Non-Markovian dynamics beyond the Gaussian ansatz

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Outline

- Open quantum systems: Markovian vs non-Markovian

- Gaussian non-Markovian map and master equation

- Beyond the Gaussian ansatz: a recursive approach

Open quantum systems

- Interaction between the system and the environment

$$\hat{\rho}_{SE} = \hat{\rho}_S \otimes \hat{\rho}_E \qquad \hat{H} = \hat{H}_S + \hat{H}_E + \hat{V}$$

$$\frac{d\hat{\rho}_{SE}(t)}{dt} = -i\left[\hat{V}_t, \hat{\rho}_{SE}(t)\right] \equiv -iV_t^- \hat{\rho}_{SE}(t)$$

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

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- Bilinear interaction: $$\hat{V}_t = \hat{A}^j(t)\hat{\phi}_j(t)$$

Hermitian system operators

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

Gaussian non-Markovian map

Environmental degrees of freedom can be traced exactly

$$\mathcal{M}_t \hat{\rho}_S = \mathrm{Tr}_{\mathrm{E}} \left[T \left(e^{-i \int_0^t d\tau V_\tau^-} \right) \hat{\rho}_S \otimes \hat{\rho}_E \right]$$

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The general Gaussian non-Markovian map reads

$$\mathcal{M}_t = T \exp \left\{ - \int_0^t d\tau \int_0^\tau ds A_j^-(\tau) \left(D_{jk}^{\mathrm{Re}}(\tau, s) A_j^-(s) + i D_{jk}^{\mathrm{Im}}(\tau, s) A_j^+(s) \right) \right\}$$

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

Gaussian master equation

Linear Heisenberg equations of motion for $\hat{A}^j(t)$ $\longrightarrow$ Wick's theorem

Gaussian master equation

Linear Heisenberg equations of motion for $\hat{A}^j(t)$ ⟶ Wick's theorem

$$\frac{d\hat{\rho}_S(t)}{dt} = -A_i^-(t)\left[\int_0^t d\tau \mathbb{D}_{ij}^{\mathrm{Re}}(t,\tau)A_j^-(\tau) + i\mathbb{D}_{ij}^{\mathrm{Im}}(t,\tau)A_j^+(\tau)\right]\hat{\rho}_S(t)$$

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

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

→ Bath correlation function

→ Wick's contractions

↓ Recursive definition

Beyond Gaussian

Perturbative techniques

- Projection operator technique
- Cumulant expansion
- Path integral
- ...

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Perturbative techniques →

- Projection operator technique
- Cumulant expansion
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Two drawbacks →

- Repeated application of the whole formalism in order to obtain the n-th expansion order
- No clear evidence of the mathematical structure in terms of [,] and { , }

Projection operator technique

$$\mathcal{P}\hat{\rho}_{SE}(t) = \hat{\rho}_S(t) \otimes \hat{\rho}_E$$

$$\frac{d\hat{\rho}_S(t)}{dt} = \mathbb{L}(t)\hat{\rho}_S(t)$$

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$$\mathbb{L}(t) = \sum_{k=0} L_k(t) = \sum_{k=0} \alpha \mathcal{P} V_t^{-} \Sigma(t)^k$$

$$\hat{V}_t = \hat{A}^j(t)\hat{\phi}_j(t)$$

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$$L_2(t) = \alpha^2 \int_0^t d\tau \mathcal{P} V_t^- V_\tau^- \mathcal{P}$$

$$L_4(t) = \alpha^4 \int_0^t d\vec{\tau} \mathcal{P} V_t^- V_{\tau_1}^- (1-\mathcal{P}) V_{\tau_2}^- V_{\tau_3}^- \mathcal{P}$$

$$-\mathcal{P} V_t^- V_{\tau_2}^- \mathcal{P} V_{\tau_1}^- V_{\tau_3}^- \mathcal{P} - \mathcal{P} V_t^- V_{\tau_3}^- \mathcal{P} V_{\tau_1}^- V_{\tau_2}^- \mathcal{P}$$

Recursive approach: map

$$\mathcal{M}_t \hat{\rho}_S = \mathrm{Tr}_{\mathrm{E}} \left[T \left(e^{-i \int_0^t d\tau V_\tau^-} \right) \hat{\rho}_S \otimes \hat{\rho}_E \right] = \sum_{n=0}^{\infty} (-i)^n \mu_n(t) \hat{\rho}_S$$

$$\mu_n(t) \hat{\rho}_S = \frac{1}{n!} \mathrm{Tr}_E \left[T \left(\int_0^t d\tau V_\tau^- \right)^n \hat{\rho}_S \otimes \hat{\rho}_E \right]$$

