



## DOCTOR OF PHILOSOPHY

### Simulation, characterisation and control of open quantum systems dynamics

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# **Simulation, characterisation and control of open quantum systems dynamics**

Thesis submitted for the degree of

*Doctor of Philosophy*

in the

Faculty of Engineering and Physical Sciences

by

**Giorgio Zicari**

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# Abstract

In this Thesis, we discuss aspects of the simulation, characterisation, and control of the dynamics of open quantum systems. The latter are systems governed by quantum mechanical laws and interacting with an environment, which is typically much larger than the system itself. According to the standard approach, one is usually able to perform a suitable average over the environmental degrees of freedom, resulting in an effective description of the main system dynamics, which accounts for the effects of the interaction with the surroundings. In standard scenarios, usually studied within the so-called Born-Markov approximation, the system-environment coupling is weak and such that we can perform a neat separation of timescales: the environmental dynamics is assumed to be fast compared to the typical evolution timescale of the system of interest. However, nowadays we are able to inspect physical scenarios where the usual Born-Markov approximation breaks down: the interaction between system and environment can be strong, likely leading to non-negligible memory (non-Markovian) effects.

In this work, we discuss some instances in which we cannot work in the standard Born-Markov regime. We introduce and analyse some numerical and analytical techniques to characterise and simulate non-standard scenarios. We show that, even in the Markovian regime, the traditional formulation of thermodynamic irreversibility shows flaws and inconsistencies. We thus use phase-space methods to assess the role of initial correlations shared by the two parties of a bipartite harmonic system in the entropy production rate, including non-Markovian effects. Furthermore, we show that certain interactions enable to redraw the boundaries between the system and the environment in an effective manner, resulting in a new picture where the system degrees of freedom are augmented, while the residual environment is rearranged in such a way that the Born-Markov approximation is recovered. This analytical technique, known as reaction coordinate mapping approach, is employed in this work to show that, upon an accurate choice of the parameter regime, a spin-boson model can serve as a quantum analogue simulator of non-Markovian multiphoton Jaynes-Cummings models. These systematic studies shed light on the thermodynamic characterisation of open quantum systems, as well as on their numerical simulation.

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# List of Acronyms

<b>CM</b>	Covariance Matrix
<b>CP</b>	Completely Positive
<b>CPTP</b>	Completely Positive and Trace Preserving
<b>CV</b>	Continuous Variables
<b>GKSL</b>	Gorini Kossakowski Sudarshan Lindblad
<b>GLEMS</b>	Gaussian Least Entangled Mixed States
<b>GMEMS</b>	Gaussian Maximally Entangled Mixed States
<b>HEOM</b>	Hierarchical Equations Of Motion
<b>JCM</b>	Jaynes Cummings Model
<b>KMS</b>	Kubo Martin Schwinger
<b>NZ</b>	Nakajiima Zwanzig
<b>PPT</b>	Positive Partial Transpose
<b>QRM</b>	Quantum Rabi Model
<b>RC</b>	Reaction Coordinate
<b>RHP</b>	Rivas Huelga Plenio
<b>SD</b>	Spectral Density
<b>TCL</b>	Time Convolutionless

# List of publications

- [1] Ricardo Puebla, Giorgio Zicari, Iñigo Arranzola, Enrique Solano, Mauro Paternostro, and Jorge Casanova. “Spin-boson model as a simulator of non-Markovian multiphoton Jaynes-Cummings models”. In *Symmetry* **11** (5), 695. DOI: [10.3390/sym11050695](https://doi.org/10.3390/sym11050695). arXiv: [1904.07037 \[quant-ph\]](https://arxiv.org/abs/1904.07037) (2019).
- [2] Giorgio Zicari, Matteo Brunelli, and Mauro Paternostro. “Assessing the role of initial correlations in the entropy production rate for nonequilibrium harmonic dynamics”. In *Physical Review Research* **2**, 043006. DOI: [10.1103/PhysRevResearch.2.04300](https://doi.org/10.1103/PhysRevResearch.2.04300). arXiv: [2004.10726 \[quant-ph\]](https://arxiv.org/abs/2004.10726) (2020).

# Chapter 1

## Introduction

The traditional presentation of quantum mechanics delivers a picture in which dynamical systems are usually regarded as perfectly isolated from their surroundings, and whose time evolutions are governed by the Schrödinger equation — or equivalent versions thereof. Historically, this approach to the study of physical phenomena, albeit simplified, has been responsible for unprecedented progress – both theoretical and experimental – in the understanding of physical reality. However, it is clear that a closed system is a rather crude approximation: more realistically, quantum systems are open, as they undergo the influence of the environment interacting with them. According to this picture, systems governed by quantum-mechanical laws always appear *prima facie* as many-body systems. This opens up a plethora of questions regarding their characterisation, control, and numerical simulation.

In the last decades, open quantum systems have been deeply investigated within an elegant and powerful paradigm, in which the features of the main system emerge after carefully discarding the infinitely many environmental degrees of freedom (Breuer, 2002). The latter procedure dramatically simplifies the problem: the influence of the surroundings on the main system dynamics is automatically taken into account by the dynamical equations in an effective manner. Such formalism is indeed able to capture the effect of the environment without the need of explicitly accessing it, an operation that would be formidable in some cases, but impossible in the vast majority of them. Besides, this theoretical picture is corroborated by our ability to experimentally exercise control only over a limited part of a quantum system.

The theory of open quantum systems was consistently formulated back in the 1970s by eminent scholars such as Davies, Gorini, Kossakowski, Spohn, Sudarshan, and Lindblad, among others (Chruściński, 2017). Such efforts led to the notion of *quantum dynamical semigroup*, which relies on a set of physically reasonable assumptions such as the weak coupling between the system and the environment, and a Markovian (memoryless) description of the dynamics in terms of completely positive maps. This formal apparatus, although restrictive, encompasses several interesting cases, and constitutes hitherto a reference scheme

in the theory of open quantum systems. Physical phenomena of relaxation and dissipation are naturally epitomised by this framework, as well as the genuine quantum phenomenon of *decoherence* (Zurek, 2003). In this context, one can also study the thermodynamics of quantum processes. At a fundamental level, the latter provides the natural language to phrase the problem of irreversibility that is unavoidably entailed by the coupling of a system with an environment. Such progress is not just relevant *per se*, but has also significantly contributed to design and control several experimental platforms, mostly in quantum linear optics scenarios (Scully, 1997). Over the last few decades, we have witnessed rapid advances in the ability of controlling and manipulating systems at microscopic scales, in a wider class of physical settings, ranging, e.g., from solid state devices to quantum biology (Huelga, 2013; de Vega, 2017). There are indeed novel scenarios where decoherence and dissipation occur. In many of them, the system-environment interaction typically goes beyond standard approximations, leading to previously inaccessible regimes, where memory and strong coupling effects are brought about. Furthermore, the so-called second quantum revolution has been boosting the interest towards such non-standard regimes, driven by potential technological applications (MacFarlane, 2003; Binder, 2018).

In this Thesis, we investigate issues commonly encountered in the study of open quantum systems, whenever one challenges the standard Born-Markov approximation. In these scenarios, we do not always obtain dynamical equations – known as master equations – in the so-called Lindblad form; under certain conditions, we can obtain equations that might be non-local in time. There are general techniques to derive master equations in such cases, often referred as projection operators techniques (Breuer, 2002). As, frequently, analytical solutions are not available, one has to resort to several simulation methods that have been put forth over the last few decades, depending on the specific physical regime of interest. Some of them are said to be numerically exact, in the sense that they only require numerical approximations — e.g., Hilbert space truncation. Examples of these methods are the hierarchical equations of motion (HEOM) (Tanimura, 1989) or the time-evolving density operator with orthogonal polynomials algorithm (TEDOPA) (Prior, 2010; Tamaselli, 2019). In some other approaches, the system-environment interaction is remapped in such a way that the system of interest is explicitly coupled to one or more auxiliary systems encoding the strong coupling and/or memory effects, while dissipation is modelled through a Markovian damping undergone by these auxiliary degrees of freedom. This is essentially the underpinning idea of the so-called pseudo-mode approach (Garraway, 1997; Dalton, 2001), or the reaction coordinate mapping (Garg, 1985; Martinazzo, 2011). The latter will be specifically employed in this work to show that a spin-boson model can serve to simulate multiphoton interactions. Nonetheless, the limitations of the traditional formulation of open quantum systems do not necessarily emerge when we push the dynamics beyond the Born-Markov regime. For instance, in this Thesis we discuss the drawbacks of the traditional formulation of the entropy production in terms of von Neumann entropy. These difficulties can be overcome by using phase-space methods borrowed from quantum optics (Santos, 2017; Landi, 2020). In particular, we will use this alternative formulation of the entropy production to show that quantum correlations initially shared by two parties of a given system affect the overall entropy production rate.

# Outline of the thesis

This Thesis is organised as follows. In [Chapter 2](#) we introduce the mathematical notation used throughout the Thesis, as well as the relevant notions of linear maps and their representation. Particular emphasis is given to completely positive maps and entanglement, and their respective characterisation. In [Chapter 3](#), we introduce quantum dynamical maps; we unveil the relation between the latter and the open systems dynamical equations, namely master equations. The formal construction of the so-called quantum dynamical semigroup is followed by [Chapter 4](#), where, resorting to projection operators techniques, we provide an overview about the microscopic derivation of quantum master equations. The considerations presented are rather general and they apply either to a Markovian or a non-Markovian description of the dynamics. We introduce some notions used to define, characterise, and measure non-Markovianity; likewise we discuss the assumptions that lead to the Born-Markov approximation. In [Chapter 5](#), we provide some notions for thermodynamically characterising open quantum systems. We discuss the theory of open quantum systems in terms of von-Neumann entropy, stressing on the role played by quantum coherences. After highlighting the inconsistencies and limitations of this approach, we introduce a theory of the irreversibility based on phase space-methods, and Wigner (or, equivalently, Rényi-2) entropy. We make use of this formalism to claim that, in a system of two harmonic oscillators undergoing a non-Markovian dynamics, initial correlations shared by the two parties play a role in the entropy production rate. In [Chapter 6](#) we discuss the details of the reaction coordinate mapping approach, and we apply it to the paradigmatic case of the spin-boson model. The mapping is thereupon used to show that the spin-boson model, with a suitable choice of the parameters, can serve as an analogue quantum simulator of non-Markovian multiphoton Jaynes-Cummings models. In [Chapter 7](#), we summarise the contents of the Thesis and our main findings, and we briefly comment on possible directions to pursue in future.

# Chapter 2

## Mathematical Prelude

Since the early days of quantum mechanics, a crucial issue has been to provide a consistent mathematical framework of the theory (von Neumann, 1955). On a similar note, the first question one needs to address writing about quantum mechanics is: how much mathematics do we actually need? Having this question in mind, in this Chapter, we will review some relevant mathematical concepts, whose importance is twofold: one hand, they are preparatory for what we will discuss in the next Chapters; on the other hand, they help us to fix the notation. The synthesis presented in this Chapter is mainly inspired by Refs. (Heinosaari, 2011; Smirne, 2012)

### 2.1 Trace-class operators

Let us consider a separable Hilbert space  $\mathcal{H}$ , where, for any pair of ket  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ , we will denote the scalar product as  $\langle\phi|\psi\rangle$ , while the induced norm is given by  $\|\psi\| \equiv \sqrt{\langle\psi|\psi\rangle}$ . The set of all linear operators defined on  $\mathcal{H}$  is  $\mathfrak{L}(\mathcal{H})$ . An operator  $A \in \mathfrak{L}(\mathcal{H})$  is bounded if the operator norm

$$\|A\| \equiv \sup_{\|\psi\|=1} \|A|\psi\rangle\| \quad (2.1)$$

is finite (Teschl, 2014). We will denote as  $\mathfrak{B}(\mathcal{H})$  the space of all bounded operators defined on  $\mathcal{H}$ .

Let us consider an operator  $A \in \mathfrak{B}(\mathcal{H})$  and an orthonormal basis  $\{|\varphi_k\rangle\}_{k=0}^{\infty} \subset \mathcal{H}$ , the trace of the operator  $A$  is defined as

$$\text{Tr}(A) = \sum_{k=1}^{\infty} \langle\varphi_k| A |\varphi_k\rangle. \quad (2.2)$$

In the general (infinite-dimensional) case, it is not guaranteed that the latter quantity is finite and independent of the chosen basis. However, if we assume that  $A$  is a positive operator,

i.e.,  $\langle \psi | A | \psi \rangle \geq 0$ , for any  $|\psi\rangle \in \mathcal{H}$ , it is not difficult to show that the quantity defined by [Equation \(2.2\)](#) is independent of the choice of the specific orthonormal basis  $\{|\varphi_k\rangle\}_{k=0}^\infty$  in  $\mathcal{H}$ . To this end, let us suppose that  $\{|\psi_j\rangle\}_{j=0}^\infty$  is another orthonormal basis for  $\mathcal{H}$ ; it is immediate to see that

$$\begin{aligned}\text{Tr}(A) &= \sum_{k=1}^{\infty} \langle \varphi_k | A | \varphi_k \rangle = \sum_{k=1}^{\infty} \|A^{1/2} |\varphi_k\rangle\|^2 = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} |\langle \psi_j | A^{1/2} |\varphi_k\rangle|^2 \\ &= \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} |\langle \varphi_k | A^{1/2} |\psi_j\rangle|^2 = \sum_{j=1}^{\infty} \|A^{1/2} |\psi_j\rangle\|^2 = \sum_{j=1}^{\infty} \langle \psi_j | A | \psi_j \rangle,\end{aligned}\quad (2.3)$$

where, since all the terms are non-negative, we have interchanged the order of the two sums, and we have used the so-called Parseval identity twice ([Reed, 1980](#))<sup>1</sup>.

Given three positive operators  $A, B, C \in \mathfrak{B}(\mathcal{H})$ , and  $\alpha, \beta \in \mathbb{R}$ , the following properties holds:

- linearity, i.e.,

$$\text{Tr}(\alpha A + \beta B) = \alpha \text{Tr}(A) + \beta \text{Tr}(B); \quad (2.4)$$

- invariance under cyclic permutations, i.e.,

$$\text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA). \quad (2.5)$$

In particular, if  $U$  is a unitary operator, i.e.,  $U^\dagger U = UU^\dagger = \mathbb{I}$ , one has

$$\text{Tr}(U^\dagger AU) = \text{Tr}(UAU^\dagger) = \text{Tr}(A). \quad (2.6)$$

We should notice that, on the right hand side of [Equation \(2.2\)](#), we have an infinite sum of non-negative terms: it might be the case that the latter does not converge. Therefore, we should define a proper subset of operators such that the sum given in [Equation \(2.2\)](#) is finite.

In general, given a (not necessarily positive) operator  $A \in \mathfrak{B}(\mathcal{H})$ , we can construct the positive operator  $|A| \equiv \sqrt{A^\dagger A}$ ; if  $\text{Tr}|A| < \infty$ ,  $A$  is said to be a *trace-class* operator. We will denote by  $\mathfrak{B}_1(\mathcal{H}) \subseteq \mathfrak{B}(\mathcal{H})$  the set of all trace-class operators defined over the space  $\mathcal{H}$ .

Moreover,  $\mathfrak{B}_1(\mathcal{H})$  is a Banach space with respect to the norm

$$\|A\|_1 \equiv \text{Tr}|A| = \text{Tr}\sqrt{A^\dagger A}, \quad A \in \mathfrak{B}_1(\mathcal{H}), \quad (2.7)$$

known as *trace norm*.

The space  $\mathfrak{B}_1(\mathcal{H})$  is not only a linear subspace of  $\mathfrak{B}(\mathcal{H})$ , but also a *two-sided ideal* in the Banach algebra of bounded operators on  $\mathcal{H}$  ([Heinosaari, 2011](#)), essentially meaning that, even

---

<sup>1</sup>Note that the existence and uniqueness of the square root of the operator  $A$  is guaranteed by the assumption of being positive and bounded. In what follows, these assumptions are automatically satisfied, as we will deal with trace-class operators. ([Heinosaari, 2011](#))

if  $\text{Tr}(B)$  is not well-defined (in the aforementioned sense) for an operator  $B \in \mathfrak{B}(\mathcal{H})$ , the operators  $AB$  and  $BA$  still belong to  $\mathfrak{B}_1(\mathcal{H})$ , provided that  $A$  is a trace-class operator.

There is actually a deeper connection between  $\mathfrak{B}(\mathcal{H})$  and  $\mathfrak{B}_1(\mathcal{H})$ :  $\mathfrak{B}(\mathcal{H})$  is the dual space of  $\mathfrak{B}_1(\mathcal{H})$ , i.e.,  $\mathfrak{B}_1^*(\mathcal{H}) = \mathfrak{B}(\mathcal{H})$ . The duality between these two spaces can be expressed by saying that, for any operator  $B \in \mathfrak{B}_1(\mathcal{H})$ , we can construct the linear functional  $\Psi_B$  such that<sup>2</sup>:

$$\begin{aligned}\Psi_B : \mathfrak{B}(\mathcal{H}) &\rightarrow \mathbb{C} \\ A &\mapsto \Psi_B(A) \equiv \text{Tr}(AB).\end{aligned}\tag{2.8}$$

Note that the definition above is well-posed:  $\mathfrak{B}_1(\mathcal{H})$  is an ideal, therefore  $\text{Tr}(AB)$  is finite and basis-independent. Besides, the following inequality holds:

$$|\text{Tr}(AB)| \leq \|A\| \|B\|_1,\tag{2.9}$$

with  $A \in \mathfrak{B}(\mathcal{H}), B \in \mathfrak{B}_1(\mathcal{H})$ .

Let us consider a bounded operator  $A$ ; as we have done in [Equation \(2.3\)](#), it is not difficult to show that the quantity  $\sum_{k=1}^{\infty} \langle \varphi_k | A^\dagger A | \varphi_k \rangle$  is basis-independent. If the latter is also finite, then  $A$  is a *Hilbert-Schmidt operator*. The set  $\mathfrak{B}_2(\mathcal{H})$  of all Hilbert-Schmidt operators on  $\mathcal{H}$  is a Banach space with respect to the *Hilbert-Schmidt norm*

$$\|A\|_2 \equiv \sqrt{\text{Tr}(A^\dagger A)}, \quad A \in \mathfrak{B}_2(\mathcal{H}).\tag{2.10}$$

In addition to that,  $\mathfrak{B}_2(\mathcal{H})$  is a Hilbert space, on which it is defined the so-called *Hilbert-Schmidt inner product*

$$\langle A, B \rangle_{\text{HS}} \equiv \text{Tr}(A^\dagger B),\tag{2.11}$$

where  $A, B \in \mathfrak{B}_2(\mathcal{H})$ .

The space  $\mathfrak{B}_2(\mathcal{H})$  is also a two-sided ideal of  $\mathfrak{B}(\mathcal{H})$ , in the sense that, given  $A \in \mathfrak{B}_2(\mathcal{H})$  and  $B \in \mathfrak{B}(\mathcal{H})$ , the operators  $AB, BA$  belong to the Hilbert-Schmidt class.

Let us suppose that  $A$  is self-adjoint trace-class operator  $A$ ; the three different norms that we have defined above can be straightforwardly calculated, once one knows the eigenvalues  $\{\lambda_k\}_k$  of  $A$ . Indeed, one has ([Heinosaari, 2011](#)):

$$\|A\| = \max_k \{|\lambda_k|\}, \quad \|A\|_1 = \sum_k |\lambda_k|, \quad \|A\|_2 = \sqrt{\sum_k |\lambda_k|^2}.\tag{2.12}$$

One may verify that

$$\|A\| \leq \|A\|_2 \leq \|A\|_1,\tag{2.13}$$

---

<sup>2</sup>Strictly speaking, it is a isometric isomorphism ([Conway, 1985](#)).

which holds also for non-self-adjoint trace-class operators. From [Equation \(2.13\)](#), we get that

$$\mathfrak{B}(\mathcal{H}) \subseteq \mathfrak{B}_2(\mathcal{H}) \subseteq \mathfrak{B}_1(\mathcal{H}). \quad (2.14)$$

Note that, in the finite-dimensional case, all the three norms are equivalent, therefore the equal sign holds in [Equation \(2.14\)](#).

#### Example 2.1.1: Trace of a finite-dimensional operator

Let us consider the finite-dimensional case, i.e.,  $\mathcal{H} \cong \mathbb{C}^d$ . Under this hypothesis, the trace an operator is always a meaningful quantity, as it is always basis-independent and a real number.

[Equation \(2.2\)](#) tells us that the trace of an operator  $A \in \mathfrak{B}(\mathbb{C}^d)$  can be obtained by writing  $A$  as a  $d \times d$  matrix, i.e.,  $A \in \mathcal{M}_d(\mathbb{C})$ , in some orthonormal basis  $\{|\varphi_k\rangle\}_{1 \leq k \leq d}$ , then summing up all its diagonal entries.

Besides, we know from linear algebra that  $\text{Tr}(A)$  is also given by the sum of the eigenvalues of  $A$ . Let us consider a diagonalisable operator  $A$ ; this means that there exists an invertible matrix  $P \in \mathcal{M}_d(\mathbb{C})$  such that  $P^{-1}AP = D$ , where  $D$  is a diagonal matrix, i.e.,  $D = \text{diag}(\lambda_1, \dots, \lambda_d)$ . Therefore, using property [\(2.5\)](#), one easily gets

$$\text{Tr}(A) = \text{Tr}(P^{-1}AP) = \text{Tr}(D) = \sum_{k=1}^d \lambda_k. \quad (2.15)$$

Note that, in general, we need to sum all eigenvalues of  $A$ , counting their multiplicity. It is also immediate to calculate the trace norm of  $A$

$$\|A\|_2 = \sqrt{\sum_{k=1}^d |\lambda_k|^2}. \quad (2.16)$$

## 2.2 Statistical operators

In the standard presentation of quantum mechanics, a physical system is associated to a separable Hilbert space  $\mathcal{H}$  ([Teschl, 2014](#)). The ket  $|\psi\rangle \in \mathcal{H}$  is said to be a state if it is normalised to one, i.e.,  $\|\psi\| = 1$ .

Alternatively, we can express quantum states in terms of *statistical* (or *density*) *operators*. In order to be representative of a certain quantum state, a linear operator  $\rho$  should fulfil the following requirements:

- (i) self-adjointness, i.e.,  $\rho^\dagger = \rho$ ;
- (ii) semi-positiveness<sup>3</sup>, i.e.,  $\langle \psi | \rho | \psi \rangle \geq 0$ , for all  $|\psi\rangle \in \mathcal{H}$ ;

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<sup>3</sup>For the sake of conciseness, we will often say that  $\rho$  is positive.

(iii)  $\mathrm{Tr} \rho = 1$ .

If the conditions (i),(ii),(iii) are met, then  $\rho$  is a statistical (or density) operator.

We can thus introduce the *set of statistical operators*

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathfrak{B}_1(\mathcal{H}) \mid \rho^\dagger = \rho, \rho \geq 0, \mathrm{Tr} \rho = 1\}. \quad (2.17)$$

The set  $\mathcal{S}(\mathcal{H})$  is convex, in the sense that any convex combination of elements of  $\mathcal{S}(\mathcal{H})$  still belongs to the set, i.e., given a set of statistical operators  $\{\rho_i\}_{i=1}^n \subset \mathcal{S}(\mathcal{H})$ , the linear combination

$$\sum_{i=1}^n \lambda_i \rho_i \in \mathcal{S}(\mathcal{H}), \quad (2.18)$$

where  $\lambda_i \geq 0$ , for  $i = 1, \dots, n$ , and  $\sum_i \lambda_i = 1$ . By rearranging [Equation \(2.18\)](#), i.e., by writing  $\sum_{i=1}^n \lambda_i \rho_i = \lambda_1 \rho_1 + (1 - \lambda_1) \left( \frac{\lambda_2}{1 - \lambda_1} \rho_2 + \dots + \frac{\lambda_n}{1 - \lambda_1} \rho_n \right)$ , it is not difficult to see that we can indeed consider mixtures of two elements only, i.e., the combination

$$\lambda \rho_1 + (1 - \lambda) \rho_2 \in \mathcal{S}(\mathcal{H}), \quad (2.19)$$

where  $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ , and  $0 \leq \lambda \leq 1$ . According to the general terminology of convex sets, an element  $\rho$  is said to be *extremal* if it cannot be written as in [Equation \(2.19\)](#) (with  $0 < \lambda < 1$ ), thus  $\rho_1 = \rho_2 = \rho$ . We label as *trivial* those decomposition for which  $\rho_1 = \rho_2$ . In particular, any extremal element of the convex set  $\mathcal{S}(\mathcal{H})$  is called a *pure state*, while any other element of  $\mathcal{S}(\mathcal{H})$  is a *mixed state*. Note that a mixed state has uncountably many (non-trivial) convex decompositions.

Among all possible combinations, we will consider a specific form, the so-called *canonical convex decomposition* for a statistical operator  $\rho \in \mathcal{S}(\mathcal{H})$ , according to which  $\rho$  reads as a linear combination of one-dimensional projectors, i.e.,

$$\rho = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k|, \quad (2.20)$$

where  $\lambda_k \geq 0$  are the eigenvalues of  $\rho$ , such that  $\sum_k \lambda_k = 1$ , and  $|\psi_k\rangle$  the corresponding eigenstates. We should stress again that the canonical decomposition [\(2.20\)](#) always exists, but it is unique only when the eigenvalues  $\lambda_k$  are all different.

### 2.2.1 Purity

In this Section, we would like to introduce a useful mathematical characterisation of pure states. Let us first observe that if  $\rho \in \mathcal{S}(\mathcal{H})$ , then  $\rho^2$  is a positive trace-class operator and  $\mathrm{Tr} \rho^2 \geq 0$ . By using [Equations \(2.9\)](#) and [\(2.13\)](#), one easily obtains that  $\mathrm{Tr} \rho^2 \leq \|\rho\| \mathrm{Tr} \rho = \|\rho\| \leq \mathrm{Tr} \rho = 1$ , therefore we obtain the following bound:

$$0 \leq \mathrm{Tr} \rho^2 \leq 1. \quad (2.21)$$

Now, we would like to show that the following three conditions are equivalent ([Heinosaari, 2011](#)):

- (i)  $\rho$  is a pure state;
- (ii)  $\rho$  is a one-dimensional projector;
- (iii)  $\text{Tr } \rho^2 = 1$ .

Let us first prove that (i)  $\implies$  (ii). If we assume that the state  $\rho$  is expressed according to the orthogonal decomposition (2.20), it immediate to conclude that, being  $\rho$  extremal by definition, it must be in the form  $\rho = \lambda_1 |\psi_1\rangle\langle\psi_1|$ . Moreover, since  $\rho$  has unit trace, it follows that  $\lambda_1 = 1$ , hence  $\rho = |\psi_1\rangle\langle\psi_1|$ , i.e., a one-dimensional projector.

It is trivial to prove that (ii)  $\implies$  (iii). A projector is idempotent, i.e.,  $\rho^2 = \rho$ , therefore  $\text{Tr } \rho^2 = \text{Tr } \rho = 1$ .

We also need to prove that (iii)  $\implies$  (i). Let us assume that the one-dimensional projector  $\rho$  can be decomposed as  $|\psi\rangle\langle\psi| = \lambda\rho_1 + (1 - \lambda)\rho_2$ , for some  $0 < \lambda < 1$ . Thus

$$\begin{aligned} 1 &= \text{Tr } \rho^2 = \lambda^2 \text{Tr } \rho_1^2 + (1 - \lambda)^2 \text{Tr } \rho_2^2 + 2\lambda(1 - \lambda) \text{Tr}(\rho_1\rho_2) \leq \lambda^2 \\ &\quad + (1 - \lambda)^2 + 2\lambda(1 - \lambda)|\text{Tr}(\rho_1\rho_2)| \leq 1, \end{aligned} \tag{2.22}$$

where we have used the Cauchy-Schwarz inequality, i.e.,  $|\text{Tr}(\rho_1\rho_2)| \leq \sqrt{\text{Tr } \rho_1^2} \sqrt{\text{Tr } \rho_2^2}$ . Since we have obtained 1 at the end and at the beginning, [Equation \(2.22\)](#) reduces to a chain of identities, and  $|\text{Tr}(\rho_1\rho_2)| = 1$ . This also means that the Cauchy-Schwarz inequality is saturated, hence  $\rho_1 = c\rho_2$  for some constant  $c \in \mathbb{C}$ . However,  $\text{Tr } \rho_1 = 1 = \text{Tr } \rho_2$ , thus  $c = 1$ , which means that the convex decomposition of  $\rho$  is trivial.

This characterisation not only introduces a way to identify pure states, but also to quantify the degree of mixedness for non-pure states. It naturally leads to the the definition of purity  $\mathcal{P}(\rho)$  of the state  $\rho$ :

$$\mathcal{P}(\rho) \equiv \text{Tr } \rho^2, \tag{2.23}$$

such that  $0 \leq \mathcal{P}(\rho) \leq 1$ . If we assume that  $\dim \mathcal{H} = d < \infty$ , we can provide a finer lower bound for purity, obtained by considering the totally mixed state  $\rho = \mathbb{I}/d$ , where  $\mathbb{I}$  is the  $d \times d$  identity matrix ([Heinosaari, 2011](#)). Therefore,  $\frac{1}{d} \leq \mathcal{P}(\rho) \leq 1$ .

## 2.2.2 Quantum Entropies

Historically introduced in the domain of thermodynamics and statistical mechanics, entropy plays a crucial role in both classical and quantum information theory, where it is used to measure the degree of uncertainty associated to the state of a physical system. In this Section, we will review some basic concepts of quantum entropies, that will be employed in [Chapter 5](#) to describe irreversibility in open quantum systems.

## Von Neumann entropy

Given a state  $\rho \in \mathcal{S}(\mathcal{H})$ , the *von Neumann entropy* is defined as ( $k_B = 1$ ):

$$S(\rho) \equiv -\text{Tr}(\rho \ln \rho). \quad (2.24)$$

Using the canonical decomposition (2.20), one obtains

$$S(\rho) = -\sum_i \lambda_i \ln \lambda_i, \quad (2.25)$$

where  $\{\lambda_i\}_i$  are the eigenvalues of  $\rho$ . Note that we assume the usual convention  $0 \cdot \ln 0 \equiv 0$ . Furthermore, we list some useful properties of  $S$  (Wehrl, 1978; Nielsen, 2010):

- Since  $0 \leq \lambda_i \leq 1$ , we immediately have that the von Neumann entropy is a non-negative quantity, i.e.,  $S(\rho) \geq 0$ .
- Specifically,  $S(\rho) = 0$  when  $\rho$  is a pure state, as the latter would be given by a one-dimensional projector with only one non-null eigenvalue, i.e.,  $\lambda = 1$ .
- If we assume that  $\dim \mathcal{H} = d < \infty$ , then the entropy is bounded from above, i.e.,  $S(\rho) \leq \ln d$ . It is immediate to check that the upper bound is attained by the completely mixed state  $\rho = \mathbb{I}/d$ , being  $\mathbb{I}$  the  $d \times d$  identity matrix.
- The von Neumann entropy is invariant under unitary transformations, i.e.,  $S(U\rho U^\dagger) = S(\rho)$ .

## Relative entropy

On a similar note, we can introduce the *relative entropy*, sometimes referred as *Kullback-Leibler divergence*, as it is the quantum counterpart of the classical analogue quantity that applies to two probability distributions (Kullback, 1951). In the quantum case, it is defined as

$$S(\rho||\sigma) \equiv \begin{cases} \text{Tr}[\rho(\ln \rho - \ln \sigma)] & \text{if } \text{supp } \rho \subseteq \text{supp } \sigma \\ +\infty & \text{otherwise} \end{cases}, \quad (2.26)$$

where  $\rho, \sigma \in \mathcal{S}(\mathcal{H})$ , and  $\text{supp } \rho$  ( $\text{supp } \sigma$ ) is the support of the operator  $\rho$  ( $\sigma$ ), i.e., the vector space spanned by the eigenvectors of  $\rho$  ( $\sigma$ ) corresponding to non-null eigenvalues.

For the relative entropy, the following properties hold:

- It is a non-negative quantity, i.e.,  $S(\rho||\sigma) \geq 0$ . This result is also known as *Klein's inequality*<sup>4</sup>. Specifically,  $S(\rho||\sigma) = 0$  if and only if  $\rho = \sigma$ .
- Similarly to the von Neumann entropy, it is invariant under unitary transformations, i.e.,  $S(U\rho U^\dagger||U\sigma U^\dagger) = S(\rho||\sigma)$ .

---

<sup>4</sup>This is actually a specific application of the Klein inequality, that, for a pair of operators  $A, B$ , reads as  $\text{Tr } A(\ln A - \ln B) \geq \text{Tr}(A - B)$  (Wehrl, 1978).

The relative entropy is widely used in quantum information theory as a measure of dissimilarity between quantum states, though, strictly speaking, it is not a proper mathematical distance. This is due to the fact that it is not symmetric in its two arguments, i.e.,  $S(\rho||\sigma) \neq S(\sigma||\rho)$ , and it does not satisfy the triangle inequality (Audenaert, 2014).

#### Example 2.2.1: Gibbs canonical state

We would like to introduce a state that plays an important role in open quantum system dynamics. More precisely, we would like to find the state that answer the question: given  $E \equiv \text{Tr}(\rho H)$ , what does the density matrix with maximal entropy look like?

By using variational calculus, it can be proven that such a state is given by the *canonical Gibbs state* (Haag, 1996; Morandi, 2001):

$$\rho_\beta \equiv \frac{e^{-\beta H}}{\mathcal{Z}}, \quad (2.27)$$

where  $\mathcal{Z} = \text{Tr}(e^{-\beta H})$  is the partition function of the system and  $\beta = 1/T$  the inverse temperature, such that  $\text{Tr}(\rho_\beta H) = E$ .

It is not difficult to verify that any other state  $\rho$  such that  $\text{Tr}(\rho H) \leq E$  is characterised by a smaller value of the von Neumann entropy. To this end, we can compute the following quantities:

$$\text{Tr} \rho \ln \rho_\beta = -\beta \text{Tr}(\rho H) - \ln \mathcal{Z}, \quad (2.28)$$

$$\text{Tr} \rho_\beta \ln \rho_\beta = -\beta \text{Tr}(\rho_\beta H) - \ln \mathcal{Z}. \quad (2.29)$$

By assumption, we have

$$-\text{Tr} \rho \ln \rho_\beta \leq -\text{Tr} \rho_\beta \ln \rho_\beta, \quad (2.30)$$

therefore, since  $S(\rho||\rho_\beta) = \text{Tr}[\rho(\ln \rho - \ln \rho_\beta)] \geq 0$ , we get

$$S(\rho) = -\text{Tr} \rho \ln \rho \leq -\text{Tr} \rho \ln \rho_\beta \leq -\text{Tr} \rho_\beta \ln \rho_\beta = S(\rho_\beta) \quad (2.31)$$

whence we obtain  $S(\rho) \leq S(\rho_\beta)$ , i.e., the Gibbs state is indeed the state with maximal entropy (Wehrl, 1978).

## 2.3 State space for finite-dimensional systems

Let us specialise our discussion in finite-dimensional systems, i.e., the Hilbert space associated to our system is given by  $\mathcal{H} \cong \mathbb{C}^d$ , being  $d < \infty$  the dimensionality of the system. Under this hypothesis all linear operators are bounded, hence the three Banach spaces  $\mathfrak{B}(\mathcal{H}), \mathfrak{B}_1(\mathcal{H}), \mathfrak{B}_2(\mathcal{H})$  coincide with the space of linear operators defined on  $\mathbb{C}^d$ , i.e.,  $\mathfrak{L}(\mathbb{C}^d)$ . In addition, the Banach space  $\mathfrak{L}(\mathbb{C}^d)$ , equipped with the Hilbert-Schmidt inner product

defined by Equation (2.11), is a Hilbert space.

