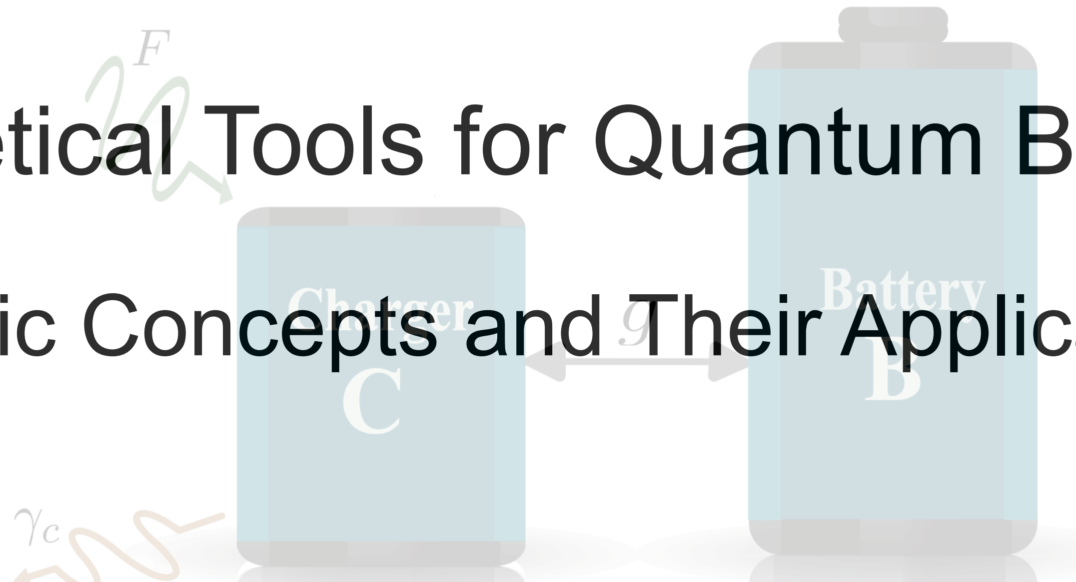
Theoretical Tools for Quantum Batteries:

Basic Concepts and Their Applications



Lecture 1

Gentaro Watanabe
(Zhejiang University)

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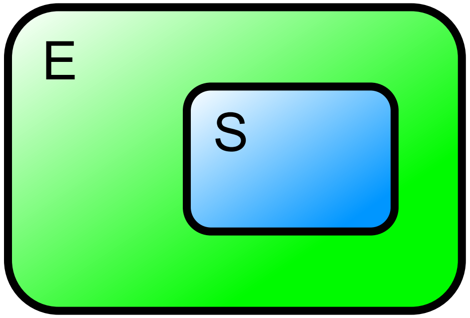
Lecture 1: Theory of open quantum systems 101

I. Kraus operator & Kraus map

Setup of the problem: Combined quantum sys.

Quantum sys. coupled to the environment



(total) = (system) + (environment)

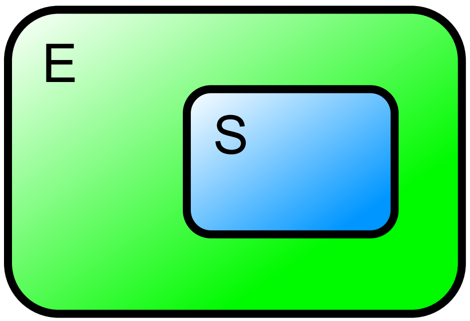
Strategy

The total sys. $S+E$ is isolated and undergoes unitary evolution.

Effective evolution of S is obtained by tracing out DOFs of E.

Setup of the problem: Combined quantum sys.

Quantum sys. coupled to the environment



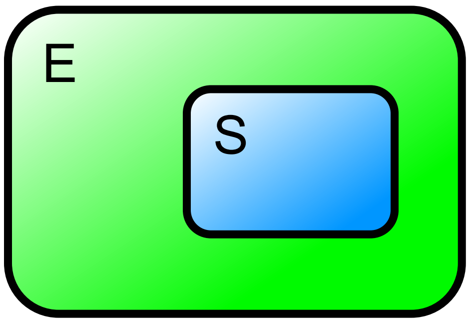
(total) = (system) + (environment)

	Hilbert space	CONS of $\mathcal{H}_i$
S: System of our interest	$\mathcal{H}_S$	$\{\vert\psi_i\rangle\}$ with $\vert\psi_i\rangle \in \mathcal{H}_S$
E: Environment	$\mathcal{H}_E$	$\{\vert\phi_i\rangle\}$ with $\vert\phi_i\rangle \in \mathcal{H}_E$
Total sys. of $S + E$	$\mathcal{H}_S \otimes \mathcal{H}_E$	$\{\vert\psi_i\rangle \otimes \vert\phi_j\rangle\} \equiv \{\vert\psi_i\rangle\vert\phi_j\rangle\}$

Arbitrary state $|\Psi\rangle$ in $S + E$ can be written as:

$$|\Psi\rangle = \sum_{i,j} c_{ij} \, |\psi_i\rangle \otimes |\phi_j\rangle$$

Quantum sys. coupled to the environment



(total) = (system) + (environment)

Introduce the density op. $\hat{\rho}$ to describe the mixed state.

$\hat{\rho}_{SE}$: total density operator (sys. + env.)

partial density op. of S : $\hat{\rho} \equiv \hat{\rho}_S = \mathrm{Tr}_E[\hat{\rho}_{SE}]$

partial density op. of E : $\hat{\rho}_E = \mathrm{Tr}_S[\hat{\rho}_{SE}]$

Density operators & partial trace

- If the state of the total sys. is a separable pure state:

$$|\Psi\rangle = |\psi_S\rangle \otimes |\phi_E\rangle \longrightarrow \hat{\rho}_{SE} = |\Psi\rangle\langle\Psi| = |\psi_S\rangle\langle\psi_S| \otimes |\phi_E\rangle\langle\phi_E|$$

➡ State of the partial sys. S is also a pure state:

$$\hat{\rho}_S = \mathrm{Tr}_E[\hat{\rho}_{SE}] = |\psi_S\rangle\langle\psi_S| \, \mathrm{Tr}_E[|\phi_E\rangle\langle\phi_E|] = |\psi_S\rangle\langle\psi_S|$$

- However, if the state of the total sys. is a non-separable pure state:

$$|\Psi\rangle = \sum_i c_i \, |\psi_i\rangle \otimes |\phi_i\rangle \longrightarrow \hat{\rho}_{SE} = |\Psi\rangle\langle\Psi|$$

$$= \sum_{i,j} c_i \, c_j^* |\psi_i\rangle\langle\psi_j| \otimes |\phi_i\rangle\langle\phi_j|$$

➡ State of the partial sys. S can be a mixed state:

$$\hat{\rho}_S = \mathrm{Tr}_E[\hat{\rho}_{SE}] = \sum_{i,j} c_i \, c_j^* |\psi_i\rangle\langle\psi_j| \, \mathrm{Tr}_E\big[|\phi_i\rangle\langle\phi_j|\big]$$

$$= \sum_i |c_i|^2 |\psi_i\rangle\langle\psi_i|$$: mixed state

Kraus operator & Kraus map (1)

Suppose the total sys. $S + E$ is isolated.

➡ Unitary evolution: $\hat{\rho}'_{SE} = \hat{U}\hat{\rho}_{SE}\hat{U}^\dagger$

($\hat{U}$: unitary op.)

Assumption

No correlation btwn. S & E in the initial st.: $\hat{\rho}_{SE} = \hat{\rho} \otimes \hat{\rho}_E$

System st. $\hat{\rho}'$ after the evolution: $\hat{\rho}' = \mathrm{Tr}_E[\hat{\rho}'_{SE}] = \mathrm{Tr}_E\left[\hat{U}\hat{\rho}_{SE}\hat{U}^\dagger\right]$

Spectral decomp. of the initial env. st.: $\hat{\rho}_E = \sum_i q_i^{(0)} \left|\phi_i^{(0)}\right\rangle\left\langle\phi_i^{(0)}\right|$

$\left\{\left|\phi_i^{(0)}\right\rangle\right\}$: eigenbasis of $\hat{\rho}_E$

Kraus operator & Kraus map (2)

Assumption

No correlation btwn. S & E in the initial st.: $\hat{\rho}_{SE} = \hat{\rho} \otimes \hat{\rho}_E$

System st. $\hat{\rho}'$ after the evolution: $\hat{\rho}' = \mathrm{Tr}_E[\hat{\rho}'_{SE}] = \mathrm{Tr}_E\left[\hat{U}\hat{\rho}_{SE}\hat{U}^\dagger\right]$

Spectral decomp. of the initial env. st.: $\hat{\rho}_E = \sum_i q_i^{(0)} \left|\phi_i^{(0)}\right\rangle\left\langle\phi_i^{(0)}\right|$

$$\hat{\rho}' = \mathrm{Tr}_E\left[\hat{U}\hat{\rho}_{SE}\hat{U}^\dagger\right]$$

$$= \sum_{i,j} q_i^{(0)} \underbrace{\left\langle\phi_j\middle|\hat{U}\middle|\phi_i^{(0)}\right\rangle}\,\hat{\rho}\,\underbrace{\left\langle\phi_i^{(0)}\middle|\hat{U}^\dagger\middle|\phi_j\right\rangle}$$

$\{|\phi_i\rangle\}$: arbitrary basis of E

operators in S

$$= \sum_{i,j} \hat{M}_{i,j}\,\hat{\rho}\,\hat{M}_{i,j}^\dagger \qquad \text{(Kraus map)}$$

Kraus op. $\hat{M}_{i,j} \equiv \left(q_i^{(0)}\right)^{\frac{1}{2}} \left\langle\phi_j\middle|\hat{U}\middle|\phi_i^{(0)}\right\rangle$

Kraus operator & Kraus map (3)

Kraus map: Effective evolution of open quantum system S

$$\hat{\rho}' = \sum_k \widehat{M}_k \, \hat{\rho} \, \widehat{M}_k^\dagger$$

with Kraus op. $\widehat{M}_k \equiv \left(q_i^{(0)}\right)^{\frac{1}{2}} \left\langle \phi_j \middle| \widehat{U} \middle| \phi_i^{(0)} \right\rangle$

$$k \equiv (i, j)$$

Completeness: $\sum_k \widehat{M}_k^\dagger \, \widehat{M}_k = \hat{I}_S$ ($\hat{I}_S$: Identity in $\mathcal{H}_S$)

→ Probability conservation.

