

TCM315 Fall 2022: Introduction to Open Quantum Systems

Lecture 14: The Nakajima–Zwanzig projection operator technique

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1. INTRODUCTION

In these notes we follow chapter 5 of [4] although the same material is also expounded in § 3 of chapter 3 of [1].

The projection of the Liouville-von Neumann equation onto the Hilbert space of the system is described in chapter 9 of [1]. In § 3.3, [1] does not make use of the Nakajima–Zwanzig projection operator technique.

The properties of the canonical form of the time-local master equation is discussed in [3]. Its derivation is based on ideas introduced in [2].

2. DECOMPOSITION OF THE LIOUVILLE–VON NEUMANN EQUATION

We consider a system S that is *weakly coupled* to an environment E (or equivalently, “bath”). The quantum dynamics in the “universe” Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$ obeys the Liouville–von Neumann equation (in universal units $\hbar = 1$),

$$i\partial_t \rho_t = [\mathbb{H}, \rho_t]$$

The Hamiltonian of the “universe” \mathbb{H} is time independent as it describes an **isolated system**. The Liouville–von Neumann equation is first order in time and must be complemented by one initial condition.

Hypothesis. We suppose that we can prepare the system at an initial time t_ι in the form of a **tensor product**

$$\rho_{t_\iota} = \rho_{t_\iota}^{(S)} \otimes \rho_{t_\iota}^{(E)} \tag{1}$$

between a state operator $\rho_{t_\iota}^{(S)}$ acting on \mathcal{H}_S and a state operator $\rho_{t_\iota}^{(E)}$ acting on \mathcal{H}_E .

We need the “tensor product” hypothesis to insure that the evolution of

$$\rho_t^{(S)} \equiv \text{Tr}_{\mathcal{H}_E} \rho_t \quad t \geq t_\iota$$

is governed by a **universal dynamical map**. An universal dynamical map depends on the environment initial data and evolution but is independent of the initial value of the state operator of the system $\rho_{t_i}^{(S)}$ (see e.g. § 3.2 and § 3.5 of [4] for more details).

We split the Hamiltonian of the combined system in three parts:

$$\mathbb{H} = \mathbb{H}^{(S)} \otimes \mathbb{1}_{\mathcal{H}_E} + \mathbb{1}_{\mathcal{H}_S} \otimes \mathbb{H}^{(E)} + \mathbb{H}^{(I)}, \quad (2)$$

where $\mathbb{H}^{(S)}$ acts only on \mathcal{H}_S , $\mathbb{H}^{(E)}$ only acts \mathcal{H}_E , and $\mathbb{H}^{(I)}$ describes the system-environment interaction. We also make the following hypothesis about the initial state of the environment.

Hypothesis. *We suppose that at $t = t_i$ the state operator of the environment satisfies*

$$[\mathbb{H}^{(E)}, \rho_{t_i}^{(E)}] = 0 \quad (3)$$

The hypothesis holds, for instance, if $\rho_{t_i}^{(E)}$ describes thermal equilibrium

$$\rho_{t_i}^{(E)} = \frac{1}{Z} e^{-\beta \mathbb{H}^{(E)}}$$

or a pure state corresponding to an energy eigenstate of $\mathbb{H}^{(E)}$ i.e.

$$\rho_{t_i}^{(E)} = \mathbf{e} \mathbf{e}^\dagger$$

with \mathbf{e}

$$\mathbb{H}^{(E)} \mathbf{e} = \epsilon \mathbf{e}$$

Finally, we write the interaction as

$$\mathbb{H}^{(I)} = \mathbb{V} \otimes \mathbb{1}_{\mathcal{H}_E} + \mathbb{W} \quad (4)$$

where \mathbb{V} is a self-interaction term of the system (i.e. \mathbb{V} is defined in the Hilbert space of the system) and \mathbb{W} denotes the interaction between the system and the environment (i.e. \mathbb{W} is defined in the joint Hilbert space of system and environment).

There are two reasons for the splitting (4). The first is that in applications it often occurs that some system self-interaction can only be treated perturbatively. The second is that

Hypothesis. *we assume that*

$$\text{Tr}_{\mathcal{H}_E} ([\mathbb{W}, \rho_{t_i}]) = 0 \quad (5)$$

to hold true irrespective of the initial system state of the system.

As we are assuming that the initial state is in the tensor product form (1), (5) is equivalent to

$$\text{Tr}_{\mathcal{H}_E} ([\mathbb{W}, \mathbb{1}_{\mathcal{H}_S} \otimes \rho_{t_i}^{(E)}]) = 0 \quad (6)$$

This hypothesis is not restrictive. It is in fact equivalent to make a judicious choice in the definition of $\mathbb{H}^{(S)}$ and/or \mathbb{V} .