### 2.3.1 Bloch representation of density matrices

We would like to introduce the so-called *Bloch representation* for  $d$ -dimensional systems, also known as *qudits*. We can observe that a density operator  $\rho \in \mathcal{S}(\mathbb{C}^d)$  can be decomposed in terms of a special basis, given by the orthogonal generators of the special unitary group  $SU(N)$  (with  $N = d$ ) (Byrd, 2003; Kimura, 2003). These generators are given by a set of operators  $G_i$  ( $i = 1, \dots, d^2 - 1$ ), which satisfy the following properties

- (i)  $G_i = G_i^\dagger$ ,
- (ii)  $\text{Tr } G_i = 0$ ,
- (iii)  $\langle G_i, G_j \rangle_{\text{HS}} = d\delta_{ij}$ .

They are characterised by the structure constants  $f_{ijk}$  (completely anti-symmetric tensor) and  $g_{ijk}$  (completely symmetric tensor) of the corresponding Lie Algebra  $\mathfrak{su}(N)$  (with  $N = d$ ), satisfying

$$[G_i, G_j] = i f_{ijk} G_k, \quad (2.32)$$

$$\{G_i, G_j\} = \frac{2}{d} \delta_{ij} \mathbb{I} + g_{ijk} G_k. \quad (2.33)$$

There is a general procedure to systematically construct the  $SU(N)$  generators. Given a complete orthonormal basis  $\{|m\rangle\}_{1 \leq m \leq d} \subset \mathbb{C}^d$ , the generators are given by

$$\{G_i\}_{1 \leq i \leq d^2-1} = \{u_{jk}, v_{jk}, w_l\}/\sqrt{2}, \quad (2.34)$$

where

$$u_{jk} = |j\rangle\langle k| + |k\rangle\langle j|, \quad (2.35)$$

$$v_{jk} = -i(|j\rangle\langle k| - |k\rangle\langle j|), \quad (2.36)$$

$$w_l = \sqrt{\frac{2}{l(l+1)}} \sum_{j=1}^l (|j\rangle\langle j| - l|l+1\rangle\langle l+1|), \quad (2.37)$$

with  $1 \leq j \leq k \leq d$  and  $1 \leq l \leq d-1$ . Any other set of generators  $\mathbf{G}' \equiv \{G'_i\}_{1 \leq i \leq d^2-1}$  with structure constants  $f'_{ijk}$  and  $g'_{ijk}$  are connected with the generators  $\mathbf{G} \equiv \{G_i\}_{1 \leq i \leq d^2-1}$  by an orthogonal matrix  $V \in O(d^2 - 1)$ , with  $G'_i = V_{ij} G_i$  and

$$f'_{ijk} = V_{il} V_{jm} V_{kn} f_{lmn}, \quad g'_{ijk} = V_{il} V_{jm} V_{kn} g_{lmn} \quad (2.38)$$

Note that, the set of generators  $\mathbf{G} \equiv \{G_i\}_{1 \leq i \leq d^2-1}$  and the  $d$ -dimensional identity operator  $\mathbb{I}$  form a complete orthogonal basis for  $\mathcal{L}(\mathbb{C}^d)$ , with respect to the Hilbert-Schmidt inner product.

Therefore, given  $\rho \in \mathcal{S}(\mathbb{C}^d)$ , it can be decomposed using the operator basis  $\{G_\alpha\}_{0 \leq \alpha \leq 1}$ , where  $G_0 = \mathbb{I}$ , while the remaining vectors are given by the set of generators  $\mathbf{G}$ . We obtain

$$\rho = \frac{1}{d} \sum_{\alpha=0}^{d^2-1} \langle G_\alpha, \rho \rangle_{\text{HS}} G_\alpha = \frac{1}{d} \sum_{\alpha=0}^{d^2-1} \text{Tr}(G_\alpha \rho) G_\alpha = \frac{1}{d} \sum_{\alpha=0}^{d^2-1} r_\alpha G_\alpha, \quad (2.39)$$

with  $r_\alpha = \text{Tr}(G_\alpha \rho)$ , whence

$$\rho = \frac{1}{d} (\mathbb{I} + \mathbf{r} \cdot \mathbf{G}), \quad (2.40)$$

where  $\mathbf{r}$  is the *generalised Bloch vector*, also known as *coherence vector* (Hioe, 1981). Using this parametrisation – usually dubbed *Bloch parametrisation* – the set of quantum states  $\mathcal{S}(\mathbb{C}^d)$  can be regarded as a convex subset of  $\mathbb{R}^{d^2-1}$ , denoted as  $\mathcal{B}(\mathbb{R}^{d^2-1})$ .

If we impose the requirement regarding the purity of the state, i.e.,  $\text{Tr } \rho^2 \leq 1$ , we immediately get the constraint

$$|\mathbf{r}| \equiv \sqrt{\sum_{i=1}^{d^2-1} r_i^2} \leq \sqrt{d-1}. \quad (2.41)$$

Therefore, for pure states, the generalised Bloch vector has to fulfil the condition

$$|\mathbf{r}| = \sqrt{d-1}. \quad (2.42)$$

In other terms, one can say that the state space is embedded in the hyper-sphere  $D_R(\mathbb{R}^{d^2-1})$ , whose radius is given by Equation (2.42). However, not all operators  $\rho$  satisfying the constraint of Equation (2.41) represent physical state (i.e., are positive-definite); this means that (de Vicente, 2007):

$$\mathcal{B}(\mathbb{R}^{d^2-1}) \subseteq D_R(\mathbb{R}^{d^2-1}). \quad (2.43)$$

### Example 2.3.1: Bloch representation of a qubit

Let us consider the case of a two-dimensional system, i.e., a *qubit*. In this case, we can consider the orthonormal basis  $\{|0\rangle, |1\rangle\}$  in  $\mathcal{H} \cong \mathbb{C}^2$ . By using the general formulas given by Equations (2.35) to (2.37), we easily get the  $SU(2)$  generators

$$G_1 = u_{12}/\sqrt{2} = (|0\rangle\langle 1| + |1\rangle\langle 0|)/\sqrt{2} \equiv \sigma_1/\sqrt{2}, \quad (2.44)$$

$$G_2 = v_{12}/\sqrt{2} = -i(|0\rangle\langle 1| - |1\rangle\langle 0|)/\sqrt{2} \equiv \sigma_2/\sqrt{2}, \quad (2.45)$$

$$G_3 = w_1/\sqrt{2} = (|0\rangle\langle 0| - |1\rangle\langle 1|)/\sqrt{2} \equiv \sigma_3/\sqrt{2}, \quad (2.46)$$

where  $\vec{\sigma} = \{\sigma_1, \sigma_2, \sigma_3\}$  is the vector containing the three Pauli operators<sup>a</sup>, whose

standard matrix representation is:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.47)$$

being  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

It is easy to verify that  $[\sigma_1, \sigma_2] = 2i \sigma_3$ , therefore, by comparing with [Equation \(2.32\)](#), we have  $f_{ijk} = \sqrt{2}\epsilon_{ijk}$ , i.e., the Levi-Civita tensor<sup>b</sup>. Similarly, one can check that  $\{\sigma_i, \sigma_j\} = 0$ , if  $i \neq j$ , whereas  $\{\sigma_i, \sigma_i\} = 2\mathbb{I}_2$ , where  $i, j = 1, 2, 3$ ; therefore, in [Equation \(2.33\)](#), we have  $g_{ijk} = 0$ . It is worth mentioning that the Levi-Civita tensor is rotationally invariant, therefore in [Equation \(2.38\)](#) one has  $V_{il}V_{jm}V_{kn}\epsilon_{ijk} = \det V\epsilon_{ijk} = \pm\epsilon_{ijk}$ . Note that this property holds specifically for  $SU(2)$ , but not in general for  $SU(N)$ , with  $N \geq 3$  ([Kimura, 2003](#)).

For  $d = 2$ , [Equation \(2.40\)](#) gives the most general density operator  $\rho$  for a qubit, i.e.,

$$\rho = \frac{1}{2} (\mathbb{I}_2 + \vec{\tau} \cdot \vec{\sigma}), \quad (2.48)$$

where  $\vec{\tau} \equiv \{\tau_x, \tau_y, \tau_z\}$  is the *Bloch vector*. Note that for  $d = 2$ , the condition  $\text{Tr } \rho^2 \leq 1$  is both necessary and sufficient for the positivity of  $\rho$ . As a consequence, any  $\rho \in \mathcal{S}(\mathbb{C}^2)$  is uniquely characterised by a three-dimensional real vector  $\vec{\tau} \in \mathbb{R}^3$ ; in other terms, there is a one-to-one correspondence between states of a qubit and a point in the so-called *Bloch sphere* (cf. [Figure 2.1](#))<sup>c</sup>

$$\mathcal{B}(\mathbb{R}^3) = \{\vec{\tau} = (\tau_x, \tau_y, \tau_z) \in \mathbb{R}^3 : |\vec{\tau}| \leq 1\}. \quad (2.49)$$

This correspondence can be easily checked by determining the eigenvalues of the statistical operator given by [Equation \(2.48\)](#). They are  $\lambda_{\pm} = \frac{1}{2}(1 \pm |\vec{\tau}|)$ , where  $|\vec{\tau}| \equiv (\tau_x^2 + \tau_y^2 + \tau_z^2)^{1/2}$ . Thus,  $\rho$  is positive if and only if  $|\vec{\tau}| \leq 1$ , which coincides with the condition of [Equation \(2.42\)](#) for  $d = 2$ . This means that  $\mathcal{B}(\mathbb{R}^3) = D_R(\mathbb{R}^3)$ . Therefore, pure states are those represented by a point on the surface of the Bloch sphere, i.e., those characterised by a unit Bloch vector.

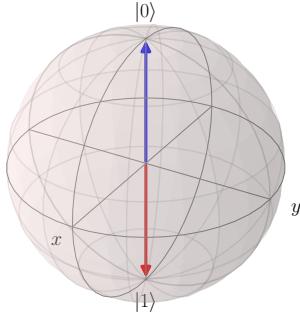
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<sup>a</sup>Note that we will use the notation  $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$  as well.

<sup>b</sup>defined as

$$\epsilon_{ijk} = \begin{cases} +1 & \text{for even permutations of } (1, 2, 3) \\ -1 & \text{for odd permutations of } (1, 2, 3) \\ 0 & \text{for repeated indices.} \end{cases}$$

<sup>c</sup>We should actually call it *Bloch ball*, as we consider points that do not lie on the surface as well. Note that this also reminds the so-called *Poincaré sphere* of optics, the latter being a geometrical representation of the so-called Stokes parameters for polarisation ([Born, 1999](#)).



**Figure 2.1:** The Bloch sphere represents the state space for a two-dimensional quantum system (qubit). Pure states are represented by points lying on the surface, while mixed states correspond to interior points. Note that the two orthogonal states  $|0\rangle, |1\rangle$  are associated with two antipodal Bloch vectors. This picture is realised using QuTip (Johansson, 2013).

### Example 2.3.2: Bloch representation of a qutrit

A further example is provided by a three-dimensional system, i.e., a *qutrit*. In this case, the corresponding Hilbert space is  $\mathcal{H} \cong \mathbb{C}^3$ . By resorting to Equations (2.35) to (2.37) once more, we can construct the generators of  $SU(3)$  (Kimura, 2003). We eventually get  $G_1 = u_{12}/\sqrt{2} = \lambda_1/\sqrt{2}$ ,  $G_2 = v_{12}/\sqrt{2} = \lambda_2/\sqrt{2}$ ,  $G_3 = w_{12}/\sqrt{2} = \lambda_3/\sqrt{2}$ ,  $G_4 = u_{13}/\sqrt{2} = \lambda_4/\sqrt{2}$ ,  $G_5 = v_{13}/\sqrt{2} = \lambda_5/\sqrt{2}$ ,  $G_6 = w_{13}/\sqrt{2} = \lambda_6/\sqrt{2}$ ,  $G_7 = v_{23}/\sqrt{2} = \lambda_7/\sqrt{2}$ ,  $G_8 = w_{23}/\sqrt{2} = \lambda_8/\sqrt{2}$ , where  $\lambda_i$  ( $i = 1, \dots, 8$ ) are the eight so-called *Gell-Mann operators*.

If we consider the orthonormal basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (2.50)$$

we would obtain

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \end{aligned} \quad (2.51)$$

known as *Gell-Mann matrices*.

If  $\rho \in \mathcal{S}(\mathbb{C}^3)$ , [Equation \(2.40\)](#) (with  $d = 3$ ) gives the following Bloch representation:

$$\rho = \frac{1}{3} (\mathbb{I}_3 + \mathbf{r} \cdot \mathbf{G}) \quad (2.52)$$

where  $\mathbf{r}$  is an eight-dimensional real vector, while  $\mathbf{G}$  is the vector containing the  $SU(3)$  generators. The remark about the general case  $d \geq 3$  also applies in this specific case: [Equation \(2.52\)](#) establishes a one-to-one correspondence between the possible density matrices of a qutrit and a proper subset of the hyperball defined by the condition  $|\mathbf{r}| \leq \sqrt{2}$ , i.e.,

$$\mathcal{B}(\mathbb{R}^8) \subseteq D_R(\mathbb{R}^8). \quad (2.53)$$

### 2.3.2 Linear maps representations

Let us consider the space of linear maps defined on  $\mathfrak{L}(\mathbb{C}^d)$ , denoted as  $\mathfrak{LL}(\mathbb{C}^d)$ . Given  $\Lambda \in \mathfrak{LL}(\mathbb{C}^d)$ ,  $\Lambda$  is said to be a *self-adjoint* operator if it equals its adjoint  $\Lambda^\dagger$ , defined as

$$\langle \Lambda^\dagger(\chi), \omega \rangle_{\text{HS}} = \langle \chi, \Lambda(\omega) \rangle_{\text{HS}}, \quad (2.54)$$

for all  $\chi, \omega \in \mathfrak{L}(\mathbb{C}^d)$ . Moreover, if  $\Lambda$  also fulfils the requirement

$$\langle \omega, \Lambda(\omega) \rangle_{\text{HS}} \geq 0 \quad (2.55)$$

for all  $\omega \in \mathfrak{L}(\mathbb{C}^d)$ , then  $\Lambda$  is *positive-definite*.

It is worth mentioning that, in the general, infinite-dimensional case, besides the concept of adjoint map there is also that of dual map. Given a linear map  $\Lambda$ , defined on  $\mathfrak{L}(\mathcal{H})$ , one can define the *dual map*  $\Lambda^*$  through the relation

$$\langle \Lambda^*(A), \sigma \rangle_{\text{HS}} = \langle A, \Lambda(\sigma) \rangle_{\text{HS}}, \quad (2.56)$$

for all  $A \in \mathfrak{B}(\mathcal{H})$  and  $\sigma \in \mathfrak{B}_1(\mathcal{H})$ . However, the notions of adjoint and dual map coincide in the finite-dimensional case that we are analysing here.

Now, we would like to introduce a matrix representation for a linear map. To this end, let us consider a basis  $\{\sigma_\alpha\}_{\alpha=1,\dots,d^2}$  in  $\mathfrak{L}(\mathbb{C}^d)$ , orthonormal with respect to the Hilbert-Schmidt inner product, i.e.,

$$\langle \sigma_\alpha, \sigma_\beta \rangle_{\text{HS}} = \text{Tr} (\sigma_\alpha^\dagger \sigma_\beta) = \delta_{\alpha\beta} \quad (2.57)$$

Given an operator  $\omega \in \mathfrak{L}(\mathbb{C}^d)$ , the latter can be identified with a vector, whose components

are  $\omega_\beta = \langle \sigma_\beta, \omega \rangle_{\text{HS}} = \text{Tr}(\sigma_\beta^\dagger \omega)$ . We can express the linear map as<sup>5</sup>

$$\Lambda(\omega) = \sum_{\alpha, \beta=1}^{d^2} \langle \sigma_\alpha, \Lambda(\sigma_\beta) \rangle_{\text{HS}} \langle \sigma_\beta, \omega \rangle_{\text{HS}} \sigma_\alpha, \quad (2.58)$$

hence, if we define the matrix  $(\Lambda_{\alpha\beta})_{1 \leq \alpha, \beta \leq d^2}$ , whose coefficients are

$$\Lambda_{\alpha\beta} \equiv \langle \sigma_\alpha, \Lambda(\sigma_\beta) \rangle_{\text{HS}} = \text{Tr}(\sigma_\alpha^\dagger \Lambda(\sigma_\beta)), \quad (2.59)$$

we eventually obtain

$$\Lambda(\omega) = \sum_{\alpha, \beta=1}^{d^2} \Lambda_{\alpha\beta} \omega_\beta \sigma_\alpha. \quad (2.60)$$

Working along the same lines, one can obtain a similar decomposition for the adjoint map  $\Lambda^*$ , i.e.,

$$\Lambda^*(\omega) = \sum_{\alpha, \beta=1}^{d^2} \Lambda_{\alpha\beta}^* \omega_\alpha \sigma_\beta, \quad (2.61)$$

where  $\Lambda_{\alpha\beta}^*$  represents the complex conjugate of the entry  $\Lambda_{\alpha\beta}$ <sup>6</sup>.

The representation (2.60) ensures remarkable advantages.

- The action of the map  $\Lambda$  on an operator  $\omega$  can be regarded as a simple multiplication between a matrix and a vector

$$\begin{aligned} (\Lambda(\omega))_\alpha &= \text{Tr}(\sigma_\alpha^\dagger \Lambda(\omega)) = \text{Tr}\left(\sigma_\alpha^\dagger \sum_{\beta, \gamma=1}^{d^2} \Lambda_{\beta\gamma} \omega_\gamma \sigma_\beta\right) = \sum_{\alpha, \beta=1}^{d^2} \text{Tr}(\sigma_\alpha^\dagger \Lambda_{\beta\gamma} \omega_\gamma \sigma_\beta) \\ &= \sum_{\alpha, \beta=1}^{d^2} \Lambda_{\beta\gamma} \omega_\gamma \text{Tr}(\sigma_\alpha^\dagger \sigma_\beta) = \sum_{\gamma=1}^{d^2} \Lambda_{\alpha\gamma} \omega_\gamma. \end{aligned} \quad (2.62)$$

- The composition of maps is nothing but a product of matrices

$$\begin{aligned} (\Lambda \circ \Xi)_{\alpha\beta} &= \text{Tr}[\sigma_\alpha^\dagger (\Lambda \circ \Xi)(\sigma_\beta)] = \text{Tr}[\sigma_\alpha^\dagger \Lambda(\Xi(\sigma_\beta))] \\ &= \sum_{\delta, \gamma=1}^{d^2} \text{Tr}\left[\sigma_\alpha^\dagger \Lambda_{\gamma\delta} \text{Tr}(\sigma_\delta^\dagger \Xi(\sigma_\beta)) \sigma_\gamma\right] = \sum_{\delta=1}^{d^2} \Lambda_{\alpha\delta} \Xi_{\delta\beta}. \end{aligned} \quad (2.63)$$

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<sup>5</sup>To catch the spirit of the decomposition in Equation (2.58), we can draw an analogy. Let us consider a linear operator  $A$  acting on  $|\psi\rangle$ ; given an orthonormal basis  $\{|\psi_k\rangle\}_k$ , we easily obtain  $A|\psi\rangle = \sum_{k,l} \langle \psi_l | A |\psi_k\rangle \langle \psi_k | \psi \rangle |\psi_l\rangle$ . In Equation (2.58), we are doing something similar, as far as we identify the appropriate spaces and inner products.

<sup>6</sup>Note that, for the finite-dimensional case considered here, this decomposition holds also for the adjoint map.

Similarly, one can check that the linear map  $\Lambda \in \mathfrak{LL}(\mathbb{C}^d)$  is positive (or Hermitian), if and only if so is it the corresponding matrix  $(\Lambda_{\alpha\beta})_{0 \leq \alpha, \beta \leq d^2}$ .

In the [Example 2.3.3](#), we consider the case of the Bloch representation of a linear map, while in [Example 2.3.4](#), we discuss the case of the so-called damping basis, that are sometimes useful in the study of open quantum systems.

### Example 2.3.3: Bloch representation of a linear map

Let us apply the decomposition given by [Equation \(2.60\)](#) using the operator basis given by the  $SU(N)$  generators. Using the quantities defined in [Section 2.3.1](#), and the Bloch representation of a density matrix – cf. [Equations \(2.39\)](#) and [\(2.40\)](#) – one can obtain

$$\Lambda(\rho) = \sum_{\alpha=0}^{d^2-1} \Lambda_{\alpha\beta} r_\beta G_\alpha \equiv \sum_{\alpha=0}^{d^2-1} r'_\alpha G_\alpha, \quad (2.64)$$

where  $\Lambda_{\alpha\beta} = \text{Tr}[G_\alpha \Lambda(G_\beta)]$ ,  $r'_\alpha = \sum_\beta \Lambda_{\alpha\beta} r_\beta$ , while we have suitably rescaled the coefficients  $r_\beta$ , such that  $r_\beta = \text{Tr}(\rho G_\beta)/d$ . By requiring the map  $\Lambda$  to be trace preserving, we get that  $r_0 = r'_0$ . Thus, in the parameter space a trace preserving linear map can be represented by the affine transformation

$$\begin{aligned} r_0 &\mapsto r'_0 = \Lambda_{00} r_0 = r_0, \\ r_j &\mapsto r'_j = \Lambda_{jk} r_k + \Lambda_{j0} r_0, \end{aligned} \quad (2.65)$$

or, equivalently, by the matrix

$$\Lambda = \begin{pmatrix} 1 & 0 \\ \mathbf{q} & \mathbf{A} \end{pmatrix}, \quad (2.66)$$

where  $A \in \mathcal{M}_{d^2-1}(\mathbb{R})$ , such that  $A_{ij} = \Lambda_{ij}$ , for all  $i, j = 1, \dots, d^2 - 1$ , whereas  $\mathbf{q}$  is a  $(d^2 - 1)$ -dimensional vector, such that  $q_j = \Lambda_{j0}$ .

### Example 2.3.4: Damping bases

The matrix representation of maps that we have put forward in [Section 2.3.2](#) can be employed to introduce the so-called *damping* (or *bi-orthogonal*) basis ([Briegel, 1993; Chruściński, 2010; Megier, 2020](#)). Specifically, we would like to see what the decomposition given by [Equation \(2.60\)](#) looks like whenever we assume that the linear map  $\Lambda$  is diagonalisable. According to the general representation given in [Section 2.3.2](#), the linear map  $\Lambda \in \mathfrak{LL}(\mathbb{C}^d)$  is diagonalisable if so is the matrix  $M^\Lambda \equiv (\Lambda_{\alpha\beta})_{0 \leq \alpha, \beta \leq d^2}$ , i.e., if there exists  $P \in \mathcal{M}_d(\mathbb{C})$  such that  $PM^\Lambda P^{-1} = D$ , where  $D = \text{diag}\{\lambda_\alpha\}_{\alpha=1, \dots, d^2}$ . Equivalently, one can write

$$\langle \sigma_\alpha, D(\sigma_\beta) \rangle_{\text{HS}} = \lambda_\alpha \delta_{\alpha\beta}, \quad (2.67)$$

being  $\{\sigma_\alpha\}_{\alpha=1,\dots,d^2}$  an orthonormal basis with respect to the Hilbert-Schmidt product. As a result, one gets  $\Lambda_{\beta\beta'} = \sum_\alpha \lambda_\alpha P_{\beta\alpha}(P^{-1})_{\alpha\beta'}$ , thus [Equation \(2.60\)](#) yields

$$\Lambda(\omega) = \sum_{\alpha=1}^{d^2} \lambda_\alpha \operatorname{Tr}(\zeta_\alpha^\dagger \omega) \tau_\alpha, \quad (2.68)$$

where  $\omega \in \mathfrak{L}(\mathbb{C}^d)$ , and  $\tau_\alpha = \sum_{\beta=1}^{d^2} P_{\beta\alpha} \sigma_\beta$ ,  $\zeta_\alpha = \sum_{\beta'=1}^{d^2} (P^{-1})_{\alpha\beta'}$ . We have thus introduced two families of operators  $\{\tau_\alpha\}_{\alpha=1,\dots,d^2}$  and  $\{\zeta_\alpha\}_{\alpha=1,\dots,d^2}$ , that, using the definitions above and [Equation \(2.57\)](#), can be proven to be orthogonal, i.e.,

$$\langle \zeta_\alpha, \tau_\beta \rangle_{\text{HS}} = \operatorname{Tr}(\zeta_\alpha^\dagger \tau_\beta) \delta_{\alpha\beta}. \quad (2.69)$$

[Equation \(2.69\)](#) can also be read as a duality relation between  $\{\tau_\alpha\}_{\alpha=1,\dots,d^2}$  and  $\{\zeta_\alpha\}_{\alpha=1,\dots,d^2}$ , the latter defined on the dual space. This justifies the name of *biorthogonal basis*, as the damping basis is sometimes referred to as.

By using [Equation \(2.61\)](#), one can obtain decomposition for the dual map  $\Lambda^*$ , similar to that in [Equation \(2.68\)](#),

$$\Lambda^*(\omega) = \sum_{\alpha=1}^{d^2} \lambda_\alpha^* \operatorname{Tr}(\tau_\alpha^\dagger \omega) \zeta_\alpha. \quad (2.70)$$

From [Equations \(2.68\)](#) and [\(2.70\)](#), one can see that the operators  $\{\tau_\alpha\}_{\alpha=1,\dots,d^2}$  and  $\{\zeta_\alpha\}_{\alpha=1,\dots,d^2}$  are, respectively, eigenvectors of the maps  $\Lambda$  and  $\Lambda^*$  with respect to the complex conjugate eigenvalues. Indeed, by exploiting the orthogonality relation [\(2.69\)](#), one immediately gets the following eigenvalue equations:

$$\Lambda(\tau_\alpha) = \lambda_\alpha \tau_\alpha, \quad \Lambda^*(\zeta_\alpha) = \lambda_\alpha^* \zeta_\alpha, \quad \alpha = 1, \dots, d^2. \quad (2.71)$$

## 2.4 Composite quantum systems

Let us consider the case of a composite quantum system, that is a system composed by two quantum systems,  $S_A$  and  $S_B$ , that can either represent two different quantum objects or two different degrees of freedom ([Breuer, 2002](#)). We will see that this mathematical formalism is particularly suitable for studying the case in which a quantum system is interacting with its surroundings.

### 2.4.1 Tensor product

Let us assume that  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are the Hilbert spaces associated to  $S_A$  and  $S_B$ , respectively. We can thus associate to the composite system  $S = S_A + S_B$  the tensor product Hilbert space

$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ . If  $\{|\psi_j\rangle\}_j \subset \mathcal{H}_A$  and  $\{|\varphi_k\rangle\}_k \subset \mathcal{H}_B$ , orthonormal basis in the respective spaces, then the set  $\{|\psi_j\rangle \otimes |\varphi_k\rangle\}_{jk}$  constitutes an orthornomal basis for  $\mathcal{H}$ . Therefore, a generic ket  $|\psi\rangle \in \mathcal{H}$  can be decomposed as

$$|\psi\rangle = \sum_{j,k} \alpha_{jk} |\psi_j\rangle \otimes |\varphi_k\rangle. \quad (2.72)$$

If  $A$  and  $B$  are linear operators on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, one can define the tensor product  $A \otimes B$  by

$$(A \otimes B) (|\psi_j\rangle \otimes |\varphi_k\rangle) \equiv (A|\psi_j\rangle) \otimes (B|\varphi_k\rangle), \quad (2.73)$$

and, by linear extension, to arbitrary states as in [Equation \(2.72\)](#). Therefore, a generic operator  $O$  acting on  $\mathcal{H}$  can be expressed as a linear combination of tenor products, i.e.,

$$O = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}. \quad (2.74)$$

If  $\mathbb{I}_A$  and  $\mathbb{I}_B$  denote the identity operators in  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, an operator acting only on the subsystem  $S_A$  takes the form  $A \otimes \mathbb{I}_B$ ; analogously,  $\mathbb{I}_A \otimes B$  acts on the subsystem  $S_B$  only.

The set of states of the composite system  $S$  is given by  $\mathcal{S}(\mathcal{H})$ . If the two subsystem  $S_A$  and  $S_B$  are uncorrelated, the total density operator is given by the following tensor product:

$$\rho = \rho_A \otimes \rho_B, \quad (2.75)$$

where  $\rho_A \in \mathcal{S}(\mathcal{H}_A)$  and  $\rho_B \in \mathcal{S}(\mathcal{H}_B)$ .

## 2.4.2 Partial trace

As we are often interested in one of the two subsystems, i.e., either  $S_A$  or  $S_B$ , we would like to formally address the issue of considering one system, e.g.,  $S_A$ , while we discard those degrees of freedom that are associated to the other, e.g.,  $S_B$ . This intuitive operation can be performed by applying the *partial trace*.

Let us define the partial trace over the system  $S_B$  by the unique linear mapping<sup>7</sup>:

$$\begin{aligned} \text{tr}_B : \mathfrak{B}_1(\mathcal{H}) &\rightarrow \mathfrak{B}_1(\mathcal{H}_A) \\ T &\mapsto \text{tr}_B T, \end{aligned} \quad (2.76)$$

such that, for all  $A \in \mathfrak{B}(\mathcal{H}_A)$  and  $T \in \mathfrak{B}(\mathcal{H})$ , it satisfies the condition

$$\text{Tr} [T (A \otimes \mathbb{I}_B)] = \text{tr}_A [(\text{tr}_B T) A]. \quad (2.77)$$

---

<sup>7</sup>Note that, in principle, we could rephrase everything that follows swapping the roles of subsystem  $S_A$  and  $S_B$ .

Moreover, if we use the orthornormal basis  $\{|\psi_j \otimes \varphi_k\rangle \equiv |\psi_j\rangle \otimes |\varphi_k\rangle\}_{jk} \subset \mathcal{H}$ , we obtain the following decomposition:

$$T = \mathbb{I}_{AB} T \mathbb{I}_{AB} = \sum_{jk} \sum_{m,n} \langle \psi_j \otimes \varphi_k | T | \psi_m \otimes \varphi_n \rangle |\psi_j\rangle \langle \psi_m| \otimes |\varphi_k\rangle \langle \varphi_n|. \quad (2.78)$$

Hence, since  $\text{tr}_B (|\psi_j\rangle \langle \psi_m| \otimes |\varphi_k\rangle \langle \varphi_n|) = |\psi_j\rangle \langle \psi_m| \delta_{kn}$ , the partial trace yields

$$\text{tr}_B T = \sum_{j,k,m} \langle \psi_j \otimes \varphi_k | T | \psi_m \otimes \varphi_k \rangle |\psi_j\rangle \langle \psi_m|. \quad (2.79)$$

Specifically, in the case of a factorised operator, i.e.,  $T = T_A \otimes T_B$ , we have

$$\text{tr}_B (T_A \otimes T_B) = (\text{tr}_B T_B) T_A, \quad (2.80)$$

therefore, in this special case, [Equation \(2.79\)](#) reads as

$$\text{tr}_B (T_A \otimes T_B) = \sum_k \langle \varphi_k | T_B | \varphi_k \rangle T_A, \quad (2.81)$$

providing a useful formula to compute the partial trace.

## Reduced states

Now, we would like to apply the general formalism outlined above to density operators. Let us consider a state  $\rho \in \mathcal{S}(\mathcal{H})$  and check what happens if we trace out one of the two subsystems, e.g.,  $S_B$ . In other words, we ask ourselves whether or not  $\rho_A \equiv \text{tr}_B \rho$  represents a physical state.

In order to answer this question, we need to check that the partial trace preserves both trace and positive-definiteness.

- Let us compute the trace of  $\rho_A$

$$\text{tr}_A \rho_A = \text{tr}_A (\text{tr}_B \rho) = \text{Tr} [\rho (\mathbb{I}_A \otimes \mathbb{I}_B)] = \text{Tr} \rho = 1, \quad (2.82)$$

where we have resorted to [Equation \(2.77\)](#), with  $A = \mathbb{I}_A$ .

- Let us consider  $|\psi\rangle \in \mathcal{H}_A$  and compute

$$\begin{aligned} \langle \psi | \rho_A | \psi \rangle &= \text{tr}_A [\text{tr}_B (\rho P_\psi)] = \text{Tr} [\rho (P_\psi \otimes \mathbb{I}_B)] = \text{Tr} [(P_\psi \otimes \mathbb{I}_B) \rho (P_\psi \otimes \mathbb{I}_B)] \\ &= \text{Tr} \{[\rho^{1/2} (P_\psi \otimes \mathbb{I}_B)]^\dagger [(P_\psi \otimes \mathbb{I}_B) \rho^{1/2}] \} \geq 0, \end{aligned} \quad (2.83)$$

where we have introduced the one-dimensional projector operator  $P_\psi = |\psi\rangle \langle \psi|$  and used [Equation \(2.77\)](#), with  $A = P_\psi$ .

Therefore

$$\rho_A = \text{tr}_B \rho \quad (2.84)$$

represents a state, i.e.,  $\rho_A \in \mathcal{S}(\mathcal{H}_A)$ , and it is called *reduced* (or *marginal*) *state*. Analogously, one can obtain the reduced state  $\rho_B = \text{tr}_A \rho$ , by tracing out the subsystem  $S_A$ .

### 2.4.3 Schmidt decomposition

Let us assume that  $\rho_A \in \mathcal{S}(\mathcal{H}_A)$  and  $\rho_B \in \mathcal{S}(\mathcal{H}_B)$  are two density operators describing the states of the system  $S_A$  and  $S_B$ , respectively. We ask ourselves: how can be the possible joint states  $\rho \in \mathcal{S}(\mathcal{H})$  of the composite system expressed?

One possible answer is given by a product state, i.e., a state in the form

$$\rho = \rho_A \otimes \rho_B, \quad (2.85)$$

which physically correspond to the case to the case of two *uncorrelated* systems  $S_A$  and  $S_B$ . In general, there are more possible answers, essentially meaning that, the knowledge of the two subsystems does not enable us to specify the state of the corresponding composite system.

In this regard, an important characterisation of the states of a composite system is provided by the so-called Schmidt decomposition theorem (Breuer, 2002). Let us assume that, given  $|\psi\rangle \in \mathcal{H}$ , can be expressed by Equation (2.72). For simplicity's sake, let us suppose that  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are both  $d$ -dimensional systems, therefore the coefficients appearing in Equation (2.72) define the square matrix  $A = (\alpha_{jk})_{1 \leq j,k \leq d}$ . We can apply a singular value decomposition of the matrix  $A$ , i.e.,

$$A = UDV, \quad (2.86)$$

where  $U = (u_{ij})_{1 \leq i,j \leq d}$ ,  $V = (v_{ij})_{1 \leq i,j \leq d}$  are unitary matrices, while  $D$  is a diagonal matrix with non negative entries  $\alpha_i \geq 0$ . Let us introduce  $\alpha_i \equiv \sqrt{\lambda_i}$ , therefore, from Equation (2.72), we get:

$$|\psi\rangle = \sum_{i,j,k} u_{ji} \sqrt{\lambda_i} v_{ik} |\psi_j\rangle \otimes |\varphi_k\rangle. \quad (2.87)$$

We can introduce the so-called *Schmidt bases*

$$|\chi_i\rangle \equiv \sum_{j=1}^d u_{ji} |\psi_j\rangle, \quad |\xi_i\rangle \equiv \sum_{j=1}^d v_{ki} |\varphi_k\rangle, \quad (2.88)$$

orthogonal in  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively. Hence, we obtain the *Schmidt decomposition*

$$|\psi\rangle = \sum_{i=1}^d \sqrt{\lambda_i} |\chi_i\rangle \otimes |\xi_i\rangle, \quad (2.89)$$

where  $\sqrt{\lambda_i}$  are called *Schmidt coefficients*. It is easy to check that the latter coincide with the square root of the eigenvalues of the partial states, obtained by tracing out one of the subsystems. By direct computation, one obtains indeed  $\rho_A = \text{tr}_B(|\psi\rangle\langle\psi|) = \sum_i \lambda_i |\chi_i\rangle\langle\chi_i|$ , and  $\rho_B = \text{tr}_A(|\psi\rangle\langle\psi|) = \sum_i \lambda_i |\xi_i\rangle\langle\xi_i|$ . Thus, we recover the canonical decomposition of Equation (2.20) for each reduced state. This justifies the identification  $\alpha_i \equiv \sqrt{\lambda_i}$ : the

latter quantities define a probability amplitude, therefore [Equation \(2.89\)](#) naturally encodes the probabilistic interpretation of a density matrix. Note that, in the general case,  $d = \min\{d_A, d_B\}$ , with  $d_A = \dim \mathcal{H}_A$ ,  $d_B = \dim \mathcal{H}_B$ .