Properties of the Kraus map

Kraus map is a CPTP map
("Completely-Positive & Trace-Preserving")

Positivity → Positivity of the probability.

Complete positivity → Positivity for extended system with arbitrary ancillary systems.

Trace preservation → Probability conservation.

Properties of the Kraus map: Trace-preserving

Kraus operators satisfy the completeness:

$$\sum_k \hat{M}_k^\dagger \hat{M}_k = \hat{I}_S \qquad (\ \hat{I}_S :\ \text{Identity in } \mathcal{H}_S\ )$$

Proof

$$\sum_k \hat{M}_k^\dagger \hat{M}_k = \sum_{i,j} \left(q_i^{(0)}\right)^{\frac{1}{2}} \left\langle \phi_i^{(0)} \middle| \hat{U}^\dagger \middle| \phi_j \right\rangle \left(q_i^{(0)}\right)^{\frac{1}{2}} \left\langle \phi_j \middle| \hat{U} \middle| \phi_i^{(0)} \right\rangle$$

$$= \sum_i q_i^{(0)} \left\langle \phi_i^{(0)} \middle| \underbrace{\hat{U}^\dagger \hat{U}}_{=\hat{I}_{SE}} \middle| \phi_i^{(0)} \right\rangle = \sum_i q_i^{(0)} \hat{I}_S = \hat{I}_S$$

$\hat{I}_{SE}$ (Identity in $\mathcal{H}_S \otimes \mathcal{H}_E$)

Completeness ➡ Kraus map is trace-preserving. (prob. conservation)

$$\mathrm{Tr}_S[\hat{\rho}'] = \mathrm{Tr}_S\left[\sum_k \hat{M}_k\, \hat{\rho}\, \hat{M}_k^\dagger\right] = \mathrm{Tr}_S\left[\underbrace{\sum_k \hat{M}_k^\dagger \hat{M}_k}_{= \hat{I}_S}\, \hat{\rho}\right] = \mathrm{Tr}_S[\hat{\rho}]$$

Positivity & complete positivity

Positive operator : An operator $\hat{A}$ such that $\langle\psi|\hat{A}|\psi\rangle \geq 0$

"$\hat{A} \geq 0$"

for any state vector $|\psi\rangle$.

- Any positive operator is Hermitian.
- All eigenvalues of positive operator are ≥ 0.

Positive map : A map keeps the positivity of the operator.

(i.e., a map which maps from a positive op. to a positive op.)

Kraus map is a positive map.

Proof

1. $\hat{\rho}_{SE} \geq 0$ ➡ $\hat{\rho}'_{SE} = \hat{U}\hat{\rho}_{SE}\hat{U}^\dagger \geq 0$

∵ For $\forall|\psi\rangle$,

$$\langle\psi|\hat{\rho}'_{SE}|\psi\rangle = \langle\psi|\hat{U}\hat{\rho}_{SE}\hat{U}^\dagger|\psi\rangle = \langle\psi'|\hat{\rho}_{SE}|\psi'\rangle \geq 0$$

($\hat{\rho}_{SE} \geq 0$)

2. Thus, $\hat{\rho}' = \mathrm{Tr}_E[\hat{\rho}'_{SE}]$ is also positive.

∵ For $\forall|\psi_S\rangle$,

$$\langle\psi_S|\mathrm{Tr}_E[\hat{\rho}'_{SE}]|\psi_S\rangle = \sum_i [\,(\langle\psi_S|\langle\phi_i|)\hat{\rho}'_{SE}(|\psi_S\rangle|\phi_i\rangle)] \geq 0$$

≥ 0 for each i

(∵ $\hat{\rho}'_{SE} \geq 0$)

Positivity & complete positivity

Completely positive map:

Consider $\mathcal{H}_S$ and an arbitrary 2nd system $\mathcal{H}'$.

For $\forall\, \hat{\rho}_{ex} \in \mathcal{H}_S \otimes \mathcal{H}'$

$$\hat{\rho}'_{ex} \equiv \sum_k \left(\widehat{M}_k \otimes \hat{I}'\right) \hat{\rho}_{ex} \left(\widehat{M}_k^{\dagger} \otimes \hat{I}'\right)$$

($\hat{I}'$: Identity in $\mathcal{H}'$)

is also positive.

⟺ The (Kraus) map is completely positive.

Complete positivity guarantees the positivity of $\hat{\rho}'_{ex}$ for any extended system when the system S evolves according to $\hat{\rho}' = \sum_k \widehat{M}_k \hat{\rho}_{ex} \widehat{M}_k^{\dagger}$.

Kraus map is completely positive.

Proof

Since $\hat{\rho}_{ex} \in \mathcal{H}_S \otimes \mathcal{H}'$ is positive, for $\forall\ |\psi\rangle$ we have:

$$\langle\psi|\hat{\rho}'_{ex}|\psi\rangle = \langle\psi| \sum_k \left(\hat{M}_k \otimes \hat{I}'\right)\hat{\rho}_{ex}\underline{\left(\hat{M}_k^\dagger \otimes \hat{I}'\right)|\psi\rangle}$$

$$\equiv \left|\psi_{ij}\right\rangle$$

$$= \sum_{i,j} \underline{\left\langle\psi_{ij}\middle|\hat{\rho}_{ex}\middle|\psi_{ij}\right\rangle} \geq 0$$

≥ 0 for each i, j

Remarks

- Kraus operator is equivalent to the measurement operator in the quantum measurement theory.

- However, in the context of the open quantum systems, there is no observer who records the measurement results.

→ Trace over all the possible measurement results.

"non-selective measurement"

II. Lindblad master equation

Lindblad (GKLS) master equation

Lindblad master eq. (ME)
(Gorini-Kosakowski-Lindblad-Sudershan; GKLS)

Markovian master eq. describing the dynamics of open quantum sys. weakly coupled to its environment.

Markov approximation

Environment relaxes much faster than the system timescale of interest.

(Rouly speaking, the environment is reset to the steady state at each instance of time.)

→ Memoryless environment

Lindblad (GKLS) master equation

dissipation rate

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}, \hat{\rho}(t)\right] + \sum_k \frac{\Gamma_k}{2}\left(\underline{2\hat{L}_k\, \hat{\rho}(t)\, \hat{L}_k^\dagger} - \hat{L}_k^\dagger\, \hat{L}_k\, \hat{\rho}(t) - \hat{\rho}(t)\, \hat{L}_k^\dagger\, \hat{L}_k\right)$$

"quantum jump term"
(discussed later)

$$\equiv \underline{-i\left[\hat{H}, \hat{\rho}(t)\right]} + \underline{\sum_k \frac{\Gamma_k}{2}\mathcal{D}\left[\hat{L}_k\right]\hat{\rho}(t)} \qquad \left(\equiv \mathcal{L}\,\hat{\rho}(t)\right)$$

unitary evolution
(non-dissipative dyn.)

non-unitary evolution
(dissipative dyn.)

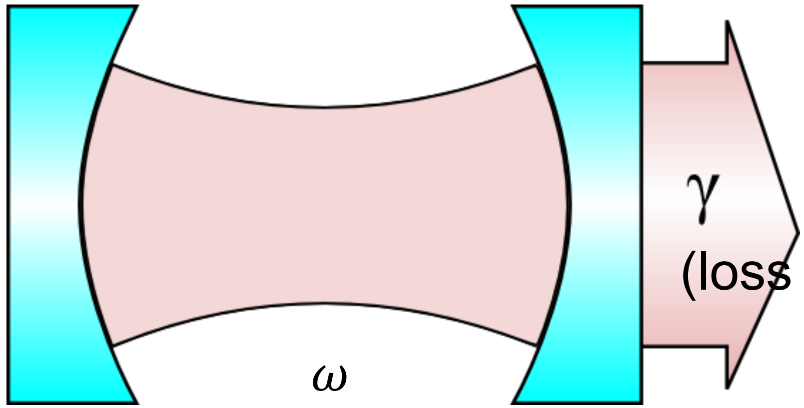
Liouville superop.
(Liouvillian)

"Dissipator" (Lindbladian) $\mathcal{D}\left[\hat{O}\right]\hat{\rho} \equiv 2\,\hat{O}\hat{\rho}\hat{O}^\dagger - \hat{O}^\dagger\hat{O}\hat{\rho} - \hat{\rho}\hat{O}^\dagger\hat{O}$

$\hat{L}_k$: Lindblad op.