Our aim is to inquire how $\mathbb{H}^{(I)}$ affects the evolution of the system S . To this end, we perform the **unitary transformation**

$$\rho_t = \mathbb{U}_{t-t_i}^{(S)} \otimes \mathbb{U}_{t-t_i}^{(E)} \tilde{\rho}_t \mathbb{U}_{t-t_i}^{(S)\dagger} \otimes \mathbb{U}_{t-t_i}^{(E)\dagger} \quad (7)$$

corresponding to a representation of the state operator of the universe in the rotating frame specified by

$$\begin{aligned} \mathbb{U}_{t-t_i}^{(S)} &= \exp \left(-i \mathbb{H}^{(S)} \otimes \mathbb{1}_{\mathcal{H}_E} (t - t_i) \right) \\ \mathbb{U}_{t-t_i}^{(E)} &= \exp \left(-i \mathbb{1}_{\mathcal{H}_S} \otimes \mathbb{H}^{(E)} (t - t_i) \right) \end{aligned}$$

The rotating frame representation is usually referred to as **interaction or Dirac's picture**.

Inserting (7) into the Liouville–von Neumann equation, we obtain

$$\partial_t \left(\mathbb{U}_{t-t_i}^{(S)} \otimes \mathbb{U}_{t-t_i}^{(E)} \tilde{\rho}_t \mathbb{U}_{t-t_i}^{(S)\dagger} \otimes \mathbb{U}_{t-t_i}^{(E)\dagger} \right) = -\imath \left[\tilde{\mathbb{H}}_t, \tilde{\rho}_t \right]$$

which we then couch into the form

$$\partial_t \tilde{\rho}_t = -\imath \left[\tilde{\mathbb{H}}_t, \tilde{\rho}_t \right] \quad (8)$$

The interaction picture Hamiltonian is **time-dependent** in consequence of

$$\tilde{\mathbb{H}}_t = \mathbb{U}_{t-t_i}^{(S)} \otimes \mathbb{U}_{t-t_i}^{(E)} \mathbb{H}^{(I)} \mathbb{U}_{t-t_i}^{(S)\dagger} \otimes \mathbb{U}_{t-t_i}^{(E)\dagger} \equiv \tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t$$

3. THE NAKAJIMA–ZWANZIG PROJECTION OPERATOR TECHNIQUE

Our aim is to obtain an exact closed equation for the evolution of state operator of the system. This expression will be the starting point for controlled perturbative treatment of the system dynamics.

3.1. The projector operators

We define the projection operator \mathbb{P} acting on the state operator on the full Hilbert space \mathcal{H}

$$\mathbb{P} \rho_t = (\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)} \equiv \rho_t^{(S)} \otimes \rho_{t_i}^{(E)}$$

As usual $\text{Tr}_{\mathcal{H}_E}$ is the partial trace over the degrees of freedom of the environment, whilst $\rho_{t_i}^{(E)} \in \mathcal{H}_E$ is the initial state of the environment. Thus, the projector \mathbb{P} extricates from the exact state operator, a tensor product of state operators respectively defined in \mathcal{H}_S and \mathcal{H}_E .

Proposition.

$$\mathbb{P}^2 = \mathbb{P}$$

Proof.

$$\mathbb{P}^2 \rho_t = \mathbb{P} \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)} \right) = \text{Tr}_{\mathcal{H}_E} \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)} \right) \otimes \rho_{t_i}^{(E)} = (\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)}$$

□

We denote the orthogonal complement of \mathbb{P} as

$$\mathbb{Q} = \mathbb{1}_{\mathcal{H}} - \mathbb{P}$$

or equivalently

$$\mathbb{Q} \rho_t = \rho_t - (\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)}$$

The definition is consistent since it is easy to verify

Proposition.

$$\mathbb{Q} \mathbb{P} = \mathbb{P} \mathbb{Q} = 0 \quad \& \quad \mathbb{Q}^2 = \mathbb{Q}$$

Proof.

Let us verify

$$0 = \mathbb{Q} \mathbb{P} \rho_t = \mathbb{Q} \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_i}^{(E)} \right)$$

Indeed, we see that

$$\begin{aligned} \mathbb{Q} \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_\iota}^{(E)} \right) &\equiv (\mathbb{1}_{\mathcal{H}} - \mathbb{P}) \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_\iota}^{(E)} \right) \\ &= (\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_\iota}^{(E)} - \mathbb{P} \left((\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_\iota}^{(E)} \right) = 0 \end{aligned}$$

Similarly, the identity

$$\mathbb{P}\mathbb{Q}\rho_t = \mathbb{P} \left(\rho_t - (\text{Tr}_{\mathcal{H}_E} \rho_t) \otimes \rho_{t_\iota}^{(E)} \right) = 0$$

completes the proof of the orthogonality of the state operators generated by the action of \mathbb{P} and \mathbb{Q} .

