TCM315 Fall 2022: Introduction to Open Quantum Systems

Lecture 15: Derivation of the Lindblad-Gorini-Kossakowski-Sudarshan equation from unitary dynamics

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CONTENTS

1. INTRODUCTION

The derivation follows § 3.3 of [1].

2. BORN APPROXIMATION AT LEADING ORDER

The system state operator obeys the exact equation

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\,[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] - \int_{t_\imath}^{t} \mathrm{d}s\ \mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t, \mathbb{G}_{t\,s}\,[\tilde{\mathbb{W}}_s, \tilde{\boldsymbol{\rho}}_s^{(S)} \otimes \boldsymbol{\rho}_{t_\imath}^{(E)}]]\right)$$

It is not closed in the sense that it requires the evaluation of the operator $\mathbb{G}$. The lowest order approximation is

$$\mathbb{G}_{t\,s} = \mathbb{1}_{\mathcal{H}} \tag{1}$$

In such a case we get into

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\,[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] - \int_{t_\imath}^{t} \mathrm{d}s\ \mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t\,,\,[\tilde{\mathbb{W}}_s, \tilde{\boldsymbol{\rho}}_s^{(S)} \otimes \boldsymbol{\rho}_{t_\imath}^{(E)}]]\right)$$

We can then avail us of

$$\mathrm{Tr}_{\mathcal{H}_E}\left([\mathbb{W}, \boldsymbol{\rho}_{t_\imath}^{(E)}]\right) = 0 \tag{2}$$

to show that the integrand does not depend explicitly upon $\tilde{\mathbb{V}}_s$:

$$\mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E}\,,\,[\tilde{\mathbb{W}}_s, \tilde{\boldsymbol{\rho}}_s^{(S)} \otimes \boldsymbol{\rho}_{t_\iota}^{(E)}]]\right) = [\tilde{\mathbb{V}}_t\,,\,\mathrm{Tr}_{\mathcal{H}_E}([\tilde{\mathbb{W}}_s, \tilde{\boldsymbol{\rho}}_s^{(S)} \otimes \boldsymbol{\rho}_{t_\iota}^{(E)}])] = 0$$

We therefore arrive at

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\,[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] - \int_{t_\iota}^{t} \mathrm{d}s\;\mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{W}}_t\,,[\tilde{\mathbb{W}}_s, \tilde{\boldsymbol{\rho}}_s^{(S)} \otimes \boldsymbol{\rho}_{t_\iota}^{(E)}]]\right) \tag{3}$$

This equation is now a closed equation for the system state operator. We emphasize that closure is attained by neglecting all terms contributing to the Born series expansion of $\mathbb{G}$.

3. TIME LOCAL APPROXIMATION

Born's approximation yields the interaction picture evolution (3). The state operator $\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)}$ specifies the state of environment at time t_ι and it is invariant under the unitary transformation defining the interaction picture

$$\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)} = \boldsymbol{\rho}_{t_\iota}^{(E)}$$

in consequence of the assumption

$$[\mathbb{H}^{(E)}\,,\boldsymbol{\rho}_{t_\iota}^{(E)}] \,=\, 0$$

The integro-differential equation (3) states that the state operator $\tilde{\boldsymbol{\rho}}_t^{(S)}$ of the system at time t depends upon its previous history from t_ι up to time t. We **assume**, however, that

Hypothesis. *memory effects are (in some average sense) weak so that we can* model *(3) by means of the time-local equation of motion obtained by replacing $\tilde{\boldsymbol{\rho}}_s^{(S)}$ with $\tilde{\boldsymbol{\rho}}_t^{(S)}$:*

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\,[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] - \int_{t_\iota}^{t} \mathrm{d}s\;\mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{W}}_t, [\tilde{\mathbb{W}}_s\,, \tilde{\boldsymbol{\rho}}_t^{(S)} \otimes \boldsymbol{\rho}_{t_\iota}^{(E)}]]\right) \tag{4}$$

This is a very strong and delicate assumption. In particular, there is no guarantee and in general it is not true that the resulting effective dynamics be state operator positivity preserving. The main advantage of the assumption is that (4) becomes time-local: its solution is fully specified upon assigning an initial data for $\tilde{\boldsymbol{\rho}}^{(S)}$ at time t_ι. Equation (4) is, however, "non-Markovian". Namely, the time dependent coefficients in (4) are function not only of the time at which we wish to evaluate the state operator of the system but also keep memory of the time t_ι when we assign the initial condition $\tilde{\boldsymbol{\rho}}_{t_\iota}^{(S)}$.