$\hat{L}_k$ describes the dissipation process caused by the coupling btwn. sys. & env.

Example 1: Lossy single-mode optical cavity



$$\hat{H} = \omega\, \hat{a}^\dagger \hat{a}$$

($\hat{a}$: annihilation op. of a cavity photon)

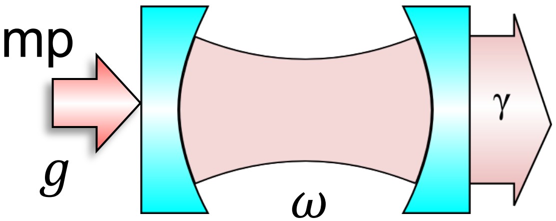
$\hat{L} = \hat{a}$: loss of a photon

$$\frac{d\hat{\rho}}{dt} = -i\left[\omega\, \hat{a}^\dagger \hat{a}, \hat{\rho}\right] + \frac{\gamma}{2}\left(2\, \hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger \hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger \hat{a}\right)$$

Example 1: Lossy single-mode cavity (with pump)

[G. S. Agarwal, J. Opt. Soc. Am. B, **5**, 1940 (1988)]

Exercise: Determine the steady state.



Pumping Hamiltonian: $\hat{H}' = \frac{g}{2}\left(\hat{a} + \hat{a}^\dagger\right)$

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}_0 + \hat{H}', \hat{\rho}\right] + \frac{\gamma}{2}\left(2\,\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}\right) \qquad \hat{H}_0 \equiv \omega\,\hat{a}^\dagger\hat{a}$$

Rotating frame w.r.t. $\hat{H}_0$: $\tilde{\rho}(t) = e^{i\hat{H}_0 t}\hat{\rho}(t)e^{-i\hat{H}_0 t}$

$$\dot{\hat{\rho}} = -i\left[\hat{H}_0, \hat{\rho}\right] + e^{-i\hat{H}_0 t}\,\dot{\tilde{\rho}}\,e^{i\hat{H}_0 t}$$

From Hausdorf: $e^{i\hat{H}_0 t}\hat{a}e^{-i\hat{H}_0 t} = \hat{a}e^{-i\omega t}$

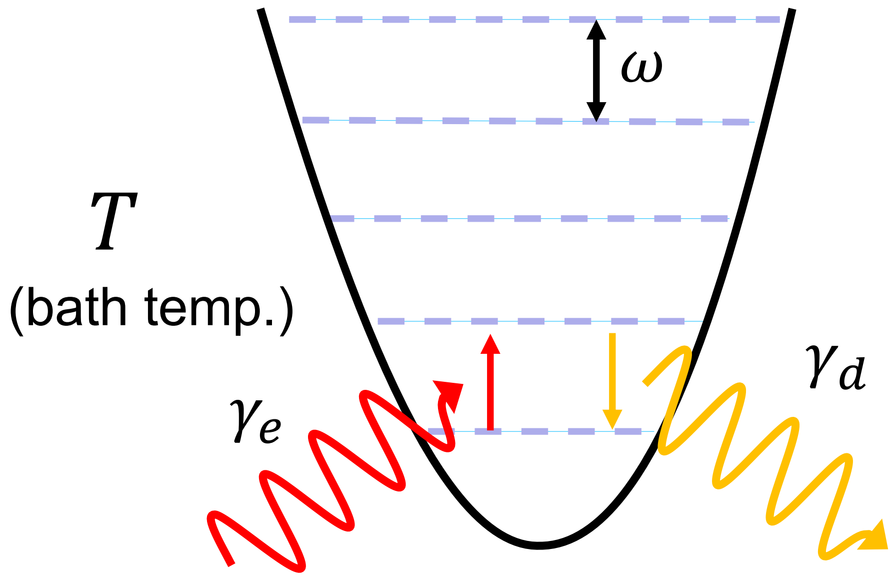
$$\dot{\tilde{\rho}} = -i\left[\frac{g}{2}\left(\hat{a}e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}\right), \tilde{\rho}\right] + \frac{\gamma}{2}\left(2\,\hat{a}\tilde{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\tilde{\rho} - \tilde{\rho}\hat{a}^\dagger\hat{a}\right)$$

$$= \frac{\gamma}{2}\left(2\,\hat{c}\tilde{\rho}\hat{c}^\dagger - \hat{c}^\dagger\hat{c}\tilde{\rho} - \tilde{\rho}\hat{c}^\dagger\hat{c}\right) \quad \text{with} \quad \hat{c} \equiv \hat{a}e^{-i\omega t} + ig/\gamma$$

$\dot{\tilde{\rho}} = 0$ if & only if $\left(\hat{a}e^{-i\omega t} + ig/\gamma\right)\tilde{\rho} = \tilde{\rho}\left(\hat{a}e^{-i\omega t} + ig/\gamma\right)^\dagger$

→ $\tilde{\rho} = \left|-ige^{i\omega t}/\gamma\right\rangle\left\langle -ige^{i\omega t}/\gamma\right|$: coherent st.

Example 2: Quantum H.O. in a heat bath



$$\hat{H} = \omega\, \hat{a}^\dagger \hat{a}$$

2 channels:

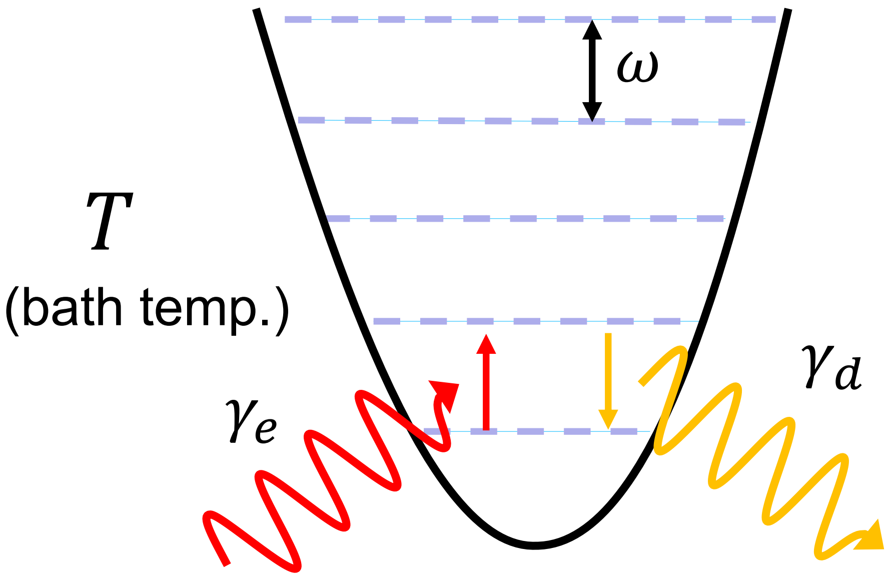
$\hat{L}_{\text{de-excite}} = \hat{a}$ with rate γ_d

$\hat{L}_{\text{excite}} = \hat{a}^\dagger$ with rate γ_e

$$\frac{d\hat{\rho}}{dt} = -i[\omega\, \hat{a}^\dagger \hat{a}, \hat{\rho}] + \underbrace{\frac{\gamma_d}{2}\left(2\, \hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}\right)}_{\text{de-excitation}}$$

$$+ \underbrace{\frac{\gamma_e}{2}\left(2\, \hat{a}^\dagger\hat{\rho}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho} - \hat{\rho}\hat{a}\hat{a}^\dagger\right)}_{\text{excitation}}$$

Example 2: Quantum H.O. in a heat bath



The rates γ_d & γ_e are not indep.

The ratio γ_d/γ_e should be determined to be consistent with thermodynamics.

The ratio γ_d/γ_e is determined by the detailed-balance condition:

$$\gamma_e \times (\text{pop. of } i\text{th level in eq.}) = \gamma_d \times (\text{pop. of } (i+1)\text{th level in eq.})$$

Equivalently, the condition such that the population $\langle \hat{a}^\dagger \hat{a} \rangle$ in the steady st. is consistent with the eq. population $n(\omega)$:

$$\langle \hat{a}^\dagger \hat{a} \rangle = n(\omega) \equiv \frac{1}{e^{\beta\omega} - 1}$$

Example 2: Quantum H.O. in a heat bath

Exercise: Determine the ratio γ_d/γ_e.

$$\frac{d}{dt}\langle \hat{a}^\dagger \hat{a}\rangle = \frac{d}{dt}\mathrm{Tr}[\hat{\rho}\,\hat{a}^\dagger\hat{a}] = \mathrm{Tr}\left[\frac{d\hat{\rho}}{dt}\hat{a}^\dagger\hat{a}\right] = \mathrm{Tr}[(\mathcal{L}\,\hat{\rho})\,\hat{a}^\dagger\hat{a}] = 0$$

(steady st.)