Finally, we verify that \mathbb{Q} is idempotent

$$\mathbb{Q}^2 = (\mathbb{1}_{\mathcal{H}} - \mathbb{P})^2 = \mathbb{1}_{\mathcal{H}} + \mathbb{P}^2 - 2\mathbb{P} = \mathbb{1}_{\mathcal{H}} - \mathbb{P}$$

□

3.2. Nakajima–Zwanzig representation of the interaction picture Liouville–von Neumann equation

We emphasize that projection operator \mathbb{P} is time independent. If we apply \mathbb{P} to the interaction picture (8) we obtain

$$\partial_t \mathbb{P} \tilde{\rho}_t = -i \mathbb{P} [\tilde{\mathbb{H}}_t, \tilde{\rho}_t] \quad (9)$$

Here, it is important to notice that

Proposition. *The projection operator \mathbb{P} commutes with the mapping to the interaction picture*

$$\mathbb{P} \tilde{\rho} = \mathbb{P} \left(\mathbb{U}^{(S)} \otimes \mathbb{U}^{(E)} \rho \mathbb{U}^{(S)\dagger} \otimes \mathbb{U}^{(E)\dagger} \right) = \mathbb{U}^{(S)} \otimes \mathbb{U}^{(E)} (\mathbb{P} \rho) \mathbb{U}^{(S)\dagger} \otimes \mathbb{U}^{(E)\dagger} = \widetilde{\mathbb{P} \rho}$$

Proof.

By definition

$$\mathbb{P} \tilde{\rho} = \text{Tr}_{\mathcal{H}_E} (\mathbb{U}^{(S)} \otimes \mathbb{U}^{(E)} \rho \mathbb{U}^{(S)\dagger} \otimes \mathbb{U}^{(E)\dagger}) \otimes \rho_{t_\iota}^{(E)}$$

As the partial trace operation does not affect $\mathbb{U}^{(S)}$ we obtain

$$\mathbb{P} \tilde{\rho} = \left(\mathbb{U}^{(S)} \otimes \mathbb{1}_{\mathcal{H}_E} \right) \left(\rho^{(S)} \otimes \rho_{t_\iota}^{(E)} \right) \left(\mathbb{U}^{(S)\dagger} \otimes \mathbb{1}_{\mathcal{H}_E} \right)$$

having set

$$\rho^{(S)} = \text{Tr}_{\mathcal{H}_E} (\mathbb{1}_{\mathcal{H}_S} \otimes \mathbb{U}^{(E)} \rho \mathbb{1}_{\mathcal{H}_S} \otimes \mathbb{U}^{(E)\dagger})$$

Finally we avail us of the hypothesis (3) to arrive at

$$\mathbb{P} \tilde{\rho} = \mathbb{U}^{(S)} \otimes \mathbb{U}^{(E)} \left(\rho^{(S)} \otimes \rho_{t_\iota}^{(E)} \right) \mathbb{U}^{(S)\dagger} \otimes \mathbb{U}^{(E)\dagger} = \mathbb{U}^{(S)} \otimes \mathbb{U}^{(E)} (\mathbb{P} \rho) \mathbb{U}^{(S)\dagger} \otimes \mathbb{U}^{(E)\dagger}$$

□

The right hand side of (9) is not closed in \mathcal{H}_S . We need therefore to solve it in conjunction to a second equation for the orthogonal complement.

$$\partial_t \mathbb{Q} \tilde{\rho}_t = -i \mathbb{Q} [\tilde{\mathbb{H}}_t, \tilde{\rho}_t] \quad (10)$$

It is expedient at this stage to neaten the notation by introducing the “adjoint action”

$$\text{ad}_{\tilde{\mathbb{H}}_t} \cdot = [\tilde{\mathbb{H}}_t, \cdot]$$

whose integral version is

$$\begin{aligned} \text{Ad}_{\tilde{\mathbb{U}}_{t_s}} \cdot &= \tilde{\mathbb{U}}_{t_s} \cdot \tilde{\mathbb{U}}_{t_s}^\dagger \\ \tilde{\mathbb{U}}_{t_s} &= \overleftarrow{\mathcal{T}} e^{-\imath \int_s^t du \tilde{\mathbb{H}}_u} = \mathbb{1}_{\mathcal{H}} - \imath \int_s^t du \tilde{\mathbb{H}}_u + (-\imath)^2 \int_s^t du_1 \int_s^{u_1} du_2 \tilde{\mathbb{H}}_{u_1} \tilde{\mathbb{H}}_{u_2} + \dots \end{aligned}$$

The symbol $\overleftarrow{\mathcal{T}}$ indicates the chronological (time-ordered) $u_1 \geq u_2 \geq \dots$ ordering of non commuting operators in the exponential series.