The number of non-zero Schmidt coefficients is called *Schmidt rank*  $r_S(\psi)$  and it is invariant under unitary transformations  $U_A$  and  $U_B$  acting on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively. As a result, this also means that the Schmidt rank does not depend on the specific Schmidt bases chosen, but it is a property uniquely determined by the state  $|\psi\rangle$ .

We will call *separable* those states that can be written in a tensor product form, as in [Equation \(2.85\)](#). All other states are called *entangled*. Therefore, it is immediate to conclude that the former are characterised by  $r_S(\psi) = 1$ , while the latter by  $r_S(\psi) > 1$ .

Furthermore, we will call *maximally entangled* those states that can be written in the form

$$|\psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |\chi_i\rangle \otimes |\xi_i\rangle, \quad (2.90)$$

i.e., those states that are characterised by the fact that all nonzero Schmidt coefficients in [Equation \(2.89\)](#) are equal to  $d^{-1/2}$ .

#### Example 2.4.1: Bell States

To illustrate the concepts that we have just introduced, let us consider the case of a pair of qubits, associated to the tensor product Hilbert space  $\mathcal{H} \cong \mathbb{C}^2 \otimes \mathbb{C}^2$ . If  $\{|0\rangle_A, |1\rangle_A\}$  and  $\{|0\rangle_B, |1\rangle_B\}$  are the two orthonormal bases in  $\mathcal{H}_A \cong \mathbb{C}^2$  and  $\mathcal{H}_B \cong \mathbb{C}^2$ , respectively, we can construct the so-called *computational basis*  $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$  in  $\mathcal{H} \cong \mathbb{C}^2 \otimes \mathbb{C}^2$ , where  $|ij\rangle \equiv |i\rangle_A \otimes |j\rangle_B$ . It is easy to check that the elements of this basis are eigenvectors of the tensor product operator  $\sigma_z \otimes \sigma_z$ .

On the other hand, we can construct the following states:

$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle), \quad (2.91)$$

$$|\psi^\pm\rangle = \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle), \quad (2.92)$$

known as *Bell states*. These states are common eigenvectors of the commuting operators  $\sigma_y \otimes \sigma_y$  and  $\sigma_z \otimes \sigma_z$ . [Equations \(2.91\)](#) and [\(2.92\)](#) define a basis of maximally entangled states, called *Bell basis* ([Benenti, 2007](#)).

#### Example 2.4.2: Bloch representation of a bipartite system

In this example, we would like to generalise [Equation \(2.40\)](#) to bipartite systems. Let us consider two systems living in the Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , whose dimensions are  $d_A$  and  $d_B$ , respectively. As in the case discussed in [Section 2.3.1](#), we can resort to the

$SU(N)$  generators to obtain suitable operator bases.

Therefore, for each system we can consider the corresponding generators, i.e.  $\mathbf{r}_A \equiv \{r_i^A\}_{1 \leq i \leq d_A^2 - 1}$  and  $\mathbf{r}_B \equiv \{r_j^B\}_{1 \leq j \leq d_B^2 - 1}$ , which serve as operator basis for density matrices in  $\mathcal{S}(\mathcal{H}_A)$  and  $\mathcal{S}(\mathcal{H}_B)$ , respectively.

A generic state of the composite system  $\rho \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$  can be expressed as

$$\rho = \frac{1}{d_A d_B} \left( \mathbb{I}_A \otimes \mathbb{I}_B + \sum_{i=1}^{d_A^2-1} \tau_i^A r_i^A \otimes \mathbb{I}_B + \sum_{j=1}^{d_B^2-1} \mathbb{I}_A \otimes \tau_j^B r_j^B + \sum_{i=1}^{d_A^2-1} \sum_{j=1}^{d_B^2-1} t_{ij} r_i^A \otimes r_j^B \right), \quad (2.93)$$

where  $\boldsymbol{\tau}_A$  and  $\boldsymbol{\tau}_B$  are generalised Bloch vectors corresponding to the reduced states  $\rho_A$  and  $\rho_B$ , respectively, whereas  $t_{ij}$  is the so-called *correlation tensor* (de Vicente, 2007; Sarbicki, 2020).

It is straightforward to see that we recover the form of [Equation \(2.40\)](#) for each of the two reduced matrices by performing a partial trace with respect to one of the two parties, i.e.,

$$\rho_A \equiv \text{tr}_B \rho = \frac{1}{d_A} (\mathbb{I}_A + \boldsymbol{\tau}_A \cdot \mathbf{r}_A), \quad (2.94)$$

$$\rho_B \equiv \text{tr}_A \rho = \frac{1}{d_B} (\mathbb{I}_B + \boldsymbol{\tau}_B \cdot \mathbf{r}_B). \quad (2.95)$$

#### Example 2.4.3: Fano form and Weyl states

Let us specialise the [Example 2.4.2](#) by explicitly considering the case of a pair of qubits. As a first example, let us consider the simplest case of a bipartite system made of two qubits. In this case,  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \cong \mathbb{C}^2 \otimes \mathbb{C}^2$ ; by taking  $d_A = d_B = 2$  and  $\mathbf{r} \equiv \vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$  in [Equation \(2.93\)](#), we eventually obtain the so-called *Fano form* for the two-qubit density operator (Fano, 1983; Friis, 2017):

$$\tilde{\rho} = \frac{1}{4} \left\{ \mathbb{I}_{AB} + (\vec{\tau}_A \cdot \vec{\sigma}) \otimes \mathbb{I}_B + \mathbb{I}_A \otimes (\vec{\tau}_B \cdot \vec{\sigma}) + \sum_{j,k=1}^3 t_{jk} \sigma_j \otimes \sigma_k \right\}. \quad (2.96)$$

Moreover, the invariance properties of  $SU(2)$  provide a remarkable advantage: the correlation tensor  $T \equiv (t_{jk})_{1 \leq j,k \leq 3}$  can be brought in a diagonal form by applying local unitary operations (Luo, 2008). To this end, we can preliminarily resort to the singular value decomposition theorem to get

$$T = O^A \text{diag}(c_1, c_2, c_3) O^B \quad (2.97)$$

or, equivalently,

$$\sum_{j,k=1}^3 O_{jm}^A t_{jk} O_{nk}^B = \delta_{mn} c_m, \quad (2.98)$$

where  $O^A = (O_{jm}^A)_{1 \leq j,m \leq 3}$  and  $O^B = (O_{jm}^B)_{1 \leq j,m \leq 3}$  are orthogonal matrices in  $O(3)$ . Moreover, there always exist unitary matrices  $U_A$  and  $U_B$  such that

$$U_A \sigma_j U_A^\dagger = \sum_{m=1}^3 O_{jm}^A \sigma_m, \quad (2.99)$$

$$U_B \sigma_k U_B^\dagger = \sum_{n=1}^3 O_{nk}^B \sigma_n. \quad (2.100)$$

Now we would like to show that the correlation tensor  $T$  can be diagonalised by a local unitary transformation acting on the state  $\tilde{\rho}$ , i.e.,

$$\rho = U_A \otimes U_B \tilde{\rho} U_A^\dagger \otimes U_B^\dagger, \quad (2.101)$$

where  $U_A$ ,  $U_B$  are unitary transformation respectively defined on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . It is useful to apply the transformation to each term appearing in [Equation \(2.96\)](#):

$$(U_A \otimes U_B) (\mathbb{I}_{AB}) \left( U_A^\dagger \otimes U_B^\dagger \right) = \mathbb{I}_{AB}. \quad (2.102)$$

The two local contributions transform as

$$\begin{aligned} (U_A \otimes U_B) \{(\vec{\tau}_A \cdot \vec{\sigma}) \otimes \mathbb{I}_B\} \left( U_A^\dagger \otimes U_B^\dagger \right) &= \sum_j (\vec{\tau}_A)_j U_A \sigma_j U_A^\dagger \otimes \mathbb{I}_B \\ &= \sum_{j,m} (\vec{\tau}_A)_j O_{jm}^A \sigma_m \otimes \mathbb{I}_B = \sum_m (\vec{\tau}_A O^A)_m \sigma_m \otimes \mathbb{I}_B \\ &= \vec{a} \cdot \vec{\sigma} \otimes \mathbb{I}_B \end{aligned} \quad (2.103)$$

and

$$(U_A \otimes U_B) \{ \mathbb{I}_A \otimes (\vec{\tau}_B \cdot \vec{\sigma}) \} \left( U_A^\dagger \otimes U_B^\dagger \right) = \mathbb{I}_A \otimes \vec{b} \cdot \vec{\sigma}, \quad (2.104)$$

where  $\vec{a} \equiv \vec{\tau}_A O^A$  and  $\vec{b} \equiv \vec{\tau}_B (O^B)^T$ . The last contribution comes from correlations:

$$\begin{aligned} (U_A \otimes U_B) \left\{ \sum_{j,k=1}^3 w_{jk} \sigma_j \otimes \sigma_k \right\} \left( U_A^\dagger \otimes U_B^\dagger \right) &= \sum_{jk} w_{jk} (U_A \sigma_j U_A^\dagger) \otimes (U_B \sigma_k U_B^\dagger) \\ &= \sum_{m,n=1}^3 \left( \sum_{j,k=1}^3 w_{jk} O_{jm}^A O_{nk}^B \right) (\sigma_m \otimes \sigma_n) = \sum_1^3 c_m (\sigma_m \otimes \sigma_m). \end{aligned} \quad (2.105)$$

Therefore, a generic two-qubit state can always be brought in the following form:

$$\rho = \frac{1}{4} \left\{ \mathbb{I}_{AB} + (\vec{a} \cdot \vec{\sigma}) \otimes \mathbb{I}_B + \mathbb{I}_A \otimes (\vec{b} \cdot \vec{\sigma}) + \sum_{j=1}^3 c_j \sigma_j \otimes \sigma_j \right\}, \quad (2.106)$$

where  $\vec{c}$  is the *correlation vector*, while  $\vec{a}$  and  $\vec{b}$  are the transformed local Bloch vectors. A special case is given by the so-called *Weyl states* (Friis, 2017), that are characterised by null local Bloch vectors. For these states, Equation (2.106) reads as

$$\rho = \frac{1}{4} \left( \mathbb{I}_4 + \sum_{j=1}^3 c_j \sigma_j \otimes \sigma_j \right). \quad (2.107)$$

Note that the marginal states are given  $\rho_a = \mathbb{I}/2$  and  $\rho_b = \mathbb{I}/2$ , representing maximally mixed states, with  $\mathbb{I}$   $d$ -dimensional identity matrix.

## 2.5 Complete Positivity and Entanglement

In Section 2.4.3, we have introduced the notion of entangled and separable states for bipartite systems. Entanglement is the non classical feature of quantum theory *par excellence*, that has informed the debate about the foundations of quantum mechanics since its early days, while, more recently, it has drawn a great deal of attention in relation to technological applications. Since a full account of this fascinating aspect of the theory is beyond the scopes of this work, we will just briefly discuss some of its main features, without going into details, that are covered, for example, in the review paper (Horodecki, 2009) (and references therein).

In general, the main issues of quantum entanglement theory concern its definition, its characterisation (in terms of suitable criteria), and its measure. For our purposes, it is sufficient to rely on the definition given in Section 2.4.3, as will focus on the bipartite case only. However, the definition given by Equation (2.89) is of very limited use, the latter being difficult to check in practical cases. It is therefore desirable to have an alternative characterisation of entanglement: this is, in general, a difficult problem to tackle, even in the simplest case of bipartite systems.

In this regard, it can be shown that positivity and complete positivity of a linear map constitute useful mathematical tools to infer properties about entanglement. Hence, besides the notion of positive map, we need to specify what we mean when we talk about complete positivity (Heinosaari, 2011). A linear map

$$\begin{aligned} \Lambda : \mathfrak{B}_1(\mathcal{H}) &\rightarrow \mathfrak{B}_1(\mathcal{H}) \\ \omega &\mapsto \Lambda(\omega) \end{aligned} \quad (2.108)$$

is *completely positive* (CP) if and only if the map

$$\begin{aligned}\Lambda \otimes \mathbb{I}_n : \mathfrak{B}_1(\mathcal{H} \otimes \mathbb{C}^n) &\rightarrow \mathfrak{B}_1(\mathcal{H} \otimes \mathbb{C}^n) \\ \omega \otimes \sigma_n &\mapsto \Lambda(\omega) \otimes \sigma_n\end{aligned}\tag{2.109}$$

is positive for any  $n \in \mathbb{N}$ , with  $\mathbb{I}_n$  identity operator on  $\mathbb{C}^n$ , and  $\sigma_n \in \mathfrak{L}(\mathbb{C}^n)$ .

It is not difficult to conclude that, if  $\Lambda$  is a positive map, and  $\rho$  is a product state, i.e.,  $\rho = \omega \otimes \chi$ , then  $(\Lambda \otimes \mathbb{I}_B)\rho = \Lambda(\omega) \otimes \chi$  is positive, even if  $\Lambda$  is not CP, as it is a tensor product of positive operators. By linearity, this can be naturally extended to all separable states. Horodecki *et al.* have recognised that the latter property is essential to detect entangled states; in other terms, it has been proven that the positivity of  $(\Lambda \otimes \mathbb{I}_B)\rho \geq 0$  is a necessary condition for the separability of the state  $\rho$ , while its non-positivity is mathematically sufficient to conclude that  $\rho$  is entangled (Horodecki, 1996).

### Example 2.5.1: Partial Transposition

An example of map that is positive, but not CP, is provided by partial transposition. Since, in order to define the partial transpose we need to fix a basis, we will consider an explicit example. Let us consider a pair of qubits in the Bell state  $|\phi^+\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ , defined by Equation (2.91). By using the computational basis, we can construct the following density operator:

$$\begin{aligned}\rho_{\phi^+} \equiv |\phi^+\rangle \langle \phi^+| &= \frac{1}{2} \left( |0\rangle \langle 0| \otimes |0\rangle \langle 0| + |1\rangle \langle 1| \otimes |1\rangle \langle 1| \right. \\ &\quad \left. + |0\rangle \langle 1| \otimes |0\rangle \langle 1| + |1\rangle \langle 0| \otimes |1\rangle \langle 0| \right)\end{aligned}\tag{2.110}$$

If we adopt the standard representation  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ ,  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , we can represent  $\rho_{\phi^+}$  as a matrix in  $\mathcal{M}_4(\mathbb{C})$

$$\rho_{\phi^+} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.\tag{2.111}$$

The spectrum of this positive-definite matrix is given by  $\{1, 0, 0, 0\}$ . Moreover, by using Equation (2.12), one obtains  $\|\rho_{\phi^+}\|_1 = 1$ , as required by the definition of density operator.

Let us apply the partial transposition with respect to the first qubit, i.e.,

$$\begin{aligned}\rho_{\phi^+}^{T_A} \equiv (T_A \otimes \mathbb{I}_B) \rho_{\phi^+} &= \frac{1}{2} \left( |0\rangle \langle 0| \otimes |0\rangle \langle 0| + |1\rangle \langle 1| \otimes |1\rangle \langle 1| \right. \\ &\quad \left. + |0\rangle \langle 1| \otimes |1\rangle \langle 0| + |1\rangle \langle 0| \otimes |0\rangle \langle 1| \right),\end{aligned}\tag{2.112}$$

or, using the corresponding matrix representation,

$$\rho_{\phi^+}^{T_A} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (2.113)$$

The spectrum of  $\rho_{\phi^+}^{T_A}$  is given by  $\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\}$ , therefore we are left with a negative object. Moreover, one has  $\|\rho_{\phi^+}^{T_A}\|_1 = 2$ .

Therefore, with the help of this example, we can conclude that partial transposition is a positive, but not CP, map. As a byproduct, we have also shown an example of non-trace-preserving map: the presence of negative eigenvalues for  $\rho_{\phi^+}^{T_A}$  leads to the increase of the trace norm.

The Example 2.5.1 can be considered as a sort of guiding line in our quest for entanglement characterisation. Indeed, Peres proved that a strong necessary condition for separability is provided by the Positive Partial Transpose (PPT) criterion (Peres, 1996). According to the latter, if  $\rho \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$  is separable, then  $\rho^{T_A}$  is a density operator itself, i.e., it has a non-negative spectrum.

The PPT criterion can also be a sufficient condition for separability, depending on the dimensions  $d_A$  and  $d_B$  of the two subsystems. Horodecki (Horodecki, 1997) proved that, if  $d_A d_B \leq 6$  (i.e., if we deal with two-qubit or qubit-qutrit systems), states are separable if and only if they are PPT. For these systems, the PPT – also known as Peres-Horodecki – criterion provides a complete characterisation of separable states.

### Entanglement negativity

As a result, the PPT criterion not only provides a necessary condition for separability of a bipartite state, but its violation constitutes also a sufficient condition for entanglement. This naturally suggests a computable measure of entanglement, based on the trace norm of the partially transposed matrix. We can indeed define the *entanglement negativity* (or simply *negativity*) of a bipartite state  $\rho$  in the following manner (Vidal, 2002):

$$\mathcal{N}(\rho) \equiv \|\rho^{T_A}\|_1 - 1, \quad (2.114)$$

that, in general, is given by the absolute value of the sum of the negative eigenvalues, i.e.,  $\mathcal{N}(\rho) = 2 |\sum_i \mu_i|$ . The rationale behind this formula can be intuitively explained as follows:  $\mathcal{N}(\rho)$  essentially measures the degree to which  $\rho^{T_A}$  fails to be positive. Indeed, if  $\rho$  is separable, then  $\rho^{T_A}$  is itself a state, thus  $\|\rho^{T_A}\|_1 = 1$ , and  $\mathcal{N}(\rho) = 0$ ; by contrast, if  $\rho$  is entangled, the condition  $\text{tr}_A(\rho^{T_A}) = 1$  still holds, but  $\mathcal{N}(\rho) \neq 0$ .

In particular,  $\mathcal{N}(\rho)$  can be employed as a good measure of entanglement for two-qubit systems, i.e.,  $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ . If  $\mu_{\min}$  is the smallest eigenvalue of  $\rho^{T_A}$ , the entanglement negativity is

given by

$$\mathcal{N}(\rho) = 2 \max\{-\mu_{\min}, 0\}. \quad (2.115)$$

### Example 2.5.2: Werner states

A Werner state is given by (Werner, 1989; Benenti, 2007):

$$\rho_W = \frac{1}{4} (1 - c) \mathbb{I} + c |\psi^-\rangle\langle\psi^-|, \quad (2.116)$$

where  $0 \leq c \leq 1$ , and  $|\psi^-\rangle$  is defined by Equation (2.92), and  $\mathbb{I}$  is the 4 identity matrix. In other terms, a Werner state  $\rho_W$  can be regarded as an incoherent mixture of the maximally entangled Bell state  $|\psi^-\rangle$  with probability  $c$  and the maximally mixed state  $\frac{1}{4}\mathbb{I}$ .

In the computational basis, the matrix  $\rho_W$  is given by:

$$\rho_W = \frac{1}{4} \begin{pmatrix} 1 - c & 0 & 0 & 0 \\ 0 & 1 + c & -2c & 0 \\ 0 & -2c & 1 + c & 0 \\ 0 & 0 & 0 & 1 - c \end{pmatrix}. \quad (2.117)$$

In order to resort the PPT criterion, we need to compute the partial transpose:

$$(\rho_W)^{T_A} = \frac{1}{4} \begin{pmatrix} 1 - c & 0 & 0 & -2c \\ 0 & 1 + c & 0 & 0 \\ 0 & 0 & 1 + c & 0 \\ -2c & 0 & 0 & 1 - c \end{pmatrix}, \quad (2.118)$$

whose eigenvalues are given by  $\mu_1 = \mu_2 = \mu_3 = \frac{1+c}{4}$ , and  $\mu_4 = \frac{1-3c}{4}$ . By using Equation (2.115), we get  $\mathcal{N}(\rho) = 2 \max\{\frac{3c-1}{4}, 0\}$ . More explicitly:

$$\mathcal{N}(\rho) = \begin{cases} 0 & \text{if } 0 \leq c \leq \frac{1}{3} \\ \frac{3c-1}{2} & \text{if } \frac{1}{3} < c \leq 1 \end{cases}. \quad (2.119)$$

Therefore,  $\rho_W$  is separable if  $0 \leq c \leq \frac{1}{3}$ , while it is entangled for  $\frac{1}{3} < c \leq 1$ .

### 2.5.1 Linear maps and complete positivity

In this Section, we would like to consider the general case of a linear map and introduce an important characterisation of CP maps. The request of complete positivity is, at the same time, mathematically crucial and physically natural when we consider the scenario in which a quantum systems is interacting with an environment. Indeed, it guarantees that

our description is physically consistent against possible couplings with finite-dimensional extensions of the main system (Kraus, 1983; Benatti, 2005).

Let us consider a finite-dimensional system, i.e.,  $\mathcal{H} = \mathbb{C}^n$ . Given the canonical basis is given by  $\{|e_j\rangle\}_{1 \leq j \leq n}$ , we can construct the corresponding basis of operators  $E_{ij} \equiv |e_j\rangle\langle e_k|$ , whose elements can be represented by matrices in  $\mathcal{M}_n(\mathbb{C})$ . Let us consider the maximally entangled state

$$|\psi\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |e_j\rangle \otimes |e_j\rangle, \quad (2.120)$$

that allows us to construct the following operator:

$$\frac{1}{n} X \equiv \frac{1}{n} \sum_{j,k=1}^n E_{jk} \otimes E_{jk} = |\psi\rangle\langle\psi|, \quad (2.121)$$

which is positive.

An important characterisation of CP maps is given by a theorem due to Choi, that rephrase the problem of checking the complete positivity of a map in terms of the positivity of a certain matrix, known a Choi matrix (Choi, 1975). In this perspective, given a linear map  $\Lambda : \mathcal{M}_n(\mathbb{C}) \rightarrow \mathcal{M}_d(\mathbb{C})$ , the following statements are equivalent (Heinosaari, 2011):

- (i)  $\Lambda$  is CP;
- (ii)  $\Lambda$  is  $n$ -positive, i.e.,  $\Lambda \otimes \mathbb{I}_n$  is a positive map;
- (iii) for any orthonormal basis  $\{|e_j\rangle\}$  in  $\mathbb{C}^n$ , the following matrix:

$$\Phi_\Lambda = \begin{pmatrix} \Lambda(|e_1\rangle\langle e_1|) & \dots & \Lambda(|e_1\rangle\langle e_n|) \\ \vdots & \ddots & \vdots \\ \Lambda(|e_n\rangle\langle e_1|) & \dots & \Lambda(|e_n\rangle\langle e_n|) \end{pmatrix}, \quad (2.122)$$

known as *Choi matrix*, is positive.

Note that the implication (i)  $\implies$  (ii) follows trivially from the definition of CP map. We can easily prove that (ii)  $\implies$  (iii), by applying the map  $\Lambda \otimes \mathbb{I}_n$  on the positive operator  $X$  defined by Equation (2.121) through a maximally entangled state. It is indeed immediate to conclude that  $\Phi_\Lambda = \Lambda \otimes \mathbb{I}_n(X)$  is positive.

The proof that the positivity of the Choi matrix implies the complete positivity of  $\Lambda$ , i.e., (iii)  $\implies$  (i), is a bit more involved. To this end, we can let  $\Phi_\Lambda$  act on the operator  $X$ :

$$\Phi_\Lambda = \Lambda \otimes \mathbb{I}_n(X) = \sum_{k,q}^n \Lambda(|e_k\rangle\langle e_q|) \otimes |e_k\rangle\langle e_q| = \sum_{k,q}^n \Lambda(E_{kq}) \otimes E_{kq}, \quad (2.123)$$

and, since we are assuming that  $\Phi_\Lambda$  is a positive matrix, we can diagonalise it and write:

$$\Phi_\Lambda = \sum_{j=1}^{nd} |v_j\rangle\langle v_j|, \quad (2.124)$$

with  $|v_j\rangle \in \mathbb{C}^n \otimes \mathbb{C}^d$  non-normalised eigenvectors. Now, bearing in mind that a  $n \times d$  matrix can be regarded as a  $n \times n$  matrix, whose entries are  $d \times d$  matrix<sup>8</sup>, the eigenvectors  $|v_j\rangle$  can be expressed as

$$|v_j\rangle = \sum_{k=1}^n |v_{ij}\rangle \otimes |e_k\rangle. \quad (2.125)$$

We can thus define the operator:

$$\begin{aligned} V_j : \mathbb{C}^n &\rightarrow \mathbb{C}^d \\ e_k &\mapsto |v_{jk}\rangle \equiv V_j |e_k\rangle, \end{aligned} \quad (2.126)$$

and obtain

$$\begin{aligned} \Phi_\Lambda &= \sum_{j=1}^{nd} \sum_{k,q=1}^n |v_{jk}\rangle\langle v_{jq}| \otimes |e_k\rangle\langle e_q| = \sum_{j=1}^{nd} \sum_{k,q=1}^n V_j |e_k\rangle\langle e_q| V_j^\dagger \otimes |e_k\rangle\langle e_q| \\ &= \sum_{j=1}^{nd} \sum_{k,q=1}^n V_j E_{kq} V_j^\dagger \otimes E_{kq} \end{aligned} \quad (2.127)$$

By comparing Equations (2.123) and (2.127), we get

$$\Lambda(E_{kq}) = \sum_{j=1}^{nd} V_j E_{kq} V_j^\dagger, \quad (2.128)$$

which is positive, thus completely positivity follows.

The Choi theorem suggests that there is a correspondence – known as *Choi-Jamiołkowski isomorphism* ([Jamiołkowski, 1972](#); [Choi, 1975](#)) – between completely positive maps  $\Lambda : \mathcal{M}_n(\mathbb{C}) \rightarrow \mathcal{M}_d(\mathbb{C})$  (represented by matrices with positive entries) and linear operators in  $\mathbb{C}^d \otimes \mathbb{C}^n$ .

Moreover, the constructive proof of the Choi theorem that we have just presented naturally leads to a useful characterisation of CP maps. Indeed, extending by linearity Equation (2.128), we obtain a similar representation for a generic map  $\Lambda$ :

$$\Lambda(\omega) = \sum_{\mu} K_{\mu} \omega K_{\mu}^\dagger, \quad (2.129)$$

---

<sup>8</sup>In other terms, we are relying on the fact that  $\mathbb{C}^{nd \times nd} \cong \mathbb{C}^{n \times n} \otimes \mathbb{C}^{d \times d}$ .

where the index  $\mu$  runs over a finite set (for finite-dimensional systems), or over a countable set (for infinite-dimensional systems). This representation is known as *Kraus-Stinespring representation* or, alternatively, *operator-sum representation*, while the operators  $K_\mu$  are called *Kraus operators* (Kraus, 1983; Benatti, 2005). The fact that  $\Lambda$  can be written in such a form constitutes a necessary and sufficient condition for  $\Lambda$  to be CP. As we will realise in [Chapter 3](#), this result is particularly useful in the theory of open quantum systems.

# Chapter 3

## Dynamical maps and master equations

In this Chapter, we review some important notions in the theory of open quantum systems, that we will employ in the next Chapters to introduce the standard tools for microscopically deriving dynamical equations ([Chapter 4](#)), and to discuss some specific problems, such as the characterisation of nonequilibrium dynamics in terms of entropy production ([Chapter 5](#)), or the simulation of the dynamics beyond standard regimes ([Chapter 6](#)). In the following Sections, we will see that a consistent description of the open system dynamics can be either expressed in terms of maps or in terms of equations. The former are particularly useful to characterise general properties of the dynamics, such as, for instance, the presence of absence of memory effects, while the latter represents a standard way to look at the system evolution and evaluate physical quantities. Although the contents presented in this Chapter are well-established results, they are presented in such a way that emphasis is given to the limitations imposed by the usual construction of a quantum dynamical semigroup. As we will see in the following Chapters, the standard approach, based on the weak coupling and memoryless approximations, is indeed quite restrictive, and fails to apply to a broader variety of processes that are physically interesting.

### 3.1 Quantum dynamical maps

In [Chapter 2](#), we have discussed some important features of abstract linear maps. Now, we would like to apply those mathematical tools to the description of the dynamics of quantum systems. If we assume the latter to be formally described by a linear map, our first concern is that physical states gets mapped into physical states. This justifies the definition of a *quantum dynamical map* as ([Alicki, 2007](#); [Asorey, 2009](#))

$$\begin{aligned}\Lambda_{t,t_0} : \mathcal{S}(\mathcal{H}) &\rightarrow \mathcal{S}(\mathcal{H}) \\ \rho(t_0) &\mapsto \rho(t) = \Lambda_{t,t_0}\rho(t_0),\end{aligned}\tag{3.1}$$

that preserves self-adjointness, positivity, and trace (i.e.,  $\mathrm{Tr} \rho(t_0) = 1 = \mathrm{Tr} \rho(t)$ ). However, these requirements are not enough, as we need to add the stronger condition of complete positivity, a genuine quantum requirement that protects us against the consequences of potential entanglement with possible extensions of our system. In [Section 2.5](#), we have seen that a necessary and sufficient condition for the complete positivity of a map is for it to be in the Kraus-Stinespring form ([Kraus, 1983](#)), i.e.,

$$\Lambda_{t,t_0} \rho(t_0) = \sum_{\mu} K_{\mu} \rho(t_0) K_{\mu}^{\dagger}, \quad \rho \in \mathcal{S}(\mathcal{H}), \quad (3.2)$$

where the operators  $K_{\mu}$  can either form a finite or infinite sequence ([Heinosaari, 2011](#)). If we impose trace preservation, we automatically get a constraint on the Kraus operators, i.e.,

$$\sum_{\mu} K_{\mu}^{\dagger} K_{\mu} = \mathbb{I}. \quad (3.3)$$

In [Section 2.1](#), we have seen that a linear mapping on  $\mathfrak{B}_1(\mathcal{H})$  induces a linear mapping on the dual space  $\mathfrak{B}(\mathcal{H})$ . In our case, the dynamical map  $\Lambda_{t,t_0}$  induces the dual map

$$\Lambda_{t,t_0}^* : \mathfrak{B}(\mathcal{H}) \rightarrow \mathfrak{B}(\mathcal{H}), \quad (3.4)$$

that are related by the following *duality relation* ([Breuer, 2002; Benatti, 2005](#))

$$\mathrm{Tr}(A \Lambda_{t,t_0} \rho(t_0)) = \mathrm{Tr}(\Lambda_{t,t_0}^*[A] \rho(t_0)), \quad (3.5)$$

where  $A$  is a bounded operator. This formula is a direct consequence of the isomorphism in [Equation \(2.8\)](#). From a physical perspective, the latter formally establishes a correspondence between states and observables. In the dual space, we have the equivalent of [Equation \(3.2\)](#), i.e.,

$$\Lambda_{t,t_0}^*[A] = \sum_{\mu} K_{\mu}^{\dagger} A K_{\mu}, \quad A \in \mathfrak{B}(\mathcal{H}), \quad (3.6)$$

whence we deduce that trace preservation is equivalent to request that  $\Lambda_{t,t_0}^*$  is *unital*, i.e.,  $\Lambda_{t,t_0}^*[\mathbb{I}] = \mathbb{I}$ .

### 3.1.1 Closed systems

In the standard presentation of quantum mechanics, we usually consider the case of a closed system, i.e., a system that is perfectly isolated from the surroundings. In this scenario, the system evolves unitarily over time according to

$$\rho(t_0) \rightarrow \rho(t) = \mathcal{U}_{t,t_0} \rho(t_0) \equiv U_{t,t_0} \rho(t_0) U_{t,t_0}^{\dagger}, \quad (3.7)$$

where  $U_{t,t_0} = e^{-iH(t-t_0)}$  is the time evolution operator (henceforth, we will always work in units such that  $\hbar = 1$ ), and  $H$  the (time-independent) system Hamiltonian. By comparing

Equations (3.2) and (3.7), one can conclude that, for closed systems, one has the simplest non-trivial dynamical map, where the only Kraus operator is given by  $U_{t,t_0}$ . Equation (3.5) defines the following dual map

$$A \mapsto \mathcal{U}_{t,t_0}^*[A] = U_{t,t_0}^\dagger A U_{t,t_0} \equiv A_H(t). \quad (3.8)$$

Hence, going from Equation (3.7) to (3.8), we are transferring the time dependence from states (density operators) to observables (i.e., bounded operators); in other terms, we are going from the Schrödinger to the Heisenberg picture.

One last comment is about irreversibility (Sudarshan, 1961; Wehrl, 1978). First, a unitary evolution transforms pure states into pure states; indeed, from Equation (2.6) it follows that  $\text{Tr}[\rho^2(t)] = \text{Tr}[\rho^2(t_0)]$ . In addition, we have  $U_{t,t_0}^\dagger = U_{t,t_0}^{-1}$ , meaning that the underlying dynamics is perfectly reversible. This feature is confirmed by looking at the von Neumann entropy: as the latter is invariant under unitary transformations, we have  $S(\rho(t)) = S(\rho(t_0))$ . This mathematical evidence needs to be contrasted with the second law of thermodynamics, according to which the entropy of a closed systems is non-decreasing. In other terms, we need to consistently treat problems of irreversibility or relaxation in the domain of quantum mechanics. The possible way out is provided by a different, more general, description of the dynamics, that includes dissipation or the genuinely quantum phenomenon of *decoherence* (Breuer, 2002; Zurek, 2003).

### 3.1.2 Open quantum systems

In order to get a more realistic description of the dynamics of a quantum system, we need to relax the hypothesis of a system dynamically isolated from the surroundings. This leads to the concept of open quantum system, i.e., a system interacting with another (usually much larger) system, that we will call environment (Breuer, 2002; Rivas, 2012). Let us suppose that  $\mathcal{H}_S$  and  $\mathcal{H}_E$  are the Hilbert spaces associated with the main system  $S$  and its environment  $E$ , respectively. The Hamiltonian of the whole system reads

$$H(t) = H_S(t) \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E(t) + H_I(t), \quad (3.9)$$

where  $H_S$  and  $H_E$  are the Hamiltonian of the system and the environment, respectively, while  $H_I$  describes the interaction between them.

A generic joint state  $\rho_{SE} \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E)$  can contain correlations between the two parties of the composite system, therefore, at time  $t = t_0$ , we can write:

$$\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0) + \chi(t_0), \quad (3.10)$$

where  $\chi(t_0)$ , accounting for correlations between  $S$  and  $E$ , is not a state and satisfies the condition  $\text{tr}_S[\chi(t_0)] = 0 = \text{tr}_E[\chi(t_0)]$ .

It is customary to assume that the joint system  $S + E$  evolves unitarily according to the following:

$$\rho_{SE}(t) = \mathcal{U}_{t,t_0} \rho_{SE}(t_0) = U_{t,t_0} \rho_{SE}(t_0) U_{t,t_0}^\dagger = U_{t,t_0} [\rho_S(t_0) \otimes \rho_E(t_0) + \chi(t_0)] U_{t,t_0}^\dagger, \quad (3.11)$$

where the time evolution operator is given by

$$U_{t,t_0} = \mathcal{T}_{\leftarrow} \exp \left[ -i \int_{t_0}^t H(\tau) d\tau \right], \quad (3.12)$$

denoting as  $\mathcal{T}_{\leftarrow}$  the chronological time operator, that orders product of time-dependent operators such that their time-arguments increase from right to left.

