Non-Markovian Quantum Master Equations

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Open Quantum Systems and Dynamical Maps

- Total system composed of 'System' and 'Bath': $\mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{B}}$
- Reduced density operator

$$\rho_{\mathrm{S}}(t_1) = \mathrm{Tr}_{\mathrm{B}}(U(t_1, t_0)\rho(t_0)U^{\dagger}(t_1, t_0))$$

- Let $\mathrm{Tr}_{\mathrm{B}}\rho(t_0) = \rho_{\mathrm{S}}(t_0)$. This consitutes a dynamical map

$$\rho_{\mathrm{S}}(t_1) = \mathcal{E}_{(t_1, t_0)}[\rho_{\mathrm{S}}(t_0)]$$

Universal Dynamical Map

$$\rho_{\mathrm{S}}(t_1) = \mathcal{E}_{(t_1,t_0)}[\rho_{\mathrm{S}}(t_0)] = \sum_{\alpha} K_\alpha(t_1,t_0)\rho_{\mathrm{S}}(t_0)K_\alpha^\dagger(t_1,t_0),$$

where

$$\sum_{\alpha} K_\alpha^\dagger(t_1,t_0)K_\alpha(t_1,t_0) = \mathbb{1}$$

- Completely Positive map (Kraus)
- This is true if

$$\rho(t_0) = \rho_{\mathrm{S}}(t_0) \otimes \rho_{\mathrm{B}}(t_0)$$

- If not, in general, $K_\alpha(t_1,t_0;\rho_{\mathrm{S}})$ depends on ρ_{S} at t_0

Markovian Evolution

- For $t_2 > t_1 > t_0$ and if $\rho(t_0) = \rho_{\rm S}(t_0) \otimes \rho_{\rm B}(t_0)$

$$\mathcal{E}_{(t_1,t_0)} : \ \text{UDM}, \qquad \mathcal{E}_{(t_2,t_0)} : \ \text{UDM}$$
$$\mathcal{E}_{(t_2,t_1)} : \ \text{not} \ \ \text{UDM} \ \ \text{in general}$$

Markovian Evolution

If UDM $\mathcal{E}$ satisfies

$$\mathcal{E}_{(t_2,t_0)} = \mathcal{E}_{(t_2,t_1)} \mathcal{E}_{(t_1,t_0)}$$

- Classical analogue: Chapman-Kolmogorov equation

$$p(x_3,t_3|x_1,t_1) \int dx_2 \; p(x_3,t_3|x_2,t_2) p(x_2,t_2|x_1,t_1)$$

- For the case of $\mathcal{E}_{(t_1,t_0)} = \mathcal{E}_{t_1-t_0}$, we have semigroup property: $\mathcal{E}_{t+s} = \mathcal{E}_t \mathcal{E}_s$

Markovian and Non-Markovian QMEs

- Markovian evolution in differential form if and only if it can be expressed as (Gorini, Kossakowski, & Sudarshan; Lindblad)

$$\frac{d\rho_{\rm S}(t)}{dt} = -i[H(t), \rho_{\rm S}(t)] + \sum_k \gamma_k(t) \left[V_k(t)\rho_{\rm S}(t)V_k^\dagger(t) - \frac{1}{2}\left\{ V_k^\dagger(t)V_k(t), \rho_{\rm S}(t) \right\} \right]$$

  where H is self-adjoint and $\gamma_k(t) \geq 0$ for all k and t
- All these are mathematical. In general, QMEs derived from physical Hamiltonian,

$$H = H_{\rm S} + H_{\rm B} + H_{\rm I}$$

  will be non-Markovian.
- To get Markovian QME, one needs to impose special assumptions (secular, ULE, etc.)
- In this lecture, we present a few general and formal methods to obtain QMEs from Hamiltonian composed of system and bath

Nakajima-Zwanzig Equation

Projection Operator Formalism

- $H = H_0 + H_{\rm I}$, where $H_0 = H_{\rm S} + H_{\rm B}$
- Projection operators: for some fixed $\rho_{\rm B}$

$$\mathcal{P}\rho = {\rm Tr}_{\rm B}(\rho) \otimes \rho_{\rm B}, \qquad \mathcal{Q}\rho = (\mathbb{1} - \mathcal{P})\rho$$
$$\mathcal{P}^2\rho = {\rm Tr}_{\rm B}[{\rm Tr}_{\rm B}(\rho) \otimes \rho_{\rm B}] \otimes \rho_{\rm B} = \mathcal{P}\rho$$

- Interaction picture: $\tilde{\rho}(t) = U_0^\dagger(t)\rho(t)U_0(t)$, $\tilde{H}_{\rm I} = U_0^\dagger(t)H_{\rm I}U_0(t)$, where $U_0(t) = e^{-iH_0t}$

$$\partial_t\tilde{\rho}(t) = -i[\tilde{H}_{\rm I}, \tilde{\rho}(t)] \equiv \mathcal{L}(t)\tilde{\rho}(t),$$

where $\mathcal{L}(t)\bullet \equiv -i[\tilde{H}_{\rm I}(t), \bullet]$.