Upon applying the new notation we couch (9), (10) in to the form

$$\partial_t \tilde{\rho}_t^{(p)} = -\imath \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(p)} - \imath \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(q)} \quad (11a)$$

$$\partial_t \tilde{\rho}_t^{(q)} = -\imath \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(p)} - \imath \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(q)} \quad (11b)$$

with

$$\tilde{\rho}_t^{(p)} \equiv \mathbb{P} \rho_t \quad \& \quad \tilde{\rho}_t^{(q)} \equiv \mathbb{Q} \rho_t$$

Our aim is to use the solution of (11b) in order to recast the original Liouville–von Neumann equations in terms of an integro-differential equation for $\tilde{\rho}^{(p)}$.

3.3. The generalized Nakajima–Zwanzig equation

Proposition. For any given $\tilde{\rho}^{(p)}$ the solution of (11b) reads

$$\tilde{\rho}_t^{(q)} = \mathbb{G}_{t t_i} \tilde{\rho}_{t_i}^{(q)} - \imath \int_{t_i}^t ds \mathbb{G}_{t s} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_s} \tilde{\rho}_s^{(p)} \quad (12)$$

where

$$\mathbb{G}_{t s} = \overleftarrow{\mathcal{T}} \exp \left(-\imath \int_s^t du \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \right) = \mathbb{1}_{\mathcal{H}} + \sum_{n=1}^{\infty} \mathbb{G}_{t s}^{(n)} \quad (13)$$

with

$$\begin{aligned} \mathbb{G}_{t s}^{(1)} &= -\imath \int_s^t du_1 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \\ \mathbb{G}_{t s}^{(2)} &= (-\imath)^2 \int_s^t du_1 \int_s^{u_1} du_2 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_2}} \\ &\vdots \\ \mathbb{G}_{t s}^{(n)} &= (-\imath)^n \int_s^t du_1 \int_s^{u_1} du_2 \cdots \int_s^{u_{n-1}} du_n \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_2}} \cdots \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_n}} \\ &\vdots \end{aligned}$$

Proof.

If $\tilde{\rho}^{(p)}$ is assigned, (11b) becomes a closed linear non-homogeneous equation whose solution (12) is fully specified by the Green function \mathbb{G} solution of

$$\begin{aligned} \partial_t \mathbb{G}_{t s} &= -\imath \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_t} \mathbb{G}_{t s} \\ \mathbb{G}_{s s} &= \mathbb{1}_{\mathcal{H}} \end{aligned}$$

The integral version of this equation is given by Duhamel's formula

$$\mathbb{G}_{t s} = \mathbb{1}_{\mathcal{H}} - \imath \int_s^t du_1 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \mathbb{G}_{u_1 s}$$

This equation admits a formal solution by iteration leading to a Born's series. The first iterate is

$$\mathbb{G}_{t s} = \mathbb{1}_{\mathcal{H}} - \iota \int_s^t du_1 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} + (-\iota)^2 \int_s^t du_1 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \int_s^{u_1} du_2 \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_2}} \mathbb{G}_{u_2 s}$$

Equation (13) is then the full expression of the series. \square

Using the formal solution of (11b) we can close equation (11a)

$$\partial_t \tilde{\rho}_t^{(p)} = -\iota \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(p)} - \iota \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \mathbb{G}_{t t_i} \tilde{\rho}_{t_i}^{(q)} + (-\iota)^2 \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \int_{t_i}^t ds \mathbb{G}_{t s} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_s} \tilde{\rho}_s^{(p)}$$

The analysis of the right hand side yields some simplifications.

- $\mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(p)}$: this addend satisfies the chain of identities

$$\mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \tilde{\rho}_t^{(p)} = \text{Tr}_{\mathcal{H}_E} \left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t, \tilde{\rho}_t^{(S)} \otimes \rho_{t_i}^{(E)}] \right) \otimes \rho_{t_i}^{(E)} = [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] \otimes \rho_{t_i}^{(E)}$$

We used here the hypothesis (5) that the interaction does not have any diagonal component on the environment.