$$\mathrm{Tr}\big[\big(-i[\omega\,\hat{a}^\dagger\hat{a},\hat{\rho}]\big)\,\hat{a}^\dagger\hat{a}\big] = 0$$

$$\mathrm{Tr}\left[\left(\frac{\gamma_d}{2}\left(2\,\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}\right)\right)\,\hat{a}^\dagger\hat{a}\right] = -\gamma_d\langle\hat{a}^\dagger\hat{a}\rangle$$

$$\mathrm{Tr}\left[\left(\frac{\gamma_e}{2}\left(2\,\hat{a}^\dagger\hat{\rho}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho} - \hat{\rho}\hat{a}\hat{a}^\dagger\right)\right)\,\hat{a}^\dagger\hat{a}\right] = \gamma_e\big(\langle\hat{a}^\dagger\hat{a}\rangle + 1\big)$$

➡ Steady st. pop.: $\langle\hat{a}^\dagger\hat{a}\rangle = \frac{\gamma_e}{\gamma_d - \gamma_e} = n(\omega)$ ➡ $\dfrac{\gamma_e}{\gamma_d} = \dfrac{n(\omega)}{n(\omega)+1}$

with $n(\omega) \equiv \left(e^{\beta\omega} - 1\right)^{-1}$

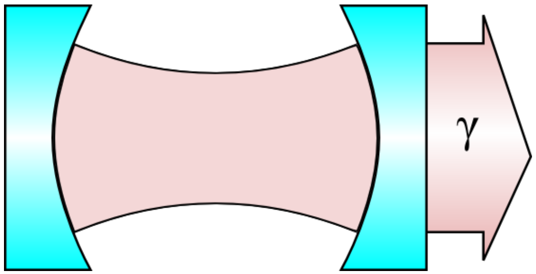
Simple derivation of the Lindblad ME

Derivation based on the Kraus map:

➡ Repetition of the Kraus map for infinitesimal time steps Δt.

For simplicity & clarity, we consider the situation in which the particle loss is the only possible dissipation process.

γ : loss rate
$\hat{a}$: annihilation op.
$\hat{H}$: system Hamiltonian



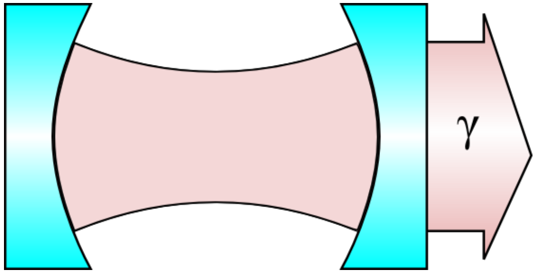
There are two possibilities (with loss or no loss) in Δt.

A set of Kraus op.

$$\begin{cases} \text{Loss: } \hat{M}_1(\Delta t) \\ \text{No loss: } \hat{M}_0(\Delta t) \end{cases}$$

Simple derivation of the Lindblad ME

γ : loss rate
$\hat{a}$: annihilation op.
$\hat{H}$: system Hamiltonian



Suppose that the sys. is in the st. $|\Psi\rangle$ at time t.

Probability of a particle escaping from the system within Δt:

$$\Delta P_1 = \gamma \langle \Psi | \hat{a}^\dagger \hat{a} | \Psi \rangle \, \Delta t$$

$$|\Psi\rangle \xrightarrow{\Delta t} \begin{cases} |\Psi_{\mathrm{loss}}\rangle & \Delta P_1 \\ |\Psi_{\mathrm{no\ loss}}\rangle & \Delta P_0 \equiv 1 - \Delta P_1 \end{cases}$$

probability

Simple derivation of the Lindblad ME

Suppose that the sys. is in the st. $|\Psi\rangle$ at time t.

1. Loss $\hat{M}_1(\Delta t) \propto \hat{a}$:

$$|\Psi\rangle \longrightarrow \frac{\hat{M}_1|\Psi\rangle}{\sqrt{\langle\Psi|\hat{M}_1^\dagger \hat{M}_1|\Psi\rangle}} \qquad \text{(quantum jump)}$$

$$\hat{M}_1(\Delta t) = \sqrt{\gamma \Delta t}\, \hat{a} \quad \Leftarrow \quad \Delta P_1 = \gamma \langle\Psi|\hat{a}^\dagger \hat{a}|\Psi\rangle \Delta t$$

2. No loss $\hat{M}_0(\Delta t)$:

$$\hat{M}_0(\Delta t) \simeq \hat{I}_S - i(\hat{H} + \Delta\hat{H}_{\text{eff}})\Delta t$$

- $\hat{H}$: unitary evolution
- $\Delta\hat{H}_{\text{eff}}$: backaction from info. gain of "no loss"

Completeness $\hat{I}_S = \sum_k \hat{M}_k^\dagger \hat{M}_k = \hat{M}_0^\dagger \hat{M}_0 + \hat{M}_1^\dagger \hat{M}_1$

$$\Rightarrow \quad \Delta\hat{H}_{\text{eff}} = -i\frac{\gamma}{2}\hat{a}^\dagger \hat{a}$$

Simple derivation of the Lindblad ME

State at $t + \Delta t$ by the Kraus map:

$$\hat{\rho}(t+\Delta t) = \hat{M}_0\, \hat{\rho}(t)\, \hat{M}_0^\dagger + \underline{\hat{M}_1\, \hat{\rho}(t)\, \hat{M}_1^\dagger}$$

$$\simeq \left[\hat{I}_S - i\left(\hat{H} - i\frac{\gamma}{2}\hat{a}^\dagger\hat{a}\right)\Delta t\right]\hat{\rho}(t)\left[\hat{I}_S + i\left(\hat{H} + i\frac{\gamma}{2}\hat{a}^\dagger\hat{a}\right)\Delta t\right]$$

$$+\underline{\gamma\, \Delta t\, \hat{a}\hat{\rho}(t)\hat{a}^\dagger}$$

$$\simeq \hat{\rho}(t) - i[\hat{H}, \hat{\rho}(t)]\Delta t - \frac{\gamma}{2}\left(\hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}\right) + \underline{\gamma\, \Delta t\, \hat{a}\hat{\rho}\hat{a}^\dagger}$$

➡ Lindblad master eq.

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}] + \frac{\gamma}{2}\left(\underline{2\hat{a}\hat{\rho}\hat{a}^\dagger}\ \underline{- \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}}\right)$$

"Quantum jump" term from $\Delta\hat{H}_{\mathrm{eff}}$

Remarks on the "Born-Markov approx."

In the derivation, we have assumed that the evolution is given by the same Kraus map at each instance of time.

The Kraus map assumes the product st. $\hat{\rho} \otimes \hat{\rho}_E$ for the init. st.

Repeating the same Kraus map at each t.

- System evolution $t \rightarrow t + \Delta t$ depends only on $\hat{\rho}$ at t and environment is reset to the same $\hat{\rho}_E$ at each t.

  No memory, indep. of the past st. ⇨ Markovian

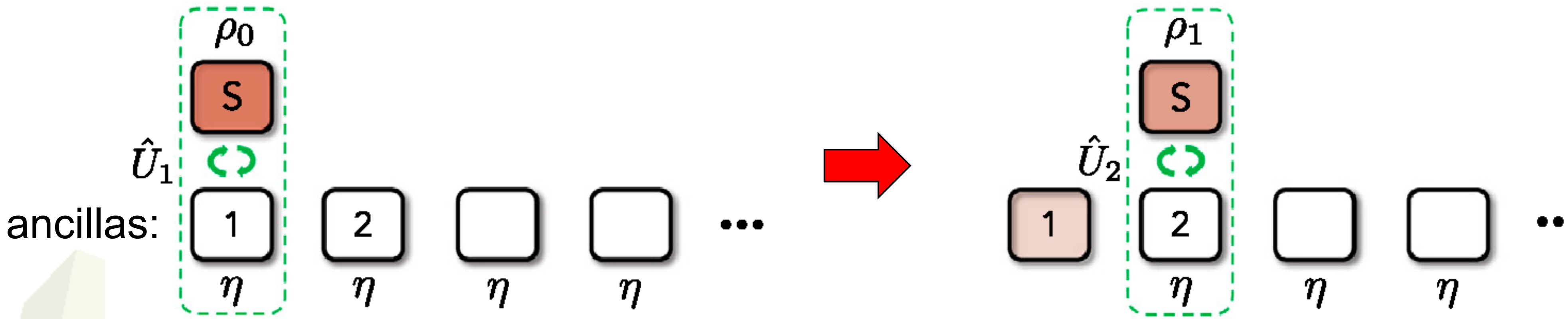
- The total density op. is set to the product st. $\hat{\rho}(t) \otimes \hat{\rho}_E$ at each t.

  Weak coupling: "Born approx."

Remarks on the collision model

The above derivation is based on the repeated applications of the Kraus map.

$$\begin{pmatrix}\text{Repeated Kraus-map} \\ \text{applications}\end{pmatrix} \cong \begin{pmatrix}\text{Sequential int. with ancillas} \\ \text{serving as the environment}\end{pmatrix}$$



Ciccarello et al., Phys. Rep. 954, 1 (2022)

"Collision model" (repeated int. scheme)

Broad applications in quantum thermodynamics

Reviews: Ciccarello *et al*., Phys. Rep. **954**, 1 (2022).
Strasberg *et al*., PRX **7**, 021003 (2017).

Other remarks

・Since the Kraus map is CPTP, the evolution by the Lindblad ME is also CPTP.

・The Lindblad ME defines the most general generator of the Markovian CPTP map.

・However, the Lindblad ME is NOT the most general formalism of open quantum systems.