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$$= \frac{1}{n!\,2^n}\mathrm{Tr}_E\left[T\left(\int_0^t d\tau(A_\tau^+\phi_\tau^- + A_\tau^-\phi_\tau^+)\right)^n\hat{\rho}_S\otimes\hat{\rho}_E\right]$$

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$$\mu_n(t)\hat{\rho}_S = \int_0^t d\bar{\tau}_n\sum_{j=1}^{n}\sum_{\mathcal{P}_j}A_{\tau_1}^-\dots A_{\tau_n}^{k_n}\,D_{\tau_1\dots\tau_n}^{+\dots\bar{k}_n}\hat{\rho}_S$$

[,] and { , } of system operators

bath ordered correlation function

$$D_{\tau_1\dots\tau_n}^{+\dots\bar{k}_n} \equiv \frac{1}{2^n}\mathrm{Tr}_E\left[\phi_{\tau_1}^+\theta_{\tau_1\tau_2}\phi_{\tau_2}^{\bar{k}_2}\dots\theta_{\tau_{n-1}\tau_n}\phi_{\tau_n}^{\bar{k}_n}\right]$$

G. Gasbarri, L. Ferialdi, arXiv:1707.06540.

Recursive approach: master equation

$$\frac{d\hat{\rho}_S(t)}{dt} = \mathbb{L}(t)\hat{\rho}_S(t)$$

$$\mathbb{L}(t) = \dot{\mathcal{M}}_t \mathcal{M}_t^{-1} = \sum_{n=1}^{\infty}(-i)^n L_n(t)$$

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$$L_1(t) = A_t^- \, D_t^+ \,,$$

$$L_2(t) = A_t^- \int_0^t d\tau_1 \left[A_{\tau_1}^+ D_{t\,\tau_1}^{+-} + A_{\tau_1}^- \left(D_{t\,\tau_1}^{++} - D_t^+ \, D_{\tau_1}^+ \right) \right]$$

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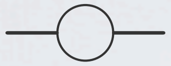
$$\begin{aligned} L_3(t) = \int_0^t d\bar{\tau}_2 \Big[& A_t^- A_{\tau_1}^- A_{\tau_2}^- \left(D_{t\,\tau_1\tau_2}^{+++} - D_t^+ D_{\tau_1\tau_2}^{++} - D_{t\,\tau_1}^{++} D_{\tau_2}^+ + D_t^+ D_{\tau_1}^+ D_{\tau_2}^+ \right) \\ & + A_t^- A_{\tau_1}^- A_{\tau_2}^+ \left(D_{t\,\tau_1\tau_2}^{++-} - D_t^+ D_{\tau_1\tau_2}^{+-} \right) \\ & + A_t^- A_{\tau_1}^+ A_{\tau_2}^- \left(D_{t\,\tau_1\tau_2}^{+-+} - D_{t\,\tau_1}^{+-} \, D_{\tau_2}^+ \right) \\ & + A_t^- A_{\tau_1}^+ A_{\tau_2}^+ D_{t\,\tau_1\tau_2}^{+--} \Big] \end{aligned}$$

G. Gasbarri, L. Ferialdi, arXiv:1707.06540.

Diagramatics

Basic elements:  $= A^+_\tau \phi^-_\tau$  $= A^-_\tau \phi^+_\tau$

Diagramatics

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Connected diagram:

$$\underbrace{\text{●—◑—}\ldots\text{—◑}}_{n} = \int_0^t d\bar{\tau}_n\, A^{-}_{\tau_1}\ldots A^{\pm}_{\tau_n}\, D^{+\cdots\mp}_{\tau_1,\ldots\tau_n}$$

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Trace preservation: $\circ\!-\!◑\!-\!◑\!-\!\ldots\!-\!◑ = 0$

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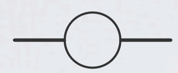
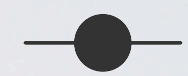
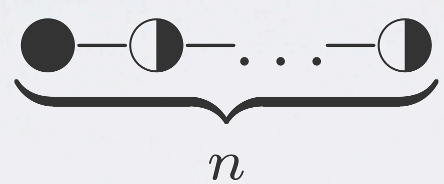
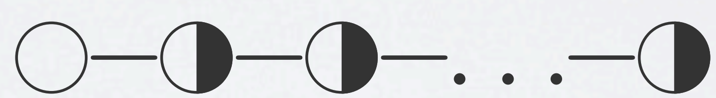
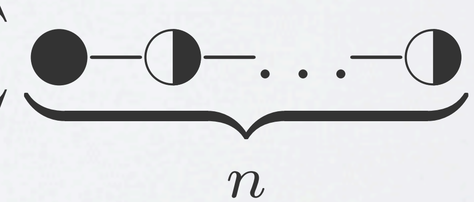
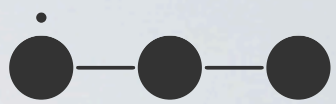
Basic elements:  $= A^+_\tau \phi^-_\tau$  $= A^-_\tau \phi^+_\tau$