- $\mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \mathbb{G}_{t t_i} \tilde{\rho}_{t_i}^{(q)}$: our hypothesis (1) sets this term to zero:

$$\tilde{\rho}_{t_i}^{(q)} = \mathbb{Q} \tilde{\rho}_{t_i} = \mathbb{Q}(\rho_{t_i}^{(S)} \otimes \rho_{t_i}^{(E)}) = 0 \quad (14)$$

3.3.1. Equation in the system Hilbert space

The equation simplifies to

$$\partial_t \tilde{\rho}_t^{(p)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] \otimes \rho_{t_i}^{(E)} + (-\iota)^2 \int_{t_i}^t ds \mathbb{P} \text{ad}_{\tilde{\mathbb{H}}_t} \mathbb{G}_{t s} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_s} \tilde{\rho}_s^{(p)}$$

We emphasize that this equation is exact. Since the projector operator acts on all terms on the right hand side we can immediately re-write it as an equation in \mathcal{H}_S . This is done by taking the trace over the environment. We obtain

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \int_{t_i}^t ds \text{Tr}_{\mathcal{H}_E} \left(\text{ad}_{\tilde{\mathbb{H}}_t} \mathbb{G}_{t s} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_s} \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)} \right)$$

or, more explicitly,

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \int_{t_i}^t ds \text{Tr}_{\mathcal{H}_E} \left([\tilde{\mathbb{H}}_t, \mathbb{G}_{t s} \mathbb{Q} [\tilde{\mathbb{H}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}]] \right)$$

The result can be further simplified. Namely, we recall that

- As \mathbb{Q} annihilates tensor product states the identity

$$\mathbb{Q}[\tilde{\mathbb{V}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}] = 0$$

holds true and thus enforces

$$\mathbb{Q}[\tilde{\mathbb{H}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}] = \mathbb{Q}[\tilde{\mathbb{W}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}]$$

- By (6)

$$\mathbb{Q}[\tilde{\mathbb{W}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}] = [\tilde{\mathbb{W}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}]$$

We get therefore into

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \int_{t_i}^t ds \text{Tr}_{\mathcal{H}_E} \left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t, \mathbb{G}_{t s} [\tilde{\mathbb{W}}_s, \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)}]] \right) \quad (15)$$

4. EXISTENCE OF THE EXACT TIME-LOCAL MASTER EQUATION

Equation (15) is time non-local as it depends upon the history of the reduced state operator of the system from the time t_i when the full system state operator is in tensor product form. The Liouville-von Neumann equation (8) is reversible. Namely if

$$\tilde{\rho}_t = \text{Ad}_{\mathbb{U}_{t_s}} \tilde{\rho}_s \quad (16)$$

then

$$\tilde{\rho}_s = \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \tilde{\rho}_t \quad (17)$$

Our aim is to use the inverse to formally derive a time-local master equation equivalent to (15). Before turning to this goal we pause to analyze the meaning of (17).

4.1. Inversion implies anti-chronological ordering

We notice that

$$\mathbb{U}_{t_s}^\dagger = \left(\overleftarrow{\mathcal{F}} \exp -\imath \int_s^t du \tilde{\mathbb{H}}_u \right)^\dagger = \left(\mathbb{1}_{\mathcal{H}} - \imath \int_s^t du \tilde{\mathbb{H}}_u + (-\imath)^2 \int_s^t du_1 \int_s^{u_1} du_2 \tilde{\mathbb{H}}_{u_1} \tilde{\mathbb{H}}_{u_2} + \dots \right)^\dagger$$

becomes

$$\mathbb{U}_{t_s}^\dagger = \mathbb{1}_{\mathcal{H}} + \imath \int_s^t du \tilde{\mathbb{H}}_u + (\imath)^2 \int_s^t du_1 \int_s^{u_1} du_2 \tilde{\mathbb{H}}_{u_2} \tilde{\mathbb{H}}_{u_1} + \dots = \overrightarrow{\mathcal{F}} \exp \imath \int_s^t du \tilde{\mathbb{H}}_u$$

i.e. an anti-chronologically ordered exponential.

4.2. Time-local closure of the dynamics

The expression (17) of the backward dynamics allows us to express the reduced state operators at any $s \leq t$ in terms of the “terminal” value

$$\tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)} = \mathbb{P} \tilde{\rho}_s = \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \tilde{\rho}_t = \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \left(\tilde{\rho}_t^{(S)} \otimes \rho_{t_i}^{(E)} + \mathbb{Q} \tilde{\rho}_t \right)$$

We now avail us of (12) and (13) to write

$$\mathbb{Q} \tilde{\rho}_t = \int_{t_i}^t du G_{t u} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_u} \tilde{\rho}_u^{(S)} \otimes \rho_{t_i}^{(E)}$$

whence we arrive at the Duhamel’s type relation

$$\tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)} = \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \left(\tilde{\rho}_t^{(S)} \otimes \rho_{t_i}^{(E)} + \int_{t_i}^t du G_{t u} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_u} \tilde{\rho}_u^{(S)} \otimes \rho_{t_i}^{(E)} \right)$$