- Take the $\mathcal{P}$-projection

$$\partial_t \underset{\sim\sim\sim}{\mathcal{P}\tilde{\rho}(t)} = \mathcal{P}\mathcal{L}(t)\tilde{\rho}(t) = \mathcal{P}\mathcal{L}(t)(\mathcal{P}+\mathcal{Q})\tilde{\rho}(t)$$
$$= \mathcal{P}\mathcal{L}(t)\underset{\sim\sim\sim}{\mathcal{P}\tilde{\rho}(t)} + \mathcal{P}\mathcal{L}(t)\underline{\underline{\mathcal{Q}\tilde{\rho}(t)}} \tag{1}$$

- Take the $\mathcal{Q}$-projection

$$\partial_t \underline{\underline{\mathcal{Q}\tilde{\rho}(t)}} = \underbrace{\mathcal{Q}\mathcal{L}(t)\mathcal{P}\tilde{\rho}(t)}_{\text{inhom.}} + \mathcal{Q}\mathcal{L}(t)\underline{\underline{\mathcal{Q}\tilde{\rho}(t)}} \tag{2}$$

- Solution to homogeneous eq. for $\mathcal{Q}\tilde{\rho}$

$$\mathcal{Q}\tilde{\rho}(t) = G(t,0)\mathcal{Q}\tilde{\rho}(0), \qquad G(t,0) = \mathbb{T}e^{\int_0^t dt'\,\mathcal{Q}\mathcal{L}(t')}$$

- Solution to full Eq. (2)

$$\mathcal{Q}\tilde{\rho}(t) = G(t,0)\mathcal{Q}\tilde{\rho}(0) + \int_0^t ds\, G(t,s)\,\underbrace{\mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s)}_{\text{inhom.}}$$

- Insert this into Eq. (1)

$$\partial_t \, \underset{\sim\sim\sim}{\mathcal{P}\tilde{\rho}(t)} = \underbrace{\mathcal{P}\mathcal{L}(t)\mathcal{P}}_{\text{(i)}} \, \tilde{\rho}(t) + \mathcal{P}\mathcal{L}(t)G(t,0) \, \underbrace{\mathcal{Q}\tilde{\rho}(0)}_{\text{(ii)}}$$

$$+ \int_0^t ds \, \mathcal{P}\mathcal{L}(t)G(t,s)\mathcal{Q}\mathcal{L}(s)\underset{\sim\sim\sim}{\mathcal{P}\tilde{\rho}(s)}$$

- Two simplifications
  - (i) If $[H_{\mathrm{B}}, \rho_{\mathrm{B}}] = 0$, one can always set

$$\mathcal{P}\mathcal{L}(t)\mathcal{P} = 0$$

  - (ii) For a product initial state $\rho(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}$,

$$\mathcal{Q}\tilde{\rho}(0) = 0$$

- We have NZ-QME in a time convolution form

$$\boxed{\partial_t \mathcal{P}\tilde{\rho}(t) = \int_0^t ds \, \underset{\sim\sim\sim}{\mathcal{P}\mathcal{L}(t)G(t,s)\mathcal{Q}\mathcal{L}(s)}\mathcal{P}\tilde{\rho}(s) \equiv \int_0^t ds \, \mathcal{K}(t,s)\mathcal{P}\tilde{\rho}(s)}$$

- Derivation of (i)
  - For any ρ

$$\begin{aligned}\mathcal{P}\mathcal{L}(t)\mathcal{P}\rho =& -i\mathrm{Tr}_{\mathrm{B}}[\tilde{H}_{\mathrm{I}}(t), \mathcal{P}\rho] \otimes \rho_{\mathrm{B}} \\ =& -i\mathrm{Tr}_{\mathrm{B}}[\tilde{H}_{\mathrm{I}}(t), \mathrm{Tr}_{\mathrm{B}}(\rho) \otimes \rho_{\mathrm{B}}] \otimes \rho_{\mathrm{B}} \\ =& -i\left[\underset{\sim\sim\sim}{\mathrm{Tr}_{\mathrm{B}}(\tilde{H}_{\mathrm{I}}(t)\rho_{\mathrm{B}})}, \mathrm{Tr}_{\mathrm{B}}(\rho)\right] \otimes \rho_{\mathrm{B}}\end{aligned}$$

