Quantum Master Equations: Methods and Properties

Joonhyun Yeo

Konkuk University

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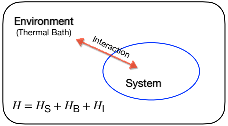
Outline

Open Systems, Classical and Quantum

- System interacting with Environment (e. g. heat bath) which has larger degrees of freedom
- How to treat (or integrate out) effect of Environment



  - Open Classical Systens
    - Langevin: Effective dynamical equation for classical states $\boldsymbol{x}(t)$ including stochastic elements
    - Fokker-Planck: Corresponding (deterministic) equation for probability density function $P(\boldsymbol{x}, t) = \langle \delta(\boldsymbol{x} - \boldsymbol{x}(t)) \rangle$
  - Open Quantum Systems
    - One can set up Quantum Langevin equations for observables $\hat{O}(t)$ (in Heisenberg picture)
    - For more complete description, one needs an equation for the density operator $\rho(t)$ describing the quantum state.

Model Hamiltonian for an Open System

- System

$$H_S = \frac{p^2}{2m} + U(x)$$

- Bath

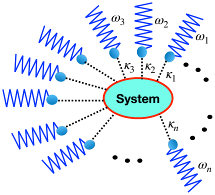
$$H_B = \sum_n \left(\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 q_n^2 \right)$$

- Interaction:

$$H_I = -x \underbrace{\sum_n \kappa_n q_n}_{\equiv B}$$

- Total Hamiltonian

$$H = \frac{p^2}{2m} + U(x) + \sum_n \left(\frac{p_n^2}{2m_n} + \frac{m_n \omega_n^2}{2} (q_n - \frac{\kappa_n}{m_n \omega_n^2} x)^2 \right)$$



Heat bath as a collection of harmonic oscillators

Equations of Motion

- Heisenberg Eqs. of motion:
  - System

$$\dot{x}(t) = \frac{i}{\hbar}[H, x(t)] = \frac{p(t)}{m},$$

$$\dot{p}(t) = \frac{i}{\hbar}[H, p(t)] = -U'(x) + \underbrace{\sum_j \kappa_j q_j(t)} - \sum_j \frac{\kappa_j^2}{m_j \omega_j^2} x(t)$$

  - Bath

$$\dot{q}_j(t) = \frac{i}{\hbar}[H, q_j(t)] = \frac{p_j(t)}{m_j}$$

$$\dot{p}_j(t) = \frac{i}{\hbar}[H, p_j(t)] = -m_j \omega_j^2 q_j(t) + \kappa_j x(t)$$

Equations of Motion

- Bath eqs. of motion are linear: Rewrite the eqs. for $\{q_j, p_j\}$ as

$$\dot{\mathtt{Q}}(t) = \mathtt{A} \cdot \mathtt{Q}(t) + \mathtt{R}(t)$$

where

$$\mathtt{Q}(t) = \begin{pmatrix} q_j(t) \\ p_j(t) \end{pmatrix}, \quad \mathtt{A} = \begin{pmatrix} 0 & 1/m_j \\ -m_j\omega_j^2 & 0 \end{pmatrix}, \quad \mathtt{R}(t) = \begin{pmatrix} 0 \\ \kappa_j x(t) \end{pmatrix}$$

- The solution to this equation is

$$\mathtt{Q}(t) = e^{\mathtt{A}t} \cdot \mathtt{Q}(0) + \int_0^t ds\; e^{\mathtt{A}(t-s)} \cdot \mathtt{R}(s)$$

- We have

$$q_j(t) = q_j(0)\cos(\omega_j t) + p_j(0)\frac{1}{m_j\omega_j}\sin(\omega_j t) + \frac{\kappa_j}{m_j\omega_j}\int_0^t ds\; \sin(\omega_j(t-s))x(s)$$

Equations of Motion

- We need

$$\sum_j \kappa_j q(t) = \underbrace{\widetilde{B}(t)}_{\text{noise}} + \underbrace{\sum_j \frac{\kappa_j^2}{m_j\omega_j} \int_0^t ds\ \sin(\omega_j(t-s))x(s)}_{\text{dissipation}},$$

where

$$\widetilde{B}(t) \equiv \sum_j \kappa_j (q_j(0)\cos(\omega_j t) + \frac{p_j(0)}{m_j\omega_j}\sin(\omega_j t))$$

$$= \sum_j \kappa_j \sqrt{\frac{\hbar}{2m_j\omega_j}}(e^{-i\omega_j t} b_j + e^{i\omega_j t} b_j^\dagger)$$

with $q_j(0) = \sqrt{\frac{\hbar}{2m_j\omega_j}}(b_j + b_j^\dagger)$, $\quad p_j(0) = -i\sqrt{\frac{\hbar m_j\omega_j}{2}}(b_j - b_j^\dagger)$

- Note that $\widetilde{B}(t)$ is $B(0) = \sum_j \kappa_j q_j(0)$ at time t in the interaction picture

$$\widetilde{B}(t) = e^{iH_B t/\hbar} B(0) e^{-iH_B t/\hbar}$$

Quantum Langevin Equation

- Plugging this into system eq, of motion, we have

$$\dot{p}(t) = -U'(x) - \sum_j \frac{\kappa_j^2}{m_j\omega_j^2} x(t) + \sum_j \frac{\kappa_j^2}{m_j\omega_j} \int_0^t ds \ \sin(\omega_j(t-s))x(s) + \tilde{B}(t)$$
$$= -U'(x) - \frac{d}{dt}\int_0^t ds \, \gamma(t-s)x(s) + \tilde{B}(t)$$
$$= -U'(x) - \int_0^t ds \, \gamma(t-s)\dot{x}(s) + \xi(t),$$

  where $\xi(t) = \tilde{B}(t) - \gamma(t)x(0)$.
- Generalized Langevin equation with dissipation kernel $\gamma(t)$

Spectral Density

- Here, the dissipation kernel is

$$\gamma(t) \equiv \sum_j \frac{\kappa_j^2}{m_j \omega_j^2} \cos(\omega_j t), \quad t > 0$$

- Properties of the bath are specified by the spectral density

$$J(\omega) \equiv \sum_n \frac{\kappa_n^2}{2 m_n \omega_n} \delta(\omega - \omega_n)$$

such that one can write

$$\gamma(t) = 2 \int_0^\infty d\omega \, \frac{J(\omega)}{\omega} \cos(\omega t)$$

Bath correlation function

- $\tilde{B}(t)$ (or $\xi(t)$) plays a role of stochastic force from the bath.
- Bath correlation function is another quantity specifying the bath

$$C(t) \equiv \langle \tilde{B}(t)B(0)\rangle = \mathrm{Tr}_{\mathrm{B}}[\tilde{B}(t)B\rho_{\mathrm{B}}]$$

where $\rho_B = (1/Z)e^{-\beta H_B}$ with $Z = \mathrm{Tr}e^{-\beta H_B}$.

