



On the assumption of initial factorization in the master equation for weakly coupled systems I: General framework

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Abstract

We analyze the dynamics of a quantum mechanical system in interaction with a reservoir when the initial state is not factorized. In the weak-coupling (van Hove) limit, the dynamics can be properly described in terms of a master equation, but a consistent application of Nakajima–Zwanzig’s projection method requires that the reference (not necessarily equilibrium) state of the reservoir be endowed with the mixing property.

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1. Introduction

The reduced dynamics of a quantum system in contact with a reservoir is generally described in terms of a master equation. According to a widely accepted lore, the physical and mathematical assumptions that are required in order to derive such an equation are of two types: the reservoir is much larger than the system (in a sense that can be made mathematically precise) and the coupling between them is very weak. In these limits, the system has a negligible influence on the reservoir and the global properties of the latter remain unaffected during the evolution. In turns, this enables one to assume that the reservoir is in an equilibrium state (which can be properly defined by virtue of its macroscopic features—the large number of degrees of freedom). One should notice that a physically clear-cut distinction between a “large” reservoir and one of its subsystems can only be made because of their (small) mutual coupling. In this respect, the two above-mentioned hypotheses are not only consistent, but also logically intertwined. Excellent introductions to this subject can be found in Refs. [1–4].

There is, however, another important requirement that is necessary in the derivation of the master equation, but that is often taken for granted: a factorized form of initial conditions is used to define the dynamics. This is a hypothesis of initial statistical independence that is certainly less easily justified. The objective of this article is to investigate the evolution of the system with *correlated* initial conditions. We shall see that in such a case Nakajima–Zwanzig’s projection method [2,4–6] requires an interesting refinement and a characterization of the reference state of the reservoir.

Several authors have addressed the question of the modifications that arise when it is not permissible to assume initially independent system–environment [7–20]. In such a case, the features of the reduced dynamics have interesting spin-offs in relation to other issues, such as the (complete) positivity of the evolution [11–18].

We will start off by introducing notation and setting up a general framework in Section 2. Nakajima–Zwanzig’s projection method is discussed in Section 3 and our main result on the evolution when the initial state is not factorized is given in Section 4. Some of the hypotheses that are necessary in order to prove our results are thoroughly discussed in Section 5. The main theorem is proved in Section 6. In Section 7, we analyze the consistency of the method and we conclude with some remarks in Section 8. In this article, in order to stress the essential features in a transparent way, we will restrict ourselves to the main arguments without emphasis on mathematical rigor. A more rigorous investigation will be presented elsewhere.

Since some of the issues discussed in this article might not be familiar to every physicist, in particular because of the mathematical background required to study nonequilibrium statistical mechanics, we added some detailed explanations, translating some more advanced mathematical concepts into rather simple physical examples. Several details of the derivations, as well as more tutorial issues, are discussed in Appendices A, B, C, D. The tutorial discussions are often adapted to the specific problems discussed in Sections 4 and 5.

This is the first of a sequel of two papers. Here, the general analysis is presented. In the following article, hereafter referred to as Article II, the main theorem on the factorization of the state, as well as the hypotheses that are necessary for its derivation, will be scrutinized in terms of two exactly solvable models, in which an oscillator is coupled to a bosonic reservoir.

2. Framework and notation

We assume that the total system consists of a “large” reservoir B and a “small” (sub)system S, so that the total Hilbert space \mathcal{H}_{tot} can be expressed as the tensor product of the Hilbert spaces of the reservoir \mathcal{H}_B and of the system \mathcal{H}_S ,

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_S \otimes \mathcal{H}_B. \quad (2.1)$$

The Liouvillian of the total system is written as

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{SB}}, \quad (2.2)$$

where λ is the coupling constant and

$$\mathcal{L}_0 = \mathcal{L}_S \otimes 1_B + 1_S \otimes \mathcal{L}_B = \mathcal{L}_S + \mathcal{L}_B \quad (2.3)$$

is the free Liouvillian, describing the free uncoupled evolutions of the system (\mathcal{L}_S) and of the reservoir (\mathcal{L}_B). In the second equality, we omitted the tensor product with the unit operator and, with an abuse of notation, identified \mathcal{L}_S and \mathcal{L}_B with their dilations $\mathcal{L}_S \otimes 1_B$ and $1_S \otimes \mathcal{L}_B$, respectively. In the following, we will always adopt such a convention, whenever no confusion can arise. It follows that

$$[\mathcal{L}_B, \mathcal{L}_S] = 0. \quad (2.4)$$

Let us write the resolution of the system Liouvillian \mathcal{L}_S in terms of its eigenprojections \tilde{Q}_m ,

$$\mathcal{L}_S = -i \sum_m \omega_m \tilde{Q}_m, \quad \sum_m \tilde{Q}_m = 1, \quad \tilde{Q}_m \tilde{Q}_n = \delta_{mn} \tilde{Q}_m. \quad (2.5)$$

This resolution will be used in the following. By making explicit use of the Hamiltonians

$$H = H_0 + \lambda H_{\text{SB}} = H_S + H_B + \lambda H_{\text{SB}} \quad (2.6)$$

and noticing that, by the definition of Liouvillian, $\mathcal{L}\rho = -i[H, \rho]$, the superoperators \tilde{Q}_m in (2.5) can be expressed in terms of the eigenprojections Q_i of the Hamiltonian H_S as

$$\tilde{Q}_m \rho = \sum_{\substack{i,j \\ E_i - E_j = \omega_m}} Q_i \rho Q_j, \quad H_S = \sum_i E_i Q_i. \quad (2.7)$$

We are assuming that system S is finite, $\dim \mathcal{H}_S < \infty$, and thus has a pure point spectrum.

Let $\rho(t)$ be the density matrix of the total system at time t . As we anticipated, the initial state of the total system, ρ_0 , is usually taken to be the tensor product of a system initial state ρ_S and a reservoir state ρ_B ,

$$\rho_0 = \rho_S \otimes \rho_B. \quad (2.8)$$

This is an *uncorrelated* initial state. The reservoir state is assumed to be *stationary* (with respect to the reservoir free evolution \mathcal{L}_B)

$$\mathcal{L}_B \rho_B = 0 \quad (2.9)$$

and thus belongs to the 0 eigenvalue of \mathcal{L}_B . In most applications, $\rho_B = Z_\beta^{-1} e^{-\beta H_B}$ is a thermal state at the inverse temperature $\beta = (k_B T)^{-1}$ with the normalization constant Z_β . However, we have in mind more general instances, such as nonequilibrium steady states [21]. The main target of the present article is the reconsideration of the assumption of the factorized initial condition (2.8).

The system state $\rho_S(t)$ at time t is given by

$$\rho_S(t) = \text{tr}_B \rho(t), \quad \rho(t) = e^{Lt} \rho_0, \tag{2.10}$$

where $\text{tr}_B : \mathcal{T}_1(\mathcal{H}_{\text{tot}}) \rightarrow \mathcal{T}_1(\mathcal{H}_S)$ is the partial trace over the reservoir degrees of freedom, a linear operator from $\mathcal{T}_1(\mathcal{H}_{\text{tot}})$, the Banach space of trace-class operators on the total Hilbert space \mathcal{H}_{tot} , onto $\mathcal{T}_1(\mathcal{H}_S)$. In general, unlike $\rho(t) = e^{-iHt} \rho_0 e^{iHt}$, $\rho_S(t)$ is not unitarily equivalent to ρ_S and the system undergoes dissipation and/or decoherence.

3. The projection method

Consider the initial-value problem

$$\frac{d}{dt} \rho(t) = \mathcal{L} \rho(t), \quad \rho(0) = \rho_0, \tag{3.1}$$

where the initial density operator ρ_0 is *not* assumed here to be factorized like (2.8). We are interested in the reduced dynamics of the system, $\rho_S(t)$ given by (2.10), with a correlated initial state ρ_0 .

The starting point of Nakajima–Zwanzig’s procedure is the introduction of the projection operators [2,4–6]

$$\mathcal{P} \rho = \text{tr}_B \{ \rho \} \otimes \Omega_B = \sigma \otimes \Omega_B, \quad \mathcal{Q} = 1 - \mathcal{P}, \tag{3.2}$$

where $\rho \in \mathcal{T}_1(\mathcal{H}_{\text{tot}})$, $\sigma \in \mathcal{T}_1(\mathcal{H}_S)$ and $\Omega_B \in \mathcal{T}_1(\mathcal{H}_B)$ is a given *reference state* of the reservoir. Note that, from the normalization condition $\text{tr}_B \Omega_B = 1$, it follows that $\mathcal{P}^2 = \mathcal{P}$ and $\mathcal{Q}^2 = \mathcal{Q}$. Therefore, \mathcal{P} is the projection onto the space of operators of the form $\sigma \otimes \Omega_B$, a subspace of $\mathcal{T}_1(\mathcal{H}_{\text{tot}})$ isometrically isomorphic to $\mathcal{T}_1(\mathcal{H}_S)$. In particular,

$$\mathcal{P} \rho(t) = \rho_S(t) \otimes \Omega_B, \quad \mathcal{Q} \rho(t) = \rho(t) - \rho_S(t) \otimes \Omega_B, \tag{3.3}$$

where we used the definition (2.10).

Since we are interested in a *correlated* initial state ρ_0 , which is not factorized like (2.8), a question arises as to which state should be taken as the reference state Ω_B [6,9,10] and whether the naive choice $\Omega_B = \text{tr}_S \rho_0$ is in principle appropriate. We shall see that the situation is much more subtle than one might naively expect: the reference state Ω_B and the reservoir dynamics cannot be independent, but must satisfy some important properties in order to yield a consistent description of the physical dynamics. One of the main subjects of this article will be the specification of the correct state Ω_B . Furthermore, our analysis will show that attention should be paid to the reference state Ω_B *even for a factorized initial state*. This corroborates and sheds additional light on the rigorous conditions for the derivation of the master equation [22]. At this moment, we take for granted only the stationarity (2.9) of Ω_B with respect to the reservoir free dynamics, namely $\mathcal{L}_B \Omega_B = 0$.

Let us project the Liouville equation (3.1) onto the two subspaces defined by \mathcal{P} and \mathcal{Q} . Notice first that

$$[\mathcal{P}, \mathcal{L}_S] = [\mathcal{Q}, \mathcal{L}_S] = 0, \quad \mathcal{P} \mathcal{L}_B = \mathcal{L}_B \mathcal{P} = 0, \quad [\mathcal{Q}, \mathcal{L}_B] = 0. \tag{3.4}$$

The first equation is a consequence of the fact that \mathcal{L}_S and \mathcal{P} essentially operate in different spaces, while the second derives from (2.9) and from the characteristic structure of the Liouvillians, $\text{tr} \{ \mathcal{L} \rho(t) \} = 0$ (a direct consequence of probability conservation). In addition, we require that

$$\mathcal{P}\mathcal{L}_{\text{SB}}\mathcal{P} = 0, \tag{3.5}$$

which is always satisfied as long as H_{SB} has vanishing diagonal elements with respect to the reservoir degrees of freedom.