Connected diagram:  $= \int_0^t d\bar{\tau}_n \, A^-_{\tau_1} \dots A^{\pm}_{\tau_n} D^{+\cdots\mp}_{\tau_1,\dots\tau_n}$

Trace preservation:  $= 0$

n-th momentum: $\mu_n = \sum_{j=1}^{n} \sum_{\mathcal{P}_j}$ 

Diagramatic rules

1. Write the n-th order "black" connected diagram: 

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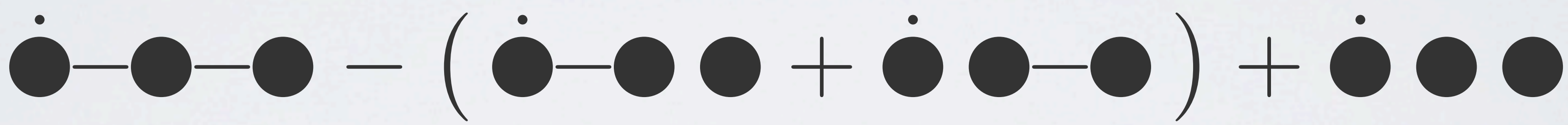
1. Write the n-th order "black" connected diagram: 

2. Remove $p \leq n-1$ lines in all possible ways and multiply by $(-1)^p$:



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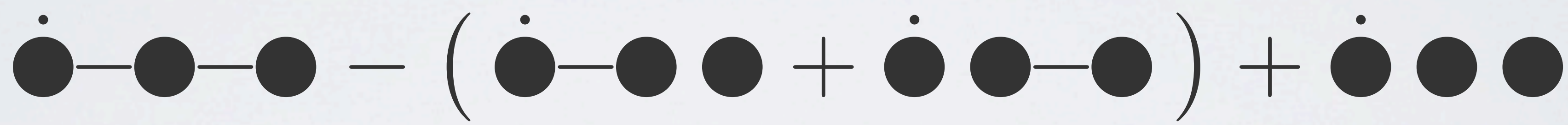

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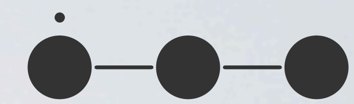
1. Write the n-th order "black" connected diagram: 

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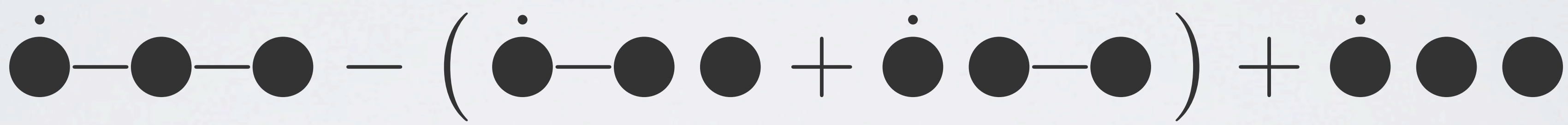

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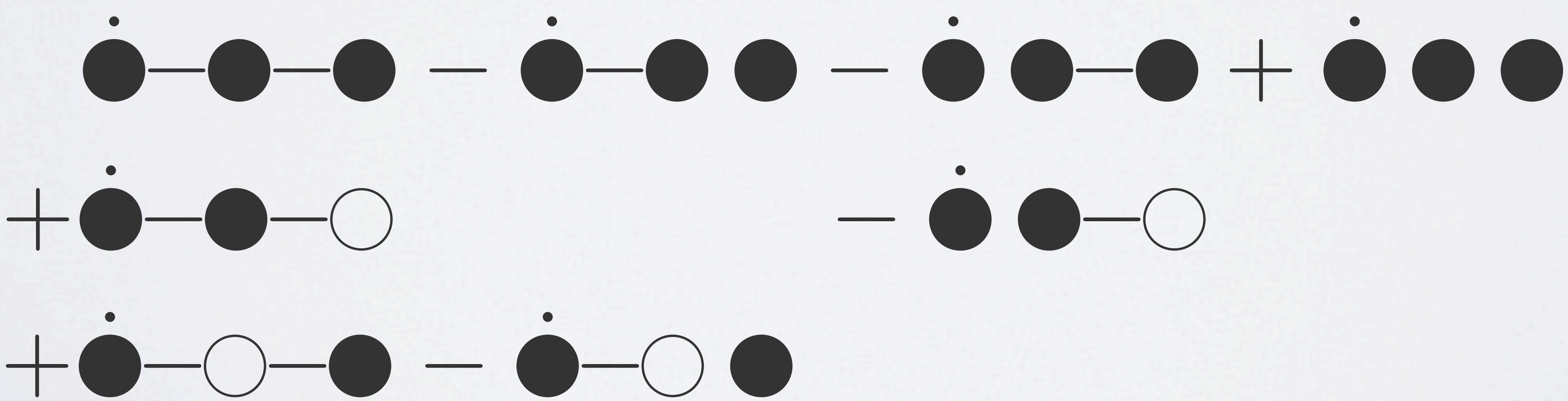