However, our interest is devoted to the reduced dynamics, for which we would like to obtain a dynamical map  $\Lambda_{t,t_0}$  acting on the state  $\rho_S(t)$ , by tracing over the environmental degrees of freedom, i.e.,

$$\rho_S(t) = \Lambda_{t,t_0} \rho_S(t_0) \equiv \text{tr}_E \{ \rho_{SE}(t) \} = \text{tr}_E \left\{ U_{t,t_0} [\rho_S(t_0) \otimes \rho_E(t_0) + \chi(t_0)] U_{t,t_0}^\dagger \right\}. \quad (3.13)$$

Note that a fixed environmental state  $\rho_E(t_0)$  can be expressed through its spectral decomposition, i.e.,  $\rho_E(t_0) = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ , thus [Equation \(3.13\)](#) can be rewritten as

$$\begin{aligned} \rho_S(t) &= \sum_j \lambda_j \text{tr}_E \left\{ U_{t,t_0} [\rho_S(t_0) \otimes |\psi_j\rangle\langle\psi_j|] U_{t,t_0}^\dagger \right\} + \text{tr}_E \left\{ U_{t,t_0} \chi(t_0) U_{t,t_0}^\dagger \right\} \\ &= \sum_{j,k} \lambda_j \langle \psi_k | U_{t,t_0} | \psi_j \rangle \rho_S(t_0) \langle \psi_j | U_{t,t_0}^\dagger | \psi_k \rangle + \text{tr}_E \left\{ U_{t,t_0} \chi(t_0) U_{t,t_0}^\dagger \right\} \end{aligned} \quad (3.14)$$

By introducing  $\delta\rho(t, t_0) \equiv \text{tr}_E \{ U_{t,t_0} \chi(t_0) U_{t,t_0}^\dagger \}$ , and the following operators:

$$K_\mu(t, t_0) \equiv \sqrt{\lambda_j} \langle \psi_k | U_{t,t_0} | \psi_j \rangle, \quad (3.15)$$

where  $\mu \equiv \{k, j\}$ , we eventually get

$$\rho_S(t) = \Lambda_{t,t_0} \rho_S(t_0) = \sum_\mu K_\mu(t, t_0) \rho_S(t_0) K_\mu^\dagger(t, t_0) + \delta\rho(t, t_0). \quad (3.16)$$

Following from the definitions, we aim at obtaining a CP dynamical map  $\Lambda_{t,t_0}$ , therefore it has to be in the Kraus form [\(3.2\)](#). In order to retrieve the latter, we need to choose states such that the inhomogeneous part  $\delta\rho(t, t_0)$  is vanishing, i.e., such that  $\chi(t_0) = 0$ . This choice also carries one more important feature: the map  $\Lambda_{t,t_0}$  is universal ([Rivas, 2012](#)), in the sense that is independent of the state it acts upon. Indeed, our map would clearly bear dependence on the particular choice of the initial state  $\rho_S(t_0)$ , were  $\chi(t_0)$  non-zero ([Štelmachovič, 2001](#)). On a more general note, it is still an open question to ascertain a general relation between the form of the initial correlated state  $\rho_{SE}$  and the corresponding open system dynamics<sup>1</sup> ([de Vega, 2017](#)).

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<sup>1</sup>Historically, this issue has raised an intense debate within the open quantum systems community, through the voices of Pechukas and Alicki ([Pechukas, 1994](#); [Alicki, 1995](#)): the former challenged the usual picture of open system dynamics, showing that initially correlated states might generate evolutions that violate the requirement of complete positivity; in response, the latter argued that all physical meaningful states lead to CP maps.

$$\begin{array}{ccc}
\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E & \xrightarrow{\text{unitary evolution}} & \rho(t) = \mathcal{U}_{t,t_0} \rho_{SE}(t_0) \\
\downarrow \text{tr}_E & & \downarrow \text{tr}_E \\
\rho_S(t_0) & \xrightarrow{\text{dynamical map}} & \rho_S(t) = \Lambda_{t,t_0} \rho_S(t_0)
\end{array}$$

**Figure 3.1:** Open quantum system evolution.

In light of the previous observations, we will consider initially non correlated states, i.e., states in the tensor product form

$$\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0), \quad (3.17)$$

so that we eventually get a legitimate dynamical map of the form

$$\rho_S(t) = \Lambda_{t,t_0} \rho_S(t_0) = \sum_{\mu} K_{\mu}(t, t_0) \rho_S(t_0) K_{\mu}^{\dagger}(t, t_0), \quad (3.18)$$

where the operators  $K_{\mu}$ , depending only on the global unitary evolution and the initial state of the environment, are Kraus operators that automatically fulfil the condition  $\sum_{\mu} K_{\mu} K_{\mu}^{\dagger} = \mathbb{I}_S$ . What we have illustrated so far can be effectively summarised by the diagram in [Figure 3.1](#).

Owing to the duality relation [Equation \(3.5\)](#), one can also define the time evolution of an operator in the Heisenberg picture by applying the dual map  $\Lambda_{t,t_0}^*$ , i.e.,

$$A_H(t) = \Lambda_{t,t_0}^* A, \quad (3.19)$$

where  $A$  is the operator in the Schrödinger picture.

In order to show how this description in terms of dynamical maps encompasses irreversibility, we should discuss the invertibility of the dynamical map  $\Lambda_{t,t_0}$ . Physically, this is associated with the possibility of going backwards in time through a well-defined dynamical map  $\Lambda_{t_0,t}$  such that

$$\Lambda_{t_0,t} \circ \Lambda_{t,t_0} = \Lambda_{t,t_0}^{-1} \circ \Lambda_{t,t_0} = \mathbb{I}. \quad (3.20)$$

The relevant point to make is that, even if the inverse map  $\Lambda_{t,t_0}^{-1}$  exists, there is no guarantee that it is a proper Completely Positive Trace Preserving (CPTP) map. In this regard, one can show ([Rivas, 2012](#)) that a CPTP dynamical map can be inverted, obtaining another CPTP map if and only if it is unitary. Since this is not always the case, the formalism outlined above naturally embeds the irreversibility of open system dynamics.

There is one more thorny issue that we cannot leave unmentioned at this stage and it has to do with the existence of a composition law for dynamical maps. Let us suppose that  $t_0 < t_1 < t_2$  and that we are given with two legitimate dynamical maps  $\Lambda_{t_1,t_0}$  and  $\Lambda_{t_2,t_1}$ , that transform reduced states of the system from  $t_0$  to  $t_1$  and from  $t_1$  to  $t_2$ , respectively. Intuitively

one would anticipate that the full evolution from  $t_0$  to  $t_1$  is given by composition of the two previous maps, i.e.,

$$\Lambda_{t_2,t_0} = \Lambda_{t_2,t_1} \circ \Lambda_{t_1,t_0}, \quad (3.21)$$

but this is not, in general, the case. To further corroborate this statement, we observe that the two maps  $\Lambda_{t_1,t_0}$  and  $\Lambda_{t_2,t_0}$  can be expressed in Kraus form of (3.18), as we are assuming that  $\rho(t_0)$  is in a product state. By contrast, we should define the map

$$\Lambda_{t_2,t_1}\rho_S(t_1) \equiv \text{tr}_E \left[ U_{t_2,t_1} \rho_{SE}(t_1) U_{t_2,t_1}^\dagger \right], \quad (3.22)$$

that, in general, is not a CP map, neither is it independent of  $\rho(t_1)$ , as we have observed about Equation (3.16). This is actually something that we would physically expect, because, as the system evolves, correlations between system and environment are inevitably built up, thus, we are no longer in the position of assuming that  $\rho_{SE}(t_1)$  is a product state.

## 3.2 From maps to equations

In the previous Section, we have seen that the evolution of a quantum system can be described in terms of a suitable dynamical map, that is completely positive and preserves the trace. This perspective offers valuable insight for characterising intrinsic properties of the dynamics, such as, for instance, its Markovian character or lack thereof (Breuer, 2016), but more often one is interested in solving dynamical equations. In the following Sections, we illustrate the way the former are related to the latter.

### 3.2.1 Unitary evolution group

Let us start with the familiar case of a closed quantum system governed by a unitary dynamics. In Section 3.1.1, we have seen that the unitary map  $\mathcal{U}_{t,t_0}$  is invertible, therefore, from Equation (3.7) we obtain

$$\dot{\rho}(t) = \dot{\mathcal{U}}_{t,t_0} \rho(t_0) = \dot{\mathcal{U}}_{t,t_0} \circ \mathcal{U}_{t,t_0}^{-1} \rho(t), \quad (3.23)$$

where  $\dot{\mathcal{U}}_{t,t_0} = \partial_t \mathcal{U}_{t,t_0}$ . A simple calculation yields the following dynamical equation:

$$\dot{\rho}(t) = -i[H, \rho(t)] \equiv \mathcal{L}_H[\rho], \quad (3.24)$$

known as *Liouville - von Neumann* (or simply *von Neumann*) *equation*, which is the equivalent – in the language of density operators – of the Schrödinger equation, while  $\mathcal{L}_H$  is the *Liouvillian* (or *Liouville operator*).

Analogously, the unitary map satisfies a similar differential equation

$$\dot{\mathcal{U}}_{t,t_0} = \mathcal{L}_H[\mathcal{U}_{t,t_0}], \quad (3.25)$$

with the initial condition  $\mathcal{U}_{t_0,t_0} = \mathbb{I}$ , whose formal solution is given by:

$$\mathcal{U}_{t,t_0} = e^{(t-t_0)\mathcal{L}_H}. \quad (3.26)$$

Since  $\mathcal{U}_{t,t_0}$  only depends on the difference  $t - t_0$ , we can define  $\mathcal{U}_t \equiv \mathcal{U}_{t,t_0}$ , or, equivalently, always assume that  $t_0 = 0$ . To summarise, using this notation, a unitary map  $\mathcal{U}_t$  satisfies the following properties:

- (i)  $\mathcal{U}_{t_1} \circ \mathcal{U}_{t_2} = \mathcal{U}_{t_1+t_2}$ ;
- (ii) there exists  $\mathcal{U}_t^{-1}$  such that  $\mathcal{U}_t^{-1} \circ \mathcal{U}_t = \mathcal{U}_t \circ \mathcal{U}_t^{-1} = \mathbb{I}$ .

Therefore, we can introduce a collection of unitary maps  $\{\mathcal{U}_t\}_{t \geq 0}$ , with  $\mathcal{U}_{t=0} = \mathbb{I}$ , that defines a one-parameter *unitary evolution group*: the existence of its generator is guaranteed by Stone's theorem (Teschl, 2014).

### Heisenberg picture

Owing to the duality relation [Equation \(3.5\)](#), we can introduce the group  $\{\mathcal{U}_t^*\}_{t \geq 0}$ , isomorphic to  $\{\mathcal{U}_t\}_{t \geq 0}$ , that describes the evolution of the physical system in the Heisenberg picture. As a consequence, the dynamical equation for an observable in the Heisenberg picture is given by

$$\dot{A}_H(t) = i[H, A_H(t)] \equiv \mathcal{L}_H^*[A_H(t)]. \quad (3.27)$$

Let us suppose that we need to track over time a certain (explicitly time-dependent) observable, say  $A(t)$ , in the Schrödinger picture. To this end, it is worth noticing that, in the Heisenberg picture, the expectation values are determined through the fixed density operator  $\rho_H(t_0)$ , hence

$$\langle A(t) \rangle = \text{Tr}(A(t)\rho(t_0)) = \text{Tr}(A_H(t)\rho_H(t_0)). \quad (3.28)$$

Taking the derivative with respect to time and using [Equation \(3.27\)](#), we get

$$\frac{d}{dt}\langle A(t) \rangle = \text{Tr} \left\{ \left( i[H, A_H(t)] + \frac{\partial A}{\partial t} \right) \rho_H(t_0) \right\}, \quad (3.29)$$

sometimes referred to as Ehrenfest theorem.

### 3.2.2 Quantum dynamical semigroup

Let us now generalise the previous discussion to the case of non-Hamiltonian dynamics linked to open systems. In the same spirit as of unitary evolution, we can introduce a one-parameter family  $\{\Lambda_t\}_{t \geq 0}$  of dynamical maps, with  $\Lambda_{t=0} = \mathbb{I}$ . We would like to assess what kind of mathematical structure can be defined for this instance.

Let us consider a two-parameter family of dynamical maps given by:

$$\Lambda_{t,s} = \Lambda_t \circ \Lambda_s^{-1}, \quad 0 \leq s \leq t, \quad (3.30)$$

such that

$$\Lambda_t = \Lambda_{t,s} \circ \Lambda_s. \quad (3.31)$$

This definition is non-trivial because of the following remarks.

- In general, the inverse map  $\Lambda_t^{-1}$  does not exist. As we will see later on, the class of processes for which  $\Lambda_t^{-1}$  exists lead to a time-local dynamical equation for the open system.
- If the inverse map exists, in general it is not even guaranteed to be positive.

This motivates the following definition: a dynamical map  $\Lambda_t$  given by [Equation \(3.31\)](#) is said to be *P-divisible* or *CP-divisible* if and only if  $\Lambda_{t,s}$  is positive or completely positive, respectively ([Breuer, 2016](#)).

In general, the divisibility property [Equation \(3.31\)](#) can be rewritten as

$$\Lambda_{t,s} = \Lambda_{t,\tau} \circ \Lambda_{\tau,s}, \quad 0 \leq s \leq \tau \leq t, \quad (3.32)$$

which represents the quantum analogue of the Chapman-Kolmogorov equation for classical stochastic processes ([Gardiner, 2009](#); [Vacchini, 2011](#)).

Although proposals based on P-divisibility have been put forward ([Wißmann, 2015](#); [Breuer, 2016](#)), for our purposes we can assume that CP-divisibility is a necessary and sufficient condition for the system dynamics to be *Markovian*, or, as sometimes referred to, *memoryless*. We can thus define a *quantum dynamical semigroup* as a collection of one-parameter CTPT maps  $\{\Lambda_t\}_{t \geq 0}$ , with  $\Lambda_{t=0} = \mathbb{I}$ , satisfying the following homogeneous composition law ([Kossakowski, 1972](#)):

$$\Lambda_{t+s} = \Lambda_t \circ \Lambda_s, \quad s, t \geq 0. \quad (3.33)$$

The semigroup structure is consistent with the irreversible character of the dynamics.

Furthermore, we have to discuss two main mathematical issues: one related to the existence of the generator of this semigroup, the other to the form of the most general generator of this semigroup. Although the formulation of the problem looks simple, the general answers to these questions still constitute open problems ([Chruściński, 2014](#)).

Let us suppose that the dynamical map  $\Lambda_t$  is invertible – i.e., there exists  $\Lambda_t^{-1}$  such that  $\Lambda_t^{-1} \circ \Lambda_t = \Lambda_t \circ \Lambda_t^{-1} = \mathbb{I}$ ; by differentiating  $\rho_t = \Lambda_t \rho(0)$ , one obtains

$$\dot{\rho}(t) = \mathcal{L}[\rho(t)], \quad (3.34)$$

where we have defined the generator  $\mathcal{L} \equiv \dot{\Lambda}_t^{-1} \circ \Lambda_t$ . [Equation \(3.34\)](#) is usually called *master equation*, which is the non-Hamiltonian counterpart of [Equation \(3.24\)](#). The corresponding map  $\Lambda_t$  satisfies the differential equation

$$\dot{\Lambda}_t = \mathcal{L}[\Lambda_t], \quad \Lambda_0 = \mathbb{I}, \quad (3.35)$$

whose formal solution is  $\Lambda_t = e^{t\mathcal{L}}$ .

Under rather general assumptions<sup>2</sup>, the Hille-Yoshida theorem (Yoshida, 1995) warrants the existence of the generator  $\mathcal{L}$ . In relation to the form of such a generator, in the subclass of CP maps, a crucial result is given by the celebrated Gorini, Kossakowski, Sudarshan, and Lindblad (GKSL) theorem (Gorini, 1976; Lindblad, 1976), that represents a cornerstone in the theory of open quantum systems<sup>3</sup>. In its finite-dimensional version ( $\dim \mathcal{H}_S = N$ ), the theorem reads as follows. A linear operator  $\mathcal{L}$  is the generator of a quantum dynamical semigroup  $\{\Lambda_t\}_{t \geq 0}$  if and only if it is in the form:

$$\mathcal{L}[\rho] = -i[H, \rho] + \sum_{k,l=1}^{N^2-1} a_{kl} \left( F_k \rho F_l^\dagger - \frac{1}{2} \{F_l^\dagger F_k, \rho\} \right), \quad (3.36)$$

where  $H = H^\dagger$ ,  $\langle F_l, F_k \rangle_{\text{HS}} = \delta_{lk}$ , with  $k, l = 1, \dots, N^2 - 1$ , while the positive-definite matrix  $A = (a_{k,l})_{k,l} \in \mathcal{M}_{N^2-1}(\mathbb{R})$  is known as *Kossakowski matrix*. Note that the operator  $H$  and  $F_l$  can be taken to be traceless, i.e.,  $\text{Tr}(H) = 0$  and  $\text{Tr}(F_l) = 0$ , yielding the canonical separation of the generator between a unitary  $\mathcal{L}_H[\rho] = -i[H, \rho]$  and non-unitary  $\mathcal{D}[\rho]$  part (Gorini, 1978).

Moreover, the dissipative part – known as dissipator – can be brought in the so-called Lindblad form upon diagonalisation of the Kossakowski matrix  $A$ , i.e.,  $A = UDU^\dagger$ , where  $U = (u_{kl})_{k,l}$  unitary matrix, whereas  $D = \text{diag}(\{\gamma_k\}_k)$ . Therefore, by introducing the *Lindblad* (or *jump*) operators  $L_k = \sum_i u_{ki} F_i$ , one has

$$\mathcal{D}[\rho] \equiv \sum_{k=1}^{N^2-1} \gamma_k \left( L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right), \quad (3.37)$$

with  $\gamma_k \geq 0$ . Note that these positive coefficients have the dimensions of an inverse time, provided that the operators  $L_k$  are dimensionless. Indeed, we will see that these are the rates with which the environmental correlation functions decay (Breuer, 2002).

We have shown that, given a open system whose dynamical maps form a quantum dynamical semigroup, the evolution is given by the following master equation:

$$\dot{\rho}(t) = -i[H, \rho] + \mathcal{D}[\rho], \quad (3.38)$$

known as *Lindblad equation*.

A more general situation occurs when, in a Lindblad-like master equation, the decoherence rates and the Lindblad operators are time-dependent, i.e.,  $\gamma_k \rightarrow \gamma_k(t)$  and  $L_k \rightarrow L_k(t)$ . In this scenario, we can recover the generator of a quantum dynamical semigroup as far as

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<sup>2</sup>Technically, the result holds for contractions semigroups.

<sup>3</sup>Historically, it is worth mentioning that the paper by Gorini, Kossakowski and Sudarshan explicitly considers the finite-dimensional case in the Schrödinger picture, while Lindblad's paper deals with the infinite-dimensional case in the Heisenberg picture (Chruściński, 2017).

the rates are non-negative, i.e.,  $\gamma_k(t) \geq 0$  (Hall, 2014; de Vega, 2017), as their negativity might be associated to a backflow of information, leading to non-Markovian dynamics – see Section 4.1.2.

### Example 3.2.1: Pure Dephasing

Let us consider the case of a qubit, given the following time-dependent generator:

$$\mathcal{L}_t[\rho] = \frac{\gamma(t)}{2} (\sigma_z \rho \sigma_z - \rho). \quad (3.39)$$

We would like to investigate under which conditions the latter is a legitimate generator of a quantum dynamical semigroup. First, we need to derive the corresponding dynamical map  $\Lambda_t$  by exponentiation, i.e.,  $\Lambda_t = \exp \left\{ \int_0^t d\tau \Lambda_\tau \right\}$ . If we introduce the orthonormal basis  $\{|0\rangle, |1\rangle\}$ , we can construct the canonical operator basis  $E_{ij} = |i\rangle\langle j|$ . Working in the standard representation, we obtain

$$E_{00} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad E_{01} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad E_{10} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad E_{11} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (3.40)$$

while the third Pauli matrix reads as

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.41)$$

A straightforward calculation yields

$$\mathcal{L}_t[E_{00}] = 0, \quad \mathcal{L}_t[E_{01}] = -\gamma(t)E_{01}, \quad \mathcal{L}_t[E_{10}] = -\gamma(t)E_{10}, \quad \mathcal{L}_t[E_{11}] = 0, \quad (3.42)$$

whence

$$\Lambda_t E_{00} = 0, \quad \Lambda_t E_{01} = e^{-\Gamma(t)} E_{01}, \quad \Lambda_t E_{10} = e^{-\Gamma(t)} E_{10}, \quad \Lambda_t E_{11} = 0, \quad (3.43)$$

with  $\Gamma(t) \equiv \int_0^t \gamma(\tau) d\tau$ . Therefore, we obtain the following matrix representation of the map

$$\Lambda_t \rho = \begin{pmatrix} \rho_{00} & \rho_{01} e^{-\Gamma(t)} \\ \rho_{10} e^{-\Gamma(t)} & \rho_{11} \end{pmatrix}. \quad (3.44)$$

We can also compute the corresponding Choi matrix, given by

$$\Phi_{\Lambda_t} = \begin{pmatrix} \Lambda_t E_{00} & \Lambda_t E_{01} \\ \Lambda_t E_{10} & \Lambda_t E_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & e^{-\Gamma(t)} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-\Gamma(t)} & 0 & 0 & 1 \end{pmatrix}. \quad (3.45)$$

The eigenvalues of  $\Phi_{\Lambda_t}$  are

$$\lambda_1 = 0, \quad \lambda_2 = 0, \quad \lambda_3 = 1 - e^{-\Gamma(t)}, \quad \lambda_4 = 1 + e^{-\Gamma(t)}. \quad (3.46)$$

Choi's theorem – cf. [Section 2.5.1](#) – states that a linear map is CP if and only if the corresponding Choi matrix is positive. Therefore, the dynamical map  $\Lambda_t$  is CP if and only if  $\lambda_3 \geq 0$ , i.e.,  $\Gamma(t) \geq 0$ . Note that, if the latter condition is fulfilled, from [Equation \(3.44\)](#), we get that – in the basis of  $\sigma_z$  eigenvectors – the diagonal elements of the density operator (i.e., the so-called *populations*) are unaffected by the dynamics, while the off-diagonal elements (called *coherences*) decrease exponentially over time. Note that, in the long time limit  $t \rightarrow +\infty$ , coherences vanish and we are left with a diagonal density matrix, that identifies the stationary state. This genuine quantum phenomenon is known as *decoherence* ([Zurek, 2003](#)); that is the reason why one says that the map [\(3.39\)](#) induces a pure dephasing dynamics.

On a similar note, we can start from [Equation \(3.39\)](#) and realise that the generator is in a Lindblad-like form, where the Lindblad operator is given by the Pauli operator  $\sigma_z$ . The evolution is Marovian when  $\gamma(t) \geq 0$ , whereas a proper Lindblad form is obtained only when  $\gamma(t)$  is given by some constant  $\gamma > 0$  ([Chruściński, 2014](#)).

## Adjoint master equation

In analogy to the case of a closed system, we can describe the irreversible dynamics of an open system in the dual space of operators. In this case, the time evolution of the dual map is governed by

$$\partial_t \Lambda_t^* = \Lambda_t^* \mathcal{L}_t^* \quad (3.47)$$

Thus, we can introduce the adjoint master equation ([Kossakowski, 1972](#))

$$\dot{A}_H(t) = \Lambda_t^* [\mathcal{L}_t^*[A]], \quad (3.48)$$

that governs the time evolution of an operator in the Heisenberg picture, and where we have assumed that the Liouville operator is time-dependent. While carefully looking at [Equation \(3.48\)](#), one can notice that, in this picture,  $\mathcal{L}_t^*$  first acts on the operator  $A$ , then the resulting operator is propagated by the means of the dual map  $\Lambda_t^*$ . A relevant special case is obtained if the Liouvillian  $\Lambda_t^*$  does not depend explicitly on time; under this assumption,  $\mathcal{L}_t^*$  and  $\Lambda_t^*$  commute, i.e.,

$$\dot{A}_H(t) = \Lambda_t^* [\mathcal{L}_t^*[A]] = \mathcal{L}_t^* [\Lambda_t^*[A]] = \mathcal{L}_t^* [A_H(t)], \quad (3.49)$$

where we have used [Equation \(3.19\)](#). As a result, the adjoint master equation eventually takes the following form:

$$\dot{A}_H(t) = i[H, A_H(t)] + \mathcal{D}^*[A_H(t)], \quad (3.50)$$

where we have introduce the dual dissipator

$$\mathcal{D}^*[A_H(t)] \equiv \sum_k \gamma_k \left( L_k A_H(t) L_k^\dagger - \frac{1}{2} \left\{ L_k^\dagger L_k, A_H(t) \right\} \right), \quad (3.51)$$

which can be recast in the so-called standard form (Gorini, 1978)

$$\mathcal{D}^*[A_H(t)] = \Psi_{\{L\}}[A_H(t)] - \frac{1}{2} \left\{ \Psi_{\{L\}}[\mathbb{I}], A_H(t) \right\}, \quad (3.52)$$

provided that one introduces the CP operator

$$\Psi_{\{L\}}[A_H(t)] \equiv \sum_k L_k^\dagger A_H(t) L_k. \quad (3.53)$$

# Chapter 4

## Microscopic Derivations

In Chapter 3, we have outlined some rather general concepts aiming at characterising the dynamics of quantum systems. These mathematical results, albeit mainly applicable in the context of a quantum dynamical semigroup, represent, to some extent, the golden standard in the bigger, overarching problem of characterising any kind of open dynamics. On the other hand, the theory of open quantum systems is also confronted with the opposite issue of microscopically modelling a system in order to result into a well-defined description – either in terms of maps or in terms of equations – of its dynamics. In Section 4.1, with the help of a simple exactly solvable model, we will introduce some general concepts, thus paving the way to more complicated scenarios. In Sections 4.2 and 4.4, we will then discuss a general approach for deriving master equations, relying on a set of successive approximations, which, in general, encompass non-Markovian features of the dynamics: the Markovian behaviour can be recovered in a suitable limit, as thoroughly discussed in Section 4.6. The presentation of general results is instrumental to the study of the quantum Brownian motion model, analysed in Sections 4.3 and 4.5; crucially, we show that, performing the secular approximation without fully going into the Markovian limit enables to capture non-Markovian effects of the dynamics.

### 4.1 Exactly solvable spin-boson model

Let us address this issue by considering a special example, in which the dynamics of the open system is analytically solvable (Luczka, 1990; Palma, 1996). Let us assume that the Hamiltonian of the composite system reads<sup>1</sup>:

$$H = H_S + H_E + H_I, \quad (4.1)$$

where  $H_S, H_E, H_I$  represent the Hamiltonian describing the system, the environment, and their interaction, respectively. The system is given by a spin, therefore

$$H_S = \frac{\omega_0}{2} \sigma_z, \quad (4.2)$$

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<sup>1</sup>Note that we are using a shorthand notation compared to the one used in Equation (3.9).

where  $\omega_0$  is the splitting between the two levels; whereas the environment is modelled as a collection of harmonic oscillators

$$H_E = \sum_k \omega_k b_k^\dagger b_k, \quad (4.3)$$

satisfying the bosonic commutation relations

$$[b_k, b_{k'}^\dagger] = \delta_{k,k}, \quad [b_k, b_{k'}] = 0, \quad [b_k^\dagger, b_{k'}^\dagger] = 0. \quad (4.4)$$

The interaction Hamiltonian reads as

$$H_I = \sigma_z \otimes \sum_k \left( g_k b_k^\dagger + g_k^* b_k \right), \quad (4.5)$$

where  $g_k$  are the (complex) coupling constants, describing the interaction between the system and the  $k$ -th bosonic mode<sup>2</sup>. Let us denote as  $\{|0\rangle, |1\rangle\}$  the basis of  $\mathcal{H}_S \cong \mathbb{C}^2$ , made of eigenstates of  $\sigma_z$ . We can immediately notice that the Hamiltonian exhibits an explicit symmetry, i.e.,  $[H, \sigma_z] = 0$ , therefore  $\sigma_z$  is a conserved quantity. As a consequence, the populations do not evolve over time, i.e.,  $\langle 0 | \rho_S(t) | 0 \rangle = \langle 0 | \rho_S(0) | 0 \rangle$  and  $\langle 1 | \rho_S(t) | 1 \rangle = \langle 1 | \rho_S(0) | 1 \rangle$ , where  $\rho_S$  is the reduced density matrix. We further assume that at time  $t = 0$  the joint state is in a tensor product form, where the environment is in a canonical Gibbs state, i.e.,

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_E, \quad \rho_E = \frac{e^{-\beta H_E}}{\mathcal{Z}_E}, \quad (4.6)$$

being  $\mathcal{Z}_E = \text{tr}_E(e^{-\beta H_E})$  the partition function of the bosonic bath, with inverse temperature  $\beta$ . Under this assumption, it can be shown (Breuer, 2002) that coherences behave as

$$\langle 0 | \rho_S(t) | 1 \rangle = \langle 0 | \rho_S(0) | 1 \rangle e^{-\Gamma(t)}, \quad (4.7)$$

$$\langle 1 | \rho_S(t) | 0 \rangle = \langle 1 | \rho_S(0) | 0 \rangle e^{-\Gamma(t)}, \quad (4.8)$$

where  $\Gamma(t)$  is the so-called decoherence function:

$$\Gamma(t) \equiv 4 \int_0^\infty d\omega J(\omega) \coth\left(\frac{\beta}{2}\omega\right) \frac{1 - \cos\omega t}{\omega^2}, \quad (4.9)$$

where  $J(\omega)$  is the *Spectral Density* (SD), defined as

$$J(\omega) \equiv \sum_k |g_k|^2 \delta(\omega - \omega_k), \quad (4.10)$$

whose physical meaning is transparent: it essentially quantifies the way the spin couples with each mode of the bath. Note that Equation (4.10) is the standard definition for the SD of a

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<sup>2</sup>Note that  $g_k^*$  denotes the complex conjugate of  $g_k$ .

discrete environment made of harmonic oscillators, whilst in [Equation \(4.9\)](#) the decoherence function is defined through an integral over all possible frequencies: it is understood that the environmental harmonic oscillators are taken to be infinitely many, so that the frequency spectrum can be assumed to form a continuum.

All in all, we have sketched the exact microscopic derivation of a specific spin-boson model dynamics; it is immediate to conclude that the latter can be expressed by a dynamical map, that, in the standard matrix representation in the basis of eigenvectors of  $\sigma_z$ , is in the form of [Equation \(3.44\)](#), i.e.,

$$\rho_S(t) = \Lambda_t \rho_S(0) = \begin{pmatrix} \rho_{00}(0) & \rho_{01}(0) e^{-\Gamma(t)} \\ \rho_{10}(0) e^{-\Gamma(t)} & \rho_{11}(0) \end{pmatrix}. \quad (4.11)$$

This simple, yet insightful, example shows that, starting from a Hamiltonian describing the interaction between the system and the environment, we can perform calculations that lead to a master equation for the reduced density matrix. As we have seen in the [Example 3.2.1](#), the generator of this map is given by

$$\mathcal{L}_t[\rho_S] = \frac{\dot{\Gamma}(t)}{2} (\sigma_z \rho_S \sigma_z - \rho_S) = -\frac{\dot{\Gamma}(t)}{4} [\sigma_z, [\sigma_z, \rho_S]], \quad (4.12)$$

that, in order to be in the GKSL form, has to fulfill the condition  $\dot{\Gamma}(t) \geq 0$ . If so, the map in [Equation \(4.11\)](#) describes a purely dephasing dynamics, where populations are left unchanged, while coherences are monotonically damped to zero.

### 4.1.1 Some remarks about the spectral density

The previous example of a spin-boson model has led to the introduction of a very important function, namely, the spectral density, that encodes information about the interaction between the system and its surroundings ([de Vega, 2017](#)). This function  $J(\omega)$ , defined by [Equation \(4.10\)](#), appears whenever the environment is modelled as a set of independent harmonic oscillators at a given inverse temperature  $\beta$ . This a common setup in an open quantum system scenario; moreover, thermal reservoirs play a special role in quantum statistical mechanics, as they are characterised by the universality of their fluctuation-dissipation relations ([Esposito, 2009](#)), and, as we will see in [Sections 4.6.1](#) and [4.6.2](#), they satisfy the celebrated Kubo-Martin-Schwinger (KMS) boundary conditions ([Kubo, 1957](#); [Martin, 1959](#)), as well as the detailed balance relations. If we consider the case of a bilinear interaction, can assume that the interaction Hamiltonian between the system and the bosonic environment is in the form

$$H_I = X \otimes B, \quad (4.13)$$

where  $X$  is an operator of the system, while  $B$  is an operator of the bath, given by

$$B = \sum_k \left( g_k b_k^\dagger + g_k^* b_k \right). \quad (4.14)$$

In the [Appendix A](#) we explicitly show that  $J(\omega)$  appears in the closed expression of the two-point bath correlation function , i.e.,

$$\alpha_\beta(\tau) \equiv \langle B(\tau)B \rangle_E = \text{tr}_E (B(\tau)B\rho_E) = \int_0^{+\infty} d\omega J(\omega) \left[ \cos \omega \tau \coth \left( \frac{\beta}{2} \omega \right) - i \sin \omega \tau \right], \quad (4.15)$$

where  $B \equiv B(0)$ . Specifically, if the environment happens to be at zero temperature (i.e.,  $\beta \rightarrow +\infty$ ), [Equation \(4.15\)](#) reduces to

$$\alpha_{\beta \rightarrow \infty}(\tau) = \int_0^{+\infty} d\omega J(\omega) e^{-i\omega\tau}, \quad (4.16)$$

i.e., the bath correlation function reads as the one-sided Fourier transform of the spectral density.

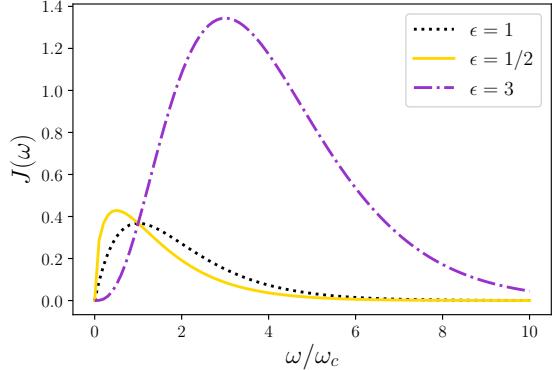
It is not redundant mentioning here that the assumption we made in [Section 4.1](#) about the continuity of the frequency spectrum is not accidental. We can indeed deduce from [Equation \(4.15\)](#) that, if the environment is made of a finite discrete set of bosonic modes, the integral reduces to a finite sum, thus  $\alpha_\beta(\tau)$  becomes a quasi-periodic function. As a consequence, the Poincaré recurrence time happens to be smaller than the typical evolution time of the system, meaning that the latter suffers revivals in the dynamics, regaining – at least partially – energy and/or coherence. It is clear that this is not exactly what we would expect from an irreversible dynamics, therefore we assume that the environment is sufficiently large so that the SD is a continuous function of the frequency. This justifies the name of *reservoir* that we often use to designate the environment; if, on top of that, the reservoir is in a thermal state as well, we can call it *heat bath*, or simply *bath* ([Breuer, 2002](#)).

Following a phenomenological approach ([Weiss, 2012](#)), one can express the SD in the quite general form

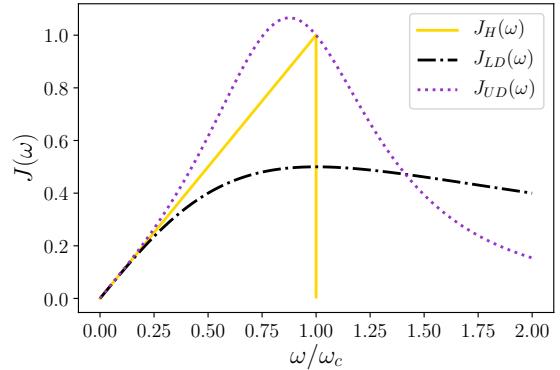
$$J(\omega) = \eta \omega_c^{1-\epsilon} \omega^\epsilon f(\omega, \omega_c), \quad (4.17)$$

where  $\epsilon > 0$  is known as the Ohmicity parameter, and  $\eta > 0$  describes the coupling strength between the system and the environment. Depending on the value of  $\epsilon$ , the SD is said to be Ohmic ( $\epsilon = 1$ ), super-Ohmic ( $\epsilon > 1$ ), or sub-Ohmic ( $\epsilon < 1$ ), each of them describing a different physical setting (see, e.g., ([de Vega, 2017](#)) and references therein). The function  $f(\omega, \omega_c)$  represents the SD cut-off and  $\omega_c$  is the cut-off frequency; they have to be conveniently chosen in accordance to other relevant scales and parameters of the problem. Possible choices are the Lorentz-Drude cut-off, i.e.,  $f(\omega, \omega_c) \equiv \omega_c^2 / (\omega_c^2 + \omega^2)$ ; the exponential cut-off  $f(\omega, \omega_c) \equiv e^{-\omega/\omega_c}$ , or the hard cut-off  $f(\omega, \omega_c) \equiv \Theta(\omega - \omega_c)$ , where  $\Theta$  is the Heaviside step function. Another common functional form is the underdamped SD

$$J(\omega) = \frac{\Gamma \omega_0^2 \omega}{(\omega_0^2 - \omega^2)^2 + \Gamma^2 \omega^2}. \quad (4.18)$$



(a)



(b)

**Figure 4.1:** Examples of commonly used spectral densities. **Panel (a):** examples of Ohmic, sub-Ohmic, super-Ohmic SDs with an exponential cut-off. Note that each of them accounts for a different physical interaction between the system and the environment. For instance, for a given cut-off  $\omega_c$ , the super-Ohmic SD covers a broader range of frequencies. **Panel (b):** examples of SD with hard cut-off  $J_H(\omega)$ , Ohmic with a Lorentz-Drude cut-off  $J_{LD}(\omega)$ , and underdamped  $J_{UD}(\omega)$ .