By making use of (3.4) and (3.5), the total Liouvillian can be decomposed as

$$\mathcal{L} = \mathcal{P}\mathcal{L}_S\mathcal{P} + \mathcal{Q}\mathcal{L}_0\mathcal{Q} + \lambda\mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{Q} + \lambda\mathcal{P}\mathcal{L}_{\text{SB}}\mathcal{Q} + \lambda\mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{P}. \tag{3.6}$$

Therefore, the free evolutions \mathcal{L}_S and \mathcal{L}_B leave invariant the two subspaces $\text{Ran}\mathcal{P}$ and $\text{Ran}\mathcal{Q}$, and all transitions are driven by the interaction \mathcal{L}_{SB} .

4. The main theorem

The main result of this article is the following theorem, that will be proved in Section 6: for a correlated initial state ρ_0 , van Hove’s “ $\lambda^2 t$ ” limit [1,23] of the \mathcal{P} -projected density operator in the system-interaction picture,

$$\rho_I(\tau) = \lim_{\lambda \rightarrow 0} \rho_I^{(\lambda)}(\tau) = \lim_{\lambda \rightarrow 0} e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \rho(\tau / \lambda^2), \tag{4.1}$$

where we assume that the above limit exists, is the solution of

$$\rho_I(\tau) = \mathcal{P} \rho_0 + \int_0^\tau dt' \mathcal{K} \rho_I(t') \tag{4.2}$$

with

$$\begin{aligned} \mathcal{K} &= \sum_m \int_0^\infty dt \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} e^{\mathcal{L}_0 t} \mathcal{L}_{\text{SB}} e^{-\mathcal{L}_0 t} \tilde{\mathcal{Q}}_m \mathcal{P} \\ &= \sum_m \int_0^\infty dt \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} e^{(\mathcal{L}_0 + i\omega_m)t} \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_m \mathcal{P} \\ &= - \sum_m \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_m \mathcal{P}, \end{aligned} \tag{4.3}$$

or equivalently,

$$\frac{d}{d\tau} \rho_I(\tau) = \mathcal{K} \rho_I(\tau), \quad \rho_I(0) = \mathcal{P} \rho_0 = \text{tr}_B \{ \rho_0 \} \otimes \Omega_B. \tag{4.4}$$

That is, even if the initial state ρ_0 is not in a factorized form, but rather there is entanglement, or simply a classical correlation, between system S and reservoir B, all correlations disappear in van Hove’s limit and system S behaves as if the total system started from the factorized initial state in (4.4) with a reservoir state Ω_B specified below.

Moreover, one shows that

$$\lim_{\lambda \rightarrow 0} \mathcal{Q} \rho(\tau / \lambda^2) = \lim_{\lambda \rightarrow 0} [\rho(\tau / \lambda^2) - \text{tr}_B \{ \rho(\tau / \lambda^2) \} \otimes \Omega_B] = 0, \tag{4.5}$$

which makes the dynamics consistent, for no spurious term develops in the master equation and no correlations can appear at later times: not only the initial state, but also the state at any moment t is factorized in van Hove’s limit. This supports the validity of the assumption of the factorized state, that is frequently applied in literature in order to derive a master equation [2–4]. The state of system S evolves according to the master equation (4.4), while reservoir B remains in the state Ω_B .

These statements are proved under the following assumptions:

- (i) 0 is a simple eigenvalue of the reservoir Liouvillian \mathcal{L}_B corresponding to the eigenvector Ω_B and the remaining part of the spectrum of \mathcal{L}_B is absolutely continuous [22,24] (strictly speaking, for infinitely extended reservoir, the spectrum of \mathcal{L}_B can be properly defined only once the sector has been specified: in our case, the relevant sector is that containing the state Ω_B);
- (ii) the initial (correlated) state of the total system is given in the form.

$$\rho_0 = \Lambda(1_S \otimes \Omega_B) = \sum_i L_i(1_S \otimes \Omega_B)L_i^\dagger, \tag{4.6}$$

where Λ is a bounded superoperator (i.e., L_i 's are bounded operators) satisfying the normalization condition $\text{tr}\rho_0 = 1$. In other words, the initial state ρ_0 is a bounded perturbation of the state $1_S \otimes \Omega_B$ (and belongs to the sector specified by it).

Several comments are in order. First, observe that the Liouvillian of an infinitely extended system can bear a point spectrum, as in hypothesis (i) (see for instance Proposition 4.3.36 of Ref. [25]).

Second, the spectral properties required in hypothesis (i) imply that Ω_B is *mixing* with respect to the reservoir dynamics $e^{\mathcal{L}_B t}$ [22,24–27], i.e.,

$$\langle X(t)Y \rangle_{\Omega_B} = \langle X e^{\mathcal{L}_B t} Y \rangle_{\Omega_B} \rightarrow \langle X \rangle_{\Omega_B} \langle Y \rangle_{\Omega_B} \text{ as } t \rightarrow \infty \tag{4.7}$$

for any bounded (super)operators X and Y of the reservoir, where $X(t) = e^{-\mathcal{L}_B t} X e^{\mathcal{L}_B t}$ and $\langle X \rangle_\rho = \text{tr}_B \{ X \rho \}$. A typical and familiar example is the thermal equilibrium state of a free boson system at a finite temperature, as explicitly recalled in Appendix A. Among other interesting mixing states, there are nonequilibrium steady states (NESS), where system B consists of several reservoirs at different temperatures and a steady current flows among them [21]. These two cases are pictorially shown in Fig. 1. Both situations are within the scope of our analysis.

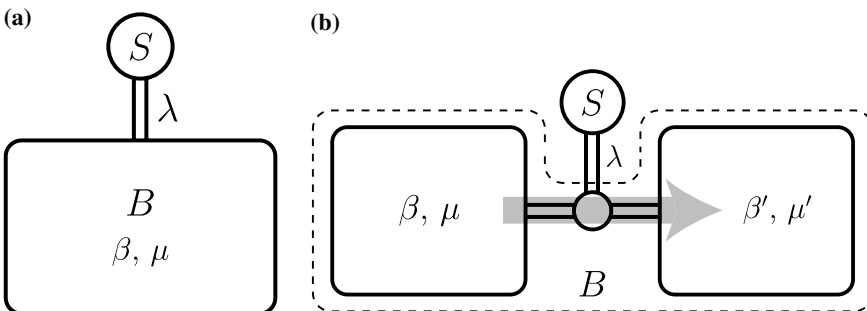


Fig. 1. Two typical examples in which the state of the reservoir is mixing: (a) system S in contact with a reservoir B in thermal equilibrium at the inverse temperature β and the chemical potential μ ; (b) system S in interaction with a reservoir B made up of two subreservoirs at different temperatures β and β' and chemical potentials μ and μ' , with a steady current flowing between them (NESS). In both cases, λ is the coupling constant: a proper application of van Hove’s “ $\lambda^2 t$ ” rescaling in the derivation of the master equation for S requires that the reference state of reservoir B be mixing.

Third, hypothesis (i) can be relaxed. In fact, the proof will make use only of the mixing property (4.7). Therefore, the remaining part of the spectrum can contain a singular continuous part: one must simply make sure that the continuous spectrum is transient (a property automatically verified by the absolutely continuous part, due to Riemann–Lebesgue’s lemma).

Fourth, the correlation between system S and reservoir B is more transparent if the initial state ρ_0 in (4.6) is written as

$$\rho_0 = \rho_S \otimes \rho_B + \delta\rho_0, \tag{4.8}$$

where

$$\rho_S = \text{tr}_B \rho_0, \quad \rho_B = \text{tr}_S \rho_0. \tag{4.9}$$

The last term $\delta\rho_0$ represents the correlation between system S and reservoir B. The important point is that each term is a bounded perturbation of the state $1_S \otimes \Omega_B$ and thus belongs to the single sector specified by it (see Appendix B for a clarification and a tutorial discussion of this issue). Indeed, the factorized part of the initial density matrix can be written as

$$\rho_S \otimes \rho_B = \Lambda'(1_S \otimes \Omega_B) = \sum_{i,m,n} L_{imn}(1_S \otimes \Omega_B)L_{imn}^\dagger, \tag{4.10a}$$

$$L_{imn} = \sqrt{\rho_S} \otimes_S \langle \phi_m | L_i | \phi_n \rangle_S, \tag{4.10b}$$

and

$$\delta\rho_0 = \delta\Lambda(1_S \otimes \Omega_B), \quad \delta\Lambda = \Lambda - \Lambda', \tag{4.10c}$$

where $\{|\phi_n\rangle_S\}$ is any complete orthonormal basis of system S. Clearly, $\delta\rho_0$ is self-adjoint, but it is not necessarily positive-definite.

Fifth, the states of the type (4.6) belong to a very general class: basically, if one deals with separable Hilbert spaces, (4.6) is of the Kraus form and therefore represents a completely positive map (that connects any two density matrices). For quantum mechanical systems (with discrete spectra), (4.6) covers all the possible states. In more general cases (with infinitely extended systems), since only bounded observables can be measured, one usually deals with a sector, i.e. a set of states which are “normal” with respect to some reference state (cf. the arguments of Sections III.2 and III.3 of Ref. [26]). In such a case, any normal states with respect to $1_S \otimes \Omega_B$ can be written as (4.6) with arbitrary precision. (See also the arguments in Ref. [24].)

Finally, the projection \mathcal{P} in (3.3) must be defined in terms of Ω_B , which is mixing and “contained” in the initial state ρ_0 in the sense of (4.6). This is the *criterion* for a *consistent choice* of the reference state Ω_B . We will see in the next section that Nakajima–Zwanzig’s projection \mathcal{P} with the correct reference state Ω_B is nothing but the eigenprojection of the Liouvillian \mathcal{L}_B belonging to the simple eigenvalue 0, as suggested by (3.4).

Note further that a state ρ_0 that refers [in the sense of (4.6)] to a coherent superposition of two (or more) different mixing states of an infinite reservoir cannot be a physical state, since it is the superposition of states belonging to different inequivalent sectors. (Imagine, for example, the superposition of states with different temperatures.) Hypothesis (ii) is therefore reasonable from this point of view and the states ρ_0 of the form (4.6) cover diverse physically interesting states, ranging from canonical equilibrium states to NESS, as far as their Ω_B ’s are mixing.

5. The diagonal projection

Before we prove the theorem, let us observe that the projection \mathcal{P} with the correct reference state Ω_B is nothing but the eigenprojection belonging to the simple eigenvalue 0 of the reservoir Liouvillian \mathcal{L}_B . To this end, we first show how the eigenprojection of 0 acts on a state of the total system.