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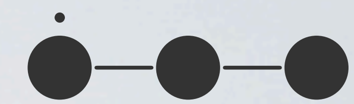

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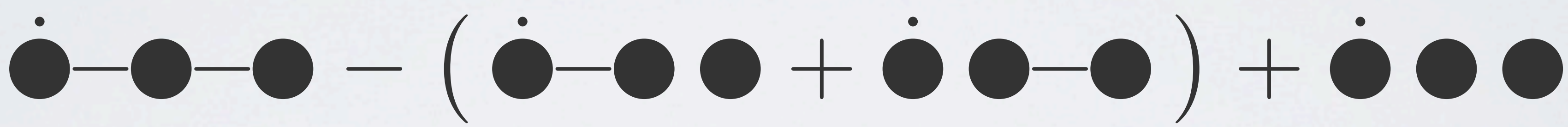

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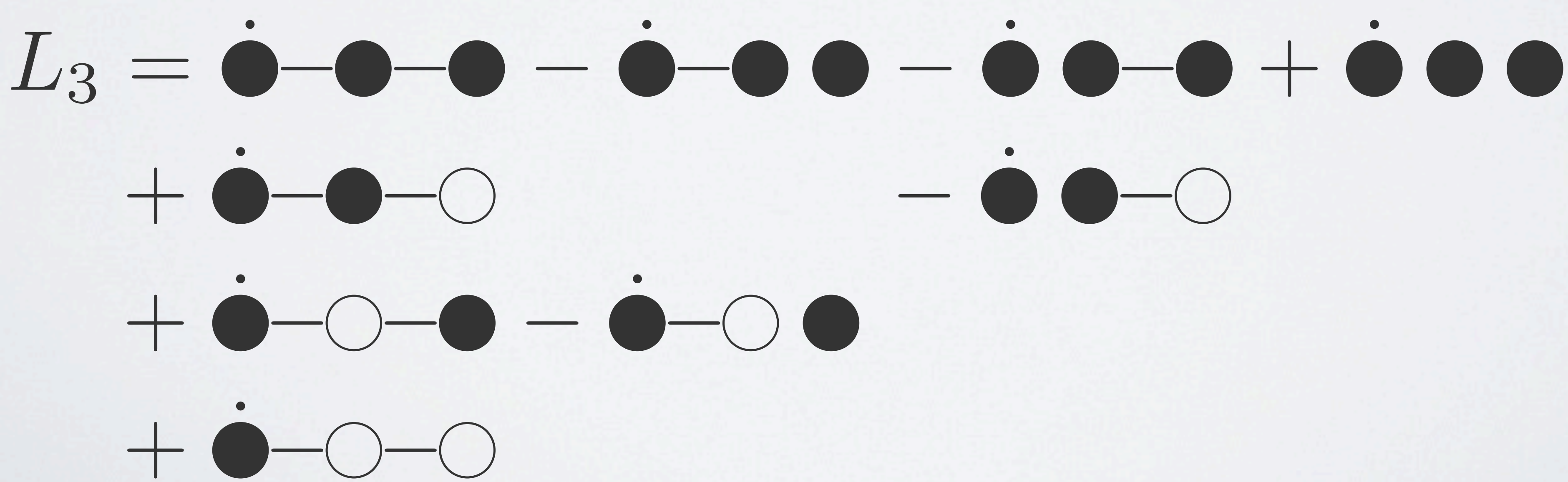
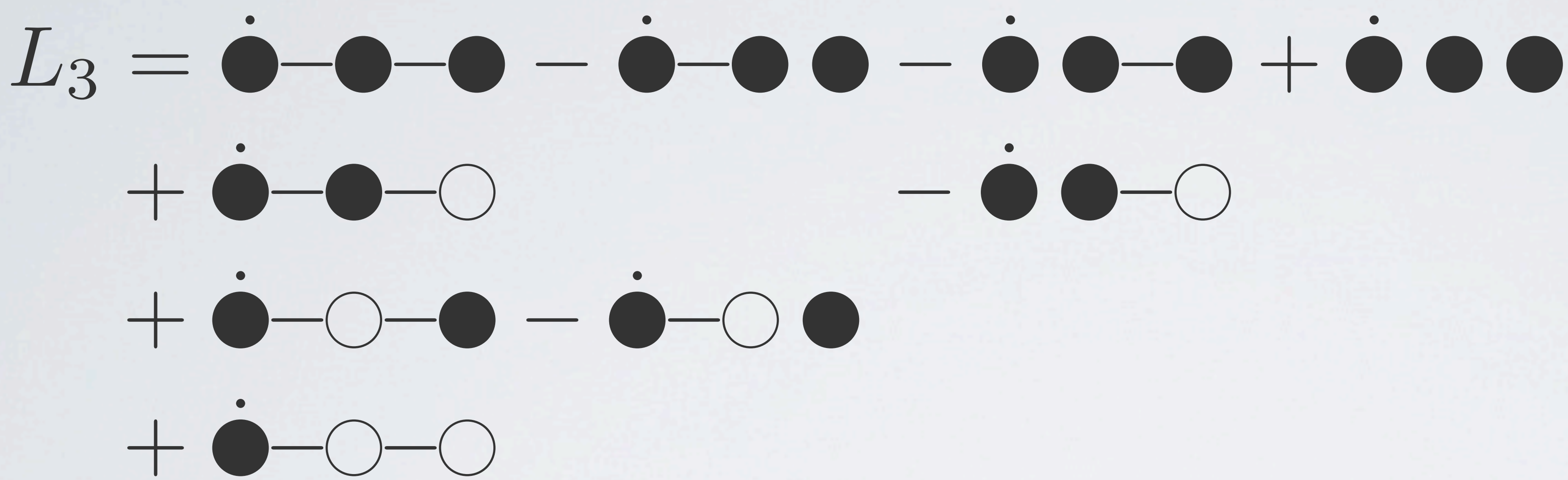