- We have

$$C(t) = \nu(t) + \frac{i}{2}\eta(t),$$

where

$$\nu(t) = \frac{1}{2}\langle\{\tilde{B}(t), B\}\rangle = \hbar\int_0^\infty d\omega\ J(\omega)\coth(\frac{1}{2}\beta\hbar\omega)\cos(\omega t),$$

$$\eta(t) = \frac{1}{i}\langle[\tilde{B}(t), B]\rangle = -2\hbar\int_0^\infty d\omega\ J(\omega)\sin(\omega t)$$

- In the classical limit $\beta\hbar\omega \ll 1$,

$$\frac{1}{2}\langle\{\tilde{B}(t), B\}\rangle = k_B T\gamma(t)$$

Connection with classical generalized Langevin equation

- Recall that $\tilde{B}(t) = \sum_j \kappa_j \left\{ q_j(0)\cos(\omega_j t) + p_j(0)\frac{1}{m_j\omega_j}\sin(\omega_j t) \right\}$
- Therefore the shifted stochastic force is

$$
\begin{aligned}
\xi(t) &\equiv \tilde{B}(t) - \gamma(t)x(0) \\
&= \sum_j \kappa_j \left\{ \left(q_j(0) - \frac{\kappa_j}{m_j\omega_j^2}x(0) \right) \cos(\omega_j t) + p_j(0)\frac{1}{m_j\omega_j}\sin(\omega_j t) \right\}.
\end{aligned}
$$

- Noting that q_j, p_i and x operator on different Hilbert space, we see that $\xi(t)$ satisfies the exactly same statistics as $\tilde{B}(t)$ when we use the shifted bath Hamiltonian, i.e. $\rho_B' = (1/Z')e^{-\beta H_B'}$, where

$$
H_B' = \sum_j \left[\frac{p_j^2(0)}{2m_j} + \frac{1}{2}m_j\omega_j^2 \left(q_j(0) - \frac{\kappa_j}{m_j\omega_j^2}x(0) \right)^2 \right]
$$

Classical Markovian vs. Non-Markovian Dynamics

- Classical Markov limit: Ohmic bath

$$J(\omega) = \gamma\omega \Rightarrow \gamma(t) = 2\gamma\delta(t)$$

Then

$$\int_0^t ds\, \gamma(t-s)\dot{x}(s) = \gamma\dot{x}(t)$$

- Classical Non-Markovian memory effect: Drude form, for example

$$J(\omega) = \gamma\omega\frac{\Omega^2}{\omega^2+\Omega^2} \Rightarrow \gamma(t) = \gamma\Omega\exp(-\Omega t)$$

Then the memory effect for the time scale $\tau \sim \Omega^{-1}$.

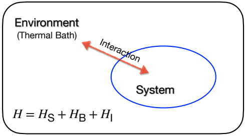
- Quantum Markovian dynamics requires more complicated conditions as we will see below.

Dynamical Maps

- Total System+Bath (SB) is a closed system:

$$\rho_{\rm SB}(t_1) = U(t_1, t_0)\rho_{\rm SB}(t_0)U^\dagger(t_1, t_0),$$
$$\frac{d}{dt}\rho_{\rm SB}(t) = -i[H, \rho_{\rm SB}(t)]$$

where
$U(t_1, t_0) = \exp[-iH(t_1 - t_0)/\hbar]$

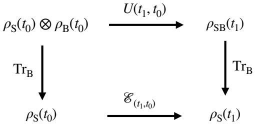


- Reduced Density Operator

$$\rho_{\rm S}(t_1) = {\rm Tr}_{\rm B}\rho_{\rm SB}(t_1)$$

- Let ${\rm Tr}_{\rm B}\rho_{\rm SB}(t_0) = \rho_{\rm S}(t_0)$.

$${\rm Dynamical\ Map}: \ \rho_{\rm S}(t_1) = \mathcal{E}_{(t_1,t_0)}[\rho_{\rm S}(t_0)]$$



Universal Dynamical Map

- If we can write $\rho_{\mathrm{S}\mathrm{B}}(t_0) = \rho_{\mathrm{S}}(t_0) \otimes \rho_{\mathrm{B}}(t_0)$ then

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

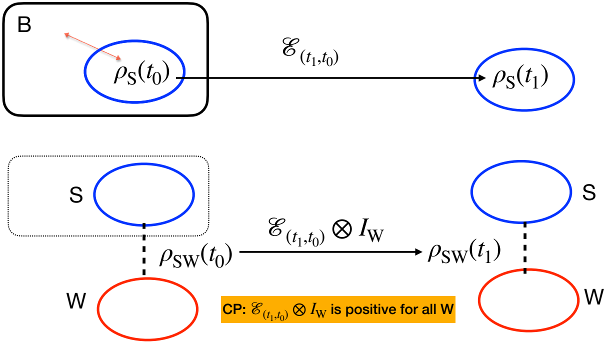
  where $\sum_\alpha K_\alpha^\dagger(t_1,t_0)K_\alpha(t_1,t_0) = \mathbb{1}$
  - Write $\rho_{\mathrm{B}}(t_0) = \sum_\nu \lambda_\nu |\nu\rangle\langle\nu|$, then

$$\begin{aligned}\rho_{\mathrm{S}}(t_1) &= \sum_{\mu} \langle\mu|U(t_1,t_0)\rho_{\mathrm{S}}(t_0) \otimes \sum_{\nu} \lambda_\nu |\nu\rangle\langle\nu| U^\dagger(t_1,t_0)|\mu\rangle \\ &= \sum_{\mu\nu} \underbrace{\sqrt{\lambda_\nu}\langle\mu|U(t_1,t_0)|\nu\rangle}_{K_{\mu\nu}(t_1,t_0)} \rho_{\mathrm{S}}(t_0) \underbrace{\sqrt{\lambda_\nu}\langle\nu|U^\dagger(t_1,t_0)|\mu\rangle}_{K^\dagger_{\mu\nu}(t_1,t_0)}\end{aligned}$$

- If not a product initial state,
  $\rho_{\mathrm{S}}(t_1) = \sum_\alpha K_\alpha(t_1,t_0)\rho_{\mathrm{S}}(t_0)K_\alpha^\dagger(t_1,t_0) + \delta\rho(t_1,t_0;\rho_{\mathrm{S}}(t_0))$

Complete Positivity

- UDM is necessary and sufficient condition for Completely Positivity (CP) (Kraus 1983)