  - Redefine H's such that $H_{\mathrm{S}} + H_{\mathrm{I}} = H'_{\mathrm{S}} + H'_{\mathrm{I}}$

$$\begin{aligned}H'_{\mathrm{I}} &\equiv H_{\mathrm{I}} - \mathrm{Tr}_{\mathrm{B}}\left(H_{\mathrm{I}}\rho_{\mathrm{B}}\right) \otimes \mathbb{1} = H_{\mathrm{I}} - \langle H_{\mathrm{I}}\rangle_{\mathrm{B}} \otimes \mathbb{1} \\ H'_{\mathrm{S}} &\equiv H_{\mathrm{S}} + \mathrm{Tr}_{\mathrm{B}}\left(H_{\mathrm{I}}\rho_{\mathrm{B}}\right) \otimes \mathbb{1} = H_{\mathrm{S}} + \langle H_{\mathrm{I}}\rangle_{\mathrm{B}} \otimes \mathbb{1}\end{aligned}$$

  - Then if $[H_{\mathrm{B}}, \rho_{\mathrm{B}}] = 0$

$$\begin{aligned}\underset{\sim\sim\sim}{\mathrm{Tr}_{\mathrm{B}}(\tilde{H}'_{\mathrm{I}}(t)\rho_{\mathrm{B}})} =& \mathrm{Tr}_{\mathrm{B}}(e^{i(H'_{\mathrm{S}}+H_{\mathrm{B}})t} H'_{\mathrm{I}} e^{-i(H'_{\mathrm{S}}+H_{\mathrm{B}})t} \rho_{\mathrm{B}}) \\ =& e^{iH'_{\mathrm{S}}t} \mathrm{Tr}_{\mathrm{B}}(e^{iH_{\mathrm{B}}t} H_{\mathrm{I}} e^{-iH_{\mathrm{B}}t} \rho_{\mathrm{B}}) e^{-iH'_{\mathrm{S}}t} \\ & - e^{iH'_{\mathrm{S}}t} \mathrm{Tr}_{\mathrm{B}}\left(H_{\mathrm{I}}\rho_{\mathrm{B}}\right) e^{-iH'_{\mathrm{S}}t} \underbrace{\mathrm{Tr}_{\mathrm{B}}(e^{iH_{\mathrm{B}}t}\rho_{\mathrm{B}} e^{-iH_{\mathrm{B}}t})}_{=1} \\ =& 0\end{aligned}$$

- Derivation of (ii)
  - For a product initial state

$$\rho(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}} \Rightarrow \tilde{\rho}(0) = \rho(0)$$

  - We then have

$$\mathcal{P}\tilde{\rho}(0) = \mathrm{Tr}_{\mathrm{B}}(\rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}) \otimes \rho_{\mathrm{B}} = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}} = \tilde{\rho}(0)$$

  - Therefore

$$\mathcal{Q}\tilde{\rho}(0) = 0$$

- NZ QME is exact, nonperturbative, non-Markovian and non-local in time (with memory kernel $\mathcal{K}(t,s)$)
- Can describe an initial state which is not a product state $\rightarrow$ inhomogeneous term
- May serve as a starting point of a perturbative study

NZ equation

Weak Coupling Limit

- Let $H_{\rm I} \to \epsilon H_{\rm I}$. Then $\mathcal{L} \to \epsilon\mathcal{L}$
- Note that $G(t,s) = \mathbb{T}\exp[\epsilon \int_s^t dt'\ \mathcal{Q}\mathcal{L}(t')] = \mathbb{1} + O(\epsilon)$
- NZ equation becomes

$$
\begin{aligned}
\partial_t \mathcal{P}\tilde{\rho}(t) =& \epsilon^2 \int_0^t ds\, \mathcal{P}\mathcal{L}(t) G(t,s) \mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s) \\
=& \epsilon^2 \int_0^t ds\, \mathcal{P}\mathcal{L}(t)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s) + O(\epsilon^3) \\
=& \epsilon^2 \int_0^t ds\, \mathcal{P}\mathcal{L}(t)\mathcal{L}(s)\mathcal{P}\tilde{\rho}(s) + O(\epsilon^3) \qquad \because\ \mathcal{P}\mathcal{L}(t)\mathcal{P} = 0 \\
=& -\epsilon^2 \mathcal{P} \int_0^t ds\, [\tilde{H}_{\rm I}(t), [\tilde{H}_{\rm I}(s), \mathcal{P}\tilde{\rho}(s)]] + O(\epsilon^3)
\end{aligned}
$$

- If we write $\mathrm{Tr}_{\rm B}(\tilde{\rho}(t)) = \tilde{\rho}_{\rm S}(t)$, we get the same result as the Born Approximation

$$
\partial_t \tilde{\rho}_{\rm S}(t) = -\epsilon^2 \mathrm{Tr}_{\rm B} \int_0^t ds\, [\tilde{H}_{\rm I}(t), [\tilde{H}_{\rm I}(s), \tilde{\rho}_{\rm S}(s) \otimes \rho_{\rm B}]] + O(\epsilon^3)
$$