Hypothesis (i) states that for any reservoir state ρ_B in question the spectral resolution of $e^{\mathcal{L}_B t} \rho_B$ reads

$$e^{\mathcal{L}_B t} \rho_B = \Pi_0 \rho_B + \int e^{-ivt} d\Pi(v) \rho_B, \tag{5.1}$$

where Π_0 and $\Pi(v)$ are the spectral projections of \mathcal{L}_B belonging to its simple eigenvalue 0 and to its absolutely continuous spectrum $\{v\}$, respectively. In particular,

$$\mathcal{L}_B \Pi_0 = \Pi_0 \mathcal{L}_B = 0, \quad \Pi_0^2 = \Pi_0. \tag{5.2}$$

By Riemann–Lebesgue’s lemma, one gets from (5.1)

$$e^{\mathcal{L}_B t} \rho_B \xrightarrow{t \rightarrow \infty} \Pi_0 \rho_B = \Omega_B \tag{5.3}$$

in a weak sense. The last equality follows from the condition that Ω_B is the eigenstate belonging to the simple eigenvalue 0. As anticipated in the previous section, the requirement of an absolutely continuous spectrum is not really necessary to prove (5.3). One needs only the mixing property (4.7). Indeed, let us consider a state of the total system belonging to the same sector of $1_S \otimes \Omega_B$, i.e., a state ρ of the kind (4.6). For any operator $D = \sum_i A_i \otimes X_i$, where A_i ’s are operators of system S and X_i ’s bounded operators of reservoir B, the mixing property (4.7) of Ω_B yields

$$\begin{aligned} \text{tr}\{D e^{\mathcal{L}_B t} \rho\} &= \sum_i \text{tr}_B[X_i e^{\mathcal{L}_B t} \text{tr}_S\{A_i \Lambda(1_S \otimes \Omega_B)\}] \\ &\xrightarrow{t \rightarrow \infty} \sum_i \text{tr}_B\{X_i \Omega_B\} \text{tr}\{A_i \Lambda(1_S \otimes \Omega_B)\} \\ &= \text{tr}[D(\text{tr}_B\{\rho\} \otimes \Omega_B)], \end{aligned} \tag{5.4}$$

and in this sense, we have

$$e^{\mathcal{L}_B t} \rho \xrightarrow{t \rightarrow \infty} \text{tr}_B\{\rho\} \otimes \Omega_B, \tag{5.5}$$

for any state ρ of the form (4.6). By comparing (5.3) and (5.5), it is clear that the eigenprojection Π_0 of the Liouvillian \mathcal{L}_B belonging to the eigenvalue 0 acts on the total system as

$$(1_S \otimes \Pi_0) \rho = \text{tr}_B\{\rho\} \otimes \Omega_B = \mathcal{P} \rho. \tag{5.6}$$

We have thus proved that (5.6) holds even when the spectrum $\{v\}$ in (5.1) contains a singular continuous part, provided that the latter be transient, i.e., Riemann–Lebesgue’s lemma hold also for it.

Furthermore, it is interesting to observe that the eigenprojection $1_S \otimes \Pi_0$ is nothing but the “diagonal projection,” that extracts the diagonal part (with respect to the reservoir degrees of freedom) of a density operator. To discuss the diagonal components of a reservoir with a continuous spectrum, consider a large parameter \mathcal{V} , corresponding to the volume, so that the Hamiltonian $H_B^{(\mathcal{V})}$ admits a discrete spectrum $\{E_\mu^{(\mathcal{V})}\}$, i.e.,

$$H_B^{(\nu)} = \sum_{\mu} E_{\mu}^{(\nu)} P_{\mu}^{(\nu)}, \quad \sum_{\mu} P_{\mu}^{(\nu)} = 1, \quad P_{\mu}^{(\nu)} P_{\nu}^{(\nu)} = P_{\mu}^{(\nu)} \delta_{\mu\nu}, \tag{5.7}$$

with $E_{\mu}^{(\nu)} \neq E_{\nu}^{(\nu)}$ for $\mu \neq \nu$. Then, it is easy to define the diagonal part (with respect to the reservoir degrees of freedom) of a density matrix of the total system, $\rho^{(\nu)}$,

$$\rho_D^{(\nu)} = \sum_{\mu} P_{\mu}^{(\nu)} \rho^{(\nu)} P_{\mu}^{(\nu)}. \tag{5.8}$$

Since $E_{\mu}^{(\nu)}$'s are discrete, one easily sees that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{-i(E_{\mu}^{(\nu)} - E_{\mu'}^{(\nu)})t} = \delta_{\mu\mu'}, \tag{5.9}$$

and thus,

$$\begin{aligned} \rho_D^{(\nu)} &= \sum_{\mu, \mu'} P_{\mu}^{(\nu)} \rho^{(\nu)} P_{\mu'}^{(\nu)} \delta_{\mu\mu'} \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \sum_{\mu, \mu'} e^{-iE_{\mu}^{(\nu)}t} P_{\mu}^{(\nu)} \rho^{(\nu)} P_{\mu'}^{(\nu)} e^{iE_{\mu'}^{(\nu)}t} \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{-iH_B^{(\nu)}t} \rho^{(\nu)} e^{iH_B^{(\nu)}t} \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{\mathcal{L}_B^{(\nu)}t} \rho^{(\nu)}. \end{aligned} \tag{5.10}$$

We now define the diagonal part of ρ via

$$\rho_D = \lim_{\nu \rightarrow \infty} \rho_D^{(\nu)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{\mathcal{L}_B t} \rho, \tag{5.11}$$

assuming that the two limits can be interchanged. Then, under the assumption of the ergodicity of Ω_B [which follows from the mixing of Ω_B : see Eq. (A.4)], one has, for any state ρ of the type (4.6),

$$\rho_D = \text{tr}_B\{\rho\} \otimes \Omega_B, \tag{5.12}$$

which is the right-hand side of (5.6). Indeed, for any bounded operator $D = \sum_i A_i \otimes X_i$ considered in (5.4),

$$\begin{aligned} \text{tr}\{D\rho_D\} &= \sum_i \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \text{tr}_B[X_i e^{\mathcal{L}_B t} \text{tr}_S\{A_i \Lambda(1_S \otimes \Omega_B)\}] \\ &= \sum_i \text{tr}_B\{X_i \Omega_B\} \text{tr}\{A_i \Lambda(1_S \otimes \Omega_B)\} \\ &= \text{tr}[D(\text{tr}_B\{\rho\} \otimes \Omega_B)], \end{aligned} \tag{5.13}$$

which proves (5.12), and the eigenprojection of \mathcal{L}_B belonging to the discrete eigenvalue 0 is the diagonal projection. Notice that the ergodicity of Ω_B is sufficient to show that $1_S \otimes \Pi_0$ is the diagonal projection. A direct demonstration of the diagonal projection (5.12) in a simple model is given in Appendix C.

It is now clear that the eigenprojection $1_S \otimes \Pi_0$ in (5.6) acts like the projection \mathcal{P} defined in (3.3), provided the state $\rho(t)$ is of the form $\Lambda_t(1_S \otimes \Omega_B)$, with a bounded superoperator

Λ_t . Since $\rho(t)$ has evolved from the initial state (4.6), it always satisfies this criterion. As we will discuss in the following, the eigenprojection $1_S \otimes \Pi_0$ enables us to deal with the point spectrum and yields the right choice for the projection \mathcal{P} in order to derive a master equation in van Hove's limit.

Summarizing, the initial state ρ_0 “contains,” in the sense of (4.6) and (5.5), the mixing state Ω_B . The theorem stated in Section 4 will be proved in Section 6 with the projection operator

$$\mathcal{P} = 1_S \otimes \Pi_0, \quad (5.14)$$

which is the eigenprojection of $1_S \otimes \mathcal{L}_B$ belonging to the unique simple eigenvalue 0. In the following, with an abuse of notation, $1_S \otimes \Pi_0$ will be written simply as Π_0 , as far as no confusion can arise.

Some additional comments are in order. If we assume only the ergodicity of Ω_B , rather than mixing, there can be other eigenvalues different from 0. The point spectrum other than 0 is out of control and, as we shall see in the following section, provokes the appearance of a secular term.

It is worth noting that the mixing property of Ω_B is crucial even for a *factorized* initial state like (2.8), although this point is usually not thoroughly discussed. (This is an interesting byproduct of our analysis, that is rather motivated by the study of nonfactorized initial states.) As we shall see, a wrong projection \mathcal{P} would give rise to a divergence that has nothing to do with the initial correlation.

In the standard derivations of the master equation for a factorized initial state, the projection (3.3) is defined in terms of the same Ω_B which is contained in the factorized initial state (2.8) and is usually the canonical state at temperature T , that is a mixing state. The criteria listed in Section 4 are thus satisfied and the projection is properly chosen to be $\mathcal{P} = 1_S \otimes \Pi_0$, provoking no problem. In this standard situation, the choice of the reference state is obvious: probably this often induces one to assume that Nakajima–Zwanzig's reference state is simply the canonical one (and therefore need not be characterized). However, in more articulated situations, such as those of NESS (see Fig. 1), the reference state must be chosen with care: our analysis shows that a correct reference state must in general be mixing.

6. Proof of the theorem

Let us now prove the theorem stated in Section 4. By projecting the Liouville equation (3.1) onto the two subspaces defined by \mathcal{P} and \mathcal{Q} , and using (3.6), one gets

$$\frac{d}{dt} \mathcal{P}\rho = \mathcal{L}_S \mathcal{P}\rho + \lambda \mathcal{P} \mathcal{L}_{SB} \mathcal{Q}\rho, \quad (6.1a)$$

$$\frac{d}{dt} \mathcal{Q}\rho = \mathcal{L}'_0 \mathcal{Q}\rho + \lambda \mathcal{Q} \mathcal{L}_{SB} \mathcal{P}\rho, \quad (6.1b)$$

respectively, where

$$\mathcal{L}'_0 = \mathcal{L}_0 + \lambda \mathcal{Q} \mathcal{L}_{SB} \mathcal{Q}. \quad (6.2)$$

By formally integrating out the second equation and plugging the result into the first one, one gets the following *exact* equation for the \mathcal{P} -projected operator in the interaction picture [6]

$$\frac{d}{dt} e^{-\mathcal{L}_S t} \mathcal{P} \rho(t) = \lambda^2 \int_0^t dt' e^{-\mathcal{L}_S t'} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(t-t')} \mathcal{L}_{SB} \mathcal{P} \rho(t') + \lambda e^{-\mathcal{L}_S t} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0 t} \mathcal{Q} \rho_0. \quad (6.3)$$