Complete Positivity

- UDM is positive

$$\langle\nu|\mathcal{E}[\rho_{\rm S}(t_0)]|\nu\rangle = \sum_\alpha \langle\nu|K_\alpha\rho_{\rm S}(t_0)\underbrace{K_\alpha^\dagger|\nu\rangle}_{=|\mu_\alpha\rangle} = \sum_\alpha \langle\mu_\alpha|\underbrace{\rho_{\rm S}(t_0)}_{=\sum_i \lambda_i|i\rangle\langle i|}|\mu_\alpha\rangle$$
$$= \sum_{\alpha,i} \lambda_i |\langle\mu_\alpha|i\rangle|^2 > 0$$

- UDM is CP

$$\langle\nu|(\mathcal{E}\otimes I_W)[\rho_{\rm SW}(t_0)]|\nu\rangle = \sum_\alpha \langle\nu|(K_\alpha\otimes\mathcal{I}_W)\rho_{\rm SW}(t_0)\underbrace{(K^\dagger\otimes\mathcal{I}_W)|\nu\rangle}_{=|\mu_\alpha\rangle}$$
$$= \sum_\alpha \langle\mu_\alpha|\underbrace{\rho_{\rm SW}(t_0)}_{=\sum_i \lambda_i|i\rangle\langle i|}|\mu_\alpha\rangle = \sum_{\alpha,i} \lambda_i|\langle\mu_\alpha|i\rangle|^2 > 0$$

- Every CP map is UDM: Proof is more difficult (Kraus 1983)

Divisibility of a Quantum Dynamical Map

- For a quantum map $\mathcal{E}_t \equiv \mathcal{E}_{(t,0)}$, if $\mathcal{E}_t^{-1}$ exists for all $t > 0$, one can define $\mathcal{E}_{(t_2,t_1)} \equiv \mathcal{E}_{t_2}\mathcal{E}_{t_1}^{-1}$ and have the property

$$\mathcal{E}_{(t_2,0)} = \mathcal{E}_{(t_2,t_1)}\mathcal{E}_{(t_1,0)}$$

- Then

$$\begin{aligned}\rho_{\mathrm{S}}(t+\epsilon) - \rho_{\mathrm{S}}(t) =& [\mathcal{E}_{(t+\epsilon,0)} - \mathcal{E}_{(t,0)}]\rho_{\mathrm{S}}(0) \\ =& [\mathcal{E}_{(t+\epsilon,t)} - \mathbb{1}]\mathcal{E}_{(t,0)}\rho_{\mathrm{S}}(0) = [\mathcal{E}_{(t+\epsilon,t)} - \mathbb{1}]\rho_{\mathrm{S}}(t)\end{aligned}$$

and we have time-local QME

$$\frac{d\rho_{\mathrm{S}}(t)}{dt} = \lim_{\epsilon\to 0}\frac{\mathcal{E}_{(t+\epsilon,t)} - \mathbb{1}}{\epsilon}\rho_{\mathrm{S}}(t) \equiv \mathcal{L}_t[\rho_{\mathrm{S}}(t)]$$

Dynamical Semigroup

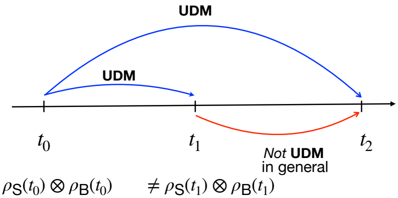
- If it further satisfies $\mathcal{E}_{(t_2,t_1)} = \mathcal{E}_{t_2-t_1}$, we have a semigroup:

$$\mathcal{E}_{t+s} = \mathcal{E}_t \mathcal{E}_s$$

Then one can write for a time-independent generator $\mathcal{L}$

$$\mathcal{E}_t = e^{\mathcal{L}t}, \qquad \frac{d\rho_{\mathrm{S}}(t)}{dt} = \mathcal{L}[\rho_{\mathrm{S}}(t)]$$

CP divisibility and Quantum Markovianity



- Even if $\mathcal{E}_t \equiv \mathcal{E}_{(t,t_0)}$ is CP by construction for all t, in general, $\mathcal{E}_{(t_2,t_1)}$ need not be CP (not even positive) since $\mathcal{E}_t^{-1}$ need not be positive.
- A dynamical map is CP-divisible (Markovian) if $\mathcal{E}_{(t_2,t_1)}$ is UDM (i.e. CP) for all $t_2 \geq t_1$.
- Classical analogue: Chapman-Kolmogorov equation $p(x_3, t_3|x_1, t_1) = \int dx_2 \; p(x_3, t_3|x_2, t_2)p(x_2, t_2|x_1, t_1)$

Gorini-Kossakowski-Sudarshan-Lindblad Equation

- A dynamical map $\mathcal{E}$ satisfying the semigroup property is CP *iff* the generator $\mathcal{L}$ can be expressed as

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

$$\equiv \underbrace{-i[\mathcal{H}, \rho_{\mathrm{S}}(t)]}_{\text{unitary}} + \underbrace{\mathcal{D}[\rho_{\mathrm{S}}(t)]}_{\text{dissipator}}$$

where $\mathcal{H}$ is hermitian and $\boxed{\gamma_k \geq 0}$ for all k

Lindblad Equation with Time-dependent Generator

- A dynamical map is CP-divisible *iff* the time-dependent generator $\mathcal{L}_t$ takes the form

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

  with $\boxed{\gamma_k(t) \geq 0}$ for all k and t

- Open Problem: What is the condition for $\mathcal{E}_{(t_2,t_1)} = \mathbb{T}\exp[\int_{t_1}^{t_2} \mathcal{L}_t dt]$ to be CP?
  - Sufficient condition: $\gamma_k(t) \geq 0$; Necessary condition: unknown
  - $\exists$ examples of $\gamma_k(t)$ becoming negative for some t, but the resulting $\mathcal{E}_{(t_2,t_1)}$ is CP

Derivation of QME from Hamiltonian

- Interaction Hamiltonian

$$H_{\mathrm{I}} = \epsilon \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}$$

- Total system is closed; (interaction picture: $H = H_0 + H_{\mathrm{I}}$, $H_0 = H_{\mathrm{S}} + H_{\mathrm{B}}$)

$$\frac{d}{dt}\tilde{\rho}_{\mathrm{SB}}(t) = -i\left[\tilde{H}_{\mathrm{I}}(t), \tilde{\rho}_{\mathrm{SB}}(t)\right]$$

or

$$\tilde{\rho}_{\mathrm{SB}}(t) = \tilde{\rho}_{\mathrm{SB}}(0) - i\int_0^t ds\ \left[\tilde{H}_{\mathrm{I}}(s), \tilde{\rho}_{\mathrm{SB}}(s)\right]$$