We solve the relation by recursion. The first iterate is

$$\begin{aligned} \tilde{\rho}_s^{(S)} \otimes \rho_{t_i}^{(E)} &= \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \tilde{\rho}_t^{(S)} \otimes \rho_{t_i}^{(E)} \\ &+ \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \int_{t_i}^t du_1 G_{t u_1} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_1}} \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \left(\tilde{\rho}_t^{(S)} \otimes \rho_{t_i}^{(E)} + \int_{t_i}^t du_2 G_{t u_2} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_{u_2}} \tilde{\rho}_{u_2}^{(S)} \otimes \rho_{t_i}^{(E)} \right) \end{aligned}$$

Thus upon defining

$$\mathbb{S}_{t t_i} = \int_{t_i}^t du G_{t u} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_u} \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger}$$

we get

$$\tilde{\rho}_s^{(S)} \otimes \rho_{t_\iota}^{(E)} = \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} \left(\tilde{\rho}_t^{(S)} \otimes \rho_{t_\iota}^{(E)} + \mathbb{S}_{t t_\iota} \tilde{\rho}_t^{(S)} \otimes \rho_{t_\iota}^{(E)} + \mathbb{S}_{t t_\iota} \int_{t_\iota}^t du \mathbb{G}_{t u} \mathbb{Q} \text{ad}_{\tilde{\mathbb{H}}_u} \tilde{\rho}_u^{(S)} \otimes \rho_{t_\iota}^{(E)} \right)$$

we arrive at the geometric series

$$\tilde{\rho}_s^{(S)} \otimes \rho_{t_\iota}^{(E)} = \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} (1 - \mathbb{S}_t)^{-1} \tilde{\rho}_t^{(S)} \otimes \rho_{t_\iota}^{(E)}$$

Next, we insert the result in (15)

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \int_{t_\iota}^t ds \text{Tr}_{\mathcal{H}_E} \left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t, \mathbb{G}_{t s} [\tilde{\mathbb{W}}_s, \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} (1 - \mathbb{S}_t)^{-1} \tilde{\rho}_t^{(S)} \otimes \rho_{t_\iota}^{(E)}]] \right) \quad (18)$$

4.3. Reduction to the canonical form

The equation is time-local as it depends upon the reduced state operator only at time t . The equation is also manifestly

1. trace preserving

$$\partial_t \text{Tr}_{\mathcal{H}_S} \tilde{\rho}_t^{(S)} = -\iota \text{Tr}_{\mathcal{H}_S} [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \int_{t_\iota}^t ds \text{Tr}_{\mathcal{H}} \left([\tilde{\mathbb{V}}_t \otimes \mathbb{1}_{\mathcal{H}_E} + \tilde{\mathbb{W}}_t, \mathbb{G}_{t s} [\tilde{\mathbb{W}}_s, \mathbb{P} \text{Ad}_{\mathbb{U}_{t_s}^\dagger} (1 - \mathbb{S}_t)^{-1} \tilde{\rho}_t^{(S)} \otimes \rho_{t_\iota}^{(E)}]] \right) = 0$$

2. self-adjoint-ness preserving: the ad-operator is anti-self adjoint: its even iterations or the product by ι are thus self-adjoint.

It must be, however, added that from the mathematical point of view the time local master equation, is **not** equivalent to a system of ordinary differential equations. The reason is that the right hand side of (18) carries a parametric dependence upon the “initial” time t_ι . It can be interpreted as a system of ordinary differential equations only if the physical interpretation of t_ι is neglected. Neglecting the physical meaning of t_ι comes, however, at a price: completely positive maps generically originate from the assignment at t_ι of a state operator in tensor product form. Hence, the assignment of reduced state operators at time $t \neq t_\iota$ will in general only give rise to a completely bounded dynamics.