The last term in the right-hand side represents the contribution arising from a possible initial correlation between system S and reservoir B. We will show that this term dies out in the weak-coupling limit $\lambda \rightarrow 0$ with the scaled time $\tau = \lambda^2 t (> 0)$ fixed, provided the projection \mathcal{P} is chosen to be the eigenprojection $I_S \otimes \Pi_0$ belonging to the simple eigenvalue 0 of \mathcal{L}_B . To this end, consider the density operator

$$\rho_I^{(\lambda)}(\tau) = e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \rho(\tau / \lambda^2), \quad (6.4)$$

introduced in (4.1), that for any nonvanishing λ satisfies

$$\begin{aligned} \frac{d}{d\tau} \rho_I^{(\lambda)}(\tau) &= \int_0^{\tau / \lambda^2} dt e^{-\mathcal{L}_S t / \lambda^2} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(\tau / \lambda^2 - t)} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S t} \rho_I^{(\lambda)}(\lambda^2 t) \\ &\quad + \frac{1}{\lambda} e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0 \tau / \lambda^2} \mathcal{Q} \rho_0, \end{aligned} \quad (6.5)$$

with the initial condition

$$\rho_I^{(\lambda)}(0) = \mathcal{P} \rho_0. \quad (6.6)$$

By integrating (6.5) and (6.6), one gets

$$\begin{aligned} \rho_I^{(\lambda)}(\tau) &= \mathcal{P} \rho_0 + \int_0^\tau d\tau' \int_0^{\tau' / \lambda^2} dt e^{-\mathcal{L}_S t' / \lambda^2} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(\tau' / \lambda^2 - t)} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S t} \rho_I^{(\lambda)}(\lambda^2 t) \\ &\quad + \frac{1}{\lambda} \int_0^\tau d\tau' e^{-\mathcal{L}_S \tau' / \lambda^2} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0 \tau' / \lambda^2} \mathcal{Q} \rho_0. \end{aligned} \quad (6.7)$$

The second term is rearranged as

$$\begin{aligned} &\int_0^\tau d\tau' \int_0^{\tau' / \lambda^2} dt e^{-\mathcal{L}_S t' / \lambda^2} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(\tau' / \lambda^2 - t)} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S t} \rho_I^{(\lambda)}(\lambda^2 t) \\ &= \int_0^{\tau / \lambda^2} dt \int_0^{\lambda^2 t} d\tau' e^{-\mathcal{L}_S t'} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(t - \tau' / \lambda^2)} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S \tau' / \lambda^2} \rho_I^{(\lambda)}(\tau') \\ &= \int_0^\tau d\tau' \int_{\tau' / \lambda^2}^{\tau / \lambda^2} dt e^{-\mathcal{L}_S t'} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0(t - \tau' / \lambda^2)} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S \tau' / \lambda^2} \rho_I^{(\lambda)}(\tau') \\ &= \int_0^\tau d\tau' \int_0^{(\tau - \tau') / \lambda^2} dt e^{-\mathcal{L}_S(t + \tau' / \lambda^2)} \mathcal{P} \mathcal{L}_{SB} e^{\mathcal{L}'_0 t} \mathcal{L}_{SB} \mathcal{P} e^{\mathcal{L}_S \tau' / \lambda^2} \rho_I^{(\lambda)}(\tau') \\ &= \sum_{m,n} \int_0^\tau d\tau' e^{i(\omega_m - \omega_n)\tau' / \lambda^2} \mathcal{K}_{mn}^{(\lambda)}(\tau - \tau') \rho_I^{(\lambda)}(\tau'), \end{aligned} \quad (6.8)$$

with the memory kernel

$$\mathcal{K}_{mn}^{(\lambda)}(\tau) = \int_0^{\tau / \lambda^2} dt \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{SB} \mathcal{Q} e^{(\mathcal{L}'_0 + i\omega_m)t} \mathcal{L}_{SB} \tilde{\mathcal{Q}}_n \mathcal{P}. \quad (6.9)$$

The last term in Eq. (6.7), which is relevant to the initial correlation, reads

$$\begin{aligned} \mathcal{I}^{(\lambda)}(\tau) &= \frac{1}{\lambda} \int_0^\tau dt' e^{-\mathcal{L}_S t'/\lambda^2} \mathcal{P} \mathcal{L}_{\text{SB}} e^{\mathcal{L}'_0 t'/\lambda^2} \mathcal{Q} \rho_0 \\ &= \lambda \sum_m \int_0^{\tau/\lambda^2} dt \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} e^{(\mathcal{L}'_0 + i\omega_m)t} \mathcal{Q} \rho_0. \end{aligned} \tag{6.10}$$

In conclusion,

$$\rho_I^{(\lambda)}(\tau) = \mathcal{P} \rho_0 + \sum_{m,n} \int_0^\tau dt' e^{i(\omega_m - \omega_n)t'/\lambda^2} \mathcal{K}_{mn}^{(\lambda)}(\tau - t') \rho_I^{(\lambda)}(t') + \mathcal{I}^{(\lambda)}(\tau). \tag{6.11}$$

We can now analyze the van Hove limits of the memory kernel $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ and of the initial correlation $\mathcal{I}^{(\lambda)}(\tau)$. Both limits can be computed at the same time if we consider the van Hove limit of the operator

$$\mathcal{R}_m^{(\lambda)}(\tau) = \int_0^{\tau/\lambda^2} dt \mathcal{Q} e^{(\mathcal{L}'_0 + i\omega_m)t}, \tag{6.12}$$

since both $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ and $\mathcal{I}^{(\lambda)}(\tau)$ contain it. The analysis of the properties of $\mathcal{R}_m^{(\lambda)}(\tau)$ is given in Appendix D, where it is shown that, irrespectively of the point spectrum of \mathcal{L}'_0 , one obtains

$$\mathcal{R}_m^{(0)} = \lim_{\lambda \rightarrow 0} \mathcal{R}_m^{(\lambda)}(\tau) = -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \quad (\tau > 0), \tag{6.13}$$

provided that $\mathcal{P} = 1_S \otimes \Pi_0$. The expression (6.13) is our key formula: it immediately leads us to the conclusion that, in van Hove’s limit, the memory kernel $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ in (6.9) is reduced to a Markovian generator

$$\begin{aligned} \mathcal{K}_{mn}^{(\lambda)}(\tau) &= \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_n \mathcal{P} \\ \xrightarrow{\lambda \rightarrow 0} \mathcal{K}_{mn}^{(0)} &= -\mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_n \mathcal{P}, \end{aligned} \tag{6.14}$$

while the correlation term $\mathcal{I}^{(\lambda)}(\tau)$ in (6.10) disappears

$$\mathcal{I}^{(\lambda)}(\tau) = \lambda \sum_m \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \mathcal{Q} \rho_0 \xrightarrow{\lambda \rightarrow 0} 0, \tag{6.15}$$

so that the reduced dynamics (6.11) becomes

$$\begin{aligned} \rho_I^{(\lambda)}(\tau) &\xrightarrow{\lambda \rightarrow 0} \mathcal{P} \rho_0 + \sum_{m,n} \int_0^\tau dt' \delta_{mn} \mathcal{K}_{mn}^{(0)} \rho_I(t') \\ &= \mathcal{P} \rho_0 + \int_0^\tau dt' \mathcal{K} \rho_I(t'). \end{aligned} \tag{6.16}$$

The master equation in van Hove’s limit therefore reads

$$\frac{d}{dt} \rho_I(\tau) = \mathcal{K} \rho_I(\tau), \tag{6.17a}$$

$$\mathcal{K} = \sum_m \mathcal{K}_{mm}^{(0)} = -\sum_m \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_m \mathcal{P}. \tag{6.17b}$$

We have thus proved (4.2)–(4.4), the first part of the theorem in Section 4. In van Hove’s limit, the density matrix evolves as if it started from the initial condition $\mathcal{P} \rho_0$, even when

$\mathcal{Q}\rho_0 \neq 0$: the initial correlation dies out immediately (at $\tau = 0^+$) in the scaled time τ . The contribution originating from the initial correlation between the system and the reservoir disappears in the scaling limit and one is allowed to start from an initial density matrix in the factorized form (4.4). From a physical point of view, the factorization Ansatz described above simply means that the “initial” correlations between the system and its environment are “forgotten” on a time scale of order λ^2 in τ (which is very small when compared to the timescale of the evolution of the system). We shall see in Article II, by looking at a specific example, that the problem of the relevant timescales must be tackled with care, as it also involves locality issues related to the “size” of the local observables of the reservoir.

It is important to note that, if we choose a different projection \mathcal{P} from the eigenprojection of \mathcal{L}_B belonging to its vanishing eigenvalue, and fail to appropriately remove the point spectrum of \mathcal{L}_B , Eq. (6.13) does not hold anymore, and $\mathcal{R}_m^{(\lambda)}(\tau)$ diverges in van Hove’s limit. [See, for example, Eq. (D.6) in Appendix D.] $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ and $\mathcal{I}^{(\lambda)}(\tau)$ accordingly diverge and the van Hove limit of the master equation does not exist. This is because a “wrong” projection \mathcal{P} would project the reservoir onto a wrong (in general non-stationary) state, so that the system evolution would develop a secular term in τ/λ^2 [like in Eq. (D.6)]. It is remarkable that such a secular term appears as a consequence of a sloppy application of Nakajima–Zwanzig’s projection method: in a sense, the very method makes sense only if applied to the “correct” mixing state.

As stressed at the end of the previous section, the reference state of the reservoir must be mixing (and not, e.g., simply ergodic), in order that no discrete eigenvalue different from 0 exists. Otherwise, the point spectrum (except 0) is out of control and again the emergence of secular terms is inevitable. Moreover, the mixing property of the reservoir is crucial even for a *factorized* initial state like (2.8). Indeed, careful scrutiny of the proof shown in this section shows that the divergence of $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ has nothing to do with the initial correlation. In this sense, although our original motivation was the study of the factorization Ansatz, the results have more general validity. The reason why this was unnoticed so far is the following. In the standard textbook derivations of the master equation, a factorized initial state is assumed and the projection (3.3) is defined in terms of the same reference state Ω_B that is contained in the factorized initial state (2.8): in practically all examples, this is taken to be the canonical state at temperature T , which is clearly mixing, and all the criteria listed in Section 4 are satisfied. However, recently, more complicated physical situations are attracting increasing interest, such as those related to NESS shown in Fig. 1(b). These cases call for a characterization of the state of the reservoir, that is mixing and satisfies the hypotheses in Section 4 required to prove the theorem [21].

7. Factorization at all times

Time $t = 0$ has no particular status: one can prove the same master equation (4.4) with a factorized initial state for any “initial” time t_0 . This means that the limiting dynamics is such that the density matrix remains *factorized at all times*: the reservoir state does not evolve, while the system state follows the master equation (4.4). In order to show this, one must prove the validity of Eq. (4.5) in van Hove’s limit. Then, clearly, no spurious term will develop in the master equation and no correlations can appear.