- Eq. for reduced density operator (exact)

$$\frac{d}{dt}\tilde{\rho}_{\mathrm{S}}(t) = -\mathrm{Tr}_{\mathrm{B}}\int_0^t ds\ \left[\tilde{H}_{\mathrm{I}}(t), \left[\tilde{H}_{\mathrm{I}}(t-s), \underset{\sim}{\tilde{\rho}_{\mathrm{SB}}(t-s)}\right]\right]$$

- One can always make

$$\mathrm{Tr}_{\mathrm{B}}\left[\tilde{H}_{\mathrm{I}}(t), \tilde{\rho}_{\mathrm{SB}}(0)\right] = 0$$

Born-Markov Approximation and Redfield Equation

- Born-Markov approximation

$$\frac{d\tilde{\rho}_{\rm S}(t)}{dt} = -\int_0^{\infty} ds\, {\rm Tr}_{\rm B}[\tilde{H}_{\rm I}(\underline{t}), [\tilde{H}_{\rm I}(\underline{t-s}), \tilde{\rho}_{\rm S}(t) \otimes \rho_{\rm B}]].$$

  - Weak Coupling (Born): $\tilde{\rho}_{\rm SB}(t-s) \simeq \tilde{\rho}_{\rm S}(t-s) \otimes \rho_{\rm B}$
  - Short bath correlation time (Markov): $\tilde{\rho}_{\rm S}(t-s) \simeq \tilde{\rho}_{\rm S}(t)$ inside ${\rm Tr}_{\rm B}$
- Redfield Equation (in interaction picture) ($\tilde{A}_\alpha(t) \equiv e^{iH_{\rm S}t} A_\alpha e^{-iH_{\rm S}t}$)

$$\frac{d\tilde{\rho}_{\rm S}(t)}{dt} = -\epsilon^2 \sum_{\alpha,\beta} \int_0^{\infty} ds \left(C_{\alpha\beta}(s)[\tilde{A}_\alpha(t), \tilde{A}_\beta(t-s)\tilde{\rho}_{\rm S}(t)] + {\rm h.c.} \right)$$

- Bath correlation function ($\tilde{B}_\alpha(t) \equiv e^{iH_{\rm B}t} B_\alpha e^{-iH_{\rm B}t}$)

$$C_{\alpha\beta}(s) \equiv {\rm Tr}_B[\tilde{B}_\alpha(s) B_\beta \rho_B]$$

Projection Operator Formalism

Nakajima-Zwanzig Equation

- Let us try more systematic derivation
- Projection operators: for some fixed ρ_{B} (write ρ_{SB} as ρ for simplicity)

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

- Start again from interaction picture equation:

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

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

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

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

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

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

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

- 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)

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

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

- 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 Nakajima-Zwanzig-QME in a time convolution form

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

- Derivation of (i)
  - For any ρ

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

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

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

- 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

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

  - Therefore

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

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)

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

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

- 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 $\mathcal{P}\tilde{\rho}$

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

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

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

- Collecting coeffs. of ϵ^m

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

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

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

TCL ME

Lowest order contribution

From above expressions, we have

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

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

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

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

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

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

Weak Coupling Limit

- Note that $\mathcal{L}$ carries a factor of ϵ: $\mathcal{L} \to \epsilon\mathcal{L}$
- Note that

$$G(t,s) = \mathbb{T}\exp[\epsilon \int_s^t dt' \, \mathcal{QL}(t')] = \mathbb{1} + O(\epsilon)$$

- NZ equation becomes

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

Weak Coupling Limit

Born-Markov Approximation

- Since $\mathrm{Tr}_{\mathrm{B}}(\tilde{\rho}(t)) = \tilde{\rho}_{\mathrm{S}}(t)$, we get the Born Approximation

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

- Note that

$$\tilde{\rho}_{\mathrm{S}}(t) = \mathbb{T} \exp[\epsilon \int_s^t dt'\, \mathcal{L}(t')] \tilde{\rho}_{\mathrm{S}}(s) \simeq \tilde{\rho}_{\mathrm{S}}(s) + O(\epsilon)$$

- To $O(\epsilon^2)$, we can write

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

- After changing integration variable $s \to t - s$ and sending the upper limit to ∞, we get Born-Markov approximation

Eigenfrequency Expansion

- Let us keep the upper limit at t.
- Expansion in Bohr frequencies ($\omega = E_m - E_n$) with eigenvalues E_n of H_S: Define $A_\alpha(\omega)$ such that

$$\tilde{A}_\alpha(t) \equiv e^{iH_\mathrm{S}t} A_\alpha e^{-iH_\mathrm{S}t} = \sum_\omega A_\alpha(\omega) e^{-i\omega t}$$

- "Redfield" Equation (in interaction picture)

$$\frac{d\tilde{\rho}_\mathrm{S}(t)}{dt} = -\epsilon^2 \sum_{\alpha,\beta} \sum_{\omega,\omega'} \left(\Gamma^t_{\alpha\beta}(\omega) e^{i(\omega'-\omega)t} [A^\dagger_\alpha(\omega'), A_\beta(\omega)\tilde{\rho}_\mathrm{S}(t)] + \mathrm{h.c.} \right),$$

where

$$\Gamma^t_{\alpha\beta}(\omega) \equiv \int_0^t ds\, e^{i\omega s} C_{\alpha\beta}(s)$$

- Redfield equation is not of GKSL form; Known to be not positive.

Ultraweak Coupling Limit / Davies Theory

- Integrating we have

$$\tilde{\rho}_{\mathrm{S}}(t) = \tilde{\rho}_{\mathrm{S}}(0) - \epsilon^2 \sum_{\alpha,\beta} \sum_{\omega,\omega'} \int_0^t ds \left(\Gamma^s_{\alpha\beta}(\omega) e^{i(\omega'-\omega)s} [A^\dagger_\alpha(\omega'), A_\beta(\omega)\tilde{\rho}_{\mathrm{S}}(s)] + \mathrm{h.c.} \right),$$

- Take $\epsilon \to 0$ limit. We only see the effect of the vanishing coupling in $\tilde{\rho}(t)$ in the $t \to \infty$ limit, or in the rescaled time $\epsilon^2 t \equiv \tau$.
- Similar rescaling in the integration variable $\sigma \equiv \epsilon^2 s$

$$\tilde{\rho}_{\mathrm{S}}(\tau) = \tilde{\rho}_{\mathrm{S}}(0) - \sum_{\alpha,\beta} \sum_{\omega,\omega'} \int_0^\tau d\sigma \left(\Gamma^{\sigma/\epsilon^2}_{\alpha\beta}(\omega) e^{i(\omega'-\omega)(\sigma/\epsilon^2)} [A^\dagger_\alpha(\omega'), A_\beta(\omega)\tilde{\rho}_{\mathrm{S}}(\sigma)] + \mathrm{h.c.} \right),$$

Ultraweak Coupling Limit

- Using
$$\lim_{x\to\infty}\int_a^b dt\ e^{ixt}f(t)=0$$
we find that the terms with $\omega \neq \omega'$ vanish in the $\epsilon \to 0$ limit.
- We have
$$\tilde{\rho}_{\mathrm{S}}(\tau)=\tilde{\rho}_{\mathrm{S}}(0)-\sum_{\alpha,\beta}\sum_{\omega}\int_0^{\tau} d\sigma\ \Big(\Gamma^{\infty}_{\alpha\beta}(\omega)[A^{\dagger}_{\alpha}(\omega),A_{\beta}(\omega)\tilde{\rho}_{\mathrm{S}}(\sigma)]+\mathrm{h.c.}\Big),$$
- This is equivalent to the usual rotating wave or secular approximation.