Based on the above observations (18) is always amenable to the form

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] + \sum_{k=1}^{\mathcal{N}} \mathbb{A}_{t t_\iota}^{(k)} \tilde{\rho}_t^{(S)} \mathbb{B}_{t t_\iota}^{(k)\dagger}$$

for some integer \mathcal{N} . The operators $\left\{ \mathbb{A}_{t t_\iota}^{(k)} \right\}_{k=1}^{\mathcal{N}}$, $\left\{ \mathbb{B}_{t t_\iota}^{(k)} \right\}_{k=1}^{\mathcal{N}}$ must then enjoy the following properties

P-i trace preservation

$$\sum_{k=1}^{\mathcal{N}} \mathbb{B}_{t t_\iota}^{(k)\dagger} \mathbb{A}_{t t_\iota}^{(k)} = 0$$

P-ii self adjoint preservation: for any $\rho = \rho^\dagger$ the equality

$$\sum_{k=1}^{\mathcal{N}} \mathbb{A}_{t t_\iota}^{(k)} \rho \mathbb{B}_{t t_\iota}^{(k)\dagger} = \sum_{k=1}^{\mathcal{N}} \mathbb{B}_{t t_\iota}^{(k)} \rho \mathbb{A}_{t t_\iota}^{(k)\dagger}$$

The reduction to canonical form follows from the same considerations used in the axiomatic derivation of the Lindblad-Gorini-Kossakowski-Sudarshan completely positive master equation. Namely, it is always possible to construct a basis $\{\mathbb{F}_i\}_{i=0}^{d^2-1}$ of the Hilbert space \mathcal{M}_d of matrices on a d -dimensional Hilbert space orthonormal with respect to the

Hilbert-Schmidt inner product, and of which the first element is proportional to the identity matrix. In such a basis, we get

$$\begin{aligned}\mathbb{A}_{tt_t}^{(k)} &= \sum_{i=0}^{d^2-1} \mathbb{F}_i \text{Tr} \left(\mathbb{F}_i^\dagger \mathbb{A}_{tt_t}^{(k)} \right) = \sum_{i=0}^{d^2-1} \mathbb{F}_i \alpha_{tt_t}^{(i,k)} \\ \mathbb{B}_{tt_t}^{(k)} &= \sum_{i=0}^{d^2-1} \mathbb{F}_i \text{Tr} \left(\mathbb{F}_i^\dagger \mathbb{B}_{tt_t}^{(k)} \right) = \sum_{i=0}^{d^2-1} \mathbb{F}_i \beta_{tt_t}^{(i,k)}\end{aligned}$$

and correspondingly

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] + \sum_{i,j=0}^{d^2-1} \sum_{k=1}^{\mathcal{N}} \alpha_{tt_t}^{(i,k)} \bar{\beta}_{tt_t}^{(k,j)} \mathbb{F}_i \tilde{\rho}_t^{(S)} \mathbb{F}_j^\dagger$$

It is expedient to define the $d^2 \times d^2$ matrix \mathbb{C}_{tt_t} with components

$$\mathbf{c}_{tt_t}^{(i,j)} = \sum_{k=1}^{\mathcal{N}} \alpha_{tt_t}^{(i,k)} \bar{\beta}_{tt_t}^{(k,j)}$$

By **(P-ii)** the matrix \mathbb{C}_{tt_t} must be self-adjoint:

$$\mathbf{c}_{tt_t}^{(i,j)} = \bar{\mathbf{c}}_{tt_t}^{(j,i)}$$

We thus arrive at

$$\partial_t \tilde{\rho}_t^{(S)} = -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] + \frac{\mathbf{c}_{tt_t}^{(0,0)} \tilde{\rho}_t^{(S)}}{d} + \sum_{i=1}^{d^2-1} \frac{\mathbf{c}_{tt_t}^{(0,i)} \mathbb{F}_i \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} \mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)}}{\sqrt{d}} + \sum_{i,j=1}^{d^2-1} \mathbf{c}_{tt_t}^{(i,j)} \mathbb{F}_i \tilde{\rho}_t^{(S)} \mathbb{F}_j^\dagger$$

and therefore

$$\begin{aligned}\partial_t \tilde{\rho}_t^{(S)} &= -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] + \frac{\mathbf{c}_{tt_t}^{(0,0)} \tilde{\rho}_t^{(S)}}{d} + \sum_{i=1}^{d^2-1} \frac{(\mathbf{c}_{tt_t}^{(0,i)} \mathbb{F}_i + \bar{\mathbf{c}}_{tt_t}^{(0,i)} \mathbb{F}_i^\dagger) \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} (\mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)} + \mathbb{F}_i \bar{\mathbf{c}}_{tt_t}^{(i,0)})}{2\sqrt{d}} \\ &+ \sum_{i=1}^{d^2-1} \frac{(\mathbf{c}_{tt_t}^{(0,i)} \mathbb{F}_i - \bar{\mathbf{c}}_{tt_t}^{(0,i)} \mathbb{F}_i^\dagger) \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} (\mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)} - \mathbb{F}_i \bar{\mathbf{c}}_{tt_t}^{(i,0)})}{2\sqrt{d}} + \sum_{i,j=1}^{d^2-1} \mathbf{c}_{tt_t}^{(i,j)} \mathbb{F}_i \tilde{\rho}_t^{(S)} \mathbb{F}_j^\dagger\end{aligned}$$

