\rho} \hat{A}^k - \frac{1}{2} \left\{ \hat{A}^k \hat{A}^j, \hat{\rho} \right\} \right)$$

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- Non-Markovian dynamics



solid state (PBG materials)

ultrafast chemical  
reactions (OLEDs, FMO)

quantum optics



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$$\hat{\phi}_j(t) = \int \kappa_j^l(\omega) \hat{b}_{l\omega} e^{-i\omega t} d\omega + \text{h.c.}$$

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The general Gaussian non-Markovian map reads

$$\mathcal{M}_t = T \exp \left\{ \int_0^t d\tau \int_0^t ds D_{jk}(\tau, s) \left( \hat{A}_L^k(s) \hat{A}_R^j(\tau) - \theta_{\tau s} \hat{A}_L^j(\tau) \hat{A}_L^k(s) - \theta_{s\tau} \hat{A}_R^k(s) \hat{A}_R^j(\tau) \right) \right\}$$



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 $\downarrow$

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# Derivation of the master equation

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

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I. 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

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odd T-product



# Derivation of the master equation

3. Exploit Wick's theorem

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

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

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

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4. Iterate Wick's theorem

# Non-Markovian master equation

$$\dot{\hat{\rho}}_t = - \left( \hat{A}_L^i(t) - \hat{A}_R^i(t) \right) \left[ \int_0^t ds \mathbb{D}_{ij}(t, s) \hat{A}_L^j(s) - \mathbb{D}_{ij}^*(t, s) \hat{A}_R^j(s) \right] \hat{\rho}_t$$

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

Bath correlation function

Wick's contractions

Recursive definition

```
graph TD; A["\mathbb{D}_{ij}(t, s) = \sum_{n=1}^{\infty} (-1)^{n-1} D_{ij(n)}(t, s)"] --> B["Bath correlation function"]; A --> C["Wick's contractions"]; A --> D["Recursive definition"];
```

# Master equation for bosonic systems

We exploit the solution of Heisenberg equations:

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



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$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -i [\hat{H}, \hat{\rho}] + \Gamma_{jk}(t) [\hat{A}^j, [\hat{A}^k, \hat{\rho}]] + \Theta_{jk}(t) [\hat{A}^j, [\dot{\hat{A}}^k, \hat{\rho}]] \\ & + i\Xi_{jk}(t) [\hat{A}^j, \{\hat{A}^k, \hat{\rho}\}] + i\Upsilon_{jk}(t) [\hat{A}^j, \{\dot{\hat{A}}^k, \hat{\rho}\}] \end{aligned}$$

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

# Hu-Paz-Zhang Master Equation

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

# Hu-Paz-Zhang Master Equation

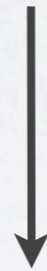
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$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -i [\hat{H}, \hat{\rho}] + \Gamma(t) [\hat{q}, [\hat{q}, \hat{\rho}]] + \Theta(t) [\hat{q}, [\hat{p}, \hat{\rho}]] \\ & + i\Xi(t) [\hat{q}^2, \hat{\rho}] + i\Upsilon(t) [\hat{q}, \{\hat{p}, \hat{\rho}\}] \end{aligned}$$

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

# 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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$$\mathcal{M}_t = T \exp \left\{ \int_0^t d\tau \int_0^\tau ds D(\tau, s) \left( \hat{A}_L^k(s) \hat{A}_R^j(\tau) - \theta_{\tau s} \hat{A}_L^j(\tau) \hat{A}_L^k(s) - \theta_{\tau s} \hat{A}_R^k(s) \hat{A}_R^j(\tau) \right) \right\}$$

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

# Non-Markovian dissipative QMUPL

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

# Non-Markovian dissipative QMUPL

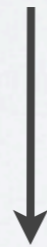
$$\frac{d|\psi_t\rangle}{dt} = \left[ -i \left( H_0 + \frac{\lambda\mu}{2} \{\hat{q}, \hat{p}\} \right) + \sqrt{\lambda} (\hat{q} + i\mu\hat{p}) \phi(t) - 2\sqrt{\lambda}\hat{q} \int_0^t ds D(t,s) \frac{\delta}{\delta\phi(s)} \right] |\psi_t\rangle$$

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

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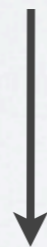


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$$+ \Gamma_\mu(t) [\hat{q}, [\hat{q}, \hat{\rho}]] + \Theta_\mu(t) [\hat{q}, [\hat{p}, \hat{\rho}]] + \gamma_\mu(t) [\hat{p}, [\hat{p}, \hat{\rho}]]$$

# Conclusions

- We have derived the most general Gaussian, completely positive, trace preserving, non-Markovian master equation.
- Stochastic unraveling allows to investigate the non-Markovian QMUPL model



# Momentum coupling

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



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

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# Momentum coupling

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}(t) - \hbar\Xi_{\mu}(t)\hat{q}^2 - \hbar\Upsilon_{\mu}(t)\{\hat{q}, \hat{p}\}, \hat{\rho}] \\ + \sum_{i,j} a_{ij}(t) \left( \hat{F}_i \hat{\rho} \hat{F}_j - \frac{1}{2} \left\{ \hat{F}_j \hat{F}_i, \hat{\rho} \right\} \right)$$

$$\hat{F}_1 = \hat{q}$$

$$\hat{F}_2 = \hat{p}$$

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

# Non-Markovianity

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

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$$\begin{aligned}\det[a(t)] &= 4\Gamma_{\mu}(t)\gamma_{\mu}(t) - (\Theta_{\mu}(t)^2 + \Upsilon_{\mu}(t)^2) \\ &= - \left[ (\Theta_{\mu}(t) + \mu\Gamma_{\mu}(t))^2 + \Upsilon_{\mu}(t)^2 \right] < 0\end{aligned}$$

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

# Caldeira-Leggett master equation

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

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

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

divergent



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divergent

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

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