Secular (Rotating Wave) Approximation

- Take further approximation on Redfield equation: Take only $\omega = \omega'$ term in

$$\frac{d\tilde{\rho}(t)}{dt} = -\epsilon^2 \sum_{\alpha,\beta} \sum_{\omega,\omega'} \left(e^{i(\omega'-\omega)t} \Gamma^{\infty}_{\alpha\beta}(\omega) [A^{\dagger}_{\alpha}(\omega'), A_{\beta}(\omega)\tilde{\rho}(t)] + \mathrm{h.c.} \right)$$

  - Valid when $|\omega - \omega'| \gg t^{-1}$. Since $t \gg \tau_{\mathrm{B}}$, it means $\min|\omega - \omega'| > \tau_{\mathrm{B}}^{-1}$
  - It breaks down when there are energy gaps small than τ_{B}^{-1}
- Write $\Gamma(\omega)$ for $\Gamma^{\infty}(\omega)$ for simplicity and define

$$\gamma_{\alpha\beta}(\omega) \equiv \Gamma_{\alpha\beta}(\omega) + \Gamma^{*}_{\beta\alpha}(\omega) = \int_{-\infty}^{\infty} ds\, e^{i\omega s} C_{\alpha\beta}(s)$$

$$S_{\alpha\beta}(\omega) \equiv \frac{1}{2i}(\Gamma_{\alpha\beta}(\omega) - \Gamma^{*}_{\beta\alpha}(\omega)) = \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\gamma_{\alpha\beta}(\omega')}{\omega - \omega'}$$

Lindblad Equation

- After secular approximation (in Schrödinger picture)

$$\frac{d\rho_{\mathrm{S}}(t)}{dt} = -i[H_{\mathrm{S}}, \rho_{\mathrm{S}}(t)] + \mathcal{L}^{(S)}_{\mathrm{sec}}[\rho_{\mathrm{S}}(t)] + \mathcal{L}^{(\gamma)}_{\mathrm{sec}}[\rho_{\mathrm{S}}(t)]$$

- S-part becomes unitary evolution (Lamb shift term)

$$\mathcal{L}^{(S)}_{\mathrm{sec}}[\rho_{\mathrm{S}}(t)] = -i[H_{\mathrm{LS}}, \rho_{\mathrm{S}}(t)], \qquad H_{\mathrm{LS}} = \sum_{\alpha,\beta}\sum_{\omega} S_{\alpha\beta}(\omega) A^{\dagger}_{\alpha}(\omega) A_{\beta}(\omega)$$

- γ-part takes the GKSL form (One can show $\gamma_{\alpha\beta}(\omega)$ is positive definite)

$$\mathcal{L}^{(\gamma)}_{\mathrm{sec}}[\rho_{\mathrm{S}}(t)] = \sum_{\alpha,\beta}\sum_{\omega} \gamma_{\alpha\beta}(\omega) \Big(A_{\beta}(\omega) \rho_{\mathrm{S}}(t) A^{\dagger}_{\alpha}(\omega) - \frac{1}{2} \left\{ A^{\dagger}_{\alpha}(\omega) A_{\beta}(\omega), \rho_{\mathrm{S}}(t) \right\} \Big).$$

Example

Damped Harmonic Oscillator

- Consider a harmonic oscillator

$$H_{\mathrm{S}} = \omega_0 a^\dagger a, \qquad H_{\mathrm{I}} = \underbrace{(a + a^\dagger)}_{A} \sum_k g_k (c_k + c_k^\dagger)$$

- Only nonvanishing terms are

$$A(\omega_0) = a, \qquad A(-\omega_0) = A^\dagger(\omega_0) = a^\dagger$$

- Comment: Another popular coupling

$$\begin{aligned} H_{\mathrm{I}}' =& a R^\dagger + a^\dagger R \quad \left(R \equiv \sum_k g_k c_k\right) \\ =& \frac{a + a^\dagger}{\sqrt{2}} \frac{R + R^\dagger}{\sqrt{2}} + \frac{a - a^\dagger}{i\sqrt{2}} \frac{R - R^\dagger}{i\sqrt{2}} = A_1' B_1' + A_2' B_2' \end{aligned}$$

For this interaction, nonsecular terms vanish automatically

Damped Harmonic Oscillator

- After following the procedure above, the Redfield dissipator is given by

$$
\begin{aligned}
\mathcal{L}^{(2)}_{\mathrm{Red}}[\rho(t)] &= \underset{\sim\sim\sim}{-i(S(\omega_0)+S(-\omega_0))[a^\dagger a,\rho(t)]} \\
&\underset{\sim\sim\sim}{+\gamma(-\omega_0)\left(a^\dagger\rho(t)a-\frac{1}{2}\{aa^\dagger,\rho(t)\}\right)+\gamma(\omega_0)\left(a\rho(t)a^\dagger-\frac{1}{2}\{a^\dagger a,\rho(t)\}\right)} \\
&+i(S(\omega_0)-S(-\omega_0))\left(a\rho(t)a-\frac{1}{2}\{a^2,\rho(t)\}-a^\dagger\rho(t)a^\dagger+\frac{1}{2}\{a^{\dagger 2},\rho(t)\}\right) \\
&+\frac{1}{2}(\gamma(\omega_0)+\gamma(-\omega_0))\left(a\rho(t)a-\frac{1}{2}\{a^2,\rho(t)\}+a^\dagger\rho(t)a^\dagger-\frac{1}{2}\{a^{\dagger 2},\rho(t)\}\right) \\
&+\frac{1}{4}(\gamma(\omega_0)-\gamma(-\omega_0))\left(-[a^2,\rho(t)]+[a^{\dagger 2},\rho(t)]\right) \\
&-\frac{i}{2}(S(\omega_0)+S(-\omega_0))\left([a^2,\rho(t)]+[a^{\dagger 2},\rho(t)]\right)
\end{aligned}
$$