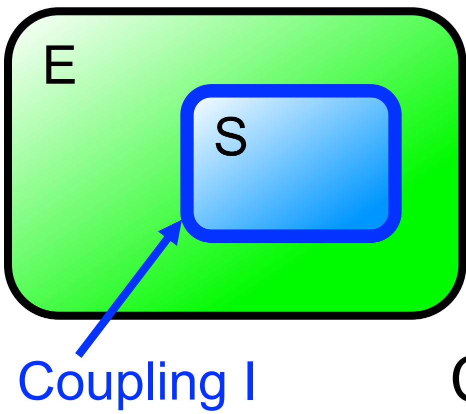
The Lindblad ME is valid only in the weak coupling regime and the coarse-grained time scale.

(time scale of interest) $\gg$ (relaxation time of the env.)

III. Microscopic derivation of the Lindblad ME

Microscopic derivation of the Lindblad ME

Based on the microscopic coupling Hamiltonian $\hat{H}_I$ btwn. sys. & env., an expression for the dissipation rate γ can be obtained.



$$\hat{H}_{tot} \equiv \underset{\text{sys.}}{\hat{H}_S} + \underset{\text{env.}}{\hat{H}_E} + \underset{\text{coupling}}{\hat{H}_I}$$

Coupling Hamiltonian: $$\hat{H}_I = \sum_i \hat{A}_i \otimes \hat{B}_i$$

- i: label of particles/sites
- $\hat{A}_i$: sys. coupling op.
- $\hat{B}_i$: env. coupling op.

In the int. picture: $$\hat{H}_I^{(I)}(t) \equiv e^{i(\hat{H}_S+\hat{H}_E)t}\hat{H}_I e^{-i(\hat{H}_S+\hat{H}_E)t}$$

$$\Rightarrow \quad \hat{H}_I^{(I)}(t) = \sum_i \hat{A}_i^{(I)}(t) \otimes \hat{B}_i^{(I)}(t)$$

$$\hat{A}_i^{(I)}(t) \equiv e^{i\hat{H}_S t}\hat{A}_i e^{-i\hat{H}_S t}$$ (same for $\hat{B}_i$)

Assumptions & approximations

- initial st.: $\hat{\rho}_{tot}(0) = \hat{\rho}(0) \otimes \hat{\rho}_E$ (product st.)

- "Born-Markov-secular approximation"

  Born approx. (weak coupling): $\hat{\rho}_{tot}(t) \approx \hat{\rho}(t) \otimes \hat{\rho}_E$ for $\forall t$.

  Markov approx.: Evolution of $\hat{\rho}(t)$ only determined by the state at current t. (S & E are memoryless)

  Secular approx. (rotating wave): Coarse-graining of time.

Born + Markov ➡ Redfield ME (non-CPTP)

Born + Markov + Secular ➡ Lindblad ME (CPTP)

Trade-off btwn. secular approx. & CPTP.

Resulting master eq.: 1st standard form

$$\dot{\hat{\rho}}(t) = -i\left[\hat{H}_S + \hat{H}_{LS}, \hat{\rho}(t)\right] + \sum_{i,j}\sum_{\omega}\frac{\gamma_{ij}(\omega)}{2}\left[2\hat{A}_j(\omega)\hat{\rho}\hat{A}_i^\dagger(\omega) - \hat{A}_i^\dagger(\omega)\hat{A}_j(\omega)\hat{\rho} - \hat{\rho}\hat{A}_i^\dagger(\omega)\hat{A}_j(\omega)\right]$$

$$\gamma_{ij}(\omega) \equiv \int_{-\infty}^{\infty} dt \left\langle \hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\right\rangle e^{i\omega t}$$

$$\hat{A}_i(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, \hat{A}_i^{(I)}(t)e^{i\omega t} = \sum_{\varepsilon'-\varepsilon=\omega}\hat{\Pi}_S(\varepsilon)\hat{A}_i\hat{\Pi}_S(\varepsilon')$$

$$\hat{H}_S = \sum_\varepsilon \varepsilon\, \hat{\Pi}_S(\varepsilon)$$

$$\hat{H}_{LS} \equiv \sum_{i,j}\sum_\omega S_{ij}(\omega)\hat{A}_i^\dagger(\omega)\hat{A}_j(\omega)$$: Lamb shift Hamiltonian

(Energy shift by int. btwn. S&E)

$$S_{ij}(\omega) \equiv \frac{1}{2i}\left[\Gamma_{ij}^{(+)}(\omega) - \left(\Gamma_{ji}^{(+)}(\omega)\right)^*\right]$$

$$\Gamma_{ij}^{(+)}(\omega) \equiv \int_0^\infty dt \left\langle \hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\right\rangle e^{i\omega t}$$

$\gamma_{ij}(\omega)$: sym. part of $\Gamma_{ij}^{(+)}(\omega)$; $S_{ij}(\omega)$: antisym. part of $\Gamma_{ij}^{(+)}(\omega)$

From 1st standard form to Lindblad ME

Coefficient matrix $\gamma_{ij}(\omega)$ is positive semidefinite.

→ γ_{ij} can be diagonalized by an appropriate unitary u :

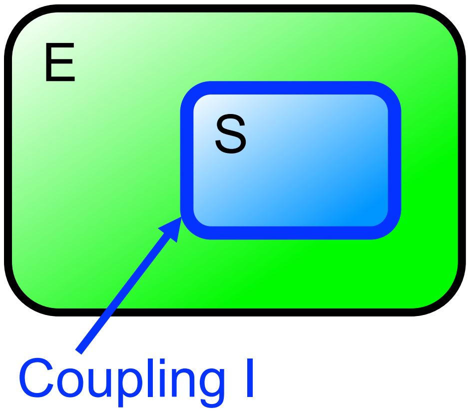
$$u\,\gamma\,u^\dagger = \begin{pmatrix} \tilde{\gamma}_1 & & & \\ & \tilde{\gamma}_2 & & \\ & & \tilde{\gamma}_3 & \\ & & & \ddots \end{pmatrix}$$

Then, the 1st standard form can always be rewritten into the Lindblad form:

$$\dot{\hat{\rho}}(t) = -i\left[\hat{H}_S + \hat{H}_{LS}\,,\hat{\rho}(t)\right]$$
$$+\sum_k \sum_\omega \frac{\tilde{\gamma}_k(\omega)}{2}\left[2\hat{L}_k(\omega)\hat{\rho}\hat{L}_k^\dagger(\omega) - \hat{L}_k^\dagger(\omega)\hat{L}_k(\omega)\hat{\rho} - \hat{\rho}\hat{L}_k^\dagger(\omega)\hat{L}_k(\omega)\right]$$

with $\hat{A}_i = \sum_k u_{ki}\,\hat{L}_k$

Derivation (1): Setup, von Neumann eq.



$$\hat{H}_{tot} \equiv \hat{H}_S + \hat{H}_E + \hat{H}_I$$

sys. env. coupling

Coupling Hamiltonian: $\hat{H}_I = \sum_i \hat{A}_i \otimes \hat{B}_i$

initial st.: $\hat{\rho}_{tot}(0) = \hat{\rho}(0) \otimes \hat{\rho}_E$ (product st.)

von Neumann eq. in the int. pict.: $\frac{d}{dt}\hat{\rho}_{tot}^{(I)}(t) = -i\left[\hat{H}_I^{(I)}(t), \hat{\rho}_{tot}^{(I)}(t)\right]$ (1)

$$\hat{\rho}_{tot}^{(I)}(t) \equiv \hat{U}_I(t)\hat{\rho}_{tot}(0)\hat{U}_I^\dagger(t) = e^{-i\hat{H}_I t}\hat{\rho}_{tot}(0)e^{i\hat{H}_I t}$$

$$\hat{H}_I^{(I)}(t) \equiv \hat{U}_0^\dagger(t)\hat{H}_I\hat{U}_0(t) = e^{i(\hat{H}_S+\hat{H}_E)t}\hat{H}_I e^{-i(\hat{H}_S+\hat{H}_E)t}$$

Formal sol.: $\hat{\rho}_{tot}^{(I)}(t) = \hat{\rho}_{tot}^{(I)}(0) - i\int_0^t dt' \left[\hat{H}_I^{(I)}(t'), \hat{\rho}_{tot}^{(I)}(t')\right]$ (2)

$$\hat{\rho}_{tot}^{(I)}(0) = \hat{\rho}_{tot}(0)$$

Derivation (2): Tracing out E

von Neumann eq. in the int. pict.: $\frac{d}{dt}\hat{\rho}_{tot}^{(I)}(t) = -i\left[\hat{H}_I^{(I)}(t), \hat{\rho}_{tot}^{(I)}(t)\right]$ (1)

Formal sol.: $\hat{\rho}_{tot}^{(I)}(t) = \hat{\rho}_{tot}^{(I)}(0) - i\int_0^t dt' \left[\hat{H}_I^{(I)}(t'), \hat{\rho}_{tot}^{(I)}(t')\right]$ (2)

Substituting (2) into (1) and tracing out E reads:

$$\frac{d}{dt}\mathrm{Tr}_E\, \hat{\rho}_{tot}^{(I)}(t) = \frac{d}{dt}\hat{\rho}^{(I)}(t) = -i\,\mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \hat{\rho}_{tot}^{(I)}(0)\right] - \int_0^t dt'\,\mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t'), \hat{\rho}_{tot}^{(I)}(t')\right]\right]$$

The 1st term (MF-shift) can be absorbed by the re-definition of $\hat{H}_S$:

$$\mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \hat{\rho}_{tot}^{(I)}(0)\right] = \sum_i \mathrm{Tr}_E\left\{\left[\hat{A}_i^{(I)}(t), \hat{\rho}(0)\right] \otimes \hat{B}_i^{(I)}(t)\hat{\rho}_E + \hat{A}_i^{(I)}(t)\hat{\rho}(0) \otimes \underbrace{\left[\hat{B}_i^{(I)}(t), \hat{\rho}_E\right]}_{0}\right\}$$

$$= \left[\underline{\sum_i b_i(t)\hat{A}_i^{(I)}(t)}, \hat{\rho}(0)\right] \qquad b_i \equiv \mathrm{Tr}_E\left[\hat{B}_i^{(I)}(t)\hat{\rho}_E\right]$$

$$\equiv \hat{H}_{MF}^{(I)}(t)$$ ("1st-order Lamb shift")

Derivation (3): Non-Markovian Redfield ME

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) = -\int_0^t dt' \, \mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t'), \hat{\rho}_{tot}^{(I)}(t')\right]\right]$$

Weak coupling approx.: $\hat{\rho}_{tot}^{(I)}(t) \approx \hat{\rho}^{(I)}(t) \otimes \hat{\rho}_E$ for $\forall t$.