By integrating (6.1a) and inserting it into (6.1b), we get the following integral equation for $\mathcal{Q}\rho(t)$:

$$\begin{aligned} \mathcal{Q}\rho(t) &= e^{\mathcal{L}'_0 t} \mathcal{Q}\rho_0 + \lambda \int_0^t dt' e^{\mathcal{L}'_0(t-t')} \mathcal{Q}\mathcal{L}_{\text{SB}} e^{\mathcal{L}'_s t'} \mathcal{P}\rho_0 \\ &\quad + \lambda^2 \int_0^t dt' \int_0^{t'} dt'' e^{\mathcal{L}'_0(t-t')} \mathcal{Q}\mathcal{L}_{\text{SB}} e^{\mathcal{L}'_s(t-t'')} \mathcal{P}\mathcal{L}_{\text{SB}} \mathcal{Q}\rho(t''), \end{aligned} \tag{7.1}$$

which is rearranged, by interchanging the integrations in the last term, to yield in the scaled time $\tau = \lambda^2 t$

$$\begin{aligned} \mathcal{Q}\rho(\tau/\lambda^2) &= \mathcal{Q}e^{\mathcal{L}'_0 \tau/\lambda^2} \left(\mathcal{Q}\rho_0 - \lambda \sum_m \mathcal{R}_m^{(\lambda)}(-\tau) \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_m \mathcal{P}\rho_0 \right. \\ &\quad \left. - \sum_m \int_0^\tau dt' e^{-\mathcal{L}'_0 t'/\lambda^2} \mathcal{R}_m^{(\lambda)}(\tau - t') \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_m \mathcal{P}\mathcal{L}_{\text{SB}} \mathcal{Q}\rho(t'/\lambda^2) \right), \end{aligned} \tag{7.2}$$

where $\mathcal{R}_m^{(\lambda)}(\tau)$ is defined in (6.12). Under the proper choice of the projection \mathcal{P} , the kernel $\mathcal{R}_m^{(\lambda)}(\tau)$ is bounded for any τ and λ (even for $\lambda \rightarrow 0$), as already discussed in the previous section and in Appendix D, and it is possible to show that (see Appendix D)

$$\lim_{\lambda \rightarrow 0} \mathcal{Q}e^{\mathcal{L}'_0 \tau/\lambda^2} = 0. \tag{7.3}$$

Then, the integrand in the last term in (7.2) is bounded, all the terms in the parentheses are finite, and the prefactor in (7.2) vanishes according to (7.3), which proves (4.5), the second part of the theorem in Section 4.

It is worth noting that the interaction between system S and reservoir B is not essential to the factorization; the free evolution eliminates the correlation, and the reservoir relaxes into the mixing state Ω_B . Indeed, for any state ρ_0 of the total system of the type (4.6), we have

$$e^{\mathcal{L}'_0 t} \rho_0 \xrightarrow{t \rightarrow \infty} e^{\mathcal{L}'_s t} \Pi_0 \rho_0 = e^{\mathcal{L}'_s t} \text{tr}_B \{ \rho_0 \} \otimes \Omega_B, \tag{7.4}$$

where the contribution of the absolutely continuous spectrum decays out due to Riemann–Lebesgue’s lemma [see Eqs. (5.1) and (5.5)]. In the rescaled time τ , the factorization is very rapid, and the total system looks factorized at any moment (if the observables that one can measure on the reservoir are local enough: a concrete example will be discussed in the following Article II). Summarizing, reservoir B relaxes into the mixing state Ω_B through its own free evolution, yielding the factorization of the state of the total system, while system S dissipates through the interaction: a remarkable and consistent global view.

It is also interesting to compare the present result with Bogoliubov’s view on the classical gas dynamics [2,28,29]. According to this view, “molecular chaos” erases a large amount of initial information and the system reaches the so-called kinetic stage, where the one-body distribution function governs the evolution of the whole system and obeys the Boltzmann equation, irrespectively of the initial conditions. In the present case, the initial loss of system-reservoir correlations corresponds to the information loss due to molecular chaos, and the stage described by the master equation in van Hove’s limit corresponds to the kinetic stage.

8. Concluding remarks

We analyzed the assumption of factorization of the initial state in the dynamics of a quantum mechanical system in interaction with a reservoir. In van Hove’s limit, the dynamics can be consistently described in terms of a master equation, but a correct

application of Nakajima–Zwanzig’s projection method requires that the reference state of the reservoir, in terms of which the projection operator is defined, be endowed with the mixing property. If the reservoir dynamics is not mixing, the evolution develops secular terms. In the above discussion, one implicitly assumes that the van Hove limit (4.1) exists and is the solution of Eqs. (4.2)–(4.4).

In the standard situation, when a small system is coupled to a reservoir at a given temperature, the choice of the reference state is obvious and is simply the canonical state (that is also mixing). In more articulated situations, such as those of NESS, the choice of the reference state requires care and need to be characterized: our analysis shows that a correct reference state must in general be mixing.

This Ansatz yields the standard procedure and the usual master equation. As a byproduct, one observes that the mixing property is crucial even when the initial state is assumed to be factorized, otherwise the presence of a secular terms is inevitable. In this respect our analysis, that was originally motivated by the study of the assumption of initial state factorization, has more general validity.

We shall see in the following Article II, by close scrutiny of some explicit examples, that Markovianity becomes a valid approximation for timescales that depend both on the form factors of the interaction and on the spatial extension of the local observables that can be measured on the reservoir. This will corroborate and complement the general findings discussed in this article. Other issues, such as the spin-offs on the complete positivity of the dynamics [11–18], the mathematical conditions at the origin of van Hove’s limit [30], as well as the consequences of higher order corrections [31] and their interplay with initial correlations will be investigated in a future paper.

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Appendix A. Mixing property

The free Liouvillian of an *infinite* reservoir \mathcal{L}_B has a point spectrum [22,25,26]. The clue for our problem is to handle it properly, by making use of the right projection \mathcal{P} . The

mixing property of the reservoir plays an important role in this context. Let us hence briefly recall these notions.

A.1. *Mixing property and spectrum of the Liouvillian*

The state Ω_B is said to be *mixing* with respect to the reservoir dynamics $e^{\mathcal{L}_B t}$, if the correlation function of any two bounded operators of the reservoir, X and Y , behaves as (4.7) [22,24–27]. The ordinary canonical equilibrium state of free bosons at a finite temperature is a typical mixing state. Other interesting examples are nonequilibrium steady states (NESS).

It is important to observe that the mixing property is strongly related to the spectral properties of the Liouvillian \mathcal{L}_B [27]. Let us consider a reservoir state $\rho_B = \Lambda_B \Omega_B$ ($\text{tr}_B \rho_B = 1$) related to a mixing state Ω_B by a bounded superoperator Λ_B , in the sense of (4.6). Then, by setting $Y \Omega_B = \Lambda_B \Omega_B = \rho_B$ in (4.7), the mixing property of Ω_B translates into

$$\langle X(t) \rangle_{\rho_B} \rightarrow \langle X \rangle_{\Omega_B} \quad \text{as } t \rightarrow \infty, \tag{A.1}$$

and in this sense,

$$e^{\mathcal{L}_B t} \rho_B \rightarrow \Omega_B \quad \text{as } t \rightarrow \infty, \tag{A.2}$$

i.e., the state ρ_B relaxes towards the mixing state Ω_B . Let us consider the spectral resolution of $e^{\mathcal{L}_B t} \rho_B$,

$$e^{\mathcal{L}_B t} \rho_B = \sum_{v_j} e^{-iv_j t} \Pi_j \rho_B + \int e^{-iv t} d\Pi(v) \rho_B, \tag{A.3}$$

where Π_j and $\Pi(v)$ are the spectral projections of \mathcal{L}_B belonging to its possible discrete eigenvalues $\{v_j\}$ and to its absolutely continuous spectrum $\{v\}$, respectively. The second term, representing the contribution of the absolutely continuous spectrum, decays out as $t \rightarrow \infty$ due to Riemann–Lebesgue’s lemma, but the first term, the contribution of the point spectrum, survives. Property (A.2) means that (within the class of states of the form $\rho_B = \Lambda_B \Omega_B$) there exists the only simple eigenvalue 0 of the Liouvillian \mathcal{L}_B with the eigenprojection Π_0 satisfying $\Pi_0 \rho_B = \Omega_B$; mixing forbids the existence of other eigenvalues than 0, reducing (A.3) to (5.1), and the eigenvalue 0 is not degenerated within the single sector specified by Ω_B . Furthermore, since $\Pi(v) \Omega_B = 0$ [remember the orthogonality $\Pi_0 \Pi(v) = \Pi(v) \Pi_0 = 0$], the mixing state Ω_B is a stationary state with respect to the reservoir dynamics $e^{\mathcal{L}_B t}$, i.e., Eq. (2.9).

If we only require that 0 be a simple eigenvalue of \mathcal{L}_B , but we do not care about the rest of the spectrum, then property (4.7) only holds in a Cesaro sense, namely

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle X(t) Y \rangle_{\Omega_B} = \langle X \rangle_{\Omega_B} \langle Y \rangle_{\Omega_B}, \tag{A.4}$$

and Ω_B is called an *ergodic* state. Ergodicity suffices to show the stationarity (2.9) of Ω_B ; the mixing property is not necessary [22,24–27]. The uniqueness of the point spectrum 0, however, is equivalent to weak mixing [22,25–27] $\int_0^T dt |\langle X(t) Y \rangle_{\Omega_B} - \langle X \rangle_{\Omega_B} \langle Y \rangle_{\Omega_B}| / T \rightarrow 0$ and this implies that the remaining part of the spectrum can also contain singular continuous components. In such a case, one might conjecture that the theorem of Section 4 is still valid, but in a weaker sense.

A.2. A solvable example

Let us demonstrate the mixing property (4.7) in a solvable example. Let us consider the reservoir Hamiltonian

$$H_B = \int d\omega \omega b_\omega^\dagger b_\omega \tag{A.5}$$

and the reservoir dynamics starting from the initial state

$$\rho_B = \tilde{\Lambda}_B \rho_{\mathcal{W}} = \int d\omega \int d\omega' w_{\omega\omega'} b_\omega^\dagger \rho_{\mathcal{W}} b_{\omega'}, \tag{A.6}$$

with

$$\rho_{\mathcal{W}} = \frac{1}{Z_{\mathcal{W}}} \exp \left(- \int d\omega \int d\omega' b_\omega^\dagger \mathcal{W}_{\omega\omega'} b_{\omega'} \right), \tag{A.7}$$

where b_ω (b_ω^\dagger) is the annihilation (creation) operator of the reservoir, satisfying the canonical commutation relation $[b_\omega, b_{\omega'}^\dagger] = \delta(\omega - \omega')$. The states ρ_B and $\rho_{\mathcal{W}}$ are normalized, $\text{tr}_B \rho_B = 1$ and $\text{tr}_B \rho_{\mathcal{W}} = 1$, with the normalization constant $Z_{\mathcal{W}}$. $w_{\omega\omega'}$ is a bounded and Hermitian positive matrix ($w_{\omega\omega'} = w_{\omega'\omega}^*$), and the Gaussian state $\rho_{\mathcal{W}}$ is perturbed by the bounded superoperator $\tilde{\Lambda}_B$. Furthermore, $\mathcal{W}_{\omega\omega'}$ is Hermitian ($\mathcal{W}_{\omega\omega'} = \mathcal{W}_{\omega'\omega}^*$) and consists of $\mathcal{W}_{\omega\omega'}^{(0)}$, that is proportional to $\delta(\omega - \omega')$, and the remaining part $\tilde{\mathcal{W}}_{\omega\omega'}$,

$$\mathcal{W}_{\omega\omega'} = \mathcal{W}_{\omega\omega'}^{(0)} + \tilde{\mathcal{W}}_{\omega\omega'}, \quad \mathcal{W}_{\omega\omega'}^{(0)} = W(\omega)\delta(\omega - \omega'). \tag{A.8}$$