Damped Harmonic Oscillator

- The wavy lines are secular approximated terms: the GKSL form
- With $\bar{n}(\omega) = 1/(e^{\beta\hbar\omega} - 1)$, we have

$$\gamma(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\mathcal{C}(t) = \begin{cases} 2\hbar J(\omega)(\bar{n}(\omega)+1), & \text{if } \omega > 0 \\ 2\hbar J(-\omega)\bar{n}(-\omega), & \text{if } \omega < 0 \end{cases}$$

- Lamb shift term (independent of $\bar{n}(\omega)$)

$$S(\omega_0) + S(-\omega_0) = -\mathcal{P}\int_0^{\infty} \frac{d\omega'}{2\pi}\left[\frac{1}{\omega' - \omega_0} + \frac{1}{\omega' + \omega_0}\right] J(\omega')$$

Lindblad equation without secular approximation 1

Universal Lindblad Equation

[Nathan and Rudner, PRB **102**, 115109 (2020)]

- Has the same level of accuracy as the Redfield equation.
- Use of a small parameter given in terms of the properties of the bath valid in the weak-coupling limit.
- $\partial_t \rho_{\rm S}(t) = -i[H_{\rm S}, \rho_{\rm S}(t)] + \epsilon^2 \mathcal{L}^{(2)}_{\rm ULE}[\rho_{\rm S}(t)]$

$$\mathcal{L}^{(2)}_{\rm ULE} = \mathcal{L}^{(a)}_{\rm ULE} + \mathcal{L}^{(b)}_{\rm ULE}$$

- $\mathcal{L}^{(a)}_{\rm ULE}[\rho_{\rm S}(t)] = -i[\Lambda, \rho_{\rm S}(t)]$ with

$$\Lambda = \sum_{\alpha,\beta} \sum_{\omega,\omega'} f_{\alpha\beta}(\omega,\omega') A_\alpha(\omega) A_\beta(\omega'),$$

- Dissipator in the GKSL form

$$\mathcal{L}^{(b)}_{\rm ULE}[\rho_{\rm S}(t)] = \sum_\alpha [L_\alpha \rho_{\rm S}(t) L_\alpha^\dagger - \frac{1}{2}\{L_\alpha^\dagger L_\alpha, \rho_{\rm S}(t)\}]$$

More on ULE

- Here the jump operator is

$$L_\alpha = \sum_\beta \sum_\omega g_{\alpha\beta}(\omega) A_\beta(\omega), \quad \text{with} \quad \gamma_{\alpha\beta}(\omega) = \sum_\mu g_{\alpha\mu}(\omega) g_{\mu\beta}(\omega).$$

- Compare with

$$\mathcal{L}^{(\gamma)}_{\rm sec}[\rho_{\rm S}(t)] = \sum_{\alpha,\beta} \sum_\omega \gamma_{\alpha\beta}(\omega) \Big(A_\beta(\omega) \rho_{\rm S}(t) A^\dagger_\alpha(\omega) - \frac{1}{2} \Big\{ A^\dagger_\alpha(\omega) A_\beta(\omega), \rho_{\rm S}(t) \Big\} \Big).$$

- $f_{\alpha\beta}(\omega, \omega')$ is given by

$$f_{\alpha\beta}(\omega, \omega') \equiv -\mathcal{P} \sum_\mu \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{1}{\tilde{\omega}} g_{\alpha\mu}(\tilde{\omega} - \omega) g_{\mu\beta}(\tilde{\omega} + \omega').$$

- Compare with

$$S_{\alpha\beta}(\omega) = -\mathcal{P} \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{1}{\tilde{\omega}} \gamma_{\alpha\beta}(\tilde{\omega} + \omega),$$

- ULE roughly corresponds to taking the square root of the Fourier transform of the bath correlation function and to distributing it to the new jump operators.

Steady State of QMEs

- Steady state ($\rho_{\rm S}(t) \to \rho^{\rm st}$ as $t \to \infty$) of $d\rho_{\rm S}(t)/dt = \mathcal{L}[\rho_{\rm S}(t)]$

$$\mathcal{L}[\rho^{\rm st}] = 0$$

- If the total system thermalizes, we expect $\rho_{\rm s} \to \rho_{\rm mfG}$, mean-force Gibbs state

$$\rho_{\rm mfG} \equiv \frac{{\rm Tr}_{\rm B}(e^{-\beta H})}{{\rm Tr}_{\rm SB}(e^{-\beta H})}.$$

- Weak coupling limit ($H = H_{\rm S} + H_{\rm B} + \epsilon H_{\rm I}$)

$$\rho_{\rm mfG} = \rho_{\rm G} + \epsilon^2 \rho_{\rm mfG}^{(2)} + \cdots , \qquad \rho_{\rm G} = \frac{e^{-\beta H_{\rm S}}}{Z_{\rm S}}$$

- One can calculate $\rho^{\rm st}$ of various QMEs perturbatively

$$\rho^{\rm st} = \rho^{(0)} + \epsilon^2 \rho^{(2)} + \cdots$$

and compare with $\rho_{\rm mfG}$.

Perturbative Steady State of QME

- Generic weak coupling QMEs

$$\frac{d\rho_{\mathrm{S}}(t)}{dt} = \mathcal{L}^{(0)}[\rho_{\mathrm{S}}(t)] + \epsilon^2 \mathcal{L}^{(2)}[\rho_{\mathrm{S}}(t)] + O(\epsilon^4)$$

with

$$\mathcal{L}^{(0)}[\rho_{\mathrm{S}}(t)] = -i[H_S, \rho_{\mathrm{S}}(t)]$$

- With $\rho^{\mathrm{st}} = \rho^{(0)} + \epsilon^2 \rho^{(2)} + O(\epsilon^4)$, we have

$$O(\epsilon^0): \ \mathcal{L}^{(0)}[\rho^{(0)}] = 0, \qquad O(\epsilon^2): \ \mathcal{L}^{(0)}[\rho^{(2)}] + \mathcal{L}^{(2)}[\rho^{(0)}] = 0$$

- Matrix elements: $\rho_{nm} = \langle n|\rho|m\rangle$ with $H_{\mathrm{S}}|n\rangle = E_n|n\rangle$

$$-i\Delta_{nm}\rho^{(0)}_{nm} = 0 \qquad \Rightarrow \qquad \boxed{\rho^{(0)}_{nm} = 0} \qquad \text{for} \quad n \neq m,$$

$$-i\Delta_{nm}\rho^{(2)}_{nm} + \left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nm} = 0, \qquad \text{where} \quad \Delta_{nm} = E_n - E_m$$

Perturbative Steady State of QME

- 0th-order: $n = m$

$$\left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nn} = 0 \qquad \Rightarrow \text{detemines} \qquad \rho^{(0)}_{nn} \qquad (\star)$$