3.1. Redfield's equation

In order to derive a genuine Markovian evolution we now turn to study the limit $t_\iota \downarrow -\infty$ of (4). A first step in this direction is simply to consider **Redfield's equation**

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\,[\tilde{\mathbb{V}}_t\,, \tilde{\boldsymbol{\rho}}_t^{(S)}] - \int_{-\infty}^{t} \mathrm{d}s\,\mathrm{Tr}_{\mathcal{H}_E}\left([\tilde{\mathbb{W}}_t\,,[\tilde{\mathbb{W}}_s\,, \tilde{\boldsymbol{\rho}}_t^{(S)} \otimes \boldsymbol{\rho}_{t_\iota}^{(E)}]]\right) \tag{5}$$

The typical time-scale of the dynamics generated by (5) is characterized by τ_R, which is the relaxation time of the system due to the interaction with the environment. The validity of the Markov approximation hinges upon a **large separation of time scales** between the relaxation times of the system τ_R and the environment τ_E:

$$\tau_R \gg \tau_E$$

For quantum optical systems, τ_E is the inverse of the optical frequency, i.e., several inverse THz, while the lifetime of an optical excitation is in the inverse MHz range. Therefore, the Markov approximation is well justified in quantum optical systems.

The dynamics specified by (5) is not equivalent to a Lindblad dynamics because, as already mentioned above, it does not guarantee positivity of the density matrix. In order to recover a quantum dynamical semi-group in Lindblad sense we need to introduce more detailed assumptions on the system-environment interaction before passing to the limit $t_\iota \downarrow -\infty$. To that goal, it is expedient to start by writing more explicitly (4)

$$\begin{aligned}&\partial_t\tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath[\tilde{\mathbb{V}}_t,\tilde{\boldsymbol{\rho}}_t^{(S)}]\\&-\int_{t_\iota}^{t}\mathrm{d}s\,\mathrm{Tr}_{\mathcal{H}_E}\left(\tilde{\mathbb{W}}_t\tilde{\mathbb{W}}_s\tilde{\boldsymbol{\rho}}_t^{(S)}\otimes\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)}-\tilde{\mathbb{W}}_t\tilde{\boldsymbol{\rho}}_t^{(S)}\otimes\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)}\tilde{\mathbb{W}}_s\right)\\&+\int_{t_\iota}^{t}\mathrm{d}s\,\mathrm{Tr}_{\mathcal{H}_E}\left(\tilde{\mathbb{W}}_s\tilde{\boldsymbol{\rho}}_t^{(S)}\otimes\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)}\tilde{\mathbb{W}}_t-\tilde{\boldsymbol{\rho}}_t^{(S)}\otimes\tilde{\boldsymbol{\rho}}_{t_\iota}^{(E)}\tilde{\mathbb{W}}_s\tilde{\mathbb{W}}_t\right)\end{aligned}\tag{6}$$

and emphasize that the integrand is in general non vanishing because the partial trace does **not** enjoy the cyclic property of the global trace operation.

4. THE SYSTEM-ENVIRONMENT INTERACTION

We surmise that the interaction Hamiltonian in the Schrödinger picture is amenable to the form

$$\mathbb{W} = \sum_a \mathbb{A}^{(a)}\otimes\mathbb{B}^{(a)}$$

with

$$\mathbb{A}^{(a)} = \mathbb{A}^{(a)\dagger} \qquad \& \qquad \mathbb{B}^{(a)} = \mathbb{B}^{(a)\dagger}\tag{7}$$

The operators $\mathbb{A}^{(a)}$ and $\mathbb{B}^{(a)}$ are respectively defined on the Hilbert space of the system and of the environment. Our working assumption (2) now translates into the condition

$$\mathrm{Tr}_{\mathcal{H}_E}\left(\left[\mathbb{B}^{(a)},\boldsymbol{\rho}_{t_\iota}^{(E)}\right]\right) = 0 \qquad \forall\, a$$

4.1. Foliation of the interaction into system energy eigenspaces

If we denote by ϵ eigenvalues of $\mathbb{H}^{(S)}$ we may write the spectral decomposition of the system Hamiltonian as

$$\mathbb{H}^{(S)} = \sum_\epsilon \epsilon\,\mathbb{P}_\epsilon$$

for $\mathbb{P}_\epsilon$ the projector on the eigenspace of $\mathbb{H}^{(S)}$ associated to the eigenvalue ϵ. We use the same notation as [1]:

$\sum_\epsilon$ means sum over all eigenvalues of $\mathbb{H}^{(S)}$.