Time Convolutionless (TCL) ME

- It is possible to obtain QME in a time local form without convolution
- Recall (We don't assume factorized init. state)

$$\partial_t \underset{\sim}{\mathcal{P}\tilde{\rho}(t)} = \epsilon \mathcal{P}\mathcal{L}(t)\underset{\sim}{\mathcal{P}\tilde{\rho}(t)} + \epsilon \mathcal{P}\mathcal{L}(t)\underline{\underline{\mathcal{Q}\tilde{\rho}(t)}}$$

$$\underline{\underline{\mathcal{Q}\tilde{\rho}(t)}} = G(t,0)\mathcal{Q}\tilde{\rho}(0) + \epsilon \int_0^t ds\, G(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\tilde{\rho}\underline{(s)}$$

- We want $\tilde{\rho}$ at t not s. Using Liouville eq. for total system+bath, can write $\tilde{\rho}(t) = \mathcal{U}_+(t,s)\tilde{\rho}(s) = \mathbb{T}_+ e^{\epsilon \int_s^t dt'\, \mathcal{L}(t')}\tilde{\rho}(s)$ and

$$\tilde{\rho}(s) = \mathcal{U}_-(t,s)\tilde{\rho}(t) = \mathbb{T}_- e^{-\epsilon \int_s^t dt'\, \mathcal{L}(t')}\tilde{\rho}(t) = \mathcal{U}_-(t,s)(\mathcal{P}+\mathcal{Q})\tilde{\rho}(t)$$

- Therefore

$$\mathcal{Q}\tilde{\rho}(t) = G(t,0)\mathcal{Q}\tilde{\rho}(0) + \underbrace{\epsilon \int_0^t ds\, G(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\mathcal{U}_-(t,s)}_{\equiv \Sigma(t)} \mathcal{P}\tilde{\rho}(t)$$
$$+ \underbrace{\epsilon \int_0^t ds\, G(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\mathcal{U}_-(t,s)}_{\equiv \Sigma(t)} \mathcal{Q}\tilde{\rho}(t)$$

- Solving this

$$\mathcal{Q}\tilde{\rho}(t) = [1 - \Sigma(t)]^{-1} G(t,0)\mathcal{Q}\tilde{\rho}(0) + [1 - \Sigma(t)]^{-1} \Sigma(t)\mathcal{P}\tilde{\rho}(t)$$

- Inserting this into eq. for $\mathcal{P}\tilde{\rho}$

$$\partial_t \mathcal{P}\tilde{\rho}(t) = \epsilon \underline{\mathcal{P}\mathcal{L}(t)}\ \underline{\mathcal{P}\tilde{\rho}(t)} + \epsilon \mathcal{P}\mathcal{L}(t)\,[1 - \Sigma(t)]^{-1} G(t,0)\mathcal{Q}\tilde{\rho}(0)$$
$$+ \epsilon \underline{\mathcal{P}\mathcal{L}(t)}[1 - \Sigma(t)]^{-1} \Sigma(t)\underline{\mathcal{P}\tilde{\rho}(t)}$$
$$= \epsilon \mathcal{P}\mathcal{L}(t)\,[1 - \Sigma(t)]^{-1} G(t,0)\mathcal{Q}\tilde{\rho}(0)$$
$$+ \epsilon \mathcal{P}\mathcal{L}(t)\,[1 - \Sigma(t)]^{-1} \mathcal{P}\tilde{\rho}(t)$$

TCL ME

$$\boxed{\partial_t \mathcal{P}\tilde{\rho}(t) = \mathcal{I}(t)\mathcal{Q}\tilde{\rho}(0) + \mathcal{K}(t)\mathcal{P}\tilde{\rho}(t)}$$

where

$$\mathcal{I}(t) = \epsilon \mathcal{P}\mathcal{L}(t)\left[1 - \Sigma(t)\right]^{-1} G(t,0)\mathcal{Q}$$
$$\mathcal{K}(t) = \epsilon \mathcal{P}\mathcal{L}(t)\left[1 - \Sigma(t)\right]^{-1} \mathcal{P}$$

- For a product initial state $\mathcal{I}(t)\mathcal{Q}\tilde{\rho}(0) = 0$

Time Convolutionless ME

Perturbative Expansion

- Consider the case of product init. state
- Write

$$[1-\Sigma(t)]^{-1} = \sum_{n=0}^{\infty} \Sigma(t)^n, \quad \Sigma(t) = \sum_{k=1}^{\infty} \epsilon^k \Sigma_k(t)$$

- We have

$$\begin{aligned}\mathcal{K}(t) =& \epsilon \mathcal{P} \mathcal{L}(t) \left[1-\Sigma(t)\right]^{-1} \mathcal{P} \\ =& \epsilon \mathcal{P} \mathcal{L}(t) \sum_{n=0}^{\infty} \left(\sum_{k=1}^{\infty} \epsilon^k \Sigma_k(t) \right)^n \mathcal{P} \\ \equiv& \sum_{m=1}^{\infty} \epsilon^m \mathcal{K}_m(t)\end{aligned}$$