Examples of common SD are plotted in Figure 4.1. In Chapter 6, we will see that the specific form of the SD is crucial in the simulation of open systems dynamics, as it can either allow or hamper certain methods or approximations, due, for instance, to the strong coupling between system and environment and/or persistent memory effects.

### 4.1.2 Memory effects

We have mentioned that some SDs can model a coupling between system and environment responsible for pronounced memory effects. In this case, we cannot rely anymore on a memoryless description of the dynamics, but we should encompass non-Markovian effects. For quantum stochastic processes, even the definition of non-Markovianity turns out to be much more involved than the classical counterpart – for a discussion on this topic, see, e.g., the reviews (Rivas, 2014; Breuer, 2016) and references therein. From a physical standpoint, memory effects are associated with a certain exchange of information between the system and the environment. In the Markovian case, being the environment practically unaffected by the coupling with a much smaller system, we witness a one-directional continuous flow of information from the open system towards the surroundings. By contrast, in a non-Markovian process, even though the environment is still inert, we can observe information flowing back to the system: the latter retrieves at a later time some of the information that was previously lost and temporarily stored in the environment. This intuitive picture can be formally defined in terms of the divisibility of the corresponding dynamical map (Wolf, 2008; Chruściński, 2014; Chruściński, 2016): without going into the mathematical details of this issue, we would like to stress that the non-Markovian character of the dynamics is a property of the corresponding dynamical map, rather than of the states. This evidence is reflected also in some measures

of non-Markovianity, which require cumbersome optimisation procedures. A plethora of measures of non-Markovianity have indeed been put forward, each of them capturing different features of these processes. For instance, the Rivas Huelga Plenio (RHP) measure aims at measuring the deviation from the divisibility requirement (Rivas, 2010), while others focus on the negativity of the decay rates of the time-local master equation (Hall, 2014), or the geometric structure of the set of accessible states (Lorenzo, 2013). Here, we limit ourselves to introduce the Breuer Laine Piilo (BLP) measure, based on the trace distance between states (Breuer, 2009). The latter provides a remarkably simple way to quantitatively express the intuitive notion of *information backflow*. Furthermore, we will see that the trace distance itself can serve as a useful quantifier of non-Markovianity, without requiring the complicated optimisation over possible pair of states implied by the BLP measure.

Let us introduce the trace distance between two states  $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$ , i.e.,

$$D(\rho_1, \rho_2) = \frac{1}{2} \|\rho_1 - \rho_2\|_1. \quad (4.19)$$

It constitutes a natural metrics on the state space  $\mathcal{S}(\mathcal{H})$ , and it is such that  $0 \leq D(\rho_1, \rho_2) \leq 1$ , for any pair of states  $\rho_1, \rho_2$ . Specifically,  $D(\rho_1, \rho_2) = 0$  if and only if  $\rho_1 = \rho_2$ , whereas  $D(\rho_1, \rho_2) = 1$  if  $\rho_1$  and  $\rho_2$  are orthogonal, i.e., their supports are orthogonal. Thanks to its mathematical and physical properties, the trace distance is widely employed in quantum information theory (Nielsen, 2010; Heinosaari, 2011); for our purposes, it is sufficient to mention two of these properties. First, the trace distance has a clear interpretation in terms of distinguishability of quantum states. The second property is that a CPTP map  $\Lambda$  is a contraction for the trace distance (Ruskai, 1994; Breuer, 2009), i.e.,

$$D(\Lambda\rho_1, \Lambda\rho_2) \leq D(\rho_1, \rho_2). \quad (4.20)$$

Therefore, from the perspective of open quantum systems, if the dynamics is Markovian, given two different initial states  $\rho_1(0)$  and  $\rho_2(0)$  of the reduced system, they becomes less and less distinguishable as the time goes by; in other words, Equation (4.20) can be expressed as

$$D(\rho_1(t), \rho_2(t)) \leq D(\rho_1(0), \rho_2(0)). \quad (4.21)$$

Physically, this means that the coupling of the system with an environment reduces our ability to discriminate two states over time. Motivated by this evidence, we are naturally led to look at the rate of change of the trace distance, i.e.,

$$\sigma(t, \rho_{1,2}(0)) = \frac{d}{dt} D(\rho_1(t), \rho_2(t)). \quad (4.22)$$

According to what we have previously discussed, a quantum Markovian process is characterised by  $\sigma \leq 0$ . Conversely, there are physical processes – that we label as non-Markovian – for which  $\sigma > 0$  for certain intervals of time, i.e., the distinguishability temporarily increases: the information backflow enhances our ability to discriminate two given states. It is interesting mentioning here that this quantifier of quantum non-Markovianity is particularly advantageous

also from an experimental point of view (Liu, 2011): one can witness non-Markovianity through state tomography rather than full process tomography.

In order to obtain a measure – i.e., roughly speaking, to attach a number to a given quantum process – one should quantify the total increase of distinguishability over the whole time evolution. As a result, one first needs to integrate over all time intervals in which  $\sigma$  is positive, then maximise over all pairs of initial states, thus, for a given process  $\Lambda_t$ , we have

$$\mathcal{N}_{\text{BLP}} = \max_{\rho_{1,2}(0)} \int_{\sigma>0} dt \sigma(t, \rho_{1,2}(0)). \quad (4.23)$$

Clearly, for Markovian evolutions, we have  $\mathcal{N}_{\text{BLP}} = 0$ .

#### Example 4.1.1: Spin-boson model: non-Markovian dynamics

Let us consider again the exactly solvable spin-boson model introduced in [Section 4.1](#). For the sake of simplicity, let us suppose that the bath is in the vacuum (i.e.,  $\beta \rightarrow +\infty$ ), thus, the decoherence function, given by [Equation \(4.9\)](#), reduces to  $\Gamma(t) = 4 \int_0^t J(\omega) \sin(\omega t) d\omega$ . In order to obtain a non-Markovian dynamics, we should choose a SD that does not lead to a decoherence function linear in  $t$ . One possible choice is given by a super-Ohmic SD (with  $\epsilon = 4$  and  $\omega_c = 1$ ) with an exponential cut-off, yielding the analytical expression

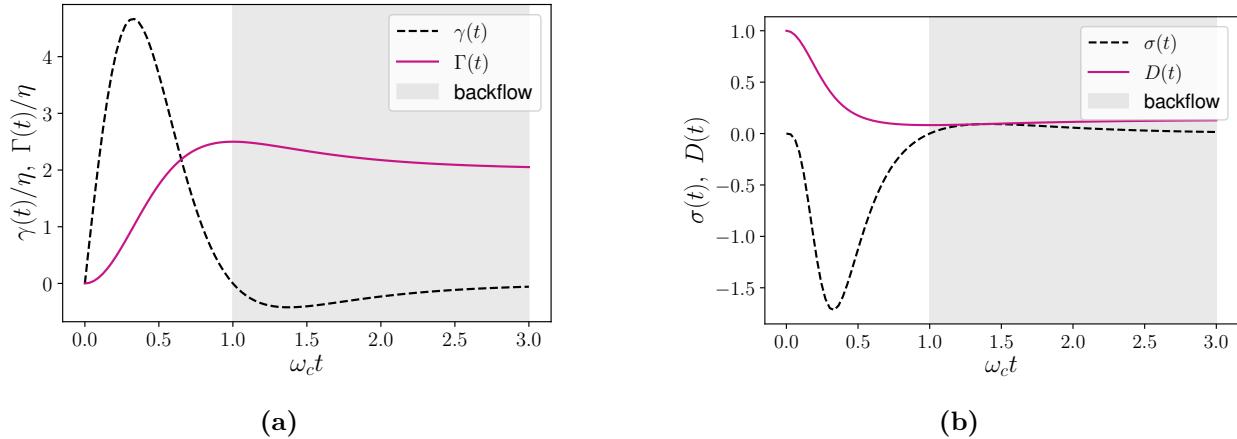
$$\Gamma(t) = 2\eta \left\{ 1 - \frac{\cos(3 \arctan t)}{(1+t^2)^{\frac{3}{2}}} \right\}, \quad (4.24)$$

whose time derivative is

$$\gamma(t) \equiv \dot{\Gamma}(t) = \frac{6\eta \sin(4 \arctan t)}{(1+t^2)^2}. \quad (4.25)$$

If we plot the  $\Gamma(t)$  and  $\gamma(t)$ , one can conclude that non-Markovian effects in the underpinning dynamics can be recorded when the dephasing factor  $\Gamma(t)$  temporarily decreases over time or, equivalently (since  $\gamma(t) = \Gamma'(t)$ ), when the dephasing rate  $\gamma(t)$  attains negative values. For our specific choice of the SD, this happens when  $t \geq \tan(\frac{\pi}{4}) = 1$  ([Addis, 2014](#)) – cf. [Figure 4.2](#). The system, then, regains some of the information that was previously lost; specifically, it is clear that the coherences do not monotonically decrease to zero over time, but the can temporarily recohore. This result is also confirmed if one looks at the trace distance; by using [Equations \(4.11\)](#) and [\(4.19\)](#), one easily obtains a closed expression for the trace distance at any time  $t$ , i.e.,

$$D(\rho_1(t), \rho_2(t)) = \sqrt{\Delta_{00}^2 + |\Delta_{01}|^2 e^{-2\Gamma(t)}}, \quad (4.26)$$



**Figure 4.2:** Non-Markovian dynamics of a spin boson model. **Panel (a):** Decoherence function  $\Gamma(t)$  and time dephasing rate  $\gamma(t)$  for a super-Ohmic SD ( $\epsilon = 1$ ) with a exponential cut-off. **Panel (b):** Trace distance  $D(\rho_1(t), \rho_2(t))$  and its time derivative  $\sigma(t, \rho_{1,2}(0))$  for the optimal pair of states  $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ . Note that all the features are compatible with a non-Markovian dynamics for  $\omega_c t > 1$ .

where  $\Delta_{ij} = (\rho_1 - \rho_2)_{ij}$ , with  $i, j = 0, 1$ . By taking the derivative w.r.t. time, i.e.,

$$\sigma(t, \rho_{1,2}(0)) = -\frac{|\Delta_{01}|^2 e^{-2\Gamma(t)} \gamma(t)}{\sqrt{\Delta_{00}^2 + |\Delta_{01}|^2 e^{-2\Gamma(t)}}}, \quad (4.27)$$

one can conclude that  $\sigma > 0$  when  $\gamma(t) < 0$ . We can actually compute the BLP measure, as we can analytically solve the optimisation problem in Equation (4.23). It has been shown indeed that the optimal pair of states is given by antipodal points on the equatorial plane of the Bloch sphere (Wißmann, 2012), e.g.,  $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ . In this case,  $\Delta_{00} = 0$  and  $\Delta_{01} = 1$ , hence  $\mathcal{N}_{\text{BLP}} = +\infty$ : this essentially means that we cannot ever resort to a Markovian approximation of the dynamics.

## 4.2 Projection operator techniques

In Section 4.1, we have analysed one specific example of microscopic derivation, which can be carried out analytically. However, this does not happen in general, so that we need to seek for a general methodological framework for microscopically deriving master equations. These methods, collectively referred as projection operator techniques, were first introduced in the domain of non-equilibrium statistical mechanics by Nakajima and Zwanzig (Nakajima, 1958; Zwanzig, 1960) and they can be rephrased in the language of open quantum systems (Breuer, 2002; Rivas, 2012). In this case, we could say that this formalism is a more refined way to look at the operation of tracing out the environmental degrees of freedom. The basic idea is

straightforward: the full density matrix contains much more information than required (or that we can handle), therefore, in order to drop such unnecessary ‘baggage’, one needs to project over a relatively smaller Hilbert space. The essence of projection operator techniques is to tell the system degrees of freedom – the so-called *relevant part* of the dynamics – from the environmental degrees of freedom —the *irrelevant part* of the dynamics. The final aim is to derive a closed equation for the former. There are two different variants of projection operators techniques leading to such equations of motion:

- The Nakajima-Zwanzig method, which yields an integro-differential equation involving a retarded time integration over the history of the reduced system;
- The time-convolutionless projection operator technique, that provide first-order differential equations which are local in time.

The former approach provides an exact equation whose integral kernel depends non-trivially on the past history of the system. Theoretically relevant, this equation is of limited practical use, being usually as difficult to solve as the Liouville - von Neumann equation; nonetheless, it is a good starting point to further simplification and approximations. By contrast, the latter technique was first introduced by Shibata *et al.* ([Shibata, 1977](#); [Chaturvedi, 1979](#); [Shibata, 1980](#)) for studying open quantum systems dynamics; it turns out to be very advantageous, as it provides a smart way to systematically expand the kernel in term of the system-environment coupling. A detailed introduction to these techniques is contained in [Appendix B](#), while here we will just state the final results.

#### 4.2.1 (Time) local *vs* non-local description of the dynamics

Let us suppose that the interaction between a system  $S$  with its environment  $E$  is modelled through the following microscopic Hamiltonian:

$$H = H_0 + \alpha H_I \tag{4.28}$$

where  $H_0 = H_S + H_E$  governs the free evolution of  $S$  and  $E$ , while  $H_I$  accounts for the interaction between them,  $\alpha$  being a dimensionless parameter that controls the interaction between the system and the environment.

The two techniques briefly introduced above offer two different perspectives: the equations we eventually obtain can be either local or non-local in time. In this paragraph, we would like to see what these equations look like in the hypothesis of weak coupling between the system and the environment. To this end, we need to make some assumptions — cf. [Appendix B](#). First, we assume that the environment is in a stationary state<sup>3</sup>, i.e.,  $[H_E, \rho_E] = 0$  and that  $\text{tr}_E(H_I(t)\rho_E) = 0$ , where  $H_I(t)$  is the interaction Hamiltonian in the interaction picture with respect to the free Hamiltonian  $H_0$ , i.e.,  $H^I(t) = e^{iH_0 t} H_I e^{-iH_0 t}$ . We can further assume that the system and the environment are initially uncorrelated, i.e.,  $\rho_{SE} = \rho_S(t_0) \otimes \rho_E$ , where  $\rho_E$  is a fixed environmental state, and that we work in the weak coupling limit. The whole set of

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<sup>3</sup>Note that this condition is trivially satisfied when the environment is a thermal reservoir.

hypothesis lead to the non-local equation ( $t_0 = 0$ )

$$\dot{\rho}_S(t) = -\alpha^2 \int_0^t ds \text{tr}_E [H_I(t), [H_I(s), \rho_S(s) \otimes \rho_E]] . \quad (4.29)$$

Moreover, under some additional assumptions that are physically reasonable in the weak coupling and short time limits, one eventually get the master equation

$$\dot{\rho}_S(t) = -\alpha^2 \int_0^t ds \text{tr}_E [H_I(t), [H_I(s), \rho_S(t) \otimes \rho_E]] . \quad (4.30)$$

Leaving all the formal details to [Appendix B](#), let us carefully discuss here the underlying physical assumptions that lead to the two equations above. In order to obtain [Equation \(4.29\)](#), we need to assume that the environment is so big that it is practically unaffected by the coupling with the system  $S$ . This is the main reason that enables to project the joint states over a smaller Hilbert space where they can be expressed in a tensor product form between the relevant part and the fixed environmental state. In other words, we are assuming that the total state of the system factorises not only at  $t = t_0$ , but at all times. By the same token, this physical scenario allows us to work in the weak coupling limit. This first approximation, known in literature as *first Born approximation*, is not sufficient to obtain a time-local master equation; it is indeed clear by looking at [Equation \(4.29\)](#) that the future evolution  $\rho_S(t)$  depends on the past history though the integration over  $\rho_S(s)$ . On the other hand, [Equation \(4.30\)](#) relies on the so-called *Markov approximation*, whose validity is based on the separation of timescales between the time  $\tau_E$  over which the environmental correlations decay and the timescale  $\tau_R$  for significant evolution of the open system  $S$ : the replacement  $\rho_S(s) \rightarrow \rho_S(t)$  is justified only if  $\tau_E \ll \tau_R$ . [Equation \(4.30\)](#) is known as *Bloch-Redfield* (or simply *Redfield*) *equation* ([Redfield, 1957](#); [Redfield, 1965](#)): though local in time, the latter is still not Markovian. Moreover, an evolution governed by a master equation of such a form do not necessarily warrants positivity, nor the more stringent requirement of complete positivity, possibly leading to non-physical predictions ([Benatti, 2003](#); [Benatti, 2005](#)).

### 4.3 *Intermezzo: non-Markovian quantum Brownian motion*

Generally speaking, there are several models microscopically accounting for dissipation and decoherence in quantum systems ([Breuer, 2002](#); [Weiss, 2012](#)). One possible example is represented by a quantum Brownian particle – namely a particle subject to a certain potential – in a bath of harmonic oscillators. This particular way of modelling the system-environment interaction has been widely discussed in literature, and it is often referred as Caldeira-Leggett model ([Caldeira, 1983a](#); [Caldeira, 1983b](#)). Usually the dynamics of a Brownian particle is presented in the Markovian regime; by contrast, in this Section, we would like to rely on

a set of assumptions that still enable to preserve some memory effects. This problem has been tackled in several ways in literature: to the best of our knowledge, the first attempt to obtain an exact master equation for a Brownian particle in a non-Markovian setting is due to Hu, Paz, and Zhang (Hu, 1992). Following this seminal paper, where the authors resort to the influence functional approach (Feynman, 1963; Breuer, 2002), different strategies have been adopted to solve this problem. For instance, in Ref. (Halliwell, 1996), a phase-space formalism is employed to derive a Fokker-Plank like evolution equation for the system, after integrating over the bath variables. The solution of the latter equation is – in general – a formidable task. The issue is thoroughly discussed, e.g., in Ref. (Ford, 2001; Ford, 2005), where the quantum Langevin equation formalism is employed; specifically, in Ref. (Ford, 2005), the authors exploit this example for challenging the utility of exact master equations, upon a careful examination of the usual assumptions required to derive them. However, in this work, we will rather tackle the problem following an operatorial approach (Breuer, 2001; Intravaia, 2003b); this amounts to take a different – somehow complementary – perspective, which is closer to the spirit of the open quantum system paradigm.

### 4.3.1 Derivation of the master equation

Let us consider a system described by a Hamiltonian  $H_S$ , coupled to an environment modelled as a collection of (infinitely many) harmonic oscillators. The total Hamiltonian reads as

$$H = H_S + H_E + \alpha H_I \equiv H_0 + \alpha H_I, \quad (4.31)$$

where the Hamiltonian  $H_S$  is that of a quantum harmonic oscillator described by the dimensionless position and momentum operators  $X, P$

$$H_S = \frac{\omega_0}{2} (X^2 + P^2), \quad (4.32)$$

with  $\omega_0$  representing the bare frequency of the harmonic oscillator, whereas

$$H_E = \sum_k \omega_k b_k^\dagger b_k. \quad (4.33)$$

The interaction Hamiltonian is given by a linear coupling of the form

$$H_I = X \otimes B \equiv X \otimes \sum_k (g_k^* b_k + g_k b_k^\dagger). \quad (4.34)$$

The starting point of our derivation is Equation (4.30), that, upon a suitable change of the integration variable, reads as

$$\dot{\rho}_S(t) = -\alpha^2 \int_0^t d\tau \text{tr}_E [H_I(t), [H_I(t-\tau), \rho_S(t) \otimes \rho_E]]. \quad (4.35)$$

Let us compute explicitly the trace over the environmental degrees of freedom of the double commutator in [Equation \(4.35\)](#)

$$\begin{aligned} \text{tr}_E [H_I(t), [H_I(t - \tau), \rho_S(t) \otimes \rho_E]] &= X(t)X(t - \tau)\rho_S(t)\langle B(t)B(t - \tau)\rangle_E \\ &\quad - X(t)\rho_S(t)X(t - \tau)\langle B(t - \tau)B(t)\rangle_E \\ &\quad - X(t - \tau)\rho_S(t)X(t)\langle B(t)B(t - \tau)\rangle_E \\ &\quad + \rho_S(t)X(t - \tau)X(t)\langle B(t - \tau)B(t)\rangle_E, \end{aligned} \quad (4.36)$$

where  $\langle \cdot \rangle_E \equiv \text{tr}_E(\cdot \rho_E)$  denotes the average over the environmental state  $\rho_E$ . We also note that, since the environmental state is stationary, the bath correlation functions are homogeneous in time, thus  $\langle B(t)B(t - \tau)\rangle_E = \langle B(\tau)B\rangle_E$ , and  $\langle B(t - \tau)B(t)\rangle_E = \langle BB(\tau)\rangle_E$ . We can introduce the *environmental noise kernel*

$$\kappa(\tau) = \alpha^2\langle\{B(\tau), B\}\rangle_E, \quad (4.37)$$

and the *dissipation kernel*

$$\mu(\tau) = i\alpha^2\langle[B(\tau), B]\rangle_E. \quad (4.38)$$

After some algebra, we can rewrite [Equation \(4.35\)](#) as follows:

$$\dot{\rho}_S(t) = -\frac{1}{2} \left\{ \int_0^t d\tau \kappa(\tau) [X(t), [X(t - \tau), \rho_S(t)]] - i \int_0^t d\tau \mu(\tau) [X(t), \{X(t - \tau), \rho_S(t)\}] \right\}. \quad (4.39)$$

Now, we would like to write [Equation \(4.39\)](#) in the Schrödinger picture. The density operator  $\rho_S(t)$ , expressed in the interaction picture with respect to  $H_0$ , is related to the operator  $\rho$  in the Schrödinger picture by the transformation  $\rho_S(t) = e^{iH_0t}\rho e^{-iH_0t}$ . Analogously, a lengthy but straightforward calculation yields

$$\begin{aligned} [X(t), [X(t - \tau), \rho_S(t)]] &= e^{iH_0t}[X, [X(-\tau), \rho]]e^{-iH_0t}, \\ [X(t), \{X(t - \tau), \rho_S(t)\}] &= e^{iH_0t}[X, \{X(-\tau), \rho\}]e^{-iH_0t}, \end{aligned} \quad (4.40)$$

where  $X(-\tau) \equiv e^{-iH_0\tau} X e^{iH_0\tau} = X \cos(\omega_0\tau) - P \sin(\omega_0\tau)$  is the interaction picture representation of the Schrödinger picture position operator  $X$ . Therefore, substituting all these quantities into [Equation \(4.39\)](#), we obtain

$$\begin{aligned} \dot{\rho}(t) &= -i[H_0, \rho] \\ &\quad - \frac{1}{2} \int_0^t d\tau \kappa(\tau) \cos(\omega_0\tau) [X, [X, \rho]] + \frac{1}{2} \int_0^t d\tau \kappa(\tau) \sin(\omega_0\tau) [X, [P, \rho]] \\ &\quad - \frac{1}{2} \int_0^t d\tau \mu(\tau) \cos(\omega_0\tau) [X, \{X, \rho\}] + \frac{i}{2} \int_0^t d\tau \mu(\tau) \sin(\omega_0\tau) [X, \{P, \rho\}] \end{aligned} \quad (4.41)$$

After noticing that  $[X, \{X, \rho\}] = [X^2, \rho]$ , we eventually obtain the following form for the master equation in the Schrödinger picture:

$$\dot{\rho}(t) = -i[H_0, \rho] - \frac{i}{2}r(t)[X^2, \rho] - \Delta(t)[X, [X, \rho]] + \Pi(t)[X, [P, \rho]] - i\gamma(t)[X, \{P, \rho\}], \quad (4.42)$$

where – following the identification put forward in Ref. (Hu, 1992) – we have introduced the following time-dependent coefficients:

$$\Delta(t) \equiv \frac{1}{2} \int_0^t \kappa(\tau) \cos(\omega_0 \tau) d\tau, \quad (4.43a)$$

$$\gamma(t) \equiv \frac{1}{2} \int_0^t \mu(\tau) \sin(\omega_0 \tau) d\tau, \quad (4.43b)$$

$$\Pi(t) \equiv \frac{1}{2} \int_0^t \kappa(\tau) \sin(\omega_0 \tau) d\tau, \quad (4.43c)$$

$$r(t) \equiv - \int_0^t \mu(\tau) \cos(\omega_0 \tau) d\tau. \quad (4.43d)$$

The time-dependent coefficient  $r(t)$  given by Equation (4.43d) does not affect the unitarity of the evolution; it is just responsible for a renormalisation of the oscillator bare frequency  $\omega_0$ . Indeed, the coupling to the environment induces a frequency shift, therefore the physically observable frequency is no longer  $\omega_0$ , and the renormalised system Hamiltonian reads as

$$\tilde{H}_0 = \frac{1}{2}\omega_0 \left( \left( 1 + \frac{r(t)}{\omega_0} \right) X^2 + P^2 \right). \quad (4.44)$$

On the other hand, the remaining time-dependent coefficients account for the different types of noise affecting the open dynamics of the system. The coefficients  $\Delta(t)$  and  $\Pi(t)$  are related to diffusive processes: the former being the *normal* diffusion coefficient, the latter is related to *anomalous* diffusion instead (Zurek, 2003). The time-dependent rate  $\gamma(t)$  is the usual damping coefficient.

Furthermore, Equation (4.42) can be rewritten in the interaction picture with respect to the renormalised Hamiltonian  $\tilde{H}_0$ , i.e.,

$$\dot{\rho}(t) = -\Delta(t)[X(t), [X(t), \rho]] + \Pi(t)[X(t), [P(t), \rho]] - i\gamma(t)[X(t), \{P(t), \rho\}], \quad (4.45)$$

where we have used the following representations:

$$X(t) = X \cos(\omega_0 t) + P \sin(\omega_0 t), \quad (4.46)$$

$$P(t) = P \cos(\omega_0 t) - X \sin(\omega_0 t). \quad (4.47)$$

## 4.4 Interaction Hamiltonian

Let us consider again [Equation \(4.30\)](#); now we would like to introduce an approximation commonly used in the study of open quantum systems — the secular approximation. The latter is a standard technique of coarse-grained averaging, that consists in neglecting fast oscillating terms in the master equation, which average to zero in the time resolution we are adopting. We will see that this approximation, in the fully Markovian limit, leads to a master equation in the Lindblad form. The applicability of this approximation is currently under debate ([Farina, 2019](#)), as it should be carefully discussed in those situations in which the system is composed of two or more interacting parties, commonly encountered in the discussion of the thermodynamic behaviour of quantum systems ([Cattaneo, 2019](#)).

### 4.4.1 Expansion in eigenoperators

First, let us notice that the interaction Hamiltonian – in its general form – can be expressed (in the Schrödinger picture) as

$$H_I = \sum_{\mu} A_{\mu} \otimes B_{\mu}, \quad (4.48)$$

where  $A_{\mu}^{\dagger} = A_{\mu}$  and  $B_{\mu}^{\dagger} = B_{\mu}$  are non-null operators acting on  $\mathcal{H}_S$  and  $\mathcal{H}_E$ , respectively.

In order to perform the so-called *secular approximation*, it is convenient to express the interaction Hamiltonian  $H_I$  into eigenoperators of the system Hamiltonian  $H_S$ . For the sake of simplicity, let us assume that the spectrum of the Hamiltonian  $H_S$  is discrete. If we denote by  $\varepsilon_i$  its eigenvalues and  $\pi(\{\varepsilon_i\})$  the projectors on the corresponding eigenspace<sup>4</sup>, the following expansion holds:

$$H_S = \sum_{\varepsilon_i} \varepsilon_i \pi(\{\varepsilon_i\}). \quad (4.49)$$

Therefore, using the resolution of the identity, one gets

$$\begin{aligned} A_{\mu} &= \mathbb{I}_S A_{\mu} \mathbb{I}_S = \left( \sum_{\varepsilon_i} \pi(\{\varepsilon_i\}) \right) A_{\mu} \left( \sum_{\varepsilon_j} \pi(\{\varepsilon_j\}) \right) \\ &= \sum_{\omega} \sum_{\varepsilon_j - \varepsilon_i = \omega} \pi(\{\varepsilon_i\}) A_{\mu} \pi(\{\varepsilon_j\}) \equiv \sum_{\omega} A_{\mu}(\omega), \end{aligned} \quad (4.50)$$

where the sum is meant to be extended over all energy eigenvalues  $\varepsilon_i$  and  $\varepsilon_j$  of  $H_S$  with a fixed energy difference  $\omega$ . Analogously, one has

$$A_{\mu} = \sum_{\omega} A_{\mu}^{\dagger}(\omega). \quad (4.51)$$

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<sup>4</sup>In the one-dimensional case, we would get  $\pi(\{\varepsilon_i\}) = |\varepsilon_i\rangle\langle\varepsilon_i|$ .

We have just defined a collection of operators:

$$A_\mu(\omega) \equiv \sum_{\varepsilon_j - \varepsilon_i = \omega} \pi(\{\varepsilon_i\}) A_\mu \pi(\{\varepsilon_j\}), \quad (4.52)$$

that fulfil the relations

$$[H_S, A_\mu(\omega)] = -\omega A_\mu(\omega), \quad (4.53)$$

$$[H_S, A_\mu^\dagger(\omega)] = +\omega A_\mu^\dagger(\omega), \quad (4.54)$$

as one can check by direct calculation, and using the property  $\pi(\{\varepsilon_i\})\pi(\{\varepsilon_j\}) = \delta_{ij}\pi(\{\varepsilon_i\})$ . In other words,  $A_\mu(\omega)$  and  $A_\mu^\dagger(\omega)$  are eigenoperators of  $H_S$  corresponding to the eigenvalue  $\mp\omega$ . In addition, the following property holds:

$$A_\mu^\dagger(\omega) = A_\mu(-\omega). \quad (4.55)$$

It is also easy to see that

$$[H_S, A_\mu^\dagger(\omega)A_\nu(\omega)] = 0. \quad (4.56)$$

This representation in terms of eigenoperators is particularly helpful when one works in the interaction picture; in this case these operators can be indeed rewritten as

$$e^{iH_S t} A_\mu(\omega) e^{-iH_S t} = e^{-i\omega t} A_\mu(\omega), \quad (4.57)$$

thus, the interaction Hamiltonian gets a particularly simple form (in the interaction picture w.r.t.  $H_0 = H_S + H_E$ ), i.e.,

$$H_I(t) = \sum_{\omega} \sum_{\mu} e^{-i\omega t} A_\mu(\omega) \otimes B_\mu(t) \quad (4.58)$$

$$= \sum_{\omega} \sum_{\mu} e^{+i\omega t} A_\mu^\dagger(\omega) \otimes B_\mu^\dagger(t), \quad (4.59)$$

where

$$B_\mu(t) = e^{iH_E t} B_\mu e^{-iH_E t}. \quad (4.60)$$

#### Example 4.4.1: Quantum Brownian motion

Let us consider the case of the quantum Brownian particle considered in [Section 4.3](#), where the interaction Hamiltonian reads as

$$H_I = X \otimes B, \quad (4.61)$$

where the position operator  $X$  can be expressed in terms of the creation and annihilation

operators  $a, a^\dagger$ , i.e.,  $X = (a+a^\dagger)/2$ ,  $a$  and  $a^\dagger$  being the eigenoperators of the Hamiltonian  $H_S$  corresponding to the eigenvalues  $\mp\omega_0$ . They indeed fulfil the relations

$$[H_S, a] = -\omega_0 a, \quad [H_S, a^\dagger] = \omega_0 a^\dagger, \quad (4.62)$$

as one can easily check recalling that  $H_S = \omega_0 a^\dagger a$ , and  $[a, a^\dagger] = 1$ . This is a special case of Equations (4.53) and (4.54). Analogously, one has  $[H_S, a^\dagger a] = 0$ , as required by Equation (4.56). In the interaction picture the creation and annihilation operators are given by

$$e^{iH_S t} a e^{-iH_S t} = a e^{-i\omega_0 t} \quad (4.63)$$

$$e^{iH_S t} a^\dagger e^{-iH_S t} = a^\dagger e^{+i\omega_0 t}. \quad (4.64)$$

Therefore, the interaction Hamiltonian reads as

$$H_I(t) = e^{-i\omega_0 t} \left( \frac{a + a^\dagger e^{2i\omega_0 t}}{\sqrt{2}} \right) \otimes B(t), \quad (4.65)$$

where

$$B(t) = \sum_k \left( g_k^* b_k e^{-i\omega_k t} + g_k b_k^\dagger e^{i\omega_k t} \right). \quad (4.66)$$

#### 4.4.2 Secular Approximation

Now, we can go back to the Redfield equation in the form of Equation (4.35); if we expand the double commutator, we get

$$\dot{\rho}_S(t) = -\alpha^2 \int_0^t d\tau \text{tr} \{ -H_I(t-\tau) \rho_S(t) \otimes \rho_E H_I(t) + H_I(t) H_I(t-\tau) \rho_S(t) \otimes \rho_E + \text{H.c.} \} \quad (4.67)$$

Now, we can use Equation (4.58) for  $H_I(t-\tau)$ , while Equation (4.59) for  $H_I(t)$ , yielding

$$\dot{\rho}_S(t) = \alpha^2 \sum_{\substack{\omega, \omega' \\ \mu, \nu}} e^{i(\omega'-\omega)t} \int_0^t d\tau e^{i\omega\tau} \langle B_\mu^\dagger(\tau) B_\nu \rangle_E \{ A_\nu(\omega) \rho_S(t) A_\mu^\dagger(\omega') - A_\mu^\dagger(\omega') A_\nu(\omega) \rho_S(t) \} + \text{H.c.}, \quad (4.68)$$

where we have exploited the homogeneity of the reservoir two-point correlation function with respect to time, thanks to the fact that the environment is stationary. We can define the

following function of the system energy differences  $\omega$ :

$$\Gamma_{\mu\nu}^t(\omega) \equiv \int_0^t d\tau e^{i\omega\tau} \langle B_\mu^\dagger(\tau) B_\nu \rangle_E, \quad (4.69)$$

which still bears dependence on time. Hence, we obtain the master equation

$$\dot{\rho}_S(t) = \sum_{\substack{\omega, \omega' \\ \mu, \nu}} e^{i(\omega' - \omega)t} \Gamma_{\mu\nu}^t(\omega) (A_\nu(\omega) \rho_S(t) A_\mu^\dagger(\omega') - A_\mu^\dagger(\omega') A_\nu(\omega) \rho_S(t)) + \text{H.c.} \quad (4.70)$$

Before performing the secular approximation, we need to pause a bit, and carefully discuss the timescales involved in the problem. We have seen that the weak coupling approximation can be applied whenever the condition  $\tau_E \ll \tau_R$  holds, meaning that the system – attached to its surroundings – relaxes slowly compared to the time interval typically required by the reservoir correlations to decay. Since we are describing the dynamics using a master equation that is accurate up to the second order in the perturbation theory, one usually heuristically set  $\tau_R = \mathcal{O}(\alpha^{-2})$ . This means that we are resolving the dynamics over a time window  $\delta t$  such that  $\tau_E \ll \delta t \ll \tau_R = \mathcal{O}(\alpha^{-2})$ . By applying the full secular approximation, we are actually providing a coarse-grained description of the dynamics such that

$$\tau_S \ll \delta t \ll \tau_R = \mathcal{O}(\alpha^{-2}), \quad (4.71)$$

where  $\tau_S$  represents the typical timescale of the free system evolution, roughly given by  $\tau_S = |\omega - \omega'|^{-1}$ .