- 2nd-order coherence: $n \neq m$

$$\rho^{(2)}_{nm} = \frac{1}{i\Delta_{nm}}\left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nm} \qquad (\star\star)$$

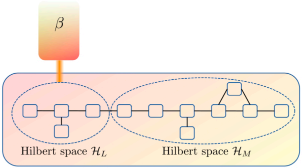
- 2nd order population $\rho^{(2)}_{nn}$ is not determined to this order. We need $\mathcal{L}^{(4)}$.
- Method of analytic continuation [Thingna et al, J. Chem. Phys. **136**, 194110 (2012)]
  – If the limit $n \to m$ exists in $(\star\star)$, we may regard this as $\rho^{(2)}_{nn}$

Perturbative Steady States of Various QMEs

	CP	$\rho^{(0)}$	$\rho^{(2)}$
Redfield	No	ρ_{G}	$\rho_{\mathrm{mG}}^{(2)}$
Secular Approximation	Yes	ρ_{G}	0
ULE	Yes	ρ_{G}	$\neq \rho_{\mathrm{mG}}^{(2)}$
TLE	Yes	$\neq \rho_{\mathrm{G}}$	$\neq \rho_{\mathrm{mG}}^{(2)}$

[J. Lee and JY, PRE **106**, 054145 (2022)]

QMEs for a System with Spatial Extent



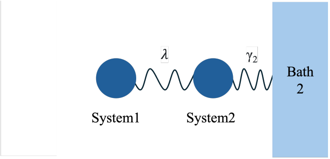
Hilbert space $\mathcal{H}_S = \mathcal{H}_L \otimes \mathcal{H}_M$, Hamiltonian H_S

- Only a part of system is coupled to heat bath
- If we try to use the method described above, this Global QME has support on the entire system Hilbert space. Recall

$$A(\omega) = \sum_{m,n,E_n - E_m = \omega} |m\rangle\langle m|A|n\rangle\langle n|$$

- Local QME uses only the spectrum of the Hilbert space that couples to the bath.

Problems of Local QME with Thermalization



- Oscillator b is in contact with the bath

$$H_{\mathrm{S}} = \omega_A a^\dagger a + \omega_B b^\dagger b + \lambda(a + a^\dagger)(b + b^\dagger)$$

- Local Lindblad equation uses the dissipater $\mathcal{D}_b$ which involves b and $b^\dagger$ only
- One can show that the zeroth order steady state is not the Gibbs state

$$\rho_{st}^{(0)} \neq \rho_{\mathrm{G}} = \frac{1}{Z_{\mathrm{S}}} e^{-\beta H_{\mathrm{S}}}$$

Global Lindblad Equation

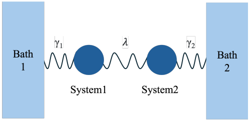
- To write global Lindblad equation, first diagonalize

$$H_{\mathrm{S}} = \omega_+ d_+^\dagger d_+ + \omega_- d_-^\dagger d_-$$

- Now the system coupling operator b can be written as a function of d_+ and d_-
- Dissipator now involves d_+ and d_-
- The zeroth-order steady state is now given by the Gibbs state
- But the dissipator which has a support on the entire Hilbert space seems unnatural.

Problems of Local QME with Nonequilibrium Transport

Levy and Kosloff, EPL, 107 (2014) 20004



- Two baths at different temperatures T_L and T_R
- Local QME

$$\partial_t \rho_S = -i[H_S, \rho_S] + \mathcal{D}_a^L[\rho_S] + \mathcal{D}_b^R[\rho_S]$$

- Heat Currents J_L and J_R ($J_L + J_R = 0$ at NESS)

$$\frac{d\langle H_S \rangle}{dt} = \underbrace{\mathrm{Tr}[H_S \mathcal{D}_a^L[\rho_S]]}_{J_L} + \underbrace{\mathrm{Tr}[H_S \mathcal{D}_b^R[\rho_S]]}_{J_R}$$

Problems with Local QME

- Using local QME, write the eqs. for

$$\frac{d}{dt}\langle a^\dagger a\rangle = \mathrm{Tr}[\frac{d\rho_S}{dt}a^\dagger a]$$

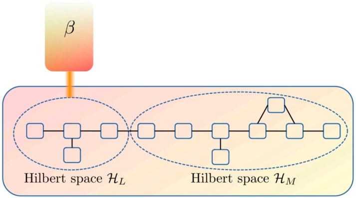
  and the same for $\langle b^\dagger b\rangle$, $\langle a^\dagger b\rangle$ and $\langle ab^\dagger\rangle$
- At NESS, $d\langle a^\dagger a\rangle/dt = 0$, etc. and we find that $\langle a^\dagger a\rangle_{ss}, \langle b^\dagger b\rangle_{ss}$, $\langle a^\dagger b\rangle_{ss}$ and $\langle ab^\dagger\rangle_{ss}$ form a closed set of equations that can be solved.
- One can express J_L ans J_R using these quantities at NESS

$$J_L^{ss} = \left(e^{\beta_L\omega_A} - e^{\beta_R\omega_B}\right)\mathcal{F}, \qquad (\mathcal{F} > 0)$$

- Even if $T_L > T_R$, one can have $J_L^{ss} < 0$

Problems of Global QME with Local Conservation Laws

D. Tupkary, et al. Phys. Rev. A **107**, 062216 (2023)



Hilbert space $\mathcal{H}_S = \mathcal{H}_L \otimes \mathcal{H}_M$, Hamiltonian H_S

$$H_\mathrm{S} = H_\mathrm{L} + H_\mathrm{M} + H_\mathrm{LM},$$

Any operator O_M acting on $\mathcal{H}_M$ satisfies

$$[O_\mathrm{M}, H_\mathrm{SB}] = 0$$

Problems of Global QME with Local Conservation Laws

- Using $[O_M, H_{SB}] = 0$

$$\frac{d}{dt}\langle I_L \otimes O_M\rangle = \mathrm{Tr}_{SB}\left(I_L \otimes O_M \dot{\rho}_{\mathrm{tot}}\right) = -i\mathrm{Tr}_{SB}\left(I_L \otimes O_M [H, \rho_{\mathrm{tot}}]\right)$$
$$= - i\mathrm{Tr}_{SB}\left([I_L \otimes O_M, H]\rho_{\mathrm{tot}}\right) = -i\mathrm{Tr}_{SB}\left([I_L \otimes O_M, H_S]\rho_{\mathrm{tot}}\right),$$
$$= - i\mathrm{Tr}_{S}\left([I_L \otimes O_M, H_S]\rho_{\mathrm{S}}\right)$$

- On the other hand,

$$\frac{d}{dt}\langle I_L \otimes O_M\rangle = \mathrm{Tr}_{S}\left(I_L \otimes O_M \dot{\rho}_{\mathrm{S}}\right) = \mathrm{Tr}_{S}\left(I_L \otimes O_M\left(\mathcal{L}^{(0)}[\rho_{\mathrm{S}}] + \epsilon^2\mathcal{L}^{(2)}[\rho_{\mathrm{S}}]\right)\right)$$
$$= - i\mathrm{Tr}_{S}\left([I_L \otimes O_M, H_S]\rho_{\mathrm{S}}\right) + \epsilon^2\mathrm{Tr}_{S}\left(I_L \otimes O_M \mathcal{L}^{(2)}[\rho_{\mathrm{S}}]\right),$$

where we have used $\mathcal{L}^{(0)}[\rho] = -i[H_S, \rho]$.