- Collecting coeffs. of ϵ^m

$$
\begin{aligned}
\mathcal{K}_1(t) &= \mathcal{P}\mathcal{L}(t)\mathcal{P} = 0 \\
\mathcal{K}_2(t) &= \mathcal{P}\mathcal{L}(t)\Sigma_1(t)\mathcal{P} \\
\mathcal{K}_3(t) &= \mathcal{P}\mathcal{L}(t)\left\{\Sigma_1(t)^2 + \Sigma_2(t)\right\}\mathcal{P} \\
\mathcal{K}_4(t) &= \mathcal{P}\mathcal{L}(t)\left\{\Sigma_1(t)^3 + \Sigma_1(t)\Sigma_2(t) + \Sigma_2(t)\Sigma_1(t) + \Sigma_3(t)\right\}\mathcal{P} \\
&\cdots
\end{aligned}
$$

- Recall $\Sigma(t) \equiv \epsilon \int_0^t ds\, G(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\mathcal{U}_-(t,s)$

$$
\begin{aligned}
G(t,s) &\equiv \mathbb{T}_+ e^{\epsilon \int_s^t dt'\ \mathcal{Q}\mathcal{L}(t')} \\
&= 1 + \epsilon \int_s^t dt'\ \mathcal{Q}\mathcal{L}(t') + \frac{\epsilon^2}{2}\int_s^t dt_1 \int_s^{t_1} dt_2\ \mathcal{Q}\mathcal{L}(t_1)\mathcal{Q}\mathcal{L}(t_2) + O(\epsilon^3) \\
\mathcal{U}_-(t,s) &\equiv \mathbb{T}_- e^{-\epsilon \int_s^t dt'\ \mathcal{L}(t')} \\
&= 1 - \epsilon \int_s^t dt'\ \mathcal{L}(t') + \frac{\epsilon^2}{2}\int_s^t dt_1 \int_s^{t_1} dt_2\ \mathcal{L}(t_2)\mathcal{L}(t_1) + O(\epsilon^3)
\end{aligned}
$$

TCL ME

Lowest order contribution

From above expressions, we have

$$\Sigma_1(t) = \int_0^t ds\ \mathcal{Q}\mathcal{L}(s)\mathcal{P}$$

$$\Rightarrow \quad \mathcal{K}_2(t) = \mathcal{P}\mathcal{L}(t)\Sigma_1(t)\mathcal{P} = \int_0^t ds\ \mathcal{P}\mathcal{L}(t)\underbrace{\mathcal{Q}}_{1-\mathcal{P}}\mathcal{L}(s)\mathcal{P}$$

$$= \int_0^t ds\ \mathcal{P}\mathcal{L}(t)\mathcal{L}(s)\mathcal{P} \qquad (\because\ \mathcal{P}\mathcal{L}\mathcal{P} = 0)$$

Lowest order TCL ME: $\partial_t \mathcal{P}\tilde{\rho}(t) = \epsilon^2 \mathcal{K}_2(t)\mathcal{P}\tilde{\rho}(t)$

$$\partial_t \tilde{\rho}_{\rm S}(t) = -\epsilon^2 \int_0^t ds\ {\rm Tr}_{\rm B}\left[\tilde{H}_{\rm I}(t), \left[\tilde{H}_{\rm I}(s), \underline{\underline{\tilde{\rho}_{\rm S}(t)}} \otimes \rho_{\rm B}\right]\right]$$

- $=$ Redfield equation (usually $\tilde{H}_{\rm I}(s) \to \tilde{H}_{\rm I}(t-s)$)
- Non-CP; Obtained usually from Born-Markov approximation
- c. f. Lowest order NZ equation contains $\tilde{\rho}_{\rm S}(s)$ at time s not t

TCL ME

The Next Order: $\mathcal{K}_3$

Note that

$$\Sigma_1(t)^2 = \int_0^t ds \int_0^t ds'\ \mathcal{Q}\mathcal{L}(s)\underset{\sim\sim}{\mathcal{P}\mathcal{Q}}\mathcal{L}(s')\mathcal{P} = 0$$

and

$$\Sigma_2(t) = \int_0^t dt_1 \int_0^{t_1} dt_2\ \Big\{\mathcal{Q}\mathcal{L}(t_1)\mathcal{Q}\mathcal{L}(t_2)\mathcal{P} - \mathcal{Q}\mathcal{L}(t_2)\mathcal{P}\mathcal{L}(t_1)\Big\}$$