Now, the eigenoperators decomposition of the interaction Hamiltonian turn out to be very helpful, as allows us to identify those terms that bring a negligible contribution to the system evolution. Under the hypothesis (4.71), we can keep in [Equation \(4.70\)](#) only those terms corresponding to  $\omega = \omega'$ , while those for which  $\omega \neq \omega'$  do not appreciably contribute in the time-scale we are resolving the system dynamics, as they oscillate very rapidly. As a result, the master equation reads as

$$\dot{\rho}_S(t) = \sum_{\omega} \sum_{\mu, \nu} \Gamma_{\mu\nu}^t(\omega) (A_\nu(\omega) \rho_S(t) A_\mu^\dagger(\omega) - A_\mu^\dagger(\omega) A_\nu(\omega) \rho_S(t)) + \text{H.c.} \quad (4.72)$$

It is convenient to decompose the function  $\Gamma_{\mu\nu}^t$  in the following way:

$$\Gamma_{\mu\nu}^t(\omega) = \frac{1}{2} \gamma_{\mu\nu}^t(\omega) + i S_{\mu\nu}^t(\omega), \quad (4.73)$$

where

$$\gamma_{\mu\nu}^t(\omega) = \Gamma_{\mu\nu}^t(\omega) + [\Gamma_{\nu\mu}^t(\omega)]^* = \int_{-t}^t d\tau e^{i\omega\tau} \langle B_\mu^\dagger(\tau) B_\nu \rangle_E, \quad (4.74)$$

and

$$S_{\mu\nu}^t = \frac{1}{2i} (\Gamma_{\mu\nu}^t(\omega) - [\Gamma_{\nu\mu}^t(\omega)]^*) . \quad (4.75)$$

Note that the matrices  $\gamma_{\mu\nu}^t(\omega)$  and  $S_{\mu\nu}^t(\omega)$  are Hermitian, i.e.,  $\gamma_{\mu\nu}^t(\omega) = [\gamma_{\nu\mu}^t(\omega)]^*$  and  $S_{\mu\nu}^t(\omega) = [S_{\nu\mu}^t(\omega)]^*$ . After some simple algebra, we eventually obtain the master equation in the secular approximation:

$$\dot{\rho}_S(t) = -i [H_{\text{LS}}(t), \rho_S(t)] + \mathcal{D}[\rho_S(t)], \quad (4.76)$$

where the Hermitian time-dependent operator

$$H_{\text{LS}}(t) = \sum_{\omega} \sum_{\mu,\nu} S_{\mu\nu}^t(\omega) A_{\mu}^{\dagger}(\omega) A_{\nu}(\omega), \quad (4.77)$$

that contributes to the Hamiltonian part of the dynamics. This term is often referred as *Lamb shift*, since it accounts for a Lamb-type renormalisation of the unperturbed energy levels due to the system-environment coupling. We further notice that the Lamb shift Hamiltonian  $H_{\text{LS}}$  commutes with the free system Hamiltonian  $H_S$ :

$$[H_S, H_{\text{LS}}(t)] = 0, \quad (4.78)$$

thanks to the property (4.56). On the other hand, we get a dissipator in the form

$$\mathcal{D}[\rho_S(t)] = \sum_{\omega} \sum_{\mu,\nu} \gamma_{\mu\nu}^t(\omega) \left[ A_{\nu}(\omega) \rho_S(t) A_{\mu}^{\dagger}(\omega) - \frac{1}{2} \{ A_{\mu}^{\dagger}(\omega) A_{\nu}(\omega), \rho_S(t) \} \right], \quad (4.79)$$

which can be brought in Lindblad-like form upon diagonalisation of the time-dependent matrices  $\gamma_{\mu\nu}^t(\omega)$ .

#### 4.4.3 Time evolution of populations and coherences

In this Section, we would like to introduce a closed form for the diagonal and off-diagonal parts of the density operator, i.e., for *populations* and *coherences*, respectively, provided that the secular approximation has been previously performed. Let us assume that the discrete spectrum of  $H_S$  is non-degenerate, so that  $\pi(\{\varepsilon_n\})$  are simply given by one-dimensional projectors, thus,

$$H_S = \sum_n \varepsilon_n |n\rangle\langle n|, \quad (4.80)$$

where  $\{\varepsilon_n\}_n$  are distinct eigenvalues. We will show that, under this hypothesis, the dynamical equations for the populations – given by  $P_n(t) = \langle n | \rho_S(t) | n \rangle$  — and the coherences – given by  $P_{mn}(t) = \langle m | \rho_S(t) | n \rangle$  — get decoupled.

One can show – see [Appendix C](#) for the details of the derivation – that the equation for the diagonal elements of the density matrix in the  $H_S$  eigenbasis satisfy the set of differential equations

$$\dot{P}_n = \sum_k [W_t(n|k)P_k(t) - W_t(k|n)P_n(t)], \quad (4.81)$$

while coherences – in the Schrödinger picture – obey

$$\dot{P}_{mn}(t) = - \left\{ i\omega_{mn} + \frac{1}{2} \sum_k [W_t(k|n) + W_t(k|m)] \right\} P_{mn}(t), \quad (4.82)$$

where  $\omega_{mn}$  are the Bohr frequencies, and we have introduced the time-dependent transition rates<sup>5</sup>

$$W_t(n|k) \equiv \sum_{\mu,\nu} \gamma_{\mu\nu}^t (\varepsilon_k - \varepsilon_n) \langle k | A_\mu | n \rangle \langle n | A_\nu | k \rangle. \quad (4.83)$$

## 4.5 *Intermezzo: non-Markovian damped harmonic oscillator*

Let us consider again the case of a Brownian particle, already discussed in [Section 4.3](#). In this Section, we would like to prove that, taking the secular approximated version of [Equation \(4.45\)](#), one ultimately obtain the master equation of a damped harmonic oscillator, displaying memory effects ([Intravaia, 2003a](#)). As we have seen in the [Example 4.1.1](#), the eigenoperators of the system free Hamiltonian  $H_S = \omega_0 a^\dagger a$  are given by the creation and annihilation operators  $a^\dagger, a$ . Furthermore, the two-point correlation function is given by  $\langle B(\tau)B \rangle_E = (\kappa(\tau) - i\mu(\tau))/2$ , where the kernels are given by [Equations \(4.37\)](#) and [\(4.38\)](#), respectively. A straightforward calculation yields the coefficients  $\gamma_{\mu\nu}^t(\omega)$  in [Equation \(4.79\)](#), as far as we observe that the kernels  $\kappa(\tau)$  and  $\mu(\tau)$  are even and odd functions of  $\tau$ , respectively. Working in the interaction picture with respect to the renormalised Hamiltonian  $\tilde{H}_S$  – cf. [Equation \(4.44\)](#), we obtain the following master equation for the reduced density operator  $\rho$ :

$$\dot{\rho}(t) = [\Delta(t) + \gamma(t)] \left( a\rho a^\dagger - \frac{1}{2} \{a^\dagger a, \rho\} \right) + [\Delta(t) - \gamma(t)] \left( a^\dagger \rho a - \frac{1}{2} \{aa^\dagger, \rho\} \right), \quad (4.84)$$

where the time-dependent rates  $\Delta(t)$  and  $\gamma(t)$  – accounting for diffusion and dissipation – are defined by [Equations \(4.43a\)](#) and [\(4.43b\)](#), respectively. It is worth mentioning that the secular approximation does not wash out all memory effects, therefore the master equation [\(4.84\)](#) still captures some non-Markovian features of the dynamics, in those time intervals in which the rate  $[\Delta(t) - \gamma(t)]$  attains negative values. These features can be observed in [Figure 4.3](#) for a specific choice of the spectral density. Moreover, these coefficients have a

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<sup>5</sup>Note that they are not, strictly speaking, transition rates, as they can be negative.

well-defined physical meaning:  $(\Delta(t) + \gamma(t))$  is the rate associated with the incoherent loss of excitations from the system, while  $(\Delta(t) - \gamma(t))$  is the rate of incoherent pumping.

If we further assume that the reservoir is made of harmonic oscillators, one can show that the noise and dissipation kernels  $\kappa(\tau)$  and  $\mu(\tau)$  – thus, in turn, the rates  $\Delta(t)$  and  $\gamma(t)$  – ultimately depend on the spectral density  $J(\omega)$  of the bath, defined as in [Equation \(4.10\)](#). We can indeed show<sup>6</sup> that

$$\begin{bmatrix} \kappa(\tau) \\ \mu(\tau) \end{bmatrix} = 2\alpha^2 \int_0^\infty J(\omega) \begin{bmatrix} \cos(\omega\tau) \coth\left(\frac{\beta}{2}\omega\right) \\ \sin(\omega\tau) \end{bmatrix} d\omega, \quad (4.85)$$

where  $\beta = (k_B T)^{-1}$  is the inverse temperature of the bath, and  $k_B$  the Boltzmann constant. It is worth mentioning that the dissipation kernel  $\mu(\tau)$  is temperature-independent, as one should expect.

#### Example 4.5.1: Ohmic spectral densities

In order to obtain the noise and the dissipation kernel, thus the time-dependent rates  $\gamma(t)$  and  $\Delta(t)$ , one has to choose explicitly the spectral density of the bath. One common choice is given by an Ohmic SD with a Lorentz-Drude cut-off

$$J(\omega) = \frac{2\omega}{\pi} \frac{\omega_c^2}{\omega_c^2 + \omega^2}, \quad (4.86)$$

where  $\omega_c$  is the cut-off frequency. With this particular choice, the noise kernel reads as

$$\kappa(\tau) = \frac{4\alpha^2 \omega_c^2}{\pi} \int_0^\infty d\omega \frac{\omega \cos(\omega\tau)}{\omega_c^2 + \omega^2} \coth\left(\frac{\beta}{2}\omega\right). \quad (4.87)$$

By using the following representation of the hyperbolic cotangent:

$$\coth\left(\frac{\beta}{2}\omega\right) = \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{\omega}{\omega^2 + \nu_n^2}, \quad (4.88)$$

[Equation \(4.87\)](#) becomes

$$\kappa(\tau) = \frac{4\alpha^2 \omega_c^2}{\pi\beta} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\omega^2 \cos(\omega\tau)}{(\omega^2 + \omega_c^2)(\omega^2 + \nu_n^2)} d\omega, \quad (4.89)$$

where we have also observed that the integrand is an even function of  $\omega$ . The integrals appearing in [Equation \(4.89\)](#) can be solved analytically using the method of residues,

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<sup>6</sup>The derivation follows the same steps as those for obtaining the thermal bath correlation function – see [Appendix A](#).

yielding the following expression for the environmental noise kernel:

$$\kappa(\tau) = \frac{4\alpha^2 \omega_c^2}{\beta} \sum_{n=-\infty}^{\infty} \frac{\omega_c e^{-\omega_c |\tau|} - |\nu_n| e^{-|\nu_n||\tau|}}{\omega_c^2 - \nu_n^2}, \quad (4.90)$$

where  $\nu_n = 2\pi n/\beta$  are known as the Matsubara frequencies (Breuer, 2002). On the other hand, by substituting Equation (4.86) into (4.85) and solving the integral, one obtains

$$\mu(\tau) = 2\alpha^2 \omega_c^2 e^{-\omega_c |\tau|} \operatorname{sign}(\tau). \quad (4.91)$$

For example, with this choice of the SD, one gets the following expression for the dissipation rate:

$$\gamma(t) = \frac{2\alpha^2 \omega_c^2}{\omega_c^2 + \omega_0^2} \left[ \omega_0 - e^{-\omega_c t} (\omega_0 \cos(\omega_0 t) + \omega_c \sin(\omega_0 t)) \right]. \quad (4.92)$$

Alternatively, one can choose an exponential cut-off (Carmichael, 1999), thus the SD reads as

$$J(\omega) = \omega e^{-\omega/\omega_c}. \quad (4.93)$$

Notwithstanding the similarity with Equation (4.86), this particular choice forecloses the pathological behaviour at  $t = 0^+$  that we would encounter dealing with a Lorentz-Drude cut-off, as the latter predicts an unphysical instantaneous dissipation (Hu, 1992). The noise kernel reads as

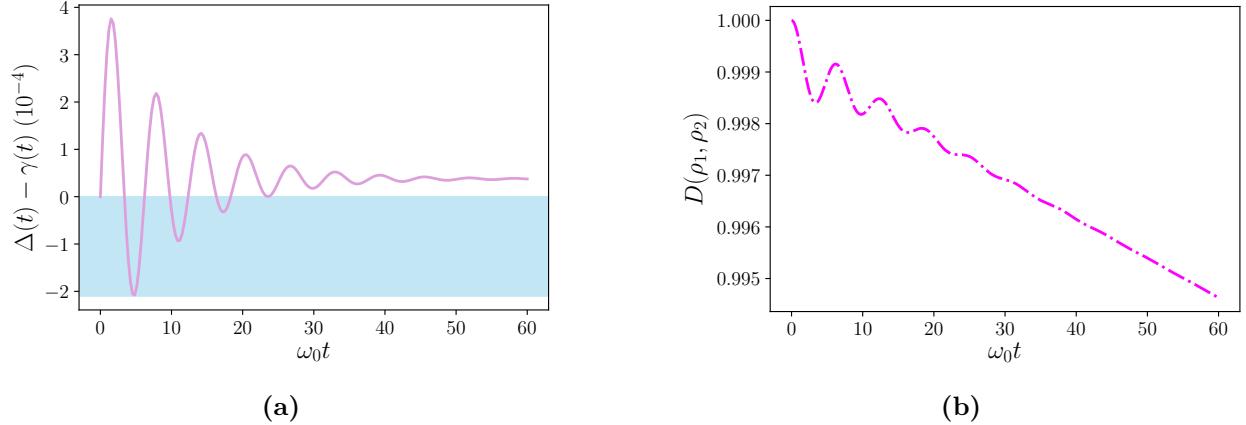
$$\kappa(\tau) = \frac{2\alpha^2 \omega_c^2 (\tau^2 \omega_c^2 - 1)}{(1 + \tau^2 \omega_c^2)^2} + \frac{2\alpha^2}{\beta^2} \left( \psi' \left( \frac{1 - i \tau \omega_c}{\beta \omega_c} \right) + \psi' \left( \frac{1 + i \tau \omega_c}{\beta \omega_c} \right) \right), \quad (4.94)$$

where  $\psi'(z) = \frac{d^2}{dz^2} \ln \Gamma(z)$  is the polygamma function of order one (also known as trigamma), while  $\Gamma(z)$  is the Gamma function (Gradshteyn, 2007). On the other hand, the dissipation kernel is given by

$$\mu(\tau) = \frac{4\alpha^2 \omega_c^3 \tau}{(1 + \tau^2 \omega_c^2)^2}. \quad (4.95)$$

#### 4.5.1 Projection of the master equation onto the Fock space basis

Let us denote as  $|n\rangle$ , with  $n = 0, 1, 2, \dots$ , the  $n$ -th eigenstate of the harmonic oscillator, satisfying the eigenvalue equation  $a^\dagger a |n\rangle = n |n\rangle$ . We would like to project Equation (4.84) onto the basis spanned by  $|n\rangle$ . A simple calculation yields the following set of differential



**Figure 4.3:** Non-Markovian damped harmonic oscillator. **Panel (a):** Time-dependent rates associated to incoherent pumping. **Panel (b):** Trace distance taking the two initial states  $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  in the two-dimensional subspace spanned by the first two levels  $|0\rangle, |1\rangle$ . The dynamics of the system is numerically simulated by solving the set of differential equations introduced in Section 4.5.1. The simulation was run choosing  $\alpha = 0.01\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ , and an Ohmic SD with a Lorentz-Drude cut-off. There is a clear correspondence between the intervals in which the decay rates become negative and those in which the trace distance increases.

equations for  $P_{mn}(t) \equiv \langle m|\rho|n\rangle$ :

$$\begin{aligned} \dot{P}_{mn}(t) = & [\Delta(t) + \gamma(t)] \left\{ \sqrt{(m+1)(n+1)} P_{(m+1)(n+1)}(t) - \frac{1}{2}(m+n) P_{mn}(t) \right\} \\ & + [\Delta(t) - \gamma(t)] \left\{ \sqrt{mn} P_{(m-1)(n-1)}(t) - \frac{1}{2}(m+n) P_{mn}(t) \right\}, \end{aligned} \quad (4.96)$$

where we have used the standard relations  $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$  and  $a|n\rangle = \sqrt{n}|n-1\rangle$ . As a byproduct, this calculation also offers a method for numerically simulating the dynamics of such a system: we essentially need to solve a Cauchy problem for a set of coupled differential equations, given a suitable set of initial conditions, i.e., the entries of the initial density matrix. We should notice that, due to the fact that the system Hamiltonian is unbounded from above, the differential equations can be, in principle, (countably) infinitely many; however, since our computational resources are limited, we need to truncate the Fock space when  $m = \bar{m}$  and  $n = \bar{n}$ , where  $\bar{m}$  and  $\bar{n}$  are fixed by the degree of accuracy one would like to reach.

### 4.5.2 Adjoint master equation

Given [Equation \(4.84\)](#), we can move in the dual space of operators and obtain the adjoint master equation for the Heisenberg operator  $A_H(t)$ , i.e.,

$$\begin{aligned}\dot{A}_H(t) &= [\Delta(t) + \gamma(t)] \left( a^\dagger A_H(t) a - \frac{1}{2} \{a^\dagger a, A_H(t)\} \right) \\ &\quad + [\Delta(t) - \gamma(t)] \left( a A_H(t) a^\dagger - \frac{1}{2} \{aa^\dagger, A_H(t)\} \right),\end{aligned}\tag{4.97}$$

We can solve the latter for the annihilation and creation operators, with the initial condition that at  $t = 0$  the Schrödinger and the Heisenberg operators coincide, obtaining

$$a_H(t) = a e^{-\Gamma(t)/2},\tag{4.98}$$

$$a_H^\dagger(t) = a^\dagger e^{-\Gamma(t)/2},\tag{4.99}$$

where  $\Gamma(t) = 2 \int_0^t \gamma(\tau) d\tau$ . Analogously, from [Equation \(4.97\)](#), one gets the differential equation

$$\frac{d}{dt} (a^\dagger a)_H(t) = -2\gamma(t)(a^\dagger a)_H(t) + \Delta(t) - \gamma(t),\tag{4.100}$$

whose solution is

$$(a^\dagger a)_H(t) = e^{-\Gamma(t)} a^\dagger a + \frac{1}{2} (e^{-\Gamma(t)} - 1) + \Delta_\Gamma(t),\tag{4.101}$$

where we have defined

$$\Delta_\Gamma(t) \equiv e^{-\Gamma(t)} \int_0^t \Delta(t_1) e^{\Gamma(t_1)} dt_1.\tag{4.102}$$

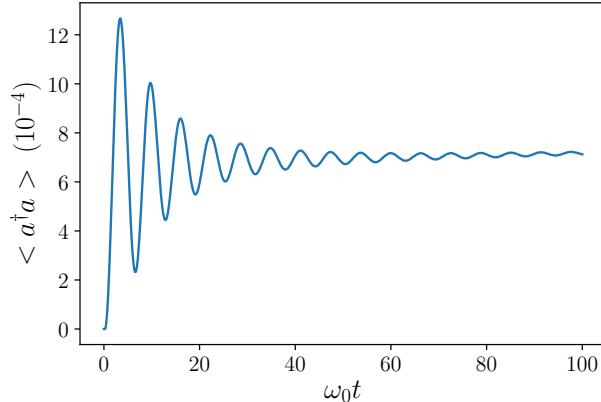
By virtue of the duality relation  $\langle a^\dagger a(t) \rangle = \text{tr}_S(a^\dagger a \rho(t)) = \text{tr}_S((a^\dagger a)_H(t) \rho(0))$ , we can derive a closed expression for the average number of excitations  $\langle a^\dagger a \rangle$ , i.e.,

$$\langle a^\dagger a(t) \rangle = e^{-\Gamma(t)} \langle a^\dagger a(0) \rangle + \frac{1}{2} (e^{-\Gamma(t)} - 1) + \Delta_\Gamma(t),\tag{4.103}$$

also known as *heating function* ([Maniscalco, 2004](#)). An example is provided in [Figure 4.4](#).

## 4.6 Microscopic derivation of the GKSL generator

The secular approximation performed onto the Redfield equation is not sufficient to guarantee that we have obtained a fully Markovian master equation; nonetheless, one can recover the semigroup property as a suitable limit of [Equation \(4.76\)](#), that sometimes is referred as *second Born approximation* ([de Vega, 2017](#)). Actually, it is customary to collectively call the whole



**Figure 4.4:** Heating function for a non-Markovian damped Harmonic oscillator. The plot refers to a Ohmic SD with an exponential cut-off. Note that the cut-off is taken to be smaller than the frequency of the oscillator, so that non-Markovian oscillation can be observed. For the numerical simulation, we took  $\alpha = 0.01\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ , assuming that the oscillator is initially in the vacuum.

set of assumptions that leads to this master equation as *Born-Markov approximation* (Breuer, 2002). The last step we need to make to obtain a generator in the GKSL form is to assume that we are resolving the dynamics over a timescale that allow us to take the limit  $t \rightarrow +\infty$  in the integrals defining the matrices  $\gamma_{\mu\nu}^t$  and  $S_{\mu\nu}^t(\omega)$ . This limit can be formally carried out by considering a technique that was first introduced by Davies, based on Van Hove's idea of rescaled time (Davies, 1976; Rivas, 2012; Chruściński, 2017; Facchi, 2017). According to the latter, we should take weaker and weaker interactions (i.e.,  $\alpha \rightarrow 0$ ), while we keep the rescaled time  $\alpha^2 t$  finite. Under this condition, we can perform the limit  $t \rightarrow +\infty$ . By so doing, we obtain

$$\gamma_{\mu\nu}(\omega) \equiv \gamma_{\mu\nu}^\infty(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} \langle B_\mu^\dagger(\tau) B_\nu \rangle_E, \quad (4.104)$$

i.e.,  $\gamma_{\mu\nu}(\omega)$  are given by the Fourier transform of the bath correlation function. One can prove that the matrices  $\gamma_{\mu\nu}$  are positive-definite for any value of  $\omega$ , i.e., they represent Kossakowski matrices, due to the fact that they are expressed as the Fourier transform of a positive-definite function — see Appendix D for a proof. As a result, we have recovered the generator of a quantum dynamical semigroup: the dynamics described by the corresponding master equation is Markovian.

From Equation (4.104), we also obtain that the two-point correlation function can be regarded as the inverse Fourier transform of the coefficients  $\gamma_{\mu\nu}(\omega)$ , i.e.,

$$\langle B_\mu^\dagger(\tau) B_\nu \rangle_E = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} e^{-i\omega'\tau} \gamma_{\mu\nu}(\omega'), \quad (4.105)$$

thus, by substituting the latter in the definition of  $S_{\mu\nu}(\omega)$  – cf. Equation (4.75) –, one eventually get that<sup>7</sup>

$$S_{\mu\nu}(\omega) = \text{P.V.} \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{\gamma_{\mu\nu}(\omega')}{\omega - \omega'}, \quad (4.106)$$

i.e.,  $S_{\mu\nu}(\omega)$  is the Hilbert transform of  $\gamma_{\mu\nu}(\omega)$ .

#### 4.6.1 Relaxation to equilibrium

In the derivation outlined in the previous Sections, we have not made any particular assumption about the environmental state, apart from requiring it to be stationary, i.e.,  $[H_E, \rho_E] = 0$ . In many applications, one assumes that the environment is a heat bath, whose inverse temperature is  $\beta$ ; in this case,  $\rho_E$  is given by

$$\rho_E = \frac{e^{-\beta H_E}}{\mathcal{Z}_E}, \quad (4.107)$$

where the environmental partition function is  $\mathcal{Z}_E = \text{tr}_E(e^{-\beta H_E})$ . Under this hypothesis, is it easy to prove that the two-point correlation function obeys the  $\beta$ -KMS boundary condition

$$\langle B_\mu^\dagger(t) B_\nu \rangle_{\text{th}} = \langle B_\nu B_\mu^\dagger(t + i\beta) \rangle_{\text{th}}, \quad (4.108)$$

where the average  $\langle \cdot \rangle_{\text{th}}$  it taken over the canonical Gibbs state (4.107). The  $\beta$ -KMS condition (4.108) carries over to the Kossakowski matrices  $\gamma_{\mu\nu}(\omega)$ , namely

$$\gamma_{\mu\nu}(-\omega) = e^{-\beta\omega} \gamma_{\nu\mu}(\omega). \quad (4.109)$$

Now, if we introduce the system canonical thermal state

$$\rho_{\text{eq}} = \frac{e^{-\beta H_S}}{\mathcal{Z}_S}, \quad (4.110)$$

where  $\mathcal{Z}_S = \text{tr}_S(e^{-\beta H_S})$ , one can prove the following properties:

$$\rho_{\text{eq}} A_\mu(\omega) = e^{\beta\omega} A_\mu(\omega) \rho_{\text{eq}}, \quad (4.111)$$

$$\rho_{\text{eq}} A_\mu^\dagger(\omega) = e^{-\beta\omega} A_\mu^\dagger(\omega) \rho_{\text{eq}}. \quad (4.112)$$

<sup>7</sup>One has to resort to the identity

$$\int_0^{+\infty} d\tau e^{-i(\omega - \omega')\tau} = \pi\delta(\omega - \omega') + i \text{ P.V.} \left( \frac{1}{\omega - \omega'} \right),$$

where P.V. stands for the Cauchy Principal Value.

If there is no external driving, i.e., there are no time-dependent fields acting on the system, we can prove that  $\rho_S(t) \rightarrow \rho_{\text{eq}}$  as  $t \rightarrow +\infty$ . The proof can be carried out by observing that, thanks to the the commutation relation given by [Equation \(4.78\)](#)<sup>8</sup>, we have  $[\rho_{\text{eq}}, H_{\text{LS}}] = 0$  for the Hamiltonian part; whereas, using [Equations \(4.109\), \(4.111\)](#) and [\(4.112\)](#), a tedious but straightforward calculation yields the result  $\mathcal{D}[\rho_{\text{eq}}] = 0$ . Thus,  $\rho_{\text{eq}}$  is a solution of the corresponding Markovian master equation.

This is actually a special instance of a more general result. A theorem by Spohn sets the conditions to have a well-defined stationary state  $\rho_{\text{ss}}$  for a system whose dynamics is described in terms of a GKSL generator ([Spohn, 1977](#); [Frigerio, 1978](#)). It states that the reduced density operator  $\rho_S(t)$  relaxes towards  $\rho_{\text{ss}}$ , if any operator  $X$  commuting with all the Lindblad operators and their adjoints is proportional to the identity. In our case, from the condition

$$[X, A_\mu(\omega)] = 0 = [X, A_\mu^\dagger(\omega)] \quad \text{for all } \mu, \omega \quad (4.113)$$

follows that  $X = c\mathbb{I}$ , with  $c \in \mathbb{C}$ . Under these assumptions, the quantum dynamical semigroup is said to be relaxing ([Rivas, 2012](#)), or ergodic ([Breuer, 2002](#)).

Nonetheless, we should stress that this peculiar property of the stationary states is a consequence of the weak coupling with the environmental degrees of freedom. For instance, if one pushes the interaction between system and thermal reservoir towards the strong coupling limit, it would not be guaranteed anymore that the steady state is given by [Equation \(4.110\)](#) — see, e.g., ([Subaşı, 2012](#); [Perarnau-Llobet, 2018](#)).

### 4.6.2 Pauli master equation

When one takes the limit  $t \rightarrow +\infty$  in the derivation of the master equation, the quantities defined by [Equation \(4.83\)](#) becomes  $W_\infty(n|k) \equiv W(n|k)$ . In this limit, as a consequence of the positive definiteness of the Kossakowski matrices  $\gamma_{\mu\nu}$ , they can be correctly interpreted as time-independent rates, and determined by means of the Fermi golden rule ([Alicki, 1977](#)). Hence, [Equation \(4.81\)](#) takes the form of a master equation for a classical probability distribution, known as *Pauli master equation*. If the environment is in a thermal state, by employing [Equation \(4.109\)](#) and the definition of the transition rates — [Equation \(4.83\)](#) in the limit  $t \rightarrow +\infty$ , one can show that the *detailed-balance condition* is satisfied

$$W(k|n) e^{-\beta\varepsilon_n} = W(n|k) e^{-\beta\varepsilon_k}. \quad (4.114)$$

This conditions ensures that the equilibrium populations  $P_n^{\text{eq}}$  follow the Boltzmann distribution, i.e.,

$$P_n^{\text{eq}} \propto e^{-\beta\varepsilon_n}. \quad (4.115)$$

Therefore, the Davies approach to the microscopic derivation of a master equation leads to a set of differential equations that govern the evolution of populations (classical part) and a separated set of equations for coherences (genuinely quantum part).

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<sup>8</sup>Note that – in the fully Markovian limit – we are using a time-independent Lamb-shift Hamiltonian.

### Example 4.6.1: Markovian damped harmonic oscillator

In this example, we would like to heuristically show that we can recover the Markovian master equation of a damped harmonic oscillator taking a suitable limit in the [Equation \(4.84\)](#). Usually, we obtain a Markovian description of the dynamics for a Brownian particle by taking simultaneously the long time and high temperature limit, i.e.,  $\omega_0 t \gg 1$  and  $\beta^{-1} \gg \omega_0$ , which is the usual physical regime in which the Caldeira-Leggett model is presented ([Breuer, 2002](#)). Since the damping coefficient – given by [Equation \(4.92\)](#) – does not depend on the reservoir temperature, one immediately obtains

$$\gamma_M \equiv 2 \lim_{t \rightarrow \infty} \gamma(t) = \frac{4\alpha^2 \omega_c^2}{\omega_c^2 + \omega_0^2} \omega_0, \quad (4.116)$$

while the diffusion coefficient  $\Delta(t)$  converges towards

$$\Delta_M(t) = \frac{\gamma_M}{2} (2\bar{n} + 1), \quad (4.117)$$

where  $\bar{n}$  is the average number of excitations with a given frequency  $\omega_0$ , i.e.,  $\bar{n} = (e^{\beta\omega_0} - 1)^{-1}$ . Therefore, in the Markovian regime, [Equation \(4.84\)](#) becomes

$$\dot{\rho}(t) = \gamma_M (\bar{n} + 1) \left( a \rho a^\dagger - \frac{1}{2} \{a^\dagger a, \rho\} \right) + \gamma_M \bar{n} \left( a^\dagger \rho a - \frac{1}{2} \{aa^\dagger, \rho\} \right), \quad (4.118)$$

which reproduces the well known result of a Markovian damped harmonic oscillator ([Breuer, 2002](#)). Moreover, taking the aforementioned limit in [Equation \(4.103\)](#), one obtains the following expression for the average number of quanta:

$$\langle a^\dagger a(t) \rangle = e^{-\gamma_M t} \langle n(0) \rangle + \bar{n} (1 - e^{-\gamma_M t}), \quad (4.119)$$

i.e., it monotonically relaxes towards  $\bar{n}$ . [Equation \(4.96\)](#) (with  $m = n$ ) allows us to write the Pauli master equation

$$\begin{aligned} \dot{P}_n(t) &= \gamma_M (\bar{n} + 1) [(n + 1)P_{n+1}(t) - nP_n(t)] \\ &\quad + \gamma_M \bar{n} [nP_{n-1}(t) - nP_n(t)], \end{aligned} \quad (4.120)$$

which is a classical equation describing a one-step stochastic process, in which, given given a state  $n$ , only jumps between neighbouring states  $n \pm 1$  are allowed ([Gardiner, 2009](#)). The stationary solution – obtained by imposing  $\dot{P}_n(t) = 0$  – can be shown to be

$$P_{ss}(n) = \frac{1}{\bar{n} + 1} \left( \frac{\bar{n}}{\bar{n} + 1} \right)^n, \quad (4.121)$$

or, equivalently,

$$P_{ss}(n) = (1 - e^{-\beta\omega_0}) e^{-n\beta\omega_0}. \quad (4.122)$$

It is easy to check that the average number of excitations in the stationary states are

$$\langle a^\dagger a \rangle_{ss} = \sum_n n P_{ss}(n) = \bar{n}, \quad (4.123)$$

as one would equally obtain by taking the long time limit  $t \rightarrow +\infty$  in [Equation \(4.119\)](#).

# Chapter 5

## Entropy production in open systems

As discussed in [Chapters 3 and 4](#), the theory of open quantum systems is an arena where irreversibility naturally comes about: this peculiar trait can be satisfactorily discussed using the language of thermodynamics, and quantified in terms of entropy. Traditionally, the theory of entropy production in the quantum domain is formulated in term of the von Neumann entropy, as we will discuss in [Section 5.2](#). On one hand, we will pinpoint the difficulties and the inconsistencies arising from the application of such a theory. We will also show that quantum coherences play a crucial role in the entropy production rate, bringing a purely quantum contribution to it. In [Section 5.3](#), we will discuss a different formulation that relies on phase-space methods. The latter will be employed in [Section 5.4](#) to assess the role of initial correlations in the entropy production rate for nonequilibrium harmonic dynamics.

### 5.1 Entropy production in classical processes

In classical thermodynamics, entropy production enables to mathematically express the second law, providing a way to characterise the irreversibility of physical processes. To be more concrete, let us suppose that we have a certain macroscopic system interacting with a reservoir. Following the splitting that was first put forth by Prigogine ([Prigogine, 1955; de Groot, 1961](#)), entropy can be expressed as a sum of two contributions

$$dS = d\Sigma - d\Phi, \quad (5.1)$$

where  $d\Phi$  is the entropy that the system exchanges with its surroundings, whereas  $d\Sigma$  is the entropy produced within the system. The second law of thermodynamics imposes a constraint on the sign of  $d\Sigma$ , i.e.,

$$d\Sigma \geq 0, \quad (5.2)$$

where  $d\Sigma = 0$  holds for reversible (or equilibrium) processes, while  $d\Sigma > 0$  for irreversible transformations. In contrast,  $d\Phi$  can be positive, negative, or null, depending on the direction

in which the entropy is flowing. Furthermore, if the system is adiabatically isolated from the reservoir, one has  $d\Phi = 0$ , thus  $dS \geq 0$ , while, if the system is allowed to exchange heat with the surroundings, in light of the Carnot-Clausius theorem, one obtains<sup>1</sup>

$$d\Phi = -\frac{dQ}{T}, \quad (5.3)$$

where  $dQ$  is the heat flowing towards the reservoir (conventionally taken to be positive), while  $T$  is the absolute temperature at which this exchange occurs. Under this hypothesis, one recovers the inequality

$$dS \geq \frac{dQ}{T}, \quad (5.4)$$

which is the standard expression of the second law of thermodynamics (Callen, 1985). From Equation (5.1) we immediately obtain the following expression for the rates

$$\frac{dS}{dt} = \dot{\Sigma}(t) - \dot{\Phi}(t), \quad (5.5)$$

where  $\dot{\Sigma}(t)$  is the *entropy production rate*, while  $\dot{\Phi}(t)$  is the *entropy flux rate*. At thermal equilibrium, we have  $\dot{\Sigma}(t) = 0 = \dot{\Phi}(t)$ . We should emphasise that, unlike entropy, which is usually regarded as a property of the system, entropy production is a quantity that characterises thermodynamic processes undergone by the system: this suggests its relevance in the domain of nonequilibrium thermodynamics, whose final goal is to relate the entropy production to the microscopic phenomena occurring within the system. Equation (5.2) implies that  $\dot{\Sigma}(t) \geq 0$ , mathematically framing the phenomenological evidence according to which entropy is always produced, never destroyed. For macroscopic systems, Equation (5.5) can be rephrased as a balance equation for the entropy density, which can be seen as the way to state locally the second law for nonequilibrium thermodynamics. However, unlike energy, entropy does not satisfy a continuity equation (de Groot, 1961).

## 5.2 Entropy production in quantum processes

Our goal is now to rewrite Equation (5.5) in the quantum domain, and identify the physical quantities upon which  $\dot{\Sigma}(t)$  and  $\dot{\Phi}(t)$  depend. In general, such a task has fostered the emergence of a variety of approaches, some of them closer to the spirit of quantum information theory (Landi, 2020). Despite this, a complete and exhaustive theory of the entropy production rate, possibly cutting across the classical-quantum boundary, is hitherto missing. As a full account of these approaches is beyond the scopes of this Thesis, we will just introduce some notions that will be useful in the following Sections, focusing on the case of weak coupling limit and thermal reservoirs.