The Gaussian state $\rho_{\mathcal{W}}$ is fully characterized by the two-point function

$$\mathcal{N}_{\omega\omega'} = \langle b_{\omega'}^\dagger b_\omega \rangle_{\rho_{\mathcal{W}}} = N(\omega)\delta(\omega - \omega') + \tilde{\mathcal{N}}_{\omega\omega'}, \tag{A.9}$$

where the first term, proportional to $\delta(\omega - \omega')$, is the expectation value of the number operator in the state $\rho_{\mathcal{W}_0}$,

$$\mathcal{N}_{\omega\omega'}^{(0)} = \langle b_{\omega'}^\dagger b_\omega \rangle_{\rho_{\mathcal{W}_0}} = N(\omega)\delta(\omega - \omega'), \quad N(\omega) = \frac{1}{e^{W(\omega)} - 1}, \tag{A.10}$$

with

$$\rho_{\mathcal{W}_0} = \frac{1}{Z_{\mathcal{W}_0}} \exp \left(- \int d\omega b_\omega^\dagger W(\omega) b_\omega \right), \quad \text{tr}_B \rho_{\mathcal{W}_0} = 1. \tag{A.11}$$

In fact, $\rho_{\mathcal{W}}$ is different from $\rho_{\mathcal{W}_0}$ by a bounded operator L_B , as

$$\rho_{\mathcal{W}} = L_B \rho_{\mathcal{W}_0} L_B^\dagger, \tag{A.12}$$

where

$$L_B = \rho_{\mathcal{W}}^{1/2} \rho_{\mathcal{W}_0}^{-1/2} = \sqrt{\frac{Z_{\mathcal{W}_0}}{Z_{\mathcal{W}}}} \bar{\mathbf{T}} \exp \left(- \int_0^{1/2} d\beta b^\dagger e^{-\beta \mathcal{W}^{(0)}} \tilde{\mathcal{W}} e^{\beta \mathcal{W}^{(0)}} b \right), \tag{A.13}$$

with $\bar{\mathbf{T}}$ denoting the anti-chronologically ordered product and

$$b^\dagger e^{-\beta \mathcal{W}^{(0)}} \tilde{\mathcal{W}} e^{\beta \mathcal{W}^{(0)}} b = \int d\omega \int d\omega' b_\omega^\dagger e^{-\beta W(\omega)} \tilde{\mathcal{W}}_{\omega\omega'} e^{\beta W(\omega')} b_{\omega'}. \tag{A.14}$$

Hence, by applying Wick's theorem, the two-point function (A.9) reads

$$\mathcal{N}_{\omega\omega'} = \langle L_B^\dagger b_{\omega'}^\dagger b_\omega L_B \rangle_{\rho_{\mathcal{W}_0}} = \langle b_{\omega'}^\dagger b_\omega \rangle_{\rho_{\mathcal{W}_0}} \langle L_B^\dagger L_B \rangle_{\rho_{\mathcal{W}_0}} + \dots \tag{A.15}$$

The first term is $\mathcal{N}_{\omega\omega'}^{(0)}$ in (A.10), since $\langle L_B^\dagger L_B \rangle_{\rho_{\mathcal{W}_0}} = \text{tr}_B \rho_{\mathcal{W}} = 1$, and the other terms, defining $\tilde{\mathcal{N}}_{\omega\omega'}$, are bounded functions, not proportional to $\delta(\omega - \omega')$.

Let us now take any two bounded operators of the reservoir, of the form

$$X = \int d\omega \int d\omega' b_\omega^\dagger \mathcal{X}_{\omega\omega'} b_{\omega'}, \quad Y = \int d\omega \int d\omega' b_\omega^\dagger \mathcal{Y}_{\omega\omega'} b_{\omega'}, \tag{A.16}$$

and observe how the mixing property (4.7) emerges. In this case, the correlation function reads

$$\begin{aligned} \langle X(t)Y \rangle_{\rho_B} &= \langle e^{iH_B t} X e^{-iH_B t} Y \rangle_{\rho_B} \\ &= \int d\omega_1 \int d\omega_2 \int d\omega_3 \int d\omega_4 \int d\omega \int d\omega' \mathcal{X}_{\omega_1\omega_2} \mathcal{Y}_{\omega_3\omega_4} w_{\omega\omega'} \\ &\quad \times \langle b_{\omega'}^\dagger b_{\omega_1}^\dagger b_{\omega_2} b_{\omega_3}^\dagger b_{\omega_4} b_\omega^\dagger \rangle_{\rho_{\mathcal{W}}} e^{i(\omega_1 - \omega_2)t}. \end{aligned} \tag{A.17}$$

By applying Wick’s theorem, $\langle b_{\omega'}^\dagger b_{\omega_1}^\dagger b_{\omega_2} b_{\omega_3}^\dagger b_{\omega_4} b_\omega^\dagger \rangle_{\rho_{\mathcal{W}}}$ can be expressed in terms of two-point functions (A.9), and by applying Riemann–Lebesgue’s lemma, only the contribution of $\delta(\omega_1 - \omega_2)$ in $\langle b_{\omega_1}^\dagger b_{\omega_2} \rangle_{\rho_{\mathcal{W}}}$ survives in the long-time limit, to yield

$$\begin{aligned} \langle X(t)Y \rangle_{\rho_B} &\xrightarrow{t \rightarrow \infty} \int d\omega_1 \int d\omega_3 \int d\omega_4 \int d\omega \int d\omega' \mathcal{X}_{\omega_1\omega_1} \mathcal{Y}_{\omega_3\omega_4} w_{\omega\omega'} \\ &\quad \times N(\omega_1) \langle b_{\omega'}^\dagger b_{\omega_3}^\dagger b_{\omega_4} b_\omega^\dagger \rangle_{\rho_{\mathcal{W}}} \\ &= \langle X \rangle_{\rho_{\mathcal{W}_0}} \langle Y \rangle_{\rho_B}. \end{aligned} \tag{A.18}$$

Therefore, if $\rho_B = \rho_{\mathcal{W}_0}$ (i.e., $\tilde{\mathcal{W}}_{\omega\omega'} = 0$ without the perturbation $\tilde{\Lambda}_B$), Eq. (A.18) is nothing but the definition of mixing in (4.7), and $\rho_{\mathcal{W}_0}$ given in (A.11) is an example of mixing state. The canonical state $\rho_{\mathcal{W}_0}$ with $W(\omega) = \beta\omega$, is thus a typical mixing state. We have demonstrated (A.18) with the specific observables X and Y in (A.16), but this example helps us understand how mixing emerges for general observables.

It is important to note that, in this appendix, we have considered only the reservoir dynamics generated by the reservoir Hamiltonian H_B , without any interaction. The free evolution is responsible for the mixing.

The mixing property (4.7) is demonstrated here with the thermal equilibrium state (A.11). It is also possible to prove it for the NESS depicted in Fig. 1(b). See Ref. [21] for details.

Appendix B. Inequivalent sectors

The main purpose of this tutorial appendix is to clarify that different mixing states belong to different sectors which are inequivalent to each other, and any bounded perturbation on a mixing state does not bring it to a different sector. Let us demonstrate the inequivalence of the sectors with an explicit example that captures the essence of the inequivalent representation.

In order to analyze an infinitely extended system, let us begin with a free bosonic gas in a 1D box whose size is specified by a parameter ℓ , and then take the continuum limit $\ell \rightarrow \infty$. We consider two canonical states Ω_β and $\Omega_{\beta'}$ with different temperatures and

compute the overlap between them through the quantity $\text{tr}_B\{\Omega_\beta^{1/2}\Omega_{\beta'}^{1/2}\}$. Note that the canonical state is a mixing state as shown in Appendix A.

In the finite box, momentum k is discrete, and the Hamiltonian of the bosonic gas is given by

$$H_B = \sum_k \omega_k b_k^{(\ell)\dagger} b_k^{(\ell)}, \tag{B.1}$$

where $b_k^{(\ell)}$ and $b_k^{(\ell)\dagger}$ satisfy the canonical commutation relation $[b_k^{(\ell)}, b_{k'}^{(\ell)\dagger}] = \delta_{kk'}$. The canonical state at the inverse temperature β is given by

$$\Omega_\beta = \frac{1}{Z_\beta} e^{-\beta H_B}, \quad Z_\beta^{-1} = \prod_k (1 - e^{-\beta\omega_k}), \tag{B.2}$$

and the overlap between Ω_β and $\Omega_{\beta'}$ reads

$$\begin{aligned} \text{tr}_B\{\Omega_\beta^{1/2}\Omega_{\beta'}^{1/2}\} &= \prod_k \frac{\sqrt{(1 - e^{-\beta\omega_k})(1 - e^{-\beta'\omega_k})}}{1 - e^{-\bar{\beta}\omega_k}} \\ &= \exp\left[-\frac{1}{2} \sum_k \ln \frac{(1 - e^{-\bar{\beta}\omega_k})^2}{(1 - e^{-\beta\omega_k})(1 - e^{-\beta'\omega_k})}\right], \end{aligned} \tag{B.3}$$

where $\bar{\beta} = (\beta + \beta')/2$. The exponent in (B.3) is easily shown to be less than zero for $\beta \neq \beta'$ and equal to zero for $\beta = \beta'$. In the continuum limit $\ell \rightarrow \infty$, the summation in the exponent is replaced with an integral as $\sum_k \rightarrow (\ell/2\pi) \int dk$, and the overlap is reduced to

$$\begin{aligned} \text{tr}_B\{\Omega_\beta^{1/2}\Omega_{\beta'}^{1/2}\} &= \exp\left[-\frac{\ell}{4\pi} \int dk \ln \frac{(1 - e^{-\bar{\beta}\omega_k})^2}{(1 - e^{-\beta\omega_k})(1 - e^{-\beta'\omega_k})}\right] \\ &\rightarrow \begin{cases} 1 & (\beta = \beta') \\ 0 & (\beta \neq \beta') \end{cases} \quad \text{as } \ell \rightarrow \infty, \end{aligned} \tag{B.4}$$

which means that canonical states with different temperatures do not overlap and belong to inequivalent sectors.