Therefore

$$\begin{aligned}
\mathcal{K}_3(t) =& \mathcal{P}\mathcal{L}(t)\left\{\cancelto{0}{\Sigma_1(t)^2} + \Sigma_2(t)\right\}\mathcal{P} \\
=& \int_0^t dt_1 \int_0^{t_1} dt_2\ \mathcal{P}\mathcal{L}(t)\Big\{\underbrace{\mathcal{Q}}_{1-\mathcal{P}}\mathcal{L}(t_1)\underbrace{\mathcal{Q}}_{1-\mathcal{P}}\mathcal{L}(t_2)\mathcal{P} - \mathcal{Q}\mathcal{L}(t_2)\underset{\sim\sim\sim\sim}{\mathcal{P}\mathcal{L}(t_1)\Big\}\mathcal{P}} \\
=& \int_0^t dt_1 \int_0^{t_1} dt_2\ \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{P}
\end{aligned}$$

- This vanishes as for odd number of $\mathcal{L}$ we can set

$$\mathcal{P}\mathcal{L}(t_1)\cdots\mathcal{L}(t_{2k-1})\mathcal{P} = 0$$

- As in proof of $\mathcal{P}\mathcal{L}\mathcal{P} = 0$, this involves setting odd moments to zero

$$\mathrm{Tr}_{\mathrm{B}}(\tilde{H}_{\mathrm{I}}(t_1)\cdots\tilde{H}_{\mathrm{I}}(t_{2k-1})\rho_{\mathrm{B}}) \Rightarrow \mathrm{Tr}_{\mathrm{B}}(\underbrace{H_{\mathrm{I}}\cdots H_{\mathrm{I}}}_{2k-1}\rho_{\mathrm{B}}) = 0$$

- First nonvanishing contribution beyond Born-Markov approximation is $\mathcal{K}_4$

TCL ME

Leading order beyond Born-Markov approximation: $\mathcal{K}_4$

- Recall

$$\mathcal{K}_4(t) = \mathcal{P}\mathcal{L}(t)\left\{\cancelto{0}{\Sigma_1(t)^3} + \cancelto{0}{\Sigma_1(t)\Sigma_2(t)} + \Sigma_2(t)\Sigma_1(t) + \Sigma_3(t)\right\}\mathcal{P}$$

- 1st term

$$\Sigma_1(t)^3 = \int_0^t ds \int_0^t ds' \int_0^t ds''\ \mathcal{Q}\mathcal{L}(s)\underset{\sim}{\mathcal{P}\mathcal{Q}}\mathcal{L}(s')\underset{\sim}{\mathcal{P}\mathcal{Q}}\mathcal{L}(s'')\mathcal{P} = 0$$

- 2nd term

$$\Sigma_1(t)\Sigma_2(t) = \int_0^t ds \int_0^t dt_1 \int_0^{t_1} dt_2$$
$$\times\ \mathcal{Q}\mathcal{L}(s)\underset{\sim}{\mathcal{P}}\Big\{\underset{\sim}{\mathcal{Q}}\mathcal{L}(t_1)\mathcal{Q}\mathcal{L}(t_2)\mathcal{P} - \underset{\sim}{\mathcal{Q}}\mathcal{L}(t_2)\mathcal{P}\mathcal{L}(t_1)\Big\} = 0$$

- We need

$$\Sigma_3(t) = \frac{1}{2}\int_0^t ds \int_s^t dt_1 \int_s^t dt_2 \left\{\mathcal{QL}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(s)\mathcal{P} + \mathcal{QL}(s)\mathcal{PL}(t_2)\mathcal{L}(t_1) - 2\mathcal{QL}(t_1)\mathcal{QL}(s)\mathcal{PL}(t_2)\right\}$$

- Using $\mathcal{Q} = 1 - \mathcal{P}$ and invoking $\mathcal{PLP} = 0$ repeatedly, we arrive at

$$\mathcal{K}_4(t) = \int_0^t ds \int_0^s dt_1 \int_0^{t_1} dt_2 \left\{\mathcal{PL}(t)\mathcal{L}(s)\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{P} - \mathcal{PL}(t)\mathcal{L}(s)\mathcal{PL}(t_1)\mathcal{L}(t_2)\mathcal{P} - \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{PL}(s)\mathcal{L}(t_2)\mathcal{P} - \mathcal{PL}(t)\mathcal{L}(t_2)\mathcal{PL}(s)\mathcal{L}(t_1)\mathcal{P}\right\}$$

Exact ME: Hu-Paz-Zhang Equation

Caldeira-Leggett Model for Quantum Brownian Motion of Harmonic Oscillator

[Hu, Paz and Zhang, Phys. Rev. D **45**, 2843 (1992)]

- System

$$H_S = \frac{p^2}{2M} + \frac{1}{2} M\Omega^2 q^2$$

- Bath

$$H_B = \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 q_j^2 \right) = \sum_j \hbar\omega_j (b_j^\dagger b_j + \frac{1}{2})$$