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<sup>1</sup>Note that is no longer true when the system can also exchange matter with its environment.

### 5.2.1 Spohn's separation of work and heat in open systems

Before discussing the way in which we can express entropy production and flux rates for open quantum systems, let us start with the identification of the suitable thermodynamic quantities (Kosloff, 2013). To this end, we can consider the usual case in which the total Hamiltonian can be expressed as

$$H(t) = H_S(t) + H_E + H_I, \quad (5.6)$$

where we let the system Hamiltonian  $H_S(t)$  be time-dependent. As we have seen in [Chapter 3](#), the joint system is closed, thus thermodynamically isolated. This means that any energy change must be identified with work. In light of this observation, the power reads as

$$\dot{W}(t) \equiv \frac{d\langle H(t) \rangle}{dt} = \text{Tr} [\dot{H}_S(t)\rho_{SE}(t)] = \text{Tr} [\dot{H}_S(t)\rho(t)], \quad (5.7)$$

where, in the last step, the trace is performed over the system degrees of freedom only, and we have also used the hypothesis of uncorrelated joint states, i.e.,  $\rho_{SE}(t) = \rho(t) \otimes \rho_E$ , as usually required by the Born-Markov approximation. Such work has to be intended as performed by, or onto, the system, as it evidently depends only on its degrees of freedom. From [Equation \(5.7\)](#), we easily deduce that no work is performed in the case of time-independent Hamiltonians.

The identification of internal energy and heat is more delicate, but, in the weak coupling limit, this task can be consistently accomplished (Rivas, 2019). Indeed, under such assumption, the interaction part of the Hamiltonian is comparatively negligible, hence

$$\langle H(t) \rangle \simeq \langle H_S(t) \rangle + \langle H_E \rangle. \quad (5.8)$$

As a consequence, the internal energy of the system is unequivocally given by  $E = \langle H_S(t) \rangle$ . Therefore, the time derivative yields

$$\frac{dE(t)}{dt} = \frac{d\langle H_S(t) \rangle}{dt} \equiv \dot{W}(t) - \dot{Q}(t), \quad (5.9)$$

where we have defined the heat flow

$$\dot{Q}(t) = -\text{Tr} [H_S(t)\dot{\rho}(t)]. \quad (5.10)$$

In [Chapter 4](#), we have seen that the weak coupling limit naturally emerges when the system's evolution is modelled in terms of a quantum dynamical semigroup. Assuming that the bath dynamics is fast compared to the typical evolution time of the system, Davies' approach leads to a Markovian master equation for the reduced dynamics  $\dot{\rho}(t) = -i[H_S(t), \rho] + \mathcal{D}[\rho] = \mathcal{L}_t[\rho]$ , where  $\mathcal{D}[\rho]$  is the dissipator in the Lindblad form — cf. [Equation \(3.37\)](#). Within this framework, one usually resorts to Spohn's separation of work and heat (Spohn, 1978; Alicki, 1979), where the former is defined as in [Equation \(5.7\)](#), while the latter is given by

$$\dot{Q}(t) = -\text{Tr} [H_S(t)\mathcal{L}_t[\rho]], \quad (5.11)$$

simply obtained by substituting the expression of  $\dot{\rho}$  given by the corresponding master equation. It should be stressed that Spohn's separation is highly non unique; it entails a certain amount of arbitrariness, as the invariance of the GKSL under certain homogeneous transformations<sup>2</sup> cannot be extended to the heat flow altogether (Kosloff, 2013).

From a more general perspective, the definitions of heat and work for the thermodynamics of quantum processes are the object of a longstanding debate within the community. Several solutions have been put forward in different scenarios (Binder, 2018), but a consistent and comprehensive definition is still lacking. For instance, in (Rivas, 2020) a general framework is presented for quantum systems in contact with a thermal reservoir, encompassing arbitrary system-reservoir coupling strengths, including possible initial correlations.

### 5.2.2 Entropy production in the weak coupling limit

We are now in the position of identifying the quantities appearing in the splitting given by Equation (5.5) for open quantum systems weakly coupled with their reservoirs. First, we need to choose which entropy we would like to use; the usual choice is to consider the von Neumann entropy and the corresponding quantum relative entropy, defined by Equations (2.24) and (2.26), respectively. It can be shown that the quantum relative entropy is monotonic under CPTP maps  $\Lambda_\tau(\cdot)$  (Lindblad, 1975), i.e.,

$$S(\Lambda_\tau\rho_1||\Lambda_\tau\rho_2) \leq S(\rho_1, \rho_2). \quad (5.12)$$

Actually, it has been shown that such monotonicity property holds if we replace the hypothesis of complete positivity with the weaker requirement of positivity (Müller-Hermes, 2017).

Let us suppose the CPTP map  $\Lambda_\tau$  is obtained from a time-dependent GKSL generator  $\mathcal{L}_t$ , i.e.,  $\Lambda_\tau = e^{\tau\mathcal{L}_t}$ , and  $\rho_{ss}(t)$  is a steady state of the map, i.e.,  $\mathcal{L}_t[\rho_{ss}(t)] = 0$ . Under these assumptions, Equation (5.12) reads

$$S(e^{\tau\mathcal{L}_t}\rho||e^{\tau\mathcal{L}_t}\rho_{ss}(t)) = S(e^{\tau\mathcal{L}_t}\rho||\rho_{ss}(t)) \leq S(\rho||\rho_{ss}(t)), \quad (5.13)$$

whence

$$\frac{d}{d\tau}S(e^{\tau\mathcal{L}_t}\rho||\rho_{ss}(t)) \leq 0. \quad (5.14)$$

Specifically, for  $\tau = 0$ , Equation (5.13) gives the so-called *Spohn inequality* (Spohn, 1978)

$$\text{Tr}(\mathcal{L}_t[\rho]\{\ln\rho - \ln\rho_{ss}(t)\}) \leq 0. \quad (5.15)$$

---

<sup>2</sup>i.e.,

$$\begin{aligned} L_k &\mapsto L'_k = L_k + \lambda_k \mathbb{I}, \\ H &\mapsto H' = H + \frac{1}{2i} \sum_k (\lambda_k^* L_k - \lambda_k L_k^\dagger) + \gamma \mathbb{I}, \end{aligned}$$

where the coefficients  $\lambda_k \in \mathbb{C}$ , while  $\gamma \in \mathbb{R}$  (Breuer, 2002).

Let us compute the time derivative of the von Neumann entropy, i.e.,

$$\dot{S}(t) = -\text{Tr}(\dot{\rho}(t) \ln \rho(t)). \quad (5.16)$$

In [Chapter 4](#), we have seen that Davies' technique provides a procedure to microscopically derive a generator  $\mathcal{L}_t$  that is automatically in the GKSL form, and enters in the master equation  $\dot{\rho}(t) = \mathcal{L}_t[\rho(t)]$ ; hence, [Equation \(5.16\)](#) reads as

$$\dot{S}(t) = -\text{Tr}(\mathcal{L}_t[\rho(t)] \ln \rho(t)). \quad (5.17)$$

Furthermore, in [Section 4.6.1](#), we have seen that, under the additional assumption that the system is coupled to a thermal reservoir, the corresponding dynamical semigroup relaxes towards the local canonical Gibbs state  $\rho_{\text{eq}} = e^{-\beta H_S}/\mathcal{Z}_S$ , thus  $\mathcal{L}_t[\rho_{\text{eq}}] = 0$ , provided that  $H_S$  is time-independent. Under this hypothesis, in full analogy with the classical case, we can identify the entropy flux with the following quantity:

$$\dot{\Phi}(t) = \beta \dot{Q}(t) = \text{Tr}(\mathcal{L}_t[\rho] \ln \rho_{\text{eq}}), \quad (5.18)$$

where, in the last step, we have invoked the definition (5.11), used the identity  $\ln \rho_{\text{eq}} = -\beta H_S - \mathbb{I} \ln \mathcal{Z}_S$ , and the fact that  $\text{Tr}(\mathcal{L}_t[\rho]) = 0$ . Now, relying on the separation given by [Equation \(5.5\)](#), and using [Equations \(5.17\)](#) and (5.18), we obtain the following expression for the entropy production rate in the weak coupling limit:

$$\dot{\Sigma}(t) = \dot{S}(t) + \dot{\Phi}(t) = -\text{Tr}(\mathcal{L}_t[\rho] \{\ln \rho - \ln \rho_{\text{eq}}\}), \quad (5.19)$$

or, equivalently,

$$\dot{\Sigma}(t) = -\frac{d}{dt} S(\rho(t) || \rho_{\text{eq}}). \quad (5.20)$$

From Spohn's inequality (5.15), it follows  $\dot{\Sigma}(t) \geq 0$  for all times. Using [Equations \(5.18\)](#) and (5.19), it is immediate to conclude that  $\dot{\Phi}(t) = 0 = \dot{\Sigma}(t)$  when the system reaches the local Gibbs state.

We should stress that this identification is valid only in the weak coupling and Markovian limits, and for thermal reservoirs. For example, as we will see, for non-Markovian dynamics is no longer true that the entropy production rate is necessarily non-negative at all times: there might be intervals of time in which the entropy production rate attains negative values ([Marcantoni, 2017](#)). This evidence is compatible with the idea of an information backflow from the environment to the system, whose features have been discussed in [Section 4.1.2](#). On a more general note, it is important to mention that, in the derivation *à la* Davies, we make use of several approximations that, although physically reasonable for deriving the reduced dynamics of the system, can lead to severe inconsistencies in terms of *thermodynamics* ([Landi, 2020](#)). For example, in Ref. ([Levy, 2014](#)), it has been argued that an approach to the thermodynamics of quantum networks based on local master equations can predict unphysical behaviours, contradicting the second law of thermodynamics. Nonetheless, this issue can

be overcome by accessing the global dynamics: in Ref. (De Chiara, 2018) it has been shown that, using an approach based on repeated collisions, a reconciliation between the local and global descriptions can be achieved.

Even in the well-established framework of a quantum dynamical semigroup, the identification introduced with the help of von Neumann entropy can be problematic in the limit of zero temperature reservoirs — i.e.,  $\beta \rightarrow +\infty$ . First, it is immediate to conclude – cf. Equation (5.18) – that the entropy flux diverges. By the same token, it is easy to see that

$$S(\rho(t)||\rho_{\text{eq}}) = -S(\rho(t)) + \beta\langle H_S \rangle + \ln \mathcal{Z}_S, \quad (5.21)$$

whence we can conclude that  $S$  is ill-defined as  $\beta \rightarrow +\infty$ , therefore  $\dot{\Sigma}(t)$  diverges. We usually face this issue whenever we compute the relative entropy using a pure reference state (Abe, 2003). However, such *zero-temperature catastrophe* is not physical, but a mere inconsistency of the theory. The limit  $T \rightarrow 0$  is indeed frequently considered in quantum optics: the resulting dynamics is well-behaved and correctly reproduces experimental data in a broad variety of physical settings (Santos, 2017).

### 5.2.3 The role of coherence

In Chapter 4, we have shown that the secular and Born-Markov approximations yield a splitting between populations and coherences in the evolution equations that mathematically expresses the occurrence of two classes of processes that are simultaneously taking place at the level of the dynamics. On one hand, there are transitions between levels of the system, causing the populations to adjust to values imposed by the bath. On the other hand, we witness the loss of coherence in the energy eigenbasis. The complete understanding of the interplay between these two processes is still an open question in quantum thermodynamics (Santos, 2019). Coherence is an essential resource for quantum processes, as it sets classical and quantum phenomena apart (Streltsov, 2017). Moreover, coherence – and thus decoherence – is a basis-dependent concept: the reduced density matrix becomes diagonal in a particular set of basis states  $\{|n\rangle\}$ , which is usually called *preferred basis*. Specifically, we will adopt the perspective according to which the emergence of a preferred basis is induced by the environment (Zurek, 1982), a general scheme that Zurek called *einselection* (Zurek, 2003).

Let us explicitly consider the case of a master equation obtained through the Davies approach. Within this framework, populations – defined as  $P_n(t) \equiv \langle n | \rho | n \rangle$  – evolve according to the classical Pauli master equation, i.e., Equation (4.81), while coherences – given by  $P_{mn}(t) \equiv \langle m | \rho | n \rangle$  – evolve according to Equation (4.82), as far as we consider time-independent transition rates satisfying the detailed balance condition

$$\frac{W(n|k)}{W(k|n)} = \frac{P_n^{\text{eq}}}{P_k^{\text{eq}}} = e^{-\beta(\varepsilon_n - \varepsilon_k)}, \quad (5.22)$$

where  $P_n^{\text{eq}}(t) \equiv \langle n | \rho_{\text{eq}} | n \rangle$ . Bearing in mind the definition of free energy  $F = E - TS$ , for the case at hand we can define the nonequilibrium free energy using the von Neumann entropy

$$F(\rho) = \text{Tr}(H_S \rho) + T \text{Tr}(\rho \ln \rho), \quad (5.23)$$

whence, for equilibrium states, we recover the well-known result of statistical mechanics

$$F_{\text{eq}} \equiv F(\rho_{\text{eq}}) = -T \ln \mathcal{Z}_S. \quad (5.24)$$

Closely following (Santos, 2019), we can define the free energy for general nonequilibrium states

$$F(\rho) = F_{\text{eq}} + TS(\rho||\rho_{\text{eq}}). \quad (5.25)$$

As we know that  $S(\rho||\rho_{\text{eq}}) \geq 0$ , we obtain the condition  $F(\rho) \geq F_{\text{eq}}$ , meaning that the equilibrium state of a system is, by definition, a system that minimises the free energy. Now, combining Equations (5.20) and (5.25), we obtain the following expression for the entropy production rate

$$\dot{\Sigma} = -\frac{1}{T} \frac{dF(\rho)}{dt}. \quad (5.26)$$

Now, we can notice that  $\rho_{\text{eq}}$  is a diagonal state in the eigenbasis  $\{|n\rangle\}$  of  $H_S$ . Since the latter is an incoherent state, we can resort to the following decomposition of von Neumann entropy (Baumgratz, 2014)

$$S(\rho||\rho_{\text{eq}}) = S(\rho_{\text{diag}}||\rho_{\text{eq}}) + C(\rho), \quad (5.27)$$

where

$$S(\rho_{\text{diag}}||\rho_{\text{eq}}) = \sum_n P_n \ln \left( \frac{P_n}{P_n^{\text{eq}}} \right), \quad (5.28)$$

which represents the Kullback-Leibler divergence of the classical probability distribution  $P \equiv \{P_n\}_n$ , relative to the equilibrium distribution  $P_{\text{eq}} \equiv \{P_n^{\text{eq}}\}_n$  (Kullback, 1951), and we have introduced the *relative entropy of coherence*

$$C(\rho) = S(\rho_{\text{diag}}) - S(\rho). \quad (5.29)$$

We can substitute Equation (5.27) back into Equation (5.25), and obtain

$$F(\rho) = F_{\text{eq}} + TS(\rho_{\text{diag}}||\rho_{\text{eq}}) + TC(\rho), \quad (5.30)$$

therefore, apart from the equilibrium contribution  $F_{\text{eq}}$ , the nonequilibrium free energy can be expressed as a sum of a classical and a genuine quantum part. The former quantifies the increase in energy due to population imbalance with respect to the equilibrium configuration, while the latter expresses the surplus in free energy carried by a nonequilibrium state with non-null coherences. From Equations (5.26) and (5.30) we easily obtain that this splitting survives for the entropy production rate altogether, i.e.,

$$\dot{\Sigma} = -\frac{d}{dt} S(\rho_{\text{diag}}||\rho_{\text{eq}}) - \frac{dC(\rho)}{dt} \equiv \dot{\Sigma}_d + \Upsilon. \quad (5.31)$$

Taking the time-derivative of [Equation \(5.28\)](#), one obtains the following expression for the diagonal part of the entropy production rate:

$$\dot{\Sigma}_d = \frac{1}{2} \sum_{n,k} [W(n|k)P_k - W(k|n)P_n] \ln \left( \frac{W(k|n)P_n}{W(n|k)P_k} \right), \quad (5.32)$$

where we have used  $\dot{P}_n$  coming from the Pauli equation, and the detailed balance condition in [Equation \(5.22\)](#). This is a result that holds for all classical stochastic processes satisfying a master equation in the Pauli form, as it can be shown by means of the so-called Schnakenberg approach ([Schnakenberg, 1976](#); [Landi, 2020](#)). Differently,  $\Upsilon$  is the rate at which entropy is dynamically produced in a process in which quantum coherence is destroyed as a result of the coupling with an environment. This splitting in the entropy production rate is not a peculiarity of Davies-Lindblad dynamical maps, but it applies more generally to maps obtained through thermal operations. The latter consist of a system that interacts with a thermal reservoir – initially prepared in an equilibrium Gibbs state – through a unitary that preserves the total (system + environment) energy ([Santos, 2019](#)).

## 5.3 Entropy production rate in phase space

In [Section 5.2.2](#), we have highlighted some of the weaknesses of the traditional formulation of entropy production in the weak coupling limit. In order to overcome this limitations, Ref. ([Santos, 2017](#)) has put forward an alternative formulation based on phase-space methods borrowed from quantum optics. The crucial step is the replacement of the von Neumann entropy with a generalised entropy function, associated with a certain probability distribution defined over the phase space. This yields a formulation of thermodynamic irreversibility that coincides with standard thermodynamics at high temperature, but helps us to gain new insight in different situations. In Ref. ([Santos, 2017](#)), the von Neumann entropy is replaced by the Wigner entropy, whose definition is based on the Wigner quasi-probability distribution.

### 5.3.1 Wigner entropy

For the sake of simplicity, let us consider a system consisting of a single bosonic mode, whose dimensionless position-like and momentum-like operators – commonly referred to as quadratures – are labelled as  $Q$  and  $P$ , respectively. The quadratures can be accommodated in a two-dimensional vector  $X = (Q, P)^T$ , and the corresponding annihilation and creation operators are defined as

$$a = \frac{Q + iP}{\sqrt{2}}, \quad a^\dagger = \frac{Q - iP}{\sqrt{2}}. \quad (5.33)$$

Given the displacement operator  $D(\lambda) = e^{\lambda a^\dagger - \lambda^* a}$  ( $\lambda \in \mathbb{C}$ ), we can define the symmetrically ordered characteristic function ([Gardiner, 2004](#))

$$\chi_W(\lambda, \lambda^*) = \text{Tr} (\rho D(\lambda)), \quad (5.34)$$

whose Fourier transform defines the Wigner function

$$\mathcal{W}(\alpha, \alpha^*) = \frac{1}{\pi^2} \int d^2\lambda e^{-\lambda\alpha^* + \lambda^*\alpha} \chi_{\mathcal{W}}(\lambda, \lambda^*), \quad (5.35)$$

where  $d^2\lambda = d\operatorname{Re}\lambda d\operatorname{Im}\lambda$ . We can also regard the Wigner function as a function of the two-dimensional vector  $\mathbf{x} = (q, p)^T$ , with  $q = (\alpha + \alpha^*)/\sqrt{2}$  and  $p = i(\alpha^* - \alpha)/\sqrt{2}$ . A particularly important class of states in the context of quantum phase space is the one embodied by Gaussian states (Ferraro, 2005), i.e., those characterised by a Gaussian characteristic function, or, equivalently, a Gaussian Wigner function<sup>3</sup>. They are fully determined by their first moments  $\bar{x}_i = \langle X_i \rangle$  and covariance matrix (CM)  $\boldsymbol{\sigma}$ , whose entries are given by

$$\sigma_{ij} = \frac{1}{2} \langle \{X_i, X_j\} \rangle - \langle X_i \rangle \langle X_j \rangle. \quad (5.36)$$

The definition of Gaussian states entails that (Ferraro, 2005)

$$\mathcal{W}(\mathbf{x}) = \frac{1}{\sqrt{2\pi \det \boldsymbol{\sigma}}} e^{-\frac{1}{2}(\mathbf{x}-\bar{\mathbf{x}})^T \boldsymbol{\sigma}^{-1}(\mathbf{x}-\bar{\mathbf{x}})}. \quad (5.37)$$

Given the Wigner function  $\mathcal{W}(\mathbf{x})$ , one can naturally associate to it the corresponding Shannon entropy, called *Wigner entropy*, which embodies a useful quantifier of information, i.e.,

$$S_{\mathcal{W}} = - \int d^2\alpha \mathcal{W}(\alpha, \alpha^*) \ln \mathcal{W}(\alpha, \alpha^*). \quad (5.38)$$

Interestingly, it can be shown that the Wigner entropy is closely related to Rényi-2 entropy<sup>4</sup>. Given a Gaussian state  $\varrho$ , its purity is given by  $\mu(\varrho) = \operatorname{Tr} \varrho^2 = (\det \boldsymbol{\sigma})^{-1/2}$ , hence  $S_2 = -\ln \mu(\varrho) = \frac{1}{2} \ln(\det \boldsymbol{\sigma})$ . It can be shown that (Adesso, 2012)

$$S_{\mathcal{W}} = S_2 + \text{const}, \quad (5.40)$$

i.e., the Wigner entropy coincide (modulo an additional constant) with the Rényi-2 entropy. Therefore, for the study of the entropy production rate there is no difference between the two quantities.

Note that, in general, for non-Gaussian states  $\mathcal{W}(\alpha, \alpha^*)$  can attain negative values, causing  $S_{\mathcal{W}}$  to take complex values, a circumstance that would make the Wigner entropy clearly unsuitable as a measure of information.

<sup>3</sup>The Fourier transform of a Gaussian function is Gaussian.

<sup>4</sup>In general, Rényi- $\alpha$  entropies are defined through the formula

$$S_{\alpha} = \frac{1}{1-\alpha} \ln \operatorname{Tr}(\rho^{\alpha}), \quad \alpha > 0, \quad (5.39)$$

and they play an important role in quantum information theory. Specifically, in the limit  $\alpha \rightarrow 1$ , we recover the von Neumann entropy, while for  $\alpha = 2$  we obtain the Rényi-2 entropy  $S_2 = -\ln \operatorname{Tr} \rho^2$ , which, being closely related to the purity  $\mathcal{P} = \operatorname{Tr} \rho^2$  of the state  $\rho$ , is easy to manipulate.

### 5.3.2 Wigner entropy production rate

We are now in a position to use  $S_{\mathcal{W}}$  to formulate a theory of the entropy production (Santos, 2017). For our purposes, it is sufficient to consider the case of a harmonic oscillator (thus, a single mode), undergoing Markovian damping [cf. Example 4.6.1]. For the sake of completeness, let us remind that the free Hamiltonian is given by  $H_S = \omega_0 a^\dagger a$ , while the dissipator in the Lindblad form reads

$$\mathcal{D}[\rho] = \gamma (\bar{n} + 1) \left( a\rho a^\dagger - \frac{1}{2} \{a^\dagger a, \rho\} \right) + \gamma \bar{n} \left( a^\dagger \rho a - \frac{1}{2} \{aa^\dagger, \rho\} \right), \quad (5.41)$$

where  $\gamma > 0$  is the damping rate of the oscillator, while  $\bar{n} = (e^{\beta\omega_0} - 1)^{-1}$  is the average number of thermal excitations in the bath. It is easy to compute the partition function  $Z_S = \text{Tr}(e^{-\beta H_S}) = (1 - e^{-\beta\omega_0})^{-1}$ , hence, using Equation (4.110), we obtain  $\rho_{\text{eq}} = (1 - e^{-\beta\omega_0})e^{-\beta\omega_0 a^\dagger a}$ . By resorting to standard methods of quantum optics, one can remap the Markovian master equation  $\dot{\rho} = -i[H_S, \rho] + \mathcal{D}[\rho]$  in the phase space, where the time evolution of the system is governed by a Fokker-Planck equation (Gardiner, 2004). To this end, we can employ the following set of correspondence rules

$$[a^\dagger a, \rho] \mapsto \partial_\alpha^*(\alpha^* \mathcal{W}) - \partial_\alpha(\alpha \mathcal{W}), \quad (5.42)$$

$$a\rho a^\dagger - \frac{1}{2} \{a^\dagger a, \rho\} \mapsto \frac{1}{2} (\alpha \partial_\alpha + \partial_{\alpha^*} \alpha^* + \partial_\alpha \partial_{\alpha^*}) \mathcal{W}, \quad (5.43)$$

$$a^\dagger \rho a - \frac{1}{2} \{aa^\dagger, \rho\} \mapsto \frac{1}{2} (-\partial_\alpha \alpha - \alpha^* \partial_{\alpha^*} + \partial_\alpha \partial_{\alpha^*}) \mathcal{W}, \quad (5.44)$$

to derive the following Fokker-Planck equation for the Wigner quasi-probability distribution

$$\partial_t \mathcal{W} = \mathcal{U}(\mathcal{W}) + \mathcal{D}(\mathcal{W}), \quad (5.45)$$

where

$$\mathcal{U}(\mathcal{W}) = -i\omega_0 [\partial_{\alpha^*}(\alpha^* \mathcal{W}) - \partial_\alpha(\alpha \mathcal{W})] \quad (5.46)$$

is the differential operator associated to the unitary part of the dynamics. On the other hand, the dissipative part is expressed through

$$\mathcal{D}(\mathcal{W}) = \partial_\alpha J(\mathcal{W}) + \partial_{\alpha^*} J^*(\mathcal{W}), \quad (5.47)$$

which reads as a divergence in the complex plane, and

$$J(\mathcal{W}) = \frac{\gamma}{2} \left[ \alpha \mathcal{W} + \left( \bar{n} + \frac{1}{2} \right) \partial_{\alpha^*} \mathcal{W} \right] \quad (5.48)$$

represents the irreversible component of the probability current. The latter vanishes if and only if  $\mathcal{W} = \mathcal{W}_{\text{eq}}$ , the Wigner function of a thermal state, i.e.,  $J(\mathcal{W}_{\text{eq}}) = 0$ . This condition is stronger than  $\mathcal{D}(\mathcal{W}_{\text{eq}}) = 0$ , as it requires that the equilibrium state is not only a fixed point of the dissipative dynamics, but the state for which all probabilities currents are identically zero.

### Example 5.3.1: Wigner function of a thermal state

Let us consider the canonical Gibbs state

$$\rho_\beta = \frac{e^{-\beta H}}{\mathcal{Z}_\beta}, \quad (5.49)$$

where  $H = \omega_0 a^\dagger a$  is the Hamiltonian of a harmonic oscillator. For the sake of this instance, the partition function is simply given by  $\mathcal{Z}_\beta = \text{Tr}(e^{-\beta H}) = (1 - e^{-\beta\omega_0})^{-1}$ , therefore, using the resolution of the identity, [Equation \(5.49\)](#) reads as

$$\rho_\beta = (1 - e^{-\beta\omega_0})^{-1} \sum_{n=0}^{\infty} (e^{-\beta\omega_0})^n |n\rangle\langle n|. \quad (5.50)$$

As  $\bar{n} = (e^{\beta\omega_0} - 1)^{-1}$ , the thermal state of a harmonic oscillator reads

$$\rho_\beta = \sum_{n=0}^{\infty} \frac{\bar{n}^n}{(\bar{n} + 1)^{n+1}} |n\rangle\langle n|. \quad (5.51)$$

The characteristic function is given by

$$\chi_W(\lambda, \lambda^*) = \text{Tr}(D(\lambda)\rho_{\text{th}}) = \sum_{n=0}^{\infty} \frac{\bar{n}^n}{(\bar{n} + 1)^{n+1}} \langle n | D(\lambda) | n \rangle \quad (5.52)$$

with  $\langle n | D(\lambda) | n \rangle = e^{-|\lambda|^2/2} L_n(|\lambda|^2)$  ([Cahill, 1969](#); [Ferraro, 2005](#)). [Equation \(5.52\)](#) thus reads

$$\chi_W(\lambda, \lambda^*) = e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\bar{n}^n}{(\bar{n} + 1)^{n+1}} L_n(|\lambda|^2). \quad (5.53)$$

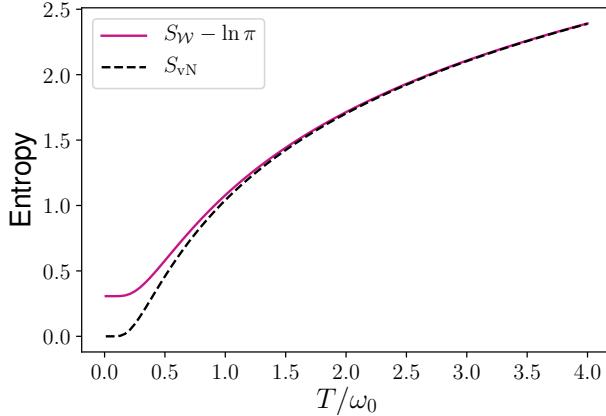
The generating function for the Laguerre polynomials fulfils the following relation ([Gradshteyn, 2007](#))

$$\sum_{n=0}^{+\infty} t^n L_n(x) = \frac{1}{1-t} e^{-tx/(1-t)}, \quad (5.54)$$

which in turn gives  $\chi_W(\lambda, \lambda^*) = e^{-(\bar{n} + \frac{1}{2})|\lambda|^2}$ .

Plugging the latter into [Equation \(5.35\)](#) and integrating, we eventually obtain the following expression for the Wigner function of a thermal state

$$\mathcal{W}_{\text{eq}} = \frac{1}{\pi(\bar{n} + \frac{1}{2})} e^{-\frac{|\alpha|^2}{\bar{n} + \frac{1}{2}}}. \quad (5.55)$$



**Figure 5.1:** Plots of the von Neumann and the Wigner entropies for a thermal state – cf. Equations (5.56) and (5.57). The picture shows that the two curves are qualitatively similar – modulo a constant  $\ln \pi$  – for a range of temperatures, while they differ in the neighbourhood of  $T = 0$ .

We can now compare the von Neumann and Wigner entropies considering Equations (5.49) and (5.55), respectively. A simple calculation yields the following expression for the Von Neumann entropy

$$S_{\text{vN}} = -\text{Tr}(\rho \ln \rho) = -\sum_{k,n=0}^{\infty} \langle n | \rho | k \rangle \langle k | \ln \rho | n \rangle = \beta \omega_0 \bar{n} - \ln(1 - e^{-\beta \omega_0}), \quad (5.56)$$

whereas, by taking into account that  $\int d^2\alpha \mathcal{W}_{\text{eq}} = 1$  and  $\int d^2\alpha |\alpha|^2 \mathcal{W}_{\text{eq}} = \bar{n} + \frac{1}{2}$ , we obtain

$$S_{\mathcal{W}} = 1 + \ln \pi + \ln \left( \bar{n} + \frac{1}{2} \right). \quad (5.57)$$

In Figure 5.1 we compare the two entropies Equations (5.56) and (5.57), explicitly showing that  $S_{\mathcal{W}}$  converges to a non-vanishing value in the limit  $T \rightarrow 0$ , while  $S_{\text{vN}}$  goes to zero.

## Entropy production rate

In the same spirit of the identification we have put forward for systems weakly coupled to their reservoirs – cf. Equation (5.20) – the *Wigner entropy production rate* is defined as

$$\dot{\Sigma}_{\mathcal{W}}(t) = -\partial_t K(\mathcal{W} || \mathcal{W}_{\text{eq}}), \quad (5.58)$$

where we have introduced the Wigner relative entropy

$$K(\mathcal{W}||\mathcal{W}_{\text{eq}}) = \int d^2\alpha \mathcal{W} \ln \left( \frac{\mathcal{W}}{\mathcal{W}_{\text{eq}}} \right). \quad (5.59)$$

At this stage, it is important mentioning that this definition is perfectly consistent in the case under scrutiny, as we are dealing with Gaussian states, for which  $\mathcal{W}$  is always positive. Inserting the definition (5.59) into Equation (5.58), we get

$$\dot{\Sigma}_{\mathcal{W}}(t) = - \int d^2\alpha \partial_t \mathcal{W} \ln \left( \frac{\mathcal{W}}{\mathcal{W}_{\text{eq}}} \right), \quad (5.60)$$

after having observed that the time derivative of  $\int \mathcal{W} d^2\alpha = 1$  vanishes. Now, we can substitute Equation (5.45) into (5.60) and integrate by parts the unitary contribution, to eventually obtain

$$\dot{\Sigma}_{\mathcal{W}}(t) = - \int d^2\alpha \mathcal{D}(\mathcal{W}) \ln \left( \frac{\mathcal{W}}{\mathcal{W}_{\text{eq}}} \right). \quad (5.61)$$

Using the expression of the dissipator in terms of probability currents – cf. Equation (5.47), we get

$$\dot{\Sigma}_{\mathcal{W}}(t) = \int d^2\alpha \left\{ J(\mathcal{W}) \left( \frac{\partial_{\alpha} \mathcal{W}}{\mathcal{W}} - \frac{\partial_{\alpha} \mathcal{W}_{\text{eq}}}{\mathcal{W}_{\text{eq}}} \right) + \alpha \rightarrow \alpha^* \right\}. \quad (5.62)$$

By inverting Equation (5.48), we obtain

$$\frac{\partial_{\alpha} \mathcal{W}}{\mathcal{W}} - \frac{\partial_{\alpha} \mathcal{W}_{\text{eq}}}{\mathcal{W}_{\text{eq}}} = \frac{2}{\gamma (\bar{n} + \frac{1}{2})} \frac{J^*(\mathcal{W})}{\mathcal{W}}, \quad (5.63)$$

where we also have taken into account that  $J(\mathcal{W}_{\text{eq}}) = J^*(\mathcal{W}_{\text{eq}})$ . This leads to the following closed expression for the Wigner entropy production rate

$$\dot{\Sigma}_{\mathcal{W}}(t) = \frac{4}{\gamma (\bar{n} + \frac{1}{2})} \int d^2\alpha \frac{|J(\mathcal{W})|^2}{\mathcal{W}}, \quad (5.64)$$

which is quadratic in the relevant probability currents. It is easy to check that this is indeed a consistent expression for the entropy production rate: on one hand, since  $\mathcal{W} > 0$ , we immediately obtain that  $\dot{\Sigma}_{\mathcal{W}}(t) \geq 0$ ; on the other hand,  $\dot{\Sigma}_{\mathcal{W}}(t) = 0$  at equilibrium, following from the condition  $J(\mathcal{W}_{\text{eq}}) = 0$ .

### Wigner entropy flux rate

Similarly, using Equation (5.5) we can derive a closed expression for the entropy flux rate. After a simple integration by parts, we can immediately obtain

$$\frac{dS_{\mathcal{W}}}{dt} = - \int d^2\alpha \mathcal{D}(\mathcal{W}) \ln \mathcal{W}, \quad (5.65)$$

whence

$$\dot{\Phi}_{\mathcal{W}}(t) = \dot{\Sigma}_{\mathcal{W}} - \frac{dS_{\mathcal{W}}}{dt} = - \int d^2\alpha \mathcal{D}(\mathcal{W}) \ln \mathcal{W}_{\text{eq}}. \quad (5.66)$$

Using the expression for  $\mathcal{W}_{\text{eq}}$  given by [Equation \(5.55\)](#) and again integrating by parts, [Equation \(5.66\)](#) becomes

$$\dot{\Phi}_{\mathcal{W}}(t) = \frac{1}{\bar{n} + \frac{1}{2}} \int d^2\alpha [\alpha^* J(\mathcal{W}) + \alpha J^*(\mathcal{W})] \quad (5.67)$$

Now, recalling that the probability current is given by [Equation \(5.48\)](#) and performing once more an integration by parts, we get

$$\dot{\Phi}_{\mathcal{W}}(t) = \frac{\gamma}{\bar{n} + \frac{1}{2}} \int d^2\alpha |\alpha|^2 \mathcal{W} - \gamma. \quad (5.68)$$

As  $\int d^2\alpha |\alpha|^2 \mathcal{W} = \langle a^\dagger a \rangle + 1/2$ , the entropy flux rate reads as

$$\dot{\Phi}_{\mathcal{W}}(t) = \frac{\gamma}{\bar{n} + \frac{1}{2}} (\langle a^\dagger a \rangle - \bar{n}), \quad (5.69)$$

which is remarkably simple, as it is given by a simple expectation value.