Any bounded perturbation does not change the situation: a state $\tilde{\Omega}_\beta$, which is different from a canonical state Ω_β only by a bounded superoperator, belongs to the same sector as that of the canonical state Ω_β and does not overlap with a canonical state $\Omega_{\beta'}$ with different temperature. Consider, for example, a state $\tilde{\Omega}_\beta$, whose square root $\tilde{\Omega}_\beta^{1/2}$ is different from $\Omega_\beta^{1/2}$ by a bounded operator K_B (or L_B) as

$$\tilde{\Omega}_\beta^{1/2} = K_B \Omega_\beta^{1/2} K_B^\dagger = L_B \Omega_\beta^{1/2} = \Omega_\beta^{1/2} L_B^\dagger, \quad L_B = K_B \Omega_\beta^{1/2} K_B^\dagger \Omega_\beta^{-1/2} \tag{B.5}$$

with the normalization conditions $\text{tr}_B \tilde{\Omega}_\beta = 1$ and $\text{tr}_B \Omega_\beta = 1$. We again begin with a finite ℓ , so that the overlap between $\tilde{\Omega}_\beta$ and $\Omega_{\beta'}$ now reads

$$\text{tr}_B\{\tilde{\Omega}_\beta^{1/2}\Omega_{\beta'}^{1/2}\} = \text{tr}_B\{L_B \Omega_\beta^{1/2}\Omega_{\beta'}^{1/2}\} = \prod_k \frac{\sqrt{(1 - e^{-\beta\omega_k})(1 - e^{-\beta'\omega_k})}}{1 - e^{-\bar{\beta}\omega_k}} \langle L_B \rangle_{\bar{\beta}}, \tag{B.6}$$

where $\langle L_B \rangle_{\bar{\beta}}$ is the expectation value of L_B in the canonical state at temperature $\bar{\beta}$. Note that $\langle L_B \rangle_{\bar{\beta}}$ is finite even in the continuum limit $\ell \rightarrow \infty$, since L_B is a bounded operator. Therefore, exactly the same argument as (B.4) applies to this case and leads to the conclusion

$$\mathrm{tr}_B\{\tilde{\Omega}_\beta^{1/2}\Omega_{\beta'}^{1/2}\} \rightarrow \begin{cases} \langle L_B \rangle_\beta & (\beta = \beta') \\ 0 & (\beta \neq \beta') \end{cases} \quad \text{as } \ell \rightarrow \infty, \quad (\text{B.7})$$

i.e., $\tilde{\Omega}_\beta$ does not overlap with $\Omega_{\beta'}$ and belongs to the sector equivalent to Ω_β .

Appendix C. Diagonal projection

Let us confirm the property of the diagonal projection in (5.12) with an explicit example. We consider the same model as in Appendix B and observe how the diagonal projection acts on a reservoir state $\tilde{\Omega}_\beta = \Lambda_B \Omega_\beta$, which is different from the canonical state Ω_β at the inverse temperature β only by a bounded superoperator Λ_B , and therefore belongs to the sector equivalent to Ω_β .

We begin with a 1D bosonic gas in a finite box, and then take the continuum limit $\ell \rightarrow \infty$. For a finite ℓ , the diagonal projection \mathcal{P}_D is defined as (5.8) and is given in this case by

$$\mathcal{P}_D \tilde{\Omega}_\beta = \sum_{\{n_k\}} |\{n_k\}\rangle \langle \{n_k\}| \tilde{\Omega}_\beta |\{n_k\}\rangle \langle \{n_k\}|, \quad (\text{C.1})$$

where $|\{n_k\}\rangle = |n_{k_1} n_{k_2} \dots\rangle$, n_k being the occupation number in mode ω_k . To be explicit, let us take a reservoir state

$$\tilde{\Omega}_\beta = \Lambda_B \Omega_\beta = \sum_{k,k'} w_{kk'}^{(\ell)} b_k^{(\ell)\dagger} \Omega_\beta b_{k'}^{(\ell)} = \sum_{k,k'} w_{kk'}^{(\ell)} e^{\beta\omega_{k'}} b_k^{(\ell)\dagger} b_{k'}^{(\ell)} \Omega_\beta \quad (\text{C.2})$$

with a Hermitian ($w_{kk'}^{(\ell)} = w_{k'k}^{(\ell)*}$) positive matrix, and consider the expectation value of a bounded operator of the reservoir

$$Y = \sum_{k,k'} \mathcal{Y}_{kk'}^{(\ell)} b_k^{(\ell)\dagger} b_{k'}^{(\ell)} \quad (\text{C.3})$$

in the projected state $\mathcal{P}_D \tilde{\Omega}_\beta$,

$$\begin{aligned} \mathrm{tr}_B\{Y \mathcal{P}_D \tilde{\Omega}_\beta\} &= \sum_{\{n_k\}} \langle \{n_k\} | Y | \{n_k\} \rangle \langle \{n_k\} | \tilde{\Omega}_\beta | \{n_k\} \rangle \\ &= \sum_{\{n_k\}} \langle \{n_k\} | Y | \{n_k\} \rangle \langle \{n_k\} | L_B | \{n_k\} \rangle \langle \{n_k\} | \Omega_\beta | \{n_k\} \rangle, \end{aligned} \quad (\text{C.4})$$

where $L_B = \sum_{k,k'} w_{kk'}^{(\ell)} e^{\beta\omega_{k'}} b_k^{(\ell)\dagger} b_{k'}^{(\ell)}$ is the bounded operator acting on the left side of Ω_β in (C.2). Note that Ω_β is diagonal with respect to the basis $|\{n_k\}\rangle$ and the diagonal elements are given by

$$\langle \{n_k\} | \Omega_\beta | \{n_k\} \rangle = \frac{1}{Z_\beta} e^{-\beta \sum_k n_k \omega_k} \quad (\text{C.5})$$

with Z_β given in (B.2). The diagonal elements of Y and L_B are easily evaluated to be

$$\langle \{n_k\} | Y | \{n_k\} \rangle = \sum_k \mathcal{Y}_{kk}^{(\ell)} n_k, \quad \langle \{n_k\} | L_B | \{n_k\} \rangle = \sum_k w_{kk}^{(\ell)} e^{\beta\omega_k} n_k, \quad (\text{C.6})$$

respectively, and Eq. (C.4) is

$$\text{tr}_B\{Y\mathcal{P}_D\tilde{\Omega}_\beta\} = \frac{1}{Z_\beta} \sum_{\{n_k\}} \sum_{k,k'} \mathcal{Y}_{kk}^{(\ell)} w_{k'k'}^{(\ell)} e^{\beta\omega_{k'}} n_k n_{k'} e^{-\beta \sum_{k''} n_{k''} \omega_{k''}}. \tag{C.7}$$

Notice here that

$$\langle n_k n_{k'} \rangle_\beta = \frac{1}{Z_\beta} \sum_{\{n_k\}} n_k n_{k'} e^{-\beta \sum_{k''} n_{k''} \omega_{k''}} = \begin{cases} \langle n_k \rangle_\beta \langle n_{k'} \rangle_\beta & (k \neq k') \\ \langle n_k^2 \rangle_\beta & (k = k'), \end{cases} \tag{C.8}$$

where

$$\langle n_k \rangle_\beta = \langle b_k^{(\ell)\dagger} b_k^{(\ell)} \rangle_\beta = \frac{1}{e^{\beta\omega_k} - 1}, \quad \langle n_k^2 \rangle_\beta = \langle (b_k^{(\ell)\dagger} b_k^{(\ell)})^2 \rangle_\beta = 2\langle n_k \rangle_\beta^2 + \langle n_k \rangle_\beta, \tag{C.9}$$

so that Eq. (C.7) is decomposed into two terms,

$$\text{tr}_B\{Y\mathcal{P}_D\tilde{\Omega}_\beta\} = \sum_{k \neq k'} \mathcal{Y}_{kk}^{(\ell)} w_{k'k'}^{(\ell)} e^{\beta\omega_{k'}} \langle n_k \rangle_\beta \langle n_{k'} \rangle_\beta + \sum_k \mathcal{Y}_{kk}^{(\ell)} w_{kk}^{(\ell)} e^{\beta\omega_k} \langle n_k^2 \rangle_\beta. \tag{C.10}$$

We are now in a position to take the continuum limit $\ell \rightarrow \infty$ by recalling the correspondence

$$\sum_k \leftrightarrow \frac{\ell}{2\pi} \int dk, \quad b_k^{(\ell)} \leftrightarrow \sqrt{\frac{2\pi}{\ell}} b_k, \quad \mathcal{Y}_{kk}^{(\ell)} \leftrightarrow \frac{2\pi}{\ell} \mathcal{Y}_{kk}, \quad w_{kk}^{(\ell)} \leftrightarrow \frac{2\pi}{\ell} w_{kk}, \tag{C.11}$$

where b_k and b_k^\dagger satisfy the canonical commutation relation $[b_k, b_{k'}^\dagger] = \delta(k - k')$, and \mathcal{Y}_{kk} and w_{kk} are assumed to be bounded functions. The relevant quantity now becomes

$$\text{tr}_B\{Y\mathcal{P}_D\tilde{\Omega}_\beta\} = \int dk \int dk' \mathcal{Y}_{kk} w_{k'k'} e^{\beta\omega_{k'}} \langle n_k \rangle_\beta \langle n_{k'} \rangle_\beta + \frac{2\pi}{\ell} \int dk \mathcal{Y}_{kk} w_{kk} e^{\beta\omega_k} \langle n_k^2 \rangle_\beta \tag{C.12}$$

for large ℓ , and the second term disappears in the continuum limit $\ell \rightarrow \infty$. We finally obtain

$$\text{tr}_B\{Y\mathcal{P}_D\tilde{\Omega}_\beta\} \rightarrow \langle Y \rangle_\beta \langle L_B \rangle_\beta = \langle Y \rangle_\beta \text{tr}_B \tilde{\Omega}_\beta \quad \text{as } \ell \rightarrow \infty, \tag{C.13}$$

which yields the formula for the diagonal projection,

$$\mathcal{P}_D \tilde{\Omega}_\beta = \Omega_\beta. \tag{C.14}$$

The action of the diagonal projection \mathcal{P}_D on the total system is now readily understood. Consider, for example, a state of the total system

$$\rho = \Lambda(1_S \otimes \Omega_\beta) = \sum_{i,j} \int dk \int dk' w_{ij,kk'} S_i b_k^\dagger (\sigma_S \otimes \Omega_\beta) b_{k'} S_j^\dagger, \tag{C.15}$$

where σ_S is any positive operator of system S, S_i 's are system operators, and Λ is a bounded superoperator acting on $1_S \otimes \Omega_\beta$. Take an operator of the system, A , and an operator of the reservoir, Y given in (C.3). Starting with a finite ℓ , the expectation value of the operator $D = A \otimes Y$ in the projected state $\mathcal{P}_D \rho$ is

$$\begin{aligned} \text{tr}\{D\mathcal{P}_D\rho\} &= \sum_{\{n_k\}} \langle \{n_k\} | Y | \{n_k\} \rangle \langle \{n_k\} | \text{tr}_S\{A\rho\} | \{n_k\} \rangle \\ &= \sum_{i,j} \sum_{k,k'} \text{tr}_S\{A S_i \sigma_S S_j^\dagger\} \mathcal{Y}_{kk}^{(\ell)} w_{ij,kk'}^{(\ell)} e^{\beta\omega_{k'}} \langle n_k n_{k'} \rangle_\beta, \end{aligned} \tag{C.16}$$

which is reduced, in the continuum limit $\ell \rightarrow \infty$, to

$$\begin{aligned} \text{tr}\{D\mathcal{P}_D\rho\} &\rightarrow \sum_{i,j} \int dk \int dk' \text{tr}_S\{AS_i\sigma_S S_j^\dagger\} \mathcal{Y}_{kk} W_{ij,k'k'} e^{\beta\omega_{k'}} \langle n_k \rangle_\beta \langle n_{k'} \rangle_\beta \\ &= \text{tr}_S[A \text{tr}_B\{\Lambda(1_S \otimes \Omega_\beta)\}] \langle Y \rangle_\beta \\ &= \text{tr}[D(\text{tr}_B\{\rho\} \otimes \Omega_\beta)], \end{aligned} \tag{C.17}$$

reproducing (5.12).