1st Markov approx.: For past t' $(< t)$ $\quad \hat{\rho}^{(I)}(t') \longrightarrow \hat{\rho}^{(I)}(t)$

$$\Rightarrow \quad \frac{d}{dt}\hat{\rho}^{(I)}(t) \simeq -\int_0^t dt' \, \mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t'), \hat{\rho}^{(I)}(t) \otimes \hat{\rho}_E\right]\right]$$

Non-Markovian Redfield ME

Derivation (4): Markov approx. & Redfield ME

non-Markovian Redfield ME: $$\frac{d}{dt}\hat{\rho}^{(I)}(t) \approx -\int_0^t dt' \, \mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t'), \hat{\rho}^{(I)}(t) \otimes \hat{\rho}_E\right]\right]$$

Introduce the elapsed time: $t'' \equiv t - t'$ $\quad (t'':\ t \sim 0)$

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) = \int_t^0 dt'' \, \mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t - t''), \hat{\rho}^{(I)}(t) \otimes \hat{\rho}_E\right]\right]$$

$t \to \infty$ (2nd Markov approx.)

2nd Markov approx.: The integrand vanishes quickly for $t'' \gg$ (correlation time τ_E of E)

This is valid when: (dynamical timescale of S) $\gg \tau_E$

2nd Markov approx. removes the initial st. dependence of $\hat{\rho}^{(I)}(t)$.

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) \approx -\int_0^\infty dt'' \, \mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t), \left[\hat{H}_I^{(I)}(t - t''), \hat{\rho}^{(I)}(t) \otimes \hat{\rho}_E\right]\right]$$

(Markovian) Redfield ME

(Here, "Markovian" means env. is memoryless; weak Markovianity.)

Derivation (5): Redfield ME

(Markovian) Redfield ME:

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) \approx -\int_0^\infty dt''\,\mathrm{Tr}_E\left[\hat{H}_I^{(I)}(t),\left[\hat{H}_I^{(I)}(t-t''),\,\hat{\rho}^{(I)}(t)\otimes\hat{\rho}_E\right]\right]$$

$$\hat{H}_I^{(I)}(t) = \sum_i \hat{A}_i^{(I)}(t)\otimes\hat{B}_i^{(I)}(t)$$

$$= \int_0^\infty dt'' \sum_{i,j}\left\{\begin{array}{c} c_{ij}(t'')\left[\hat{A}_j^{(I)}(t-t'')\,\hat{\rho}^{(I)}(t),\hat{A}_i^{(I)}(t)\right] \\ +c_{ji}(-t'')\left[\hat{A}_i^{(I)}(t),\,\hat{\rho}^{(I)}(t)\hat{A}_j^{(I)}(t-t'')\right]\end{array}\right\}$$

$$c_{ij}(\tau) \equiv \mathrm{Tr}\left[\hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\hat{\rho}_E\right] = \left\langle\hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\right\rangle$$

Fourier decomposition of $\hat{A}_i^{(I)}(t)$: $\quad \hat{A}_i^{(I)}(t) = \sum_\omega \hat{A}_i(\omega)\,e^{-i\omega t}$

$$\left[\;\hat{A}_i(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\,\hat{A}_i^{(I)}(t)e^{i\omega t} = \sum_{\varepsilon'-\varepsilon=\omega}\hat{\Pi}_S(\varepsilon)\hat{A}_i\hat{\Pi}_S(\varepsilon')\;\right]$$

Derivation (6): Secular approx.

Fourier decomposition of $\hat{A}_i^{(I)}(t)$: $\quad \hat{A}_i^{(I)}(t) = \sum_\omega \hat{A}_i(\omega)\, e^{-i\omega t}$

$$\dot{\hat{\rho}}^{(I)}(t) = \sum_{i,j} \sum_{\omega,\omega'} \left\{ \begin{array}{l} e^{-i(\omega'-\omega)t}\, \Gamma_{ij}^{(+)}(\omega') \left[\hat{A}_j(\omega')\, \hat{\rho}^{(I)}(t), \hat{A}_i^\dagger(\omega) \right] \\ + e^{-i(\omega-\omega')t}\, \Gamma_{ij}^{(-)}(-\omega') \left[\hat{A}_i(\omega),\, \hat{\rho}^{(I)}(t) \hat{A}_j^\dagger(\omega') \right] \end{array} \right\}$$

$$\Gamma_{ij}^{(+)}(\omega) \equiv \int_0^\infty dt''\, c_{ij}(t'')\, e^{i\omega t''}$$

$$\Gamma_{ij}^{(-)}(\omega) \equiv \int_0^\infty dt''\, c_{ji}(-t'')\, e^{i\omega t''}$$

Fourier transf. of the 2-time correlation func. of $\hat{B}_i^{(I)}(t)$.

Secular (rotating-wave) approx.: Keep terms only for $\omega = \omega'$.

The factor $e^{\mp i(\omega'-\omega)t}$ oscillates fast when $\omega \neq \omega'$.

$$\dot{\hat{\rho}}^{(I)}(t) \approx \sum_{i,j} \sum_{\omega} \left\{ \begin{array}{l} \Gamma_{ij}^{(+)}(\omega) \left[\hat{A}_j(\omega)\, \hat{\rho}^{(I)}(t), \hat{A}_i^\dagger(\omega) \right] \\ + \Gamma_{ij}^{(-)}(-\omega) \left[\hat{A}_i(\omega),\, \hat{\rho}^{(I)}(t) \hat{A}_j^\dagger(\omega) \right] \end{array} \right\}$$

Derivation (7): γ_{ij} & S_{ij}

$$\dot{\hat{\rho}}^{(I)}(t) \approx \sum_{i,j}\sum_{\omega}\left\{\begin{array}{c}\Gamma_{ij}^{(+)}(\omega)\left[\hat{A}_j(\omega)\,\hat{\rho}^{(I)}(t),\hat{A}_i^{\dagger}(\omega)\right] \\ +\Gamma_{ij}^{(-)}(-\omega)\left[\hat{A}_i(\omega),\,\hat{\rho}^{(I)}(t)\hat{A}_j^{\dagger}(\omega)\right]\end{array}\right\}$$

Use $\Gamma_{ji}^{(-)}(-\omega) = \left(\Gamma_{ji}^{(+)}(\omega)\right)^*$ and $i \leftrightarrow j$ in the 2nd term.

$$\dot{\hat{\rho}}^{(I)}(t) \approx \sum_{i,j}\sum_{\omega}\left\{\begin{array}{c}\Gamma_{ij}^{(+)}(\omega)\left[\hat{A}_j(\omega)\,\hat{\rho}^{(I)}(t),\hat{A}_i^{\dagger}(\omega)\right] \\ +\left(\Gamma_{ji}^{(+)}(\omega)\right)^*\left[\hat{A}_j(\omega),\,\hat{\rho}^{(I)}(t)\hat{A}_i^{\dagger}(\omega)\right]\end{array}\right\}$$

Decompose $\Gamma_{ij}^{(+)}$ into symmetric part γ_{ij} and antisymmetric part S_{ij}.

$$\gamma_{ij}(\omega) \equiv \Gamma_{ij}^{(+)}(\omega) + \left(\Gamma_{ji}^{(+)}(\omega)\right)^* \qquad \left(= \int_{-\infty}^{\infty} dt\,\left\langle \hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\right\rangle e^{i\omega t}\right)$$

$$S_{ij}(\omega) \equiv \frac{1}{2i}\left[\Gamma_{ij}^{(+)}(\omega) - \left(\Gamma_{ji}^{(+)}(\omega)\right)^*\right]$$

Lindblad ME (int. picture):

$$\dot{\hat{\rho}}^{(I)}(t) = -i\left[\hat{H}_{LS}\,, \hat{\rho}^{(I)}(t)\right]$$

$$+\sum_{i,j}\sum_{\omega}\frac{\gamma_{ij}(\omega)}{2}\left[2\hat{A}_j(\omega)\,\hat{\rho}^{(I)}\hat{A}_i^{\dagger}(\omega) - \hat{A}_i^{\dagger}(\omega)\hat{A}_j(\omega)\,\hat{\rho}^{(I)} - \hat{\rho}^{(I)}\hat{A}_i^{\dagger}(\omega)\hat{A}_j(\omega)\right]$$