Then, following [1] we can project the operators $\mathbb{A}^{(a)}$ on subspaces labeled by energy differences $\omega = \epsilon_2 - \epsilon_1$ (ϵ_1, ϵ_2 are to distinct eigenvalues in the spectrum of $\mathbb{H}^{(S)}$):

$$\mathrm{A}_\omega^{(a)} = \sum_{\epsilon_1-\epsilon_2=-\omega}\mathbb{P}_{\epsilon_1}\,\mathbb{A}^{(a)}\,\mathbb{P}_{\epsilon_2}\tag{8}$$

As the eigenvectors of $\mathbb{H}^{(S)}$ form a complete set, we recover $\mathbb{A}^{(a)}$ by summing over all frequencies

$$\mathbb{A}^{(a)} = \sum_\omega \mathrm{A}_\omega^{(a)} = \sum_\omega \mathrm{A}_\omega^{(a)\dagger}\tag{9}$$

The last identify holds since the operators associated to dynamical quantities must be self-adjoint. In consequence of these considerations, the interaction Hamiltonian admits the equivalent representation

$$\mathbb{H}_I = \sum_{\alpha,\omega}\mathrm{A}_\omega^{(a)}\otimes\mathbb{B}^{(a)}$$

The advantage is that the operators $\mathrm{A}_{\omega}^{(a)}$ are defined under the unitary evolution generated by the system Hamiltonian $\mathbb{H}^{(S)}$

$$e^{\imath\,\mathbb{H}^{(S)}t}\;\mathrm{A}_{\omega}^{(a)}\;e^{-\imath\,\mathbb{H}^{(S)}t}=e^{-\imath\,\omega t}\,\mathrm{A}_{\omega}^{(a)} \tag{10}$$

The infinitesimal version of such relation is

$$\left[\mathbb{H}^{(S)}\,,\mathrm{A}_{\omega}^{(a)}\right]=-\omega\;\mathrm{A}_{\omega}^{(a)}$$

and evinces that $\mathrm{A}_{\omega}^{(a)}$ acts as **ladder operator** on eigenstates of $\mathbb{H}^{(S)}$. This means that

Proposition. *Let $\boldsymbol{\psi}_{\epsilon}$ an eigenstate of $\mathbb{H}$ of energy ϵ. Then*

$$\mathbb{H}^{(S)}\,\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}=(\epsilon-\omega)\,\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}$$

In words $\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}$ is an eigenstate of $\mathbb{H}^{(S)}$ with energy $(\epsilon-\omega)$.

Proof.
The claim follows readily from

$$\left[\mathbb{H}^{(S)}\,,\mathrm{A}_{\omega}^{(a)}\right]\boldsymbol{\psi}_{\epsilon}=-\omega\;\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}$$

which is equivalent to

$$\mathbb{H}^{(S)}\,\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}=\left(\mathrm{A}_{\omega}^{(a)}\,\mathbb{H}^{(S)}-\omega\;\mathrm{A}_{\omega}^{(a)}\right)\boldsymbol{\psi}_{\epsilon}=(\epsilon-\omega)\,\mathrm{A}_{\omega}^{(a)}\,\boldsymbol{\psi}_{\epsilon}$$

□

Remark. *We adopted in (8) a summation convention such that for $\omega\geq 0$, $\mathrm{A}_{\omega}^{(a)}$ is a "lowering" operator (i.e. lowers the energy level ϵ by a quantum of energy ω). Correspondingly, from (9) we see that*

$$\mathrm{A}_{\omega}^{(a)\dagger}=\mathrm{A}_{-\omega}^{(a)} \tag{11}$$

specifies for $\omega\geq 0$ a raising operator.