Appendix D. Key formulas for the theorem

Here we prove the key formulas (6.13) (with its counterpart for $\tau < 0$, which is necessary in Section 7) and (7.3), and see how the proper choice of the projection \mathcal{P} is crucial.

D.1. The van Hove Limit of $\mathcal{R}_m^{(\lambda)}(\tau)$

Let us analyze the kernel $\mathcal{R}_m^{(\lambda)}(\tau)$, defined in (6.12). In this appendix, the eigenprojection $1_S \otimes \Pi_0$ is written simply as Π_0 .

We start by noting that in van Hove’s limit, for $n > 2$,

$$\lambda^n \mathcal{R}_m^{(\lambda)}(\tau) = \lambda^n \int_0^{\tau/\lambda^2} dt Q e^{(\mathcal{L}'_0 + i\omega_m)t} \rightarrow 0 \quad \text{as } \lambda \rightarrow 0 \quad (n > 2), \tag{D.1}$$

irrespectively of the spectrum of \mathcal{L}'_0 .

Second, the following observation will be important: the convolution

$$\int_0^t dt' e^{\mathcal{L}_0(t-t')} Q \mathcal{L}_{SB} Q e^{\mathcal{L}'_0 t} \tag{D.2}$$

is bounded for any t , provided the point spectrum of \mathcal{L}_0 is removed by the projection $Q = 1 - \mathcal{P}$ with $\mathcal{P} = \Pi_0$. Let us look at the Laplace transform of this convolution (for $t > 0$),

$$\frac{1}{s - \mathcal{L}_0} Q \mathcal{L}_{SB} Q \frac{1}{s - \mathcal{L}'_0}. \tag{D.3}$$

Neither $1/(s - \mathcal{L}_0)$ nor $1/(s - \mathcal{L}'_0)$ has a singularity on the right half plane $\text{Re}s > 0$. If \mathcal{L}_0 and \mathcal{L}'_0 have common eigenvalues (along the imaginary axis $\text{Re}s = 0$) that are not projected out, these would give second order poles and yield linearly diverging functions of t (for large t) after the inverse Laplace transform; otherwise, the convolution decays or just oscillates. On the other hand, if the point spectrum of \mathcal{L}_0 is removed by the projection Q , such a coincidence between the point spectra does not happen and the convolution (D.2) is bounded for $t \rightarrow \infty$, irrespectively of the point spectrum of \mathcal{L}'_0 .

Now by using

$$e^{\mathcal{L}'_0 t} = e^{\mathcal{L}_0 t} + \lambda \int_0^t dt' e^{\mathcal{L}_0(t-t')} Q \mathcal{L}_{SB} Q e^{\mathcal{L}'_0 t'}, \tag{D.4}$$

we expand the relevant quantity (6.12) as

$$\mathcal{R}_m^{(\lambda)}(\tau) = \int_0^{\tau/\lambda^2} dt \mathcal{Q}e^{(\mathcal{L}_0+i\omega_m)t} + \lambda \int_0^{\tau/\lambda^2} dt \int_0^t dt' e^{(\mathcal{L}_0+i\omega_m)t} e^{-\mathcal{L}_0 t'} \mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{Q}e^{\mathcal{L}'_0 t'}. \tag{D.5}$$

The first term is decomposed into two parts by the projections Π_0 and $\Pi_c = 1 - \Pi_0$, and the integrations are easily carried out to give (for $\tau > 0$)

$$\begin{aligned} \int_0^{\tau/\lambda^2} dt \mathcal{Q}e^{(\mathcal{L}_0+i\omega_m)t} &= \int_0^{\tau/\lambda^2} dt \mathcal{Q}\Pi_0 e^{(\mathcal{L}_0+i\omega_m)t} + \int_0^{\tau/\lambda^2} dt \mathcal{Q}\Pi_c e^{(\mathcal{L}_0+i\omega_m)t} \\ &= \sum_n \int_0^{\tau/\lambda^2} dt \mathcal{Q}\Pi_0 \tilde{\mathcal{Q}}_n e^{i(\omega_m-\omega_n)t} + \mathcal{Q}\Pi_c \frac{e^{(\mathcal{L}_0+i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+} \\ &= \frac{\tau}{\lambda^2} \mathcal{Q}\Pi_0 \tilde{\mathcal{Q}}_m + \sum_{n \neq m} \mathcal{Q}\Pi_0 \tilde{\mathcal{Q}}_n \frac{e^{i(\omega_m-\omega_n)\tau/\lambda^2} - 1}{i(\omega_m - \omega_n)} \\ &\quad + \mathcal{Q}\Pi_c \frac{e^{(\mathcal{L}_0+i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+}, \end{aligned} \tag{D.6}$$

which shows that the only possible divergence of the relevant operator in (6.12) in van Hove’s limit $\lambda \rightarrow 0$ stems from the point spectrum of \mathcal{L}_0 (i.e. the first term of the last expression). This divergence results in the divergences of both the memory kernel $\mathcal{K}_{mm}^{(\lambda)}(\tau)$ and the initial correlation $\mathcal{I}^{(\lambda)}(\tau)$. However, if $\mathcal{P} = \Pi_0$, the divergent term disappears due to $\mathcal{Q}\Pi_0 = 0$, and we have (for $\tau > 0$)

$$\int_0^{\tau/\lambda^2} dt \mathcal{Q}e^{(\mathcal{L}_0+i\omega_m)t} = \mathcal{Q} \frac{e^{(\mathcal{L}_0+i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+} \rightarrow -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \quad \text{as } \lambda \rightarrow 0, \tag{D.7}$$

by noting the formula

$$\lim_{t \rightarrow \pm\infty} \Pi_c \frac{e^{(\mathcal{L}_0+i\omega_m)t}}{\mathcal{L}_0 + i\omega_m \mp 0^+} = 0, \tag{D.8}$$

which is valid in the sense of distributions. The second term in (D.5) can be manipulated to yield

$$\begin{aligned} &\lambda \int_0^{\tau/\lambda^2} dt \int_0^t dt' e^{(\mathcal{L}_0+i\omega_m)t} e^{-\mathcal{L}_0 t'} \mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{Q}e^{\mathcal{L}'_0 t'} \\ &= \lambda \int_0^{\tau/\lambda^2} dt' \int_{t'}^{\tau/\lambda^2} dt e^{(\mathcal{L}_0+i\omega_m)t} e^{-\mathcal{L}_0 t'} \mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{Q}e^{\mathcal{L}'_0 t'} \\ &= \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} e^{i\omega_m \tau/\lambda^2} \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2-t)} \mathcal{Q}\mathcal{L}_{\text{SB}}\mathcal{Q}e^{\mathcal{L}'_0 t} \\ &\quad - \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \int_0^{\tau/\lambda^2} dt \mathcal{Q}e^{(\mathcal{L}'_0+i\omega_m)t}. \end{aligned} \tag{D.9}$$

The integral in the first term is the convolution (D.2). Since the point spectrum of \mathcal{L}_0 is removed by the projection \mathcal{Q} , this convolution is bounded for $\tau/\lambda^2 \rightarrow \infty$. In summary, with the choice of the projection $\mathcal{P} = \Pi_0$, Eq. (D.5) is arranged into the recurrence formula

$$\begin{aligned} \mathcal{R}_m^{(\lambda)}(\tau) &= \mathcal{Q} \frac{e^{(\mathcal{L}_0 + i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+} \\ &\quad + \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} e^{i\omega_m\tau/\lambda^2} \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2 - t)} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t} \\ &\quad - \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \quad (\tau > 0), \end{aligned} \tag{D.10}$$

where the first term converges to (D.7) and the second term vanishes in van Hove’s limit. Therefore, by iterating the above expansion twice, we arrive at

$$\begin{aligned} \lim_{\lambda \rightarrow 0} \mathcal{R}_m^{(\lambda)}(\tau) &= -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} - \left(\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \right)^3 \lim_{\lambda \rightarrow 0} \lambda^3 \mathcal{R}_m^{(\lambda)}(\tau) \\ &= -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \quad (\tau > 0), \end{aligned} \tag{D.11}$$

which is Eq. (6.13) of the text.

A similar argument applies to the case $\tau < 0$ to yield

$$\begin{aligned} \mathcal{R}_m^{(\lambda)}(\tau) &= \mathcal{Q} \frac{e^{(\mathcal{L}_0 + i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m + 0^+} \\ &\quad + \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m + 0^+} e^{i\omega_m\tau/\lambda^2} \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2 - t)} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t} \\ &\quad - \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m + 0^+} \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \quad (\tau < 0), \end{aligned} \tag{D.12}$$

and

$$\lim_{\lambda \rightarrow 0} \mathcal{R}_m^{(\lambda)}(\tau) = -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m + 0^+} \quad (\tau < 0). \tag{D.13}$$

D.2. The van Hove Limit of $\mathcal{Q}e^{\mathcal{L}'_0\tau/\lambda^2}$

Using the expansion (D.4), we have

$$\mathcal{Q}e^{\mathcal{L}'_0\tau/\lambda^2} = \mathcal{Q}e^{\mathcal{L}_0\tau/\lambda^2} + \lambda \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2 - t)} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t}. \tag{D.14}$$

The convolution in the second term is the same as that discussed in (D.2), which is bounded for any τ and λ , provided the projection \mathcal{P} is the eigenprojection Π_0 , and hence the second term vanishes in van Hove’s limit $\lambda \rightarrow 0$. Since the right projection $\mathcal{Q} = 1 - \Pi_0$ removes the point spectrum of \mathcal{L}_0 , the first term disappears as $\tau/\lambda^2 \rightarrow \infty$ due to Riemann–Lebesgue’s lemma. Therefore, $\mathcal{Q}e^{\mathcal{L}'_0\tau/\lambda^2}$ decays in van Hove’s limit, yielding (7.3).

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