Diagramatic rules

4. Rephrase with formulas:



$$L_3(t) = \int_0^t d\bar{\tau}_2 \Big[A^-_t A^-_{\tau_1} A^-_{\tau_2} \Big(D^{+++}_{t\,\tau_1\tau_2} - D^+_t D^{++}_{\tau_1\tau_2} - D^{++}_{t\,\tau_1} D^+_{\tau_2} + D^+_t D^+_{\tau_1} D^+_{\tau_2} \Big)$$

$$+ A^-_t A^-_{\tau_1} A^+_{\tau_2} \Big(D^{++-}_{t\,\tau_1\tau_2} - D^+_t D^{+-}_{\tau_1\tau_2} \Big)$$

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$$+ A^-_t A^+_{\tau_1} A^+_{\tau_2} D^{+--}_{t\,\tau_1\tau_2} \Big]$$

Gaussian vs non-Gaussian

Gaussian master equation:

$$\frac{d\hat{\rho}_S(t)}{dt} = -A_i^-(t)\left[\int_0^t d\tau \mathbb{D}_{ij}^{\mathrm{Re}}(t,\tau)A_j^-(\tau) + i\mathbb{D}_{ij}^{\mathrm{Im}}(t,\tau)A_j^+(\tau)\right]\hat{\rho}_S(t)$$

Non-Gaussian master equation:

$$\frac{d\hat{\rho}_S(t)}{dt} = \left[\sum_{n=1}^{\infty}(-i)^n L_n(t)\right]\hat{\rho}_S(t) \qquad L_n(t) = \dot{\mu}_n(t) - \sum_{k=1}^{n-1} L_{n-k}(t)\mu_k(t)$$

$$\mu_n(t)\hat{\rho}_S = \int_0^t d\bar{\tau}_n \sum_{j=1}^{n}\sum_{\mathcal{P}_j} A_{\tau_1}^- \ldots A_{\tau_n}^{k_n} D_{\tau_1\ldots\tau_n}^{+\ldots\bar{k}_n}\hat{\rho}_S$$

Conclusions

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

- We have provided a perturbative approach for non-Markovian master equations the Gaussian ansatz

Recursive

Clear structure in terms of [,] and { , }