By **(P-i)** the identity

$$0 = \frac{\mathbf{c}_{tt_t}^{(0,0)}}{d} \mathbb{1}_{\mathcal{H}_S} + \sum_{i=1}^{d^2-1} \frac{\mathbf{c}_{tt_t}^{(0,i)} \mathbb{F}_i + \mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)}}{\sqrt{d}} + \sum_{i,j=1}^{d^2-1} \mathbf{c}_{tt_t}^{(i,j)} \mathbb{F}_i^\dagger \mathbb{F}_j$$

must also hold true. Using $\mathbb{C}_{tt_t} = \mathbb{C}_{tt_t}^\dagger$, we can then write

$$\begin{aligned}\partial_t \tilde{\rho}_t^{(S)} &= -\iota [\tilde{\mathbb{V}}_t, \tilde{\rho}_t^{(S)}] - \sum_{i=1}^{d^2-1} \mathbf{c}_{tt_t}^{(i,j)} \frac{\mathbb{F}_i^\dagger \mathbb{F}_i \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} \mathbb{F}_i^\dagger \mathbb{F}_i}{2} \\ &+ \sum_{i=1}^{d^2-1} \frac{(\mathbf{c}_{tt_t}^{(0,i)} \mathbb{F}_i - \bar{\mathbf{c}}_{tt_t}^{(0,i)} \mathbb{F}_i^\dagger) \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} (\mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)} - \mathbb{F}_i \bar{\mathbf{c}}_{tt_t}^{(i,0)})}{2\sqrt{d}} + \sum_{i,j=1}^{d^2-1} \mathbf{c}_{tt_t}^{(i,j)} \mathbb{F}_i \tilde{\rho}_t^{(S)} \mathbb{F}_j^\dagger\end{aligned}$$

Finally, we define

$$\tilde{\mathbb{H}}_{tt_t}^{(\text{eff})} = \tilde{\mathbb{V}}_t + \sum_{i=1}^{d^2-1} \frac{\mathbb{F}_i^\dagger \mathbf{c}_{tt_t}^{(i,0)} - \mathbb{F}_i \bar{\mathbf{c}}_{tt_t}^{(i,0)}}{2\sqrt{d} \iota}$$

and arrive to

$$\partial_t \tilde{\rho}_t^{(S)} = -i [\tilde{\mathbb{H}}_{t t_i}^{(\text{eff})}, \tilde{\rho}_t^{(S)}] + \sum_{i,j=1}^{d^2-1} c_{t t_i}^{(i,j)} \left(\mathbb{F}_i \tilde{\rho}_t^{(S)} \mathbb{F}_j^\dagger - \frac{\mathbb{F}_i^\dagger \mathbb{F}_i \tilde{\rho}_t^{(S)} + \tilde{\rho}_t^{(S)} \mathbb{F}_i^\dagger \mathbb{F}_i}{2} \right)$$

Diagonalization of the reduced $(d^2 - 1) \times (d^2 - 1)$ matrix yields the completely bounded master equation in canonical form

$$\partial_t \tilde{\rho}_t^{(S)} = -i [\tilde{\mathbb{H}}_{t t_i}^{(\text{eff})}, \tilde{\rho}_t^{(S)}] + \sum_{k=1}^{d^2-1} \mathfrak{g}_t^{(k)} \left(\mathbb{G}_t^{(k)} \rho \mathbb{G}_t^{(k)\dagger} - \frac{\mathbb{G}_t^{(k)\dagger} \mathbb{G}_t^{(k)} \rho + \rho \mathbb{G}_t^{(k)\dagger} \mathbb{G}_t^{(k)}}{2} \right)$$

which is well defined [5] as long as

$$|\mathfrak{g}_t^{(l)}| < \infty \quad \forall l$$

Remark. The above definition differs from the axiomatic one because it is not based on requirements imposed on the flow. It is instead derived from formal manipulations of the exact Liouville-von Neumann equation. The manipulation are formal because for any explicit model the exact determination of the operators $\left\{ \mathbb{A}_{t t_i}^{(k)} \right\}_{k=1}^N$, $\left\{ \mathbb{B}_{t t_i}^{(k)} \right\}_{k=1}^N$ is as demanding as solving the microscopic unitary dynamics. The merit of the derivation is therefore in first place conceptual: an existence result. The result becomes of actual use when we resort to perturbative considerations to determine approximate expression of the $\left\{ \mathbb{A}_{t t_i}^{(k)} \right\}_{k=1}^N$, $\left\{ \mathbb{B}_{t t_i}^{(k)} \right\}_{k=1}^N$.

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