Equipped with these definitions we write the system-environment coupling in the interaction picture Hamiltonian as

$$\tilde{\mathbb{W}}_{t}\;\equiv\;e^{\imath\left(\mathbb{H}^{(S)}\otimes\mathbb{1}_{\mathcal{H}_E}+\mathbb{1}_{\mathcal{H}_S}\otimes\mathbb{H}^{(E)}\right)t}\,\mathbb{W}\,e^{-\imath\left(\mathbb{H}^{(S)}\otimes\mathbb{1}_{\mathcal{H}_E}+\mathbb{1}_{\mathcal{H}_S}\otimes\mathbb{H}^{(E)}\right)t}=\sum_{\alpha,\omega}e^{-\imath\,\omega\;t}\,\mathrm{A}_{\omega}^{(a)}\otimes e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t}$$

The insertion of such explicit form of the interaction into (4) yields

$$\begin{aligned}
&\partial_t\tilde{\boldsymbol{\rho}}_t^{(S)}=-\imath[\tilde{\mathbb{V}}_t,\tilde{\boldsymbol{\rho}}_t^{(S)}]\\
&-\sum_{\substack{\omega,\omega'\\a,a'}}\mathrm{A}_{\omega}^{(a)}\;\mathbb{A}_{\omega'}^{(a')}\;\tilde{\boldsymbol{\rho}}_t^{(S)}\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t+\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\right)\\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\mathrm{A}_{\omega}^{(a)}\;\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')}\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t+\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\right)\\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\mathbb{A}_{\omega'}^{(a')}\;\tilde{\boldsymbol{\rho}}_t^{(S)}\;\mathrm{A}_{\omega}^{(a)}\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t+\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left(\boldsymbol{\rho}_{t_\iota}^{(E)}\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\,(e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\right)\\
&-\sum_{\substack{\omega,\omega'\\a,a'}}\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')}\;\mathrm{A}_{\omega}^{(a)}\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t+\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,(e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\right)
\end{aligned} \tag{12}$$

We emphasize that the arguments of the trace over the Hilbert space of the environment are now operators on the same space. Hence the trace is a full and not a partial one.

4.2. Analysis of the time integrands

Our goal is to simplify (12). To achieve it, we combine the identity (11) with a suitable relabeling of one of the sums over the frequencies ω and the cyclic property of full traces. These manipulations allow us to re-write (12) as

$$\begin{aligned}
&\partial_t\tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}^{(S)}] \\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega}^{(a)\dagger}-\mathbb{A}_{\omega}^{(a)\dagger}\,\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{-\imath\,\omega\,t+\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\right) \\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega}^{(a)}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}-\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}\,\mathbb{A}_{\omega}^{(a)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t-\imath\,\omega'\,s}\,\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\right)
\end{aligned}$$

Next, the assumption

$$[\mathbb{H}^{(E)}\,,\boldsymbol{\rho}_{t_\iota}^{(E)}]=0$$

together with the cyclic property of the trace with yield the identities

$$\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\right)=\mathrm{Tr}_{\mathcal{H}_E}\left(e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,\mathbb{B}^{(a')}\right)$$

and

$$\mathrm{Tr}_{\mathcal{H}_E}\left((e^{\imath\,\mathbb{H}^{(E)}\,t}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,t})\,(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a')}e^{-\imath\,\mathbb{H}^{(E)}\,s})\,\boldsymbol{\rho}_{t_\iota}^{(E)}\right)=\mathrm{Tr}_{\mathcal{H}_E}\left(e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a')}e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\,\boldsymbol{\rho}_{t_\iota}^{(E)}\mathbb{B}^{(a)}\right)$$

It is therefore expedient to introduce the notation

$$C_{t-s}^{(a\,a')}=\mathrm{Tr}_{\mathcal{H}_E}\left(e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,\mathbb{B}^{(a')}\right)\tag{13}$$