$\hat{H}_{LS} \equiv \sum_{i,j}\sum_{\omega} S_{ij}(\omega)\hat{A}_i^{\dagger}(\omega)\hat{A}_j(\omega)$: Lamb shift Hamiltonian

Lindblad ME (Schrödinger picture):

$$\dot{\hat{\rho}}(t) = -i\left[\hat{H}_S + \hat{H}_{LS}\,, \hat{\rho}(t)\right]$$

$$+\sum_{i,j}\sum_{\omega}\frac{\gamma_{ij}(\omega)}{2}\left[2\hat{A}_j(\omega)\hat{\rho}\hat{A}_i^{\dagger}(\omega) - \hat{A}_i^{\dagger}(\omega)\hat{A}_j(\omega)\hat{\rho} - \hat{\rho}\hat{A}_i^{\dagger}(\omega)\hat{A}_j(\omega)\right]$$

$$\gamma_{ij}(\omega) \equiv \int_{-\infty}^{\infty} dt\,\left\langle \hat{B}_i^{(I)}(t)\hat{B}_j^{(I)}(0)\right\rangle e^{i\omega t}$$

$\hat{A}_i(\omega) \equiv \sum_{\varepsilon'-\varepsilon=\omega}\hat{\Pi}_S(\varepsilon)\hat{A}_i\hat{\Pi}_S(\varepsilon')$ $\qquad$ $\hat{H}_S = \sum_{\varepsilon}\varepsilon\,\hat{\Pi}_S(\varepsilon)$

Remarks on the "Markovianity"

- Here, we follow the notion of "Markovianity" used in the textbook by Breuer & Petruccione.

In this context,

"Markovian": Environment is memoryless.

(correlation time of E) $\ll$ (dynamical timescale of S)

This notion of Markovianity (sometimes called "weak Markovianity") does not require CP-divisibility.

- 2nd Markov approx. removes the explicit initial-state dependence of $\hat{\rho}(t)$ under the assumption of a memoryless environment.

In this sense, the Redfield ME after the 2nd Markov approx. is often referred to as "Markovian", although it is not Markovian in the strict (CP-divisible) sense.

Summary

	(Markovian*) Redfield ME	Lindblad ME
Markov approx.	Yes	Yes
Secular approx.	No	Yes
Positivity	Not guaranteed	Yes (CPTP)
Coherence	Preserved	Rapidly decay (averaged out)
Interference effects	Included (btwn. close Bohr freq.)	Neglected
Applicable regimes	Short-time, transient processes, quasi-degenerate sys.	Long-time, steady state, thermal processes

(*Here, "Markovian" means env. is memoryless; weak Markovianity.)

IV. Global & local MEs

Function of $\mathcal{D}[\hat{L}]$ depends on the $\hat{H}$-basis

Function of the dissipator $\mathcal{D}[\hat{L}]$ in the Lindblad ME depends on the basis of sys. Hamiltonian $\hat{H}$.

(Example) Pure dephasing (decoherence)

Decay of the off-diag. elements of $\hat{\rho}$ in $\hat{H}$-basis.

<u>For a TLS</u>

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|e\rangle + e^{i\theta}|g\rangle\right)$$

$\{|e\rangle, |g\rangle\}$: basis of $\hat{H}$

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\theta} \\ e^{i\theta} & 1 \end{pmatrix}$$

: pure st.

Dephasing →

$$\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

: statistical mix. $\begin{cases} |e\rangle & 50\% \\ |g\rangle & 50\% \end{cases}$

$\langle \hat{H}^n \rangle \equiv \mathrm{Tr}[\hat{\rho}\,\hat{H}^n]$ unchanged.

Function of $\mathcal{D}[\hat{L}]$ depends on the $\hat{H}$-basis

Function of the dissipator $\mathcal{D}[\hat{L}]$ in the Lindblad ME depends on the basis of sys. Hamiltonian $\hat{H}$.

(Example) Pure dephasing (decoherence)

Decay of the off-diag. elements of $\hat{\rho}$ in $\hat{H}$-basis.

Corresponding jump op. $\hat{L} \propto \hat{H} \quad \left(\hat{L} = \hat{H}/\varepsilon\right)$.

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}, \hat{\rho}\right] + \frac{\tilde{\Gamma}}{2}\left(2\hat{H}\hat{\rho}\hat{H}^{\dagger} - \hat{H}^{\dagger}\hat{H}\hat{\rho} - \hat{\rho}\hat{H}^{\dagger}\hat{H}\right) \qquad \left(\tilde{\Gamma} \equiv \Gamma/\varepsilon^{2}\right)$$

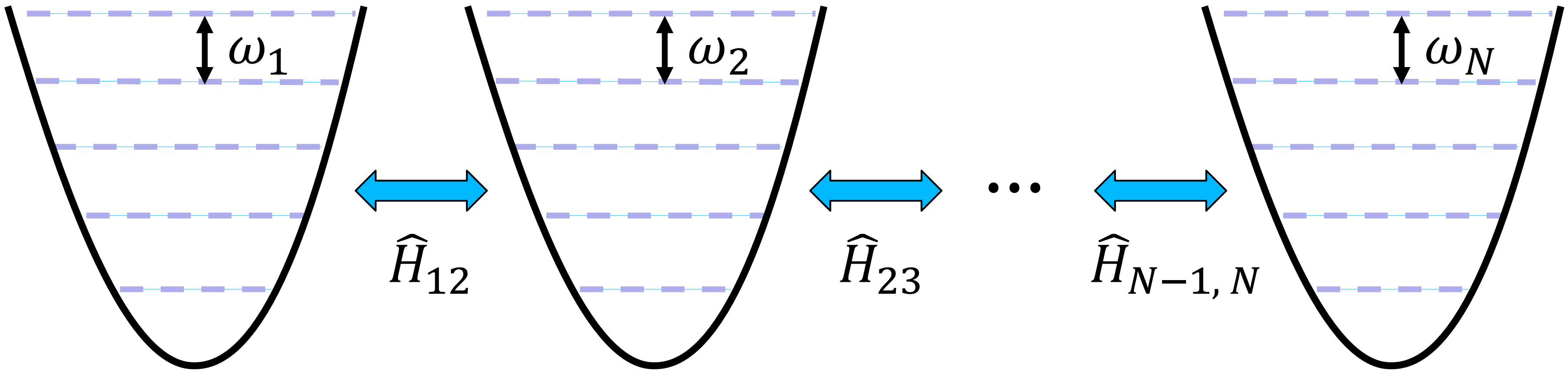
$$\hat{\rho}(t) = \sum_{i,j} \rho_{ij}(t)\left|\varepsilon_i\right\rangle\left\langle\varepsilon_j\right|$$

$$\frac{d\rho_{ij}}{dt} = -i\left(\varepsilon_i - \varepsilon_j\right)\rho_{ij} - \frac{\tilde{\Gamma}}{2}\left(\varepsilon_i - \varepsilon_j\right)^2 \rho_{ij}$$

- off-diag. $(i \neq j)$: $\rho_{ij}(t) \propto \rho_{ij}(0)\, e^{-\frac{\tilde{\Gamma}}{2}\left(\varepsilon_i - \varepsilon_j\right)^2 t}$
- diag. $(i = j)$: $\rho_{ii}(t) = \rho_{ii}(0)$

Global & local MEs: Definitions

A sys. consisting of multiple subsys.



HO-1 $\hat{H}_1 = \omega_1 \hat{a}_1^\dagger \hat{a}_1$

HO-2 $\hat{H}_2 = \omega_2 \hat{a}_2^\dagger \hat{a}_2$

HO-N $\hat{H}_N = \omega_N \hat{a}_N^\dagger \hat{a}_N$

Local ME: ME contains only local jump ops. for each subsys.

$$\hat{L} = \hat{a}_i,\ \hat{a}_i^\dagger,\ \hat{a}_i^\dagger \hat{a}_i, \text{etc.}$$

Global ME: ME contains non-local jump ops.

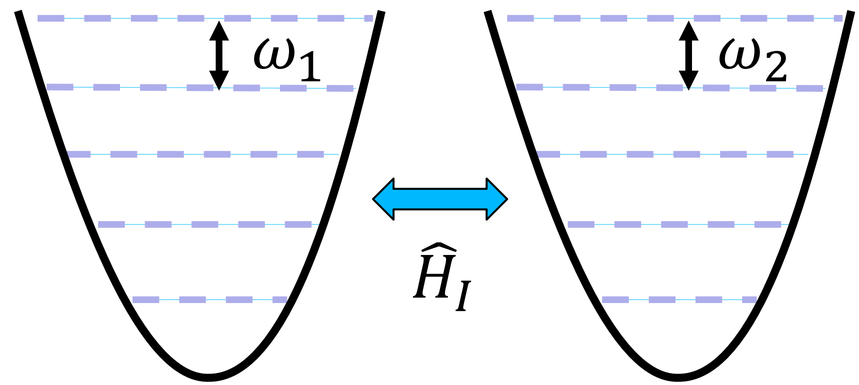
$$\hat{L} = \hat{a}_1 + \hat{a}_2,\ \hat{a}_2^\dagger \hat{a}_1, \text{etc.}$$

Thermodynamic inconsistency of the local MEs

"Local ME can be inconsistent with thermodynamics."