- Interaction: $H_I = -q \sum_j \kappa_j q_j \equiv -qB$
- Including the counterterm, total Hamiltonian is

$$H = \frac{p^2}{2M} + \frac{1}{2} M\Omega^2 q^2 + \sum_j \left(\frac{p_j^2}{2m_j} + \frac{m_j\omega_j^2}{2} (q_j - \frac{\kappa_j}{m_j\omega_j^2} q)^2 \right)$$

- Effect of counter term is the renormalization of $\tilde{\Omega}^2 = \Omega^2 + \mu/M$ where $\mu \equiv \sum_j \kappa_j^2/(m_j\omega_j^2)$

HPZ equation

Sketch of Derivation

- Original derivation by HPZ: Using Influence funtional in path integral formalism
- Simpler and more intuitive derivation by Halliwell and Yu [Phys. Rev. D **53** 2012 (1996)]
- Use Wigner function representations for $\rho_s(t) = \mathrm{Tr}_B \rho(t)$

$$W(q,p;q_n,p_n;t) = \int \frac{dy}{2\pi\hbar} \int \prod_n \frac{dy_n}{2\pi\hbar}\, e^{-ipy/\hbar - i\sum_n p_n y_n/\hbar} \times \left\langle q + \frac{y}{2}, q_n + \frac{y_n}{2} \,|\rho(t)|\, q + \frac{y}{2}, q_n + \frac{y_n}{2} \right\rangle$$

$$W_S(q,p;t) = \int \frac{dy}{2\pi\hbar} \left\langle q + \frac{y}{2} \,|\rho_S(t)|\, q + \frac{y}{2} \right\rangle = \int \prod_n dq_n dp_n\, W(q,p;q_n,p_n;t)$$

- Evolution equation for total density operator $\partial_t \rho = -(i/\hbar)[H,\rho]$ translates into

$$\frac{\partial}{\partial t} W(q,p;q_n,p_n;t) = -\frac{p}{M}\frac{\partial W}{\partial q} + M\tilde{\Omega}^2 q \frac{\partial W}{\partial p} + \sum_n \left(-\frac{p_n}{m_n}\frac{\partial W}{\partial q_n} + m_n \omega_n^2 q_n \frac{\partial W}{\partial p_n} \right) - \sum_n \kappa_n \left(q_n \frac{\partial W}{\partial p} + q \frac{\partial W}{\partial q_n} \right)$$

- Linear system $\Rightarrow$ Same as classical Liouville equation: $\partial_t W = \{H, W\}_{\rm PB}$
- Integrating over q_i, p_i,

$$\partial_t W_{\rm S}(q,p;t) = -\frac{p}{M}\frac{\partial W_{\rm S}}{\partial q} + M\tilde{\Omega}^2 q \frac{\partial W_{\rm S}}{\partial q} \underbrace{- \int \prod_i dq_i dp_i \left(\sum_n \kappa_n q_n \right) \frac{\partial W}{\partial p}}$$

- How to express $(\cdots\cdots)$ in terms of $W_{\rm S}$?

Key points in derivation

- Consider

$$\tilde{G}(k,k') = \int dq dp \, e^{ikq+ik'p} \underbrace{\int \prod_i dq_i dp_i \, (\sum_n \kappa_n q_n) W}_{\equiv G(q,p)}$$

- W satisfies classical Liouville equation

$$\begin{aligned} W(q(t),p(t);q_n(t),p_n(t);t) &= W(q(0),p(0);q_n(0),p_n(0);0) \\ &= W_{\rm S}(q(0),p(0)) \underbrace{W_{\rm B}(q_n(0),p_n(0))}_{\text{canonical at } \beta} \end{aligned}$$

- Change the integration variables $\int dq dp \prod dq_n dp_n$ to $\int dq(0) dp(0) \prod dq(0) dp(0)$
- Express everything in terms of $(q(0),p(0),q_n(0),p_n(0))$ (formally)

$$\sum_n \kappa_n q_n(t) = f(t) q(0) + g(t) p(0) + \sum_n (f_n(t) q_n(0) + g_n(t) p_n(0))$$

- Use the Gaussian property of $W_{\rm B}$. We then find that $\tilde{G}(k,k')$ is a linear combination of terms with k, k', $\partial/\partial k$ and $\partial/\partial k'$ operating on $\tilde{W}_{\rm S}(k,k')$
- Therefore for some $A(t), B(t), C(t), D(t)$,
  $G(q,p) = A(t)qW_{\rm S} + B(t)pW_{\rm S} + C(t)\partial W_{\rm S}/\partial q + D(t)\partial W_{\rm S}/\partial p$