By (7) the $C^{(a\,a')}$'s satisfy the chain of identities

$$\begin{aligned}
\overline{C_{t-s}^{(a\,a')}}&=\overline{\mathrm{Tr}_{\mathcal{H}_E}\left(e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\,\boldsymbol{\rho}_{t_\iota}^{(E)}\,\mathbb{B}^{(a')}\right)}\\
&=\mathrm{Tr}_{\mathcal{H}_E}\left(\mathbb{B}^{(a')}\,\boldsymbol{\rho}_{t_\iota}^{(E)}e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a)}e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\right)=\mathrm{Tr}_{\mathcal{H}_E}\left(e^{-\imath\,\mathbb{H}^{(E)}\,(t-s)}\mathbb{B}^{(a')}e^{\imath\,\mathbb{H}^{(E)}\,(t-s)}\,\boldsymbol{\rho}_{t_\iota}^{(E)}\mathbb{B}^{(a)}\right)=C_{s-t}^{(a'\,a)}
\end{aligned}$$

We thus write the approximate evolution equation as

$$\begin{aligned}
&\partial_t\tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] \\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega}^{(a)\dagger}-\mathbb{A}_{\omega}^{(a)\dagger}\,\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{-\imath\,\omega\,t+\imath\,\omega'\,s}C_{t-s}^{(a\,a')}\\
&+\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega}^{(a)}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}-\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}\,\mathbb{A}_{\omega}^{(a)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t-\imath\,\omega'\,s}\,\overline{C_{t-s}^{(a\,a')}}
\end{aligned}$$

We then notice that the third row of the equation is amenable to the form

$$\begin{aligned}
&\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega}^{(a)}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}-\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega'}^{(a')\dagger}\,\mathbb{A}_{\omega}^{(a)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{\imath\,\omega\,t-\imath\,\omega'\,s}\,\overline{C_{t-s}^{(a\,a')}}\\
&=\overline{\sum_{\substack{\omega,\omega'\\a,a'}}\left(\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_{\omega}^{(a)\dagger}-\mathbb{A}_{\omega}^{(a)\dagger}\,\mathbb{A}_{\omega'}^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\right)\int_{t_\iota}^{t}\mathrm{d}s\,e^{-\imath\,\omega\,t+\imath\,\omega'\,s}C_{t-s}^{(a\,a')}}
\end{aligned}$$

4.3. The approximate dynamics preserves the self-adjoint property

We therefore arrive to a form of the equation that explicitly evinces the self-adjoint property enjoyed by the reduced system state operator:

$$\begin{aligned}\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} &= -\imath[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}^{(S)}] \\ &+ \sum_{\substack{\omega,\omega' \\ a,a'}} \left(\mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)}\, \mathbb{A}_{\omega}^{(a)\dagger} - \mathbb{A}_{\omega}^{(a)\dagger}\, \mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)} \right) \int_{t_\imath}^{t} \mathrm{d}s\, e^{-\imath\,\omega\, t + \imath\,\omega'\, s} C_{t-s}^{(a\,a')} \\ &+ \overline{\sum_{\substack{\omega,\omega' \\ a,a'}} \left(\mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)}\, \mathbb{A}_{\omega}^{(a)\dagger} - \mathbb{A}_{\omega}^{(a)\dagger}\, \mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)} \right) \int_{t_\imath}^{t} \mathrm{d}s\, e^{-\imath\,\omega\, t + \imath\,\omega'\, s} C_{t-s}^{(a\,a')}}\end{aligned}$$

5. THE SECULAR APPROXIMATION

We now proceed to a careful analysis of the infinite time horizon limit. The upshot of the previous section is that we only need to control the

$$\int_{t_\imath}^{t} \mathrm{d}s\, e^{-\imath\,\omega\, t + \imath\,\omega'\, s} C_{t-s}^{(a\,a')} = e^{-\imath\,(\omega-\omega')\, t} \int_{0}^{t-t_\imath} \mathrm{d}s\, e^{-\imath\,\omega'\, s}\, C_{s}^{(a\,a')}$$

We define then the limit $t_\imath \downarrow -\infty$

$$\frac{\Gamma_{\omega}^{(a\,a')}}{2} \equiv \lim_{t_\imath \downarrow -\infty} \int_{0}^{t-t_\imath} \mathrm{d}s\, e^{-\imath\,\omega\, s}\, C_{s}^{(a\,a')}$$