Levy & Kosloff, EPL **107**, 20004 (2014)

Example: Coupled two HOs in a thermal environment (inv. temp. β).



HO-1 $\hat{H}_1 = \omega_1 \hat{a}_1^\dagger \hat{a}_1$

HO-2 $\hat{H}_2 = \omega_2 \hat{a}_2^\dagger \hat{a}_2$

Local ME: $$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}_1 + \hat{H}_2 + \hat{H}_I, \hat{\rho}\right] + \frac{\gamma_0}{2} \sum_{i=1,2} \left[\mathcal{D}[\hat{a}_i]\hat{\rho} + e^{-\beta\omega_i}\mathcal{D}\left[\hat{a}_i^\dagger\right]\hat{\rho}\right]$$

When $\hat{H}_I \neq 0$, this local ME does not satisfy (global) detailed balance.

$\because$ $\hat{a}_i^\dagger$ & $\hat{a}_i$ are not raising & lowering operators.

➡ Steady st. is not the canonical st. with inv. temp. β.

Thermodynamically consistent global ME

Exercise: Determine thermodynamically consistent global ME

for $\hat{H}_I = g\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right)$

Levy & Kosloff, EPL **107**, 20004 (2014)

Raising ops. $\hat{c}_\pm^\dagger$ & lowering ops. $\hat{c}_\pm$ satisfy:

$$[\hat{H}, \hat{c}_\pm^\dagger] = \omega_\pm \hat{c}_\pm^\dagger$$

$$[\hat{H}, \hat{c}_\pm] = -\omega_\pm \hat{c}_\pm$$

$$[\hat{c}_\pm, \hat{c}_\pm^\dagger] = 1$$

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_I$$

with $\omega_\pm = \frac{\omega_1+\omega_2}{2} \pm \sqrt{\left(\frac{\omega_1-\omega_2}{2}\right)^2 + g^2}$

$$\begin{cases} \hat{c}_+ = \hat{a}_1 \cos\theta + \hat{a}_2 \sin\theta \\ \hat{c}_- = \hat{a}_2 \cos\theta - \hat{a}_1 \sin\theta \end{cases}$$

$$\cos^2\theta = \frac{1}{2}\left(1 + \frac{\omega_1-\omega_2}{\sqrt{(\omega_1-\omega_2)^2+4g^2}}\right)$$

$$\hat{H} = \omega_+ \hat{c}_+^\dagger \hat{c}_+ + \omega_- \hat{c}_-^\dagger \hat{c}_-$$

Global ME: $$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}] + \frac{\tilde{\gamma}_0}{2} \sum_{\sigma=\pm} \left[\mathcal{D}[\hat{c}_\sigma]\hat{\rho} + e^{-\beta\omega_\sigma}\mathcal{D}[\hat{c}_\sigma^\dagger]\hat{\rho}\right]$$

References

M. A. Nielsen & I. L. Chuang,
"Quantum Computation and Quantum Information"
(Cambridge, 2010).

H.-P. Breuer & F. Petruccione,
"The Theory of Open Quantum Systems" (Oxford, 2002).

Proof of $\hat{A}_j(\omega) \equiv \sum_{\varepsilon'-\varepsilon=\omega} \hat{\Pi}_S(\varepsilon)\,\hat{A}_j \hat{\Pi}_S(\varepsilon') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\,\hat{A}_j^{(I)}(t)e^{i\omega t}$

Spectral decomp.: $\hat{H}_S = \sum_\varepsilon \varepsilon\,\hat{\Pi}_S(\varepsilon)$

$$\hat{A}_j^{(I)}(t) \equiv e^{i\hat{H}_S t}\hat{A}_j e^{-i\hat{H}_S t} = \sum_{\varepsilon,\varepsilon'} e^{i\varepsilon t}\,\hat{\Pi}_S(\varepsilon)\,\hat{A}_j \hat{\Pi}_S(\varepsilon') e^{-i\varepsilon t}$$

$$= \sum_{\varepsilon,\varepsilon'} e^{-i(\varepsilon'-\varepsilon)t}\,\hat{\Pi}_S(\varepsilon)\,\hat{A}_j \hat{\Pi}_S(\varepsilon')$$

$$= \sum_\omega e^{-i\omega t}\left(\sum_{\varepsilon'-\varepsilon=\omega} \hat{\Pi}_S(\varepsilon)\,\hat{A}_j \hat{\Pi}_S(\varepsilon')\right) \equiv \sum_\omega e^{-i\omega t}\,\hat{A}_j(\omega)$$

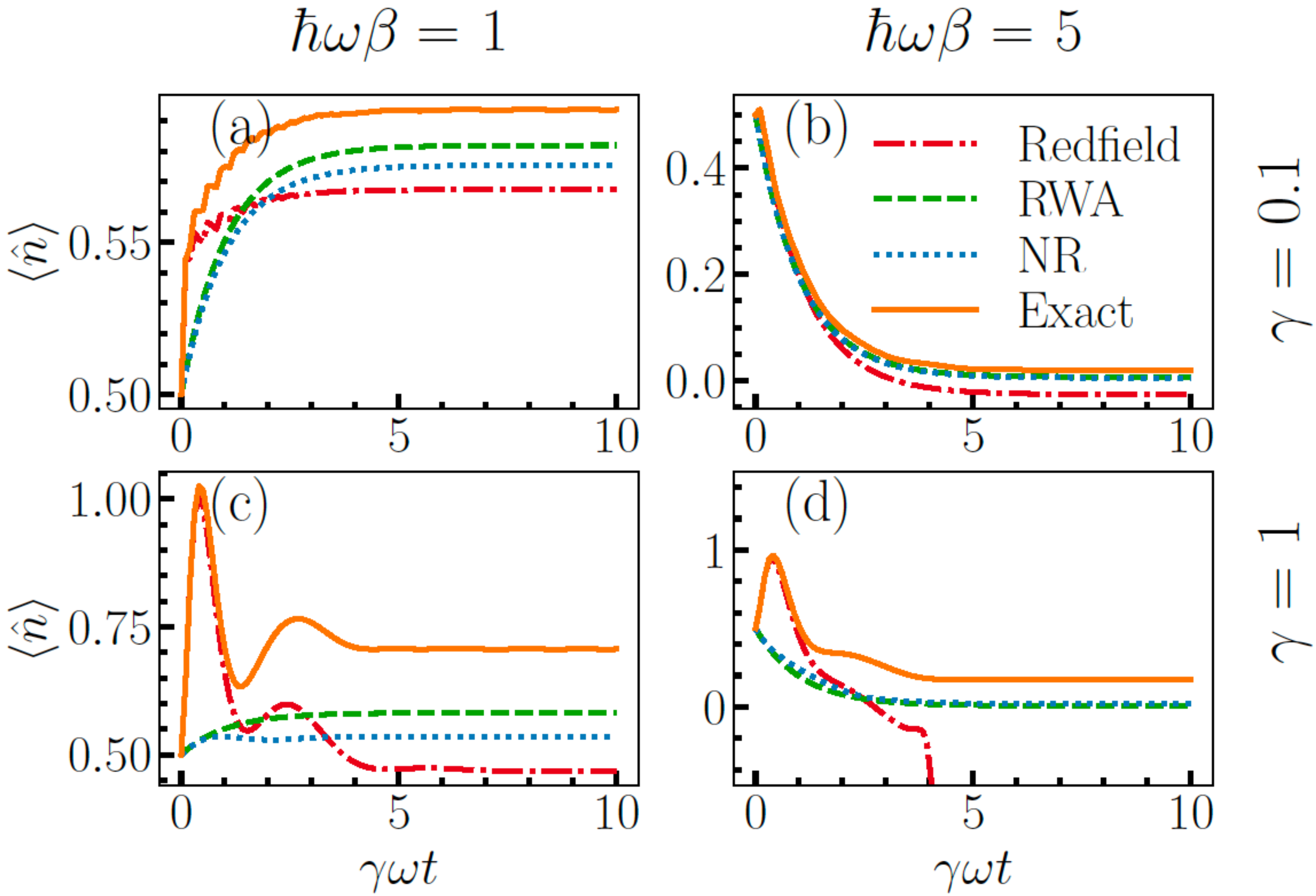
$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\,\hat{A}_j^{(I)}(t)e^{i\omega t} = \frac{1}{2\pi}\sum_{\omega'}\int_{-\infty}^{\infty} dt\,e^{i(\omega-\omega')t}\hat{A}_j(\omega')$$

$$= \sum_{\omega'} \delta(\omega-\omega')\hat{A}_j(\omega') = \hat{A}_j(\omega)$$

$$\therefore\ \hat{A}_j(\omega) \equiv \sum_{\varepsilon'-\varepsilon=\omega} \hat{\Pi}_S(\varepsilon)\,\hat{A}_j \hat{\Pi}_S(\varepsilon') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\,\hat{A}_j^{(I)}(t)e^{i\omega t}$$

Benchmark of the Redfield & Lindblad MEs

Damped HO in a thermal bath (inverse temp. β)



NR: GKSL-form ME

Tello Breuer, Becker, Eckardt, Phys. Rev. B **110**, 064319 (2024)