HPZ master equation

$$\frac{\partial}{\partial t}W_{\rm S}(q,p;t) = -\frac{p}{M}\frac{\partial W_{\rm S}}{\partial q} + M\tilde{\Omega}^2 q\frac{\partial W_{\rm S}}{\partial q} + A(t)q\frac{\partial W_{\rm S}}{\partial p} + B(t)\frac{\partial(pW_{\rm S})}{\partial p} + C(t)\frac{\partial^2 W_{\rm S}}{\partial p\partial q} + D(t)\frac{\partial^2 W_{\rm S}}{\partial p^2}$$

In the operator form

$$\frac{d}{dt}\rho_{\rm S}(t) = -\frac{i}{\hbar}\left[\frac{p^2}{2M} + \frac{1}{2}(M\tilde{\Omega}^2 + A(t))q^2, \rho_{\rm S}(t)\right] - \frac{i}{2\hbar}B(t)[q,\{p,\rho_{\rm S}(t)\}] + \frac{1}{\hbar^2}C(t)[q,[p,\rho_{\rm S}(t)]] - \frac{1}{\hbar^2}D(t)[q,[q,\rho_{\rm S}(t)]]$$

- $A(t), B(t), C(t), D(t)$ are obtained by considering time derivatives of averages $\langle q\rangle, \langle p\rangle, \langle p^2\rangle, \langle q^2\rangle, \langle qp+qp\rangle$ using equtions for both W and $W_{\rm S}$
- They are given in terms solutions of differential equations describing classical motion.

$$\ddot{u}(t) + \tilde{\Omega}^2 u(t) + \frac{1}{M}\int_0^t ds\, \eta(t-s)u(s) = 0$$

$$\frac{\partial^2}{\partial t^2}G(t,s) + \tilde{\Omega}^2 G(t,s) + \frac{1}{M}\int_0^t ds'\, \eta(t-s')G(s',s) = \delta(t-s)$$

- Two functions describing bath properties:

$$\eta(t) = -\sum_n \frac{\kappa_n^2}{m_n\omega_n}\sin(\omega_n t)$$

$$\nu(t) = \sum_n \frac{\kappa_n^2}{2m_n\omega_n}\cos(\omega_n t)\coth\left(\frac{\beta\hbar\omega_n}{2}\right)$$

- Properties of these functions have been studied only recently [see Homa et al, Phys. Rev. A **108**, 012210 (2023)]

HPZ ME

Weak Coupling Limit

- To the lowest order of coupling constant κ_n^2, we find

$$A(t) = \int_0^t ds\, \eta(s) \cos(\tilde{\Omega} s), \qquad B(t) = -\frac{1}{M\tilde{\Omega}} \int_0^t ds\, \eta(s) \sin(\tilde{\Omega} s)$$

$$C(t) = \frac{\hbar}{M\tilde{\Omega}} \int_0^t ds\, \nu(s) \sin(\tilde{\Omega} s), \qquad D(t) = \hbar \int_0^t ds\, \nu(s) \cos(\tilde{\Omega} s)$$

- Note that for $H_{\rm I} = -q \sum_n \kappa q_n \equiv q \otimes B$, where $B = -\sum_n \kappa_n q_n$, we can show that

$$G(t) \equiv {\rm Tr}_{\rm B}[B(t) B \rho_{\rm B}] = \hbar[\nu(t) + \frac{i}{2}\eta(t)]$$

- Note that for $H_{\mathrm{I}} = q \otimes B$, Redfield equation can be written as

$$\partial_t \rho_{\mathrm{S}}(t) = -\frac{i}{\hbar}[H_{\mathrm{S}}, \rho_{\mathrm{S}}] - \frac{1}{\hbar^2}\int_0^t ds\, \Big(G(s)[q, \tilde{q}(-s)\rho_{\mathrm{S}}(t)] \\ - G^*(s)[q, \rho_{\mathrm{S}}(t)\tilde{q}(-s)] \Big)$$

- $\tilde{q}$ is given by

$$\tilde{q}(-s) = q\cos(\tilde{\Omega}s) - \frac{p}{M\tilde{\Omega}}\sin(\tilde{\Omega}s)$$

- Then one can check that HPZ equation reduces to Redfield equation to this order

$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = -\frac{i}{\hbar}\left[\frac{p^2}{2M} + \frac{1}{2}(M\tilde{\Omega}^2 + A(t))q^2, \rho_{\mathrm{S}}(t)\right] - \frac{i}{2\hbar}B(t)[q, \{p, \rho_{\mathrm{S}}(t)\}] \\ + \frac{1}{\hbar^2}C(t)[q, [p, \rho_{\mathrm{S}}(t)]] - \frac{1}{\hbar^2}D(t)[q, [q, \rho_{\mathrm{S}}(t)]]$$

Summary

- Markovian and Non-Markovian QME
- We have presented some formal methods to trace out the bath part for quantum systems described by $H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}}$
  - Nakajima-Zwanzig equation
  - Time Convolutionless ME
  - Hu-Paz-Zhang exact ME