The rationale for introducing the factor two in the above definition is that when we plug it in the equation for the state operator we can conveniently cast the result in the form

$$\begin{aligned}\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} &= -\imath[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] \\ &+ \mathrm{Re}\left(\lim_{t_\imath \downarrow -\infty} \sum_{\substack{\omega,\omega' \\ a,a'}} \left(\mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)}\, \mathbb{A}_{\omega}^{(a)\dagger} - \mathbb{A}_{\omega}^{(a)\dagger}\, \mathbb{A}_{\omega'}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)} \right) e^{-\imath\,(\omega-\omega')\, t}\, \Gamma_{\omega'}^{(a\,a')} \right)\end{aligned}$$

The secular approximation consists in neglecting in the limit all terms with

$$\omega \neq \omega'$$

5.1. Riemann–Lebesgue lemma

The approximation is justified by [2] by the Riemann–Lebesgue lemma

Proposition. *Let* $f\colon [a,b] \mapsto \mathbb{R}$ *an integrable function. Then*

$$\lim_{t \uparrow \infty} \int_{a}^{b} \mathrm{d}s\, e^{\imath\, s\, t}\, f_s = 0$$

Proof.
Let θ denote the Heaviside step function. Then we define the function $g\colon \mathbb{R} \mapsto \mathbb{R}$ as

$$g_s = f_s\Big(\theta(s-a) - \theta(s-b)\Big) = \begin{cases} 0 & s < a \\ f_s & a < s < b \\ 0 & b < s \end{cases}$$

By construction g is integrable over $\mathbb{R}$. As a consequence the Fourier transform

$$\check{g}_t = \int_{\mathbb{R}} \mathrm{d}s\, e^{\imath\, s\, t}\, g_s \equiv \int_a^b \mathrm{d}s\, e^{\imath\, s\, t}\, f_s$$

is well defined. An integrable function on a finite interval is necessarily bounded. Hence, g_s is also square integrable. Parseval's identity then yields

$$\infty > \int_{\mathbb{R}} \mathrm{d}s\, |g_s|^2 = \int_{\mathbb{R}} \mathrm{d}t\, |\check{g}_t|^2$$

and therefore

$$0 = \lim_{t\uparrow\infty} \hat{g}_t = \lim_{t\uparrow\infty} \int_{\mathbb{R}} \mathrm{d}s\, e^{\imath\, s\, t}\, g_s \equiv \int_a^b \mathrm{d}s\, e^{\imath\, s\, t}\, f_s$$

□

Once we apply Riemann–Lebesgue lemma, a suitable relabeling of summation indices allows us to derive

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath[\tilde{\mathbb{V}}_t, \tilde{\boldsymbol{\rho}}_t^{(S)}] + \sum_{\omega} \sum_{\alpha,\alpha'} \mathbb{A}_{\omega}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)}\, \mathbb{A}_{\omega}^{(a)\dagger}\, \frac{\Gamma_{\omega}^{(a\,a')} + \overline{\Gamma_{\omega}^{(a'\,a)}}}{2}$$
$$- \sum_{\omega} \sum_{a,a'} \frac{\mathbb{A}_{\omega}^{(a)\dagger}\, \mathbb{A}_{\omega}^{(a')}\, \tilde{\boldsymbol{\rho}}_t^{(S)}\, \Gamma_{\omega}^{(a\,a')} + \tilde{\boldsymbol{\rho}}_t^{(S)}\, \mathbb{A}_{\omega}^{(a)\dagger}\, \mathbb{A}_{\omega}^{(a')}\, \overline{\Gamma_{\omega}^{(a'\,a)}}}{2}$$

6. LINDBLAD–GORINI–KOSSAKOWSKI–SUDARSHAN FORM OF THE WEAK COUPLING MASTER EQUATION

This master equation can now be cast into a Lindblad form. Namely, we may regard the $\Gamma_{\omega}^{(a\,a')}$ as the components of a square matrix. Next we recall that any square matrix can be written as the linear combination of two self-adjoint matrices with purely imaginary unit coefficient. This means

$$\Gamma_{\omega}^{(a\,a')} = \mathsf{G}_{\omega}^{(a\,a')} + \imath\, \mathsf{H}_{\omega}^{(a\,a')}$$

and

$$\overline{\Gamma_{\omega}^{(a'\,a)}} = \mathsf{G}_{\omega}^{(a\,a')} - \imath\, \mathsf{H}_{\omega}^{(a\,a')}$$

whence

$$\mathsf{G}_{\omega}^{(a\,a')} \equiv \frac{\Gamma_{\omega}^{(a\,a')} + \overline{\Gamma_{\omega}^{(a'\,a)}}}{2} \qquad \& \qquad \mathsf{H}_{\omega}^{(a\,a')} \equiv \frac{\Gamma_{\omega}^{(a\,a')} - \overline{\Gamma_{\omega}^{(a'\,a)}}}{2\,\imath}$$

The components of the self-adjoint matrices G and H are directly specified by the limit of the integrals over the environment operator correlations.