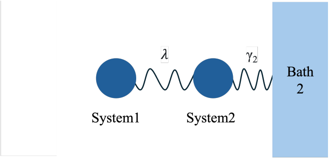
Problems of Global QME with Local Conservation Laws

- Therefore we require that

$$\boxed{\mathrm{Tr}_S\left(I_L \otimes O_M \mathcal{L}^{(2)}[\rho]\right) = 0}$$

- Global QME with the dissipator having support from global Hilbert space does not satisfiy this property
- Local QME with the dissipator having support from $\mathcal{H}_L$ satisfies this property
- Redfield equation satisfies this property

Exact Calculations for Thermalization



- System Hamiltonian :

$$H_S = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2}m\omega_0^2(x_1^2 + x_2^2) - m\lambda x_1 x_2$$

- Heisenberg equations :

$$m\ddot{x}_1(t) = -m\omega_0^2 x_1(t) + m\lambda x_2(t)$$

$$m\ddot{x}_2(t) = -m\omega_0^2 x_2(t) + m\lambda x_1(t) + \sum_n \kappa_{2,n} q_{2,n}(t) - \sum_n \frac{\kappa_{2,n}^2}{m_{2,n}\omega_{2,n}^2} x_2(t)$$

Exact Calculations for Thermalization

- Laplace transform of Heisenberg equation

$$\widehat{\boldsymbol{x}}(z) = \widehat{\boldsymbol{G}}^{(1)}(z)\boldsymbol{x}(0) + \widehat{\boldsymbol{G}}^{(2)}(z)\dot{\boldsymbol{x}}(0) + \frac{1}{m}\widehat{\boldsymbol{G}}^{(2)}(z)\widehat{\boldsymbol{B}}(z)$$

$$\begin{aligned}\frac{1}{z}\widehat{\boldsymbol{G}}^{(1)}(z) =& \widehat{\boldsymbol{G}}^{(2)}(z) \\ =& \begin{pmatrix} z^2+\omega_0^2 & -\lambda \\ -\lambda & z^2 + z\widehat{\gamma}_2(z) + \omega_0^2 \end{pmatrix}^{-1}\end{aligned}$$

$\gamma_2(t) = 2\int_0^\infty d\omega\ \frac{J_2(\omega)}{\omega}\cos(\omega t)$

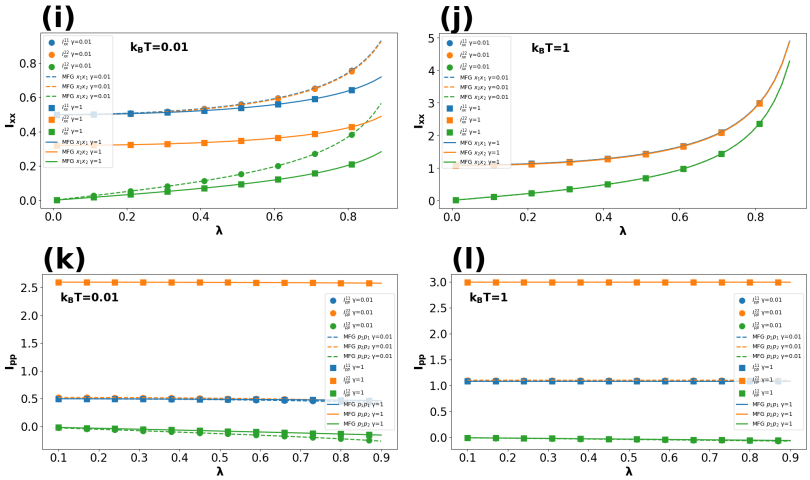
- Bath correlation function

$$\langle\{B_2(t), B_2(t')\}\rangle \equiv D_2(t-t')$$

$$D_2(t) = 2\hbar\int_0^\infty d\omega J_2(\omega)\coth(\frac{\beta\hbar\omega}{2})\cos(\omega t)$$

Exact Calculations

Long-time limit of Covariances $\langle x^2(t)\rangle$ and $\langle p^2(t)\rangle$



Exact QME

Hu-Paz-Zhang Equation [PRD **45**, 2843 (1992)]

A harmonic oscillator in contact with a heat bath:

$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = -\frac{i}{\hbar}\left[\frac{p^2}{2M} + \frac{1}{2}(M\omega_0^2 + A(t))x^2, \rho_{\mathrm{S}}(t)\right] - \frac{i}{2\hbar}B(t)[x, \{p, \rho_{\mathrm{S}}(t)\}] + \frac{1}{\hbar^2}C(t)[x, [p, \rho_{\mathrm{S}}(t)]] - \frac{1}{\hbar^2}D(t)[x, [x, \rho_{\mathrm{S}}(t)]]$$

where $A(t)$, $B(t)$, $C(t)$ and $D(t)$ are given in terms of $G^{(1)}(t)$ and $G^{(2)}(t)$.

HPZ Equation

- One can rearrange it into

$$\frac{d}{dt}\rho_{\rm S}(t) = -i[H_{\rm eff}(t), \rho_{\rm S}(t)] + \sum_{a,b=1}^{2} K_{ab}(t)\left[L_b^\dagger \rho_{\rm S}(t) L_a - \frac{1}{2}\{L_a L_b^\dagger, \rho_{\rm S}(t)\}\right]$$

  with $L_1 = x$ and $L_2 = p$.
- $K_{ab}(t)$ is not positive all the time.
- But since this is an exact equation, the dynamics is CP.
- Question: What is the steady state of the HPZ equation? If it exists, is it always eqaual to the MFG state?

Summary

- Theoretical approaches to open quantum systems
- Mathematical aspects
  - CPTP map
  - Markovian, CP divisible, semigroup : GKSL (Lindblad) form
- Physical approaches for QMEs
  - Systematic projection operator formalism
  - Weak coupling approximation: Born-Markov
  - Secular (rotating wave, ultraweak) approximation to get Lindblad equation
- Steady states of QMEs; Comparison with quantum MFG state