Proposition. *The self-adjoint matrix with elements*

$$\mathsf{G}_{\omega}^{(a\,a')} \equiv \lim_{t_\iota\downarrow-\infty} \int_{t_\iota}^{|t_\iota|} \mathrm{d}s\, e^{\imath\omega s}\ \mathrm{Tr}\left(e^{\imath\, \mathbb{H}^{(E)} s} \mathbb{B}^{(a)} e^{-\imath\, \mathbb{H}^{(E)} s}\, \mathbb{B}^{(a')} \boldsymbol{\rho}_{t_\iota}^{(E)}\right) \tag{14}$$

is ***positive definite****.*

Proof.
First, upon applying the definitions we write

$$\frac{\Gamma_{\omega}^{(a\,a')} + \overline{\Gamma_{\omega}^{(a'\,a)}}}{2} = \lim_{t_\iota\downarrow-\infty} \int_0^{t-t_\iota} \mathrm{d}s\, e^{\imath\,\omega'\, s} C_s^{(a\,a')} + \lim_{t_\iota\downarrow-\infty} \overline{\int_0^{t-t_\iota} \mathrm{d}s\, e^{\imath\,\omega'\, s} C_s^{(a'\,a)}}$$

Next, we take advantage of the chain of identities

$$\overline{\int_0^{t-t_\imath} \mathrm{d}s\, e^{\imath\,\omega'\,s} C_s^{(a'\,a)}} = \int_0^{t-t_\imath} \mathrm{d}s\, e^{-\imath\,\omega'\,s}\overline{C_s^{(a'\,a)}}$$
$$= \int_0^{t-t_\imath} \mathrm{d}s\, e^{-\imath\,\omega'\,s}\, C_{-s}^{(a\,a')} = \int_{-(t-t_\imath)}^{0} \mathrm{d}s\, e^{\imath\,\omega'\,s} C_s^{(a\,a')}$$

We therefore arrive at

$$\frac{\Gamma_\omega^{(a\,a')} + \overline{\Gamma_\omega^{(a'\,a)}}}{2} = \lim_{t_\imath \downarrow -\infty} \int_0^{t-t_\imath} \mathrm{d}s\, e^{\imath\,\omega'\,s} C_s^{(a\,a')} + \lim_{t_\imath \downarrow -\infty} \int_{-(t-t_\imath)}^{0} \mathrm{d}s\, e^{\imath\,\omega'\,s} C_s^{(a\,a')}$$

which we can immediately rewrite as (14).

Furthermore, the matrix with components specified by (14) is positive definite because for any set of c-numbers c_α we find

$$\sum_{a\,,a'} \bar{c}_a \operatorname{Tr}_{\mathcal{H}_E}\left(e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a)} e^{-\imath\,\mathbb{H}^{(E)}\,s}\,\mathbb{B}^{(a')}\boldsymbol{\rho}_{t_\imath}^{(E)}\right) c_{a'} =$$

$$\operatorname{Tr}_{\mathcal{H}_E}\left(\left(\sum_\alpha e^{\imath\,\mathbb{H}^{(E)}\,s}\mathbb{B}^{(a)}\,\bar{c}_a\right)\left(\sum_{\alpha'} e^{-\imath\,\mathbb{H}^{(E)}\,s}\,\mathbb{B}^{(a')} c_{a'}\right)\boldsymbol{\rho}_{t_\imath}^{(E)}\right) = \operatorname{Tr}_{\mathcal{H}_E}\left(\left|\sum_\alpha e^{-\imath\,\mathbb{H}^{(E)}\,s}\,\mathbb{B}^{(a)} c_a\right|^2 \boldsymbol{\rho}_{t_\imath}^{(E)}\right) \geq 0$$

□

In conclusion, we have proved that in the weak-coupling limit the reduced state operator satisfies the **Lindblad–Gorini–Kossakowski–Sudarshan equation**

$$\partial_t \tilde{\boldsymbol{\rho}}_t^{(S)} = -\imath\left[\tilde{\mathbb{V}}_t + \tilde{\mathbb{H}}_{LS}, \tilde{\boldsymbol{\rho}}_t^{(S)}\right]$$
$$+ \sum_{\omega, a\,a'} \mathsf{G}_\omega^{(a\,a')}\left(\mathbb{A}_\omega^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_\omega^{(a)\dagger} - \frac{\mathbb{A}_\omega^{(a)\dagger}\mathbb{A}_\omega^{(a')}\,\tilde{\boldsymbol{\rho}}_t^{(S)} + \tilde{\boldsymbol{\rho}}_t^{(S)}\,\mathbb{A}_\omega^{(a)\dagger}\,\mathbb{A}_\omega^{(a')}}{2}\right) \tag{15}$$

The correction term $\tilde{\mathbb{H}}_{LS}$ to the commutator in the right hand side of (15) is called the **Lamb shift Hamiltonian** and it is of the form

$$\tilde{\mathbb{H}}_{LS} = \sum_\omega \sum_{a\,a'} \mathsf{H}_\omega^{(a\,a')}\mathbb{A}_\omega^{(a)\dagger}\mathbb{A}_\omega^{(a')}$$

The **interaction picture** master equation (15) is "Markovian" in the sense that it is time-local and carries no memory of the time $t_\imath$ when exact initial data are assigned in tensor product form. Being in Lindblad–Gorini–Kossakowski–Sudarshan form guarantees that positive self adjoint initial data give rise to **completely positive** self-adjoint solutions.

A further simplification is however possible: $\mathsf{G}_\omega^{(a\,a')}$ is by construction positive definite and it is therefore amenable to diagonal form. Therefore we can always reduce the double sum over $\alpha\,\alpha'$ to a single sum by redefining the ladder operators by a unitary transformation.

6.1. Schrödinger picture time autonomous form

The interaction picture evolution (15) is in general time non-autonomous owing to the definition of the system self interaction term in the rotating frame

$$\tilde{\mathbb{V}}_t = e^{\imath\,\mathbb{H}^{(S)}\,t}\mathbb{V} e^{-\imath\,\mathbb{H}^{(S)}\,t}$$

We emphasize that the remaining addends in (15) are all quadratic in $\mathrm{A}_\omega^{(a)}$ and $\mathrm{A}_\omega^{(a')\dagger}$. As a consequence of (10) they are invariant under the unitary transformation mapping (15) into its Schrödinger picture counterpart. We thus obtain

$$\partial_t \boldsymbol{\rho}_t^{(S)} = -\imath\left[\mathbb{H}^{(S)} + \mathbb{V} + \mathbb{H}_{LS}, \boldsymbol{\rho}_t^{(S)}\right]$$
$$+ \sum_{\omega, a\,a'} \mathsf{G}_\omega^{(a\,a')}\left(\mathbb{A}_\omega^{(a')}\,\boldsymbol{\rho}_t^{(S)}\,\mathbb{A}_\omega^{(a)\dagger} - \frac{\mathbb{A}_\omega^{(a)\dagger}\mathbb{A}_\omega^{(a')}\,\boldsymbol{\rho}_t^{(S)} + \boldsymbol{\rho}_t^{(S)}\,\mathbb{A}_\omega^{(a)\dagger}\,\mathbb{A}_\omega^{(a')}}{2}\right) \tag{16}$$

Remark. *It must be stressed that the hypothesis that* ***also*** *the system self-interaction* $\mathbb{V}$ *is weak* ***impinges*** *the derivation of (15) and (16). The hypothesis is needed to truncate to leading order the Born's series expressing the exact system-environment evolution in the orthogonal complement of the system's Hilbert space defined by the Nakajima–Zwanzig projection. The perturbative nature of* $\mathbb{V}$ *is then reflected in the fact that the ladder operators* $\mathrm{A}_{\omega}^{(a)}$ *are labeled by spectral gaps in the spectrum of* $\mathbb{H}^{(S)}$ *alone.*

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