On the other hand, using the explicit form of the master equation  $\dot{\rho} = -i[H_S, \rho] + \mathcal{D}[\rho]$ , we can derive a closed expression for the energy flux rate, i.e.,

$$\dot{\Phi}_E(t) = -\frac{d\langle H_S \rangle}{dt} = -\text{Tr}(H_S \dot{\rho}) = \gamma \omega_0 (\langle a^\dagger a \rangle - \bar{n}). \quad (5.70)$$

Therefore, combining [Equations \(5.69\)](#) and [\(5.70\)](#), we get

$$\dot{\Phi}_{\mathcal{W}}(t) = \frac{\dot{\Phi}_E(t)}{\omega_0 (\bar{n} + \frac{1}{2})}. \quad (5.71)$$

In the high temperature limit, i.e.,  $T \gg \omega_0$ , the equation above yields the Clausius relation  $\dot{\Phi}_{\mathcal{W}} \simeq \dot{\Phi}_E/T$ , as  $\omega_0(\bar{n} + 1/2) \simeq T$ . Moreover, it is evident that, in the limit  $T \rightarrow 0$ , the entropy flux rate in [Equation \(5.69\)](#) stays finite, unlike the standard result obtained by means of the von Neumann entropy.

### 5.3.3 Relation with classical stochastic processes

We have seen that Gaussian states are fully described in terms of first and second moments, the latter appearing in the covariance matrix  $\sigma$ . First, we notice that the Fokker-Planck equation for the Wigner function, i.e., [Equation \(5.45\)](#), can be rewritten using rectangular coordinates  $(q, p)$ , once we recall that  $\alpha = (q + ip)/\sqrt{2}$  and  $\alpha^* = (q - ip)/\sqrt{2}$ . Hence, we

have  $\partial_\alpha = \partial_q - i\partial_p$  and  $\partial_{\alpha^*} = \partial_q + i\partial_p$ , yielding the following set of correspondence rules (Ferraro, 2005):

$$\partial_\alpha \alpha \mapsto \frac{1}{2} [\partial_q q + i(\partial_q p - \partial_p q) + \partial_p p], \quad (5.72)$$

$$\partial_{\alpha^*} \alpha^* \mapsto \frac{1}{2} [\partial_q q - i(\partial_q p - \partial_p q) + \partial_p p], \quad (5.73)$$

$$\partial_{\alpha \alpha^*}^2 \mapsto \frac{1}{2} (\partial_{qq}^2 + \partial_{pp}^2). \quad (5.74)$$

By resorting to these rules, we can recast the Fokker-Planck equation in the form of a local conservation equation (Gardiner, 2009)

$$\partial_t \mathcal{W} = -\partial_{\mathbf{x}} \mathbf{J}(\mathcal{W}), \quad (5.75)$$

where  $\partial_{\mathbf{x}} \equiv (\partial_q, \partial_p)^T$  is the phase-space gradient, with  $\mathbf{x} = (q, p)^T$ . The total probability current  $\mathbf{J}(\mathcal{W})$  is given by

$$\mathbf{J}(\mathcal{W}) = \begin{pmatrix} J_q(\mathcal{W}) \\ J_p(\mathcal{W}) \end{pmatrix} = \mathbf{A}\mathbf{x}\mathcal{W} - \frac{1}{2}\mathbf{D}\partial_{\mathbf{x}}\mathcal{W}, \quad (5.76)$$

where the drift and diffusion matrices are

$$\mathbf{A} = \begin{pmatrix} -\frac{\gamma}{2} & \omega_0 \\ -\omega_0 & -\frac{\gamma}{2} \end{pmatrix}, \quad \mathbf{D} = \gamma \left( \bar{n} + \frac{1}{2} \right) \mathbb{I}, \quad (5.77)$$

respectively. The drift matrix  $\mathbf{A}$  can be rewritten separating the irreversible part  $\mathbf{A}^{\text{irr}}$  from the reversible one  $\mathbf{A}^{\text{rev}}$ : the former is even under time reversal, while the latter is odd (Spinney, 2012; Landi, 2013). In the basis in which we are working, the time-reversal operator reads

$$\mathbf{E} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (5.78)$$

as this matrix inverts the sign of momentum. Therefore

$$\mathbf{A}^{\text{irr}} = \frac{1}{2} (\mathbf{A} + \mathbf{E}\mathbf{A}\mathbf{E}^T) = -\frac{\gamma}{2}\mathbb{I}, \quad \mathbf{A}^{\text{rev}} = \frac{1}{2} (\mathbf{A} - \mathbf{E}\mathbf{A}\mathbf{E}^T) = i\omega_0\sigma_2 \quad (5.79)$$

The splitting that we have obtained for the case at hand could have been easily anticipated: the irreversible part is associated with the damping rate  $\gamma$ , while the reversible part stems from the Hamiltonian part of the dynamics. The separation between reversible and irreversible part for the drift matrix  $\mathbf{A} = \mathbf{A}^{\text{rev}} + \mathbf{A}^{\text{irr}}$  justifies the following splitting in the probability currents

$$\mathbf{J}^{\text{rev}}(\mathcal{W}) = \mathbf{A}^{\text{rev}}\mathbf{x}\mathcal{W}, \quad (5.80)$$

$$\mathbf{J}^{\text{irr}}(\mathcal{W}) = \mathbf{A}^{\text{irr}}\mathbf{x}\mathcal{W} - \frac{1}{2}\mathbf{D}\partial_{\mathbf{x}}\mathcal{W}, \quad (5.81)$$

such that  $\mathbf{J}(\mathcal{W}) = \mathbf{J}^{\text{rev}}(\mathcal{W}) + \mathbf{J}^{\text{irr}}(\mathcal{W})$ .

## Entropy production rate

Let us now consider the Wigner entropy defined by [Equation \(5.38\)](#). By taking the derivative with respect to time and integrating by parts, we get

$$\frac{dS_{\mathcal{W}}}{dt} = \int d^2\alpha (\mathbf{J}^{\text{irr}}(\mathcal{W}))^T \left( \frac{\partial_{\mathbf{x}} \mathcal{W}}{\mathcal{W}} \right). \quad (5.82)$$

Considering the expression for  $\partial_{\mathbf{x}} \mathcal{W}$  obtained through [Equation \(5.81\)](#), we can rewrite [Equation \(5.82\)](#) in the usual form in terms of entropy production and flux rates

$$\frac{dS_{\mathcal{W}}}{dt} = \dot{\Sigma}_{\mathcal{W}}(t) - \dot{\Phi}_{\mathcal{W}}(t), \quad (5.83)$$

where we have introduced the following identification:

$$\dot{\Sigma}_{\mathcal{W}}(t) = 2 \int \frac{d^2\alpha}{\mathcal{W}} (\mathbf{J}^{\text{irr}}(\mathcal{W}))^T \mathbf{D}^{-1} \mathbf{J}^{\text{irr}}(\mathcal{W}), \quad (5.84)$$

$$\dot{\Phi}_{\mathcal{W}}(t) = 2 \int d^2\alpha (\mathbf{J}^{\text{irr}}(\mathcal{W}))^T \mathbf{D}^{-1} \mathbf{A}^{\text{irr}}(\mathcal{W}) \mathbf{x} \quad (5.85)$$

As  $\partial_{\mathbf{x}} \mathcal{W} = -\boldsymbol{\sigma}^{-1} \mathbf{x} \cdot \mathcal{W}$ , we have the irreversible current  $\mathbf{J}^{\text{irr}}(\mathcal{W}) = (\mathbf{A}^{\text{irr}} + \frac{1}{2} \mathbf{D} \boldsymbol{\sigma}^{-1}) \mathbf{x} \cdot \mathcal{W}$ ; therefore the integration in [Equation \(5.84\)](#) can be exactly carried out ([Landi, 2013](#); [Brunelli, 2016](#)), yielding the following expression for the entropy production rate

$$\dot{\Sigma}_{\mathcal{W}}(t) = \frac{1}{2} \text{Tr}[\boldsymbol{\sigma}_t^{-1} \mathbf{D}] + 2 \text{Tr}[\mathbf{A}^{\text{irr}}] + 2 \text{Tr}[(\mathbf{A}^{\text{irr}})^T \mathbf{D}^{-1} \mathbf{A}^{\text{irr}} \boldsymbol{\sigma}_t], \quad (5.86)$$

where  $\boldsymbol{\sigma}_t = \boldsymbol{\sigma}(t)$ . This allows to calculate the entropy production rate for any known process, i.e., a dynamics for which both  $\mathbf{D}$  and  $\mathbf{A}^{\text{irr}}$  are known, directly from the covariance matrix of the system<sup>5</sup>.

## Entropy flux rate

In order to derive a closed expression for the entropy flux rate, we can first notice that the evolution of a Gaussian system is governed – in terms of second moments – by a differential equation in the Lyapunov form, i.e.,

$$\dot{\boldsymbol{\sigma}}_t = \mathbf{A} \boldsymbol{\sigma}_t + \boldsymbol{\sigma}_t \mathbf{A}^T + \mathbf{D}. \quad (5.87)$$

By applying the Jacobi formula of differential calculus<sup>6</sup>, we obtain

$$\frac{dS_{\mathcal{W}}}{dt} = \frac{1}{2} \text{Tr}[\boldsymbol{\sigma}_t^{-1} \dot{\boldsymbol{\sigma}}_t] = \frac{1}{2} \text{Tr}[\boldsymbol{\sigma}_t^{-1} \mathbf{D}] + \text{Tr}[\mathbf{A}^{\text{irr}}], \quad (5.89)$$

<sup>5</sup>Note that, despite the notation used, [Equation \(5.86\)](#) is not a differential equation. This remark applies to [Equation \(5.90\)](#) as well.

<sup>6</sup>For any invertible matrix  $A(t)$ , the following formula holds

$$\frac{d}{dt} \det[A(t)] = \det[A(t)] \text{Tr}[A(t)^{-1} \dot{A}(t)]. \quad (5.88)$$

where, in the last step, we have used [Equation \(5.87\)](#) and the fact that  $\text{Tr}[\mathbf{A}^{\text{rev}}] = 0$ . Therefore, from [Equation \(5.83\)](#), we get the following expression for the entropy flux rate

$$\dot{\Phi}_W(t) = 2 \text{Tr}[(\mathbf{A}^{\text{irr}})^T \mathbf{D}^{-1} \mathbf{A}^{\text{irr}} \boldsymbol{\sigma}_t] + \text{Tr}[\mathbf{A}^{\text{irr}}]. \quad (5.90)$$

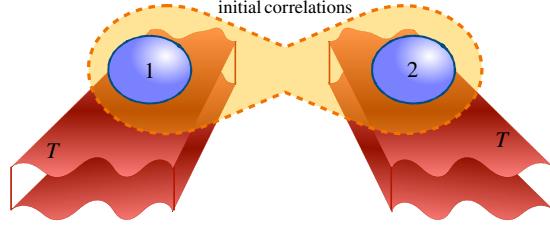
The formulation we have just introduced is particularly powerful. On one hand, it allows us to exploit all the advantages of working with Gaussian systems. The dynamics can be studied in terms of first and second moments, the latter satisfying [Equation \(5.87\)](#), and the Wigner entropy is always well-defined. On the other hand, this approach establishes a close connection between classical and quantum stochastic processes governed by linear equations: the expressions derived above are equally valid in both limits, provided that we choose the appropriate probability distribution ([Tomé, 2010](#)). More practically, [Equations \(5.86\)](#) and [\(5.90\)](#) provide a remarkably simple way to calculate entropy production and flux rates: once we know the solution  $\boldsymbol{\sigma}_t$  of the Lyapunov equation, the calculation boils down to a straightforward linear algebra problem. Moreover, this approach is not only a theoretical advance as such, as it also suitable to the interpretation of the experimental evidence gathered in some mesoscopic systems ([Brunelli, 2018](#)).

## 5.4 Assessing the role of initial correlations

In this Section, we investigate the way initial correlations affect the entropy production rate in an open quantum system by considering the case of non-Markovian Brownian motion. Specifically, we focus on the case of an uncoupled bipartite system connected to two independent baths. The rationale behind this choice is related to the fact that any interaction between the two oscillators would likely generate, during the evolution, quantum correlations between the two parties. In general, the entanglement dynamically generated through the interaction would be detrimental to the transparency of the picture we would like to deliver, as it would be difficult to isolate the contribution to  $\dot{\Sigma}(t)$  coming from the initial inter-system correlations. To circumvent this issue, in our study we choose a configuration where the inter-system dynamics is trivial (two independent relaxation processes), but the bipartite state is initially correlated.

### 5.4.1 Description of the system

Let us consider a system consisting of two quantum harmonic oscillators, each of them interacting with its own local reservoir (see [Figure 5.2](#)). Each of the two reservoirs is modelled as a system of system of  $N$  non-interacting bosonic modes (with  $N \rightarrow +\infty$ ). In order to understand the dependence of the entropy production upon the initial correlations, we choose the simplest case in which the two oscillators are identical, i.e., characterised by the same bare frequency  $\omega_0$  and the same temperature  $T$ , and they are uncoupled, so that only the initial preparation of the global state may entangle them. The Hamiltonian of the global



**Figure 5.2:** System of two uncoupled quantum harmonic oscillators interacting with their local reservoirs. The latter are characterised by the same temperature  $T$  and the same spectral properties. The two parties of the systems are initially correlated and we study their dynamics under the secular approximation so that non-Markovian effects are present.

system thus reads as

$$H = \sum_{j=1,2} \omega_0 a_j^\dagger a_j + \sum_{j=1,2} \sum_k \omega_{jk} b_{jk}^\dagger b_{jk} + \alpha \sum_{j=1,2} \sum_k \left( \frac{a_j + a_j^\dagger}{\sqrt{2}} \right) \left( g_{jk}^* b_{jk} + g_{jk} b_{jk}^\dagger \right), \quad (5.91)$$

where  $a_j^\dagger$  ( $a_j$ ) and  $b_{jk}^\dagger$  ( $b_{jk}$ ) are the system and reservoirs creation (annihilation) operators, respectively, while  $\omega_{1k}$  and  $\omega_{2k}$  are the frequencies of the reservoirs modes. The dimensionless constant  $\alpha$  represents the coupling strength between each of the two subsystems and the their local bath, while the constants  $g_{jk}$  quantify the coupling between the  $j^{\text{th}}$  oscillator ( $j = 1, 2$ ) and the  $k^{\text{th}}$  mode of its respective reservoir. These quantities therefore appear in the definition of the SD

$$J_j(\omega) = \sum_k |g_{jk}|^2 \delta(\omega - \omega_{jk}) . \quad (5.92)$$

In what follows, we will the consider the case of symmetric reservoirs, i.e.,  $J_1(\omega) = J_2(\omega) \equiv J(\omega)$ .

Following the procedure outlined in [Chapter 4](#), the dynamics of this system is governed by a time-local master equation, that, in the interaction picture with respect to the renormalised Hamiltonian, reads as

$$\dot{\rho}(t) = [\Delta(t) + \gamma(t)] \sum_{j=1,2} \left( a_j \rho a_j^\dagger - \frac{1}{2} \{ a_j^\dagger a_j, \rho \} \right) + [\Delta(t) - \gamma(t)] \sum_{j=1,2} \left( a_j^\dagger \rho a_j - \frac{1}{2} \{ a_j a_j^\dagger, \rho \} \right), \quad (5.93)$$

where  $\rho$  is the reduced density matrix of the global system, while the time dependent coefficients  $\Delta(t)$  and  $\gamma(t)$ , accounting for diffusion and dissipation, are given by [Equations \(4.43a\)](#) and [\(4.43b\)](#), respectively.

Furthermore, it can be shown that the dynamics of a harmonic system that is linearly coupled to an environment can be described in terms of a differential equation in the Lyapunov form given by [Equation \(5.87\)](#). We can indeed notice that in [Equation \(5.91\)](#) the interaction between each harmonic oscillator and the local reservoir is expressed by a Hamiltonian that is bilinear (i.e., quadratic) in the system and reservoir creation and annihilation operators. Hamiltonians of this form lead to a master equation as in [Equation \(5.93\)](#), where the dissipators are quadratic in the system creation and annihilation operators  $a_j^\dagger, a_j$ . Under these conditions, one can recast the dynamical equations in the Lyapunov form in [Equation \(5.87\)](#) ([Ferraro, 2005; Serafini, 2017](#)), where the matrices  $\mathbf{A}$  and  $\mathbf{D}$  are time-dependent, due to non-Markovianity. Indeed, we get  $\mathbf{A} = -\gamma(t)\mathbb{I}$  and  $\mathbf{D} = 2\Delta(t)\mathbb{I}$ , where  $\mathbb{I}$  is the  $4 \times 4$  identity matrix. The resulting Lyapunov equation can be analytically solved, giving the following closed expression for the CM at a time  $t$ :

$$\boldsymbol{\sigma}_t = \boldsymbol{\sigma}(0)e^{-\Gamma(t)} + 2\Delta_\Gamma(t)\mathbb{I}, \quad (5.94)$$

with

$$\Gamma(t) \equiv 2 \int_0^t d\tau \gamma(\tau) \quad \text{and} \quad \Delta_\Gamma(t) \equiv e^{-\Gamma(t)} \int_0^t d\tau \Delta(\tau) e^{\Gamma(\tau)}. \quad (5.95)$$

Moreover, a straightforward calculation allows us to determine the steady state of our two-mode system. By imposing  $\dot{\boldsymbol{\sigma}}_t \equiv 0$  in [Equation \(5.87\)](#), one obtains that the system relaxes towards a diagonal state with associated CM  $\boldsymbol{\sigma}_\infty \equiv \Delta(\infty)/\gamma(\infty)\mathbb{I}$ . By plugging  $\boldsymbol{\sigma}_\infty$  in [Equation \(5.86\)](#), we find  $\dot{\Sigma}_{\mathcal{W}}(\infty) \equiv \lim_{t \rightarrow \infty} \dot{\Sigma}_{\mathcal{W}}(t) = 0$ , showing a vanishing entropy production at the steady state. This instance can also be justified by noticing that, as  $t \rightarrow +\infty$ , we approach the Markovian limit. Therefore, the Brownian particles, exclusively driven by the interaction with their local thermal baths, will be relaxing towards the canonical Gibbs state with a vanishing associated entropy production rate.

### 5.4.2 Parametrisation of the initial states

The possibility of writing the dynamical equations in the Lyapunov form allows us to take advantage of the Continuous Variables (CV) formalism to write the initial state of our system in such a way that initial correlations can be encoded in terms of a limited number of parameters. It can be shown that the CM representing a two-mode Gaussian state can always be brought in the standard form ([Ferraro, 2005; Serafini, 2017](#)), i.e.,

$$\boldsymbol{\sigma} = \begin{pmatrix} a & 0 & c_+ & 0 \\ 0 & a & 0 & c_- \\ c_+ & 0 & b & 0 \\ 0 & c_- & 0 & b \end{pmatrix}, \quad (5.96)$$

where the entries  $a$ ,  $b$ , and  $c_\pm$  are real numbers. Note that states whose standard form fulfils the condition  $a = b$  are said to be symmetric. The global purity of the Gaussian state  $\varrho$  represented by the standard CM given by [\(5.96\)](#) is

$$\mu \equiv \mu(\varrho) = (\det \boldsymbol{\sigma})^{-1/2} = [(ab - c_+^2)(ab - c_-^2)]^{-1/2}, \quad (5.97)$$

therefore, it is easy to check that a globally pure state  $\varrho$  (i.e.,  $\mu = 1$ ) is symmetric and fulfills the relation  $c_+ = -c_- = \sqrt{a^2 - 1}$ . By contrast, the purities of the reduced states  $\varrho_i = \text{Tr}_{j \neq i} \varrho$  – also known as local purities – are given by

$$\mu_1 = (\det \boldsymbol{\alpha})^{-1/2} = \frac{1}{a}, \quad \mu_2 = (\det \boldsymbol{\beta})^{-1/2} = \frac{1}{b}, \quad (5.98)$$

where  $\boldsymbol{\alpha} = \text{diag}(a, a)$  and  $\boldsymbol{\beta} = \text{diag}(b, b)$  are the reduced CM of the two modes. Furthermore, the matrix  $\boldsymbol{\sigma}$  is a *bona fide* CM if it represents a physical state, i.e., if satisfies the so-called Robertson-Schödinger uncertainty principle, that introduces a stricter condition than the simple non-negativity of the CM (Adesso, 2005). The latter can be rephrased in terms of the symplectic spectrum of  $\boldsymbol{\sigma}$ , i.e., by computing the eigenvalues of the matrix  $|i\boldsymbol{\Omega}\boldsymbol{\sigma}|$  – called *symplectic eigenvalues* of the CM  $\boldsymbol{\sigma}$ , where  $\boldsymbol{\Omega}$  is the so-called symplectic form

$$\boldsymbol{\Omega} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \quad (5.99)$$

Specifically, we can denote the symplectic eigenvalues of a two-mode Gaussian state as  $\nu_-$ ,  $\nu_+$ , with  $\nu_- \leq \nu_+$ ; they are analytically determined through the formula

$$2\nu_{\pm}^2 = \Delta \pm \sqrt{\Delta^2 - 4 \det \boldsymbol{\sigma}}, \quad (5.100)$$

where  $\Delta \equiv \det \boldsymbol{\alpha} + \det \boldsymbol{\beta} + 2 \det \boldsymbol{\gamma} = a^2 + b^2 + 2c_+c_-$  is the so-called *seralian*, with  $\boldsymbol{\gamma} = \text{diag}(c_+, c_-)$ . A bona fide CM fulfills the condition  $\nu_- \geq 1$ .

Furthermore, we can determine a necessary and sufficient condition for the separability of a two-mode Gaussian state, provided that we observe that, in phase space, partial transposition amounts to a mirror reflection of one of the four canonical variables. For example, we can construct the partially transposed CM by inverting the momentum of the second mode, i.e.,  $\tilde{\boldsymbol{\sigma}} = \mathbf{P}\boldsymbol{\sigma}\mathbf{P}$ , being  $\mathbf{P} = \text{diag}(1, 1, 1, -1)$ . In terms of symplectic invariants partial transposition translates to a sign flip in  $\det \boldsymbol{\gamma}$ , thus it is useful to introduce  $\tilde{\Delta} \equiv \det \boldsymbol{\alpha} + \det \boldsymbol{\beta} - 2 \det \boldsymbol{\gamma} = a^2 + b^2 - 2c_+c_-$ , that enters into the closed formula of the symplectic eigenvalues of  $\tilde{\boldsymbol{\sigma}}$

$$2\tilde{\nu}_{\pm}^2 = \tilde{\Delta} \pm \sqrt{\tilde{\Delta}^2 - 4 \det \boldsymbol{\sigma}}. \quad (5.101)$$

In the same spirit of the Peres-Horodecki PPT criterion discussed in Section 2.5, a separable state is obtained when, after applying a partial transposition, we still get a physical state, therefore the CM  $\boldsymbol{\sigma}$  is representative of a separable state if and only if the smallest symplectic eigenvalue of  $\tilde{\boldsymbol{\sigma}}$  satisfies the following inequality, known as Simon's criterion (Simon, 2000):

$$\tilde{\nu}_- \geq 1. \quad (5.102)$$

Therefore, the smallest symplectic eigenvalue encodes all the information needed to quantify the entanglement for arbitrary two-modes Gaussian states. We can thus introduce a natural measure for two-mode Gaussian states that passes through the violation of [Equation \(5.102\)](#). Quantitatively, this is given by the logarithmic negativity of a quantum state  $\varrho$ , which – in the continuous variables formalism – can be computed considering the following formula ([Adesso, 2004b](#))

$$E_N(\varrho) = \max [0, -\ln \tilde{\nu}_-]. \quad (5.103)$$

Given the global state  $\varrho$  and the two single-mode states  $\varrho_i = \text{Tr}_{j \neq i} \varrho$ , global  $\mu \equiv \text{Tr} \varrho^2$  and the local  $\mu_{1,2} \equiv \text{Tr} \varrho_{1,2}^2$  purities can be used to characterise entanglement in Gaussian systems. It has been shown that two different classes of extremal states can be identified: states of maximum negativity for fixed global and local purities (GMEMS) and states of minimum negativity for fixed global and local purities (GLEMS) ([Adesso, 2004a](#))<sup>7</sup>.

In what follows, we will employ a parametrisation that covers different initial preparations ([Adesso, 2005](#)). The entries of the matrix given by [Equation \(5.96\)](#) can be expressed as

$$a = s + d, \quad b = s - d, \quad (5.104)$$

and

$$c_{\pm} = \frac{\sqrt{(4d^2 + f)^2 - 4g^2} \pm \sqrt{(4s^2 + f)^2 - 4g^2}}{4\sqrt{s^2 - d^2}}, \quad (5.105)$$

with  $f = (g^2 + 1)(\lambda - 1)/2 - (2d^2 + g)(\lambda + 1)$ . This allows us to parametrise the CM using four parameters:  $s, d, g, \lambda$ . The local purities are controlled by the parameters  $s$  and  $d$  as  $\mu_1 = (s + d)^{-1}$  and  $\mu_2 = (s - d)^{-1}$ , while the global purity is  $\mu = 1/g$ . Furthermore, in order to ensure legitimacy of a CM, the following constraints should be fulfilled:

$$s \geq 1, \quad |d| \leq s - 1, \quad g \geq 2|d| + 1. \quad (5.106)$$

Once the three aforementioned purities are given, the remaining degree of freedom required to determine the negativities is controlled by the parameter  $\lambda$ , which encompasses all the possible entangled two-modes Gaussian states. The two classes of extremal states are obtained upon suitable choice of  $\lambda$ . For  $\lambda = -1$  ( $\lambda = +1$ ) we recover the GLEMS (GMEMS). Although [Equations \(5.104\)](#) and [\(5.105\)](#) might appear rather cumbersome, they introduce a useful classification for the entanglement of a two-mode Gaussian state according to its degree of total and partial mixedness. This parametrisation indeed provides an experimentally reliable estimate of CV entanglement based on measurement of the global and local purities.

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<sup>7</sup>They are also known as Gaussian Maximally/Least Entangled Mixed States, whence the acronyms GMEMS and GLEMS.

### 5.4.3 Numerical results

We can now use our system to claim that initial correlations shared by the non-interacting oscillators do play a role in the entropy production rate. To show a preview of our results, we start with a concrete case shown in [Figure 5.3a](#). We prepare the system in a pure ( $g = 1$ ) symmetric ( $d = 0$ ) state, and investigate the effects of initial correlations on  $\dot{\Sigma}(t)$  by comparing the value taken by this quantity for such an initial preparation with what is obtained by considering the covariance matrix associated with the tensor product of the local states of the oscillators, i.e., by forcefully removing the correlations between them. Non-Markovian effects are clearly visible in the oscillations of the entropy production and lead to negative values of  $\dot{\Sigma}(t)$  in the first part of the evolution. This is in stark contrast with the Markovian case, which entails non-negativity of the entropy production rate. Crucially, we see that, for a fixed initial value of the local energies, the presence of initial correlations enhances the amount of entropy produced at later times, increasing the amplitude of its oscillations.

We now move to a more systematic investigation of  $\dot{\Sigma}(t)$  and its dependence on the specific choice of  $s, d, g, \lambda$ . In order to separate the contributions, we first study the behaviour of  $\dot{\Sigma}(t)$  when we vary one of those parameters, while all the others are fixed. We can first rule out the contribution of thermal noise by considering the case in which the reservoirs are in their vacuum state: as discussed in [Section 5.2.2](#), such zero-temperature limit can be problematic in the traditional approach based on the von Neumann entropy. By contrast, our formalism based on phase-space methods is consistent also in the liming case  $T \rightarrow 0$ , as shown in [Figure 5.3b](#), where we consider a system whose dynamics is described by [Equation \(5.93\)](#); in particular, we choose an Ohmic SD with an exponential cut-off. The map describing the dynamics converges to a stationary state characterised by a vanishing  $\dot{\Sigma}(t)$ , although the oscillations are damped to zero more slowly, as non-Markovian effects are more persistent in the presence of zero-temperature reservoirs. Furthermore, we notice that the differences between different initial states are most pronounced in correspondence of the first peak: this suggests that the maximum value for the entropy production can be reasonably chosen as an apt figure of merit to distinguish the differences due to state preparation. Supported by this evidence, we adopt the value of the first maximum of  $\dot{\Sigma}(t)$  as an indicator of the irreversibility generated in the relaxation dynamics by different initial preparations. In the inset of [Figure 5.3b](#), we show the logarithmic negativity given by [Equation \(5.103\)](#). The interaction with zero-temperature reservoirs does not cause detrimental effects to entanglement, as the latter is preserved over time ([Maniscalco, 2007; Paz, 2008; Vasile, 2009](#)).

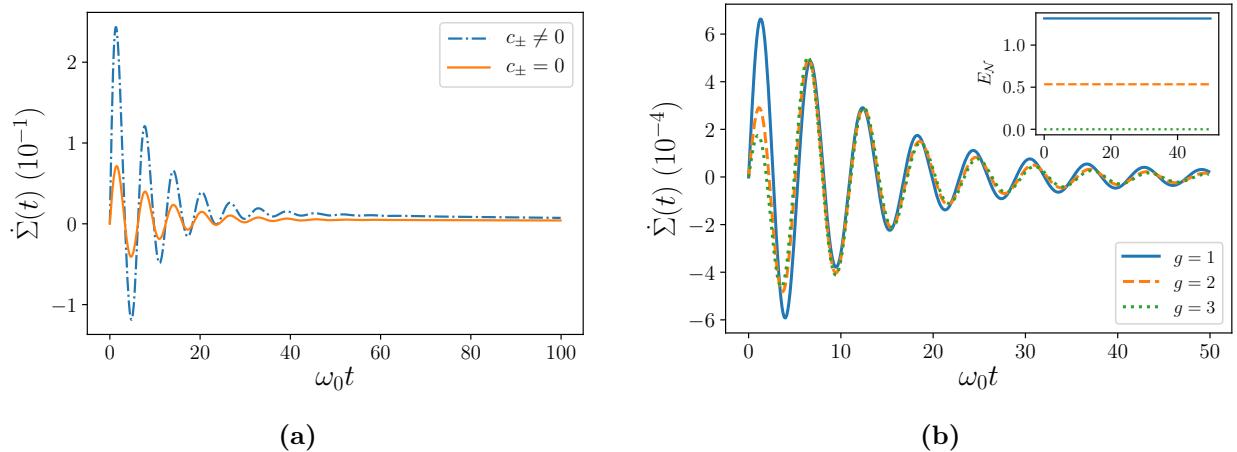
We also address the case of finite-temperature reservoirs and an Ohmic SD with Lorentz-Drude cut-off<sup>8</sup> given by

$$J(\omega) = \frac{2\omega}{\pi} \frac{\omega_c^2}{\omega_c^2 + \omega^2}. \quad (5.107)$$

Note that, in our numerical simulations, we take the cut-off frequency smaller than the

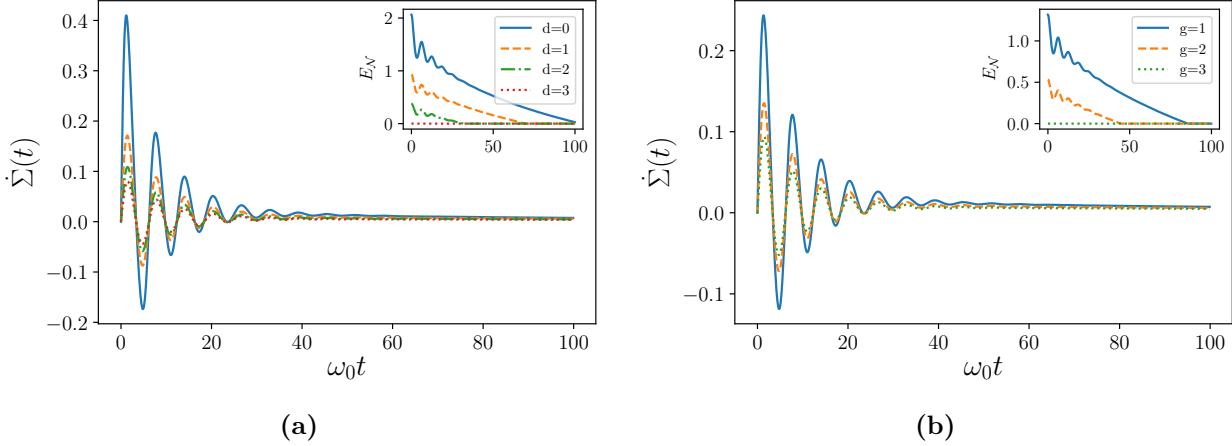
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<sup>8</sup>the analysis can easily be extended to the exponential cut-off for the Ohmic ( $\epsilon = 1$ ), super-Ohmic ( $\epsilon = 3$ ) and sub-Ohmic ( $\epsilon = 1/2$ ) case.



**Figure 5.3:** Entropy production rate in a system of two non-interacting oscillators undergoing the non-Markovian dynamics described in Section 5.4.1. **Panel (a):** We compare the behaviour of the entropy production rate resulting from a process where the system is initialised in a state with no initial correlations (solid line) to what is obtained starting from a correlated state (dashed-dotted line). The latter case refers to the preparation of a system in a pure ( $g = 1$ ), symmetric ( $d = 0$ ) squeezed state ( $\lambda = 1$ ). The former situation, instead, corresponds to taking the tensor product of the local states. In this plot we have taken  $s = 2$  and an Ohmic SD with Lorentz-Drude cut-off. The system parameters are  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ . **Panel (b):** Entropy production rates corresponding to independent zero-temperature reservoirs. We consider preparations of the initial global state corresponding to different values of parameter  $g$  (related to the global purity of the state), while fixing  $s = 2$ ,  $d = 0$ , and  $\lambda = 1$ . In the inset, we plot the logarithmic negativity for the same choice of parameters: entanglement persists over time up to the reach of a steady state of the dynamics. We have taken an Ohmic SD with an exponential cut-off with  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ .

bare frequency of the harmonic oscillators, namely  $\omega_c = 0.1\omega_0$ . This choice leads to the non-Markovian regime, where the physical quantities of interest exhibits the typical oscillating behaviour (Paavola, 2009). We thus fix  $s, d, \lambda$  and let  $g$  vary to explore the role played by the global purity. Figure 5.4a shows that, by increasing  $g$  – i.e., by reducing the purity of the global state –  $\dot{\Sigma}(t)$  decreases: an initial state with larger purity lies far from an equilibrium state at the given temperature of the environment and is associated with a larger degree of initial entanglement [cf. inset of Figure 5.4a], which translates in a larger entropy production rate. Furthermore, our particular choice of the physical parameters leads to the observation of “entanglement sudden death” (Paz, 2008; Vasile, 2009): an initial state with non-null logarithmic negativity completely disentangles in a finite time due to interaction with environment, the disentangling time being shortened by a growing  $g$  [cf. inset of Figure 5.4a]. Similarly, we can bias the local properties of the oscillators by varying  $d$  and, in turn,  $g = 2d + 1$ , while keeping  $s, \lambda$  fixed: in Figure 5.4b we can observe that, when the global energy is fixed, the asymmetry in the local energies – and purities  $\mu_1$  and  $\mu_2$  – reduces the entropy production rate. In the inset we show that, by increasing the asymmetry between the two modes, the entanglement takes less time to die out. These results are consistent



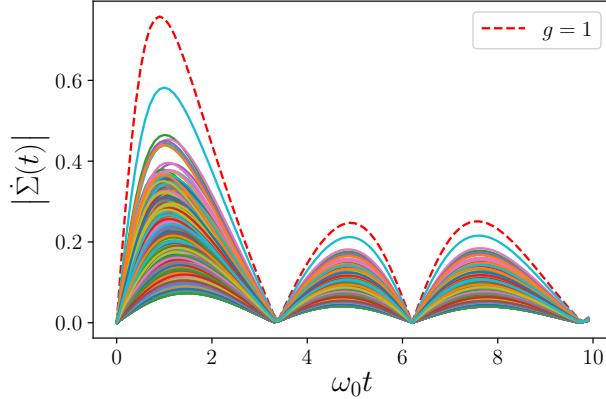
**Figure 5.4:** Entropy production rate in a system of two non-interacting oscillators undergoing the non-Markovian dynamics described in Section 5.4.1. The dynamics of the system has been simulated using an Ohmic SD with a Lorentz-Drude cut-off. The system parameters are  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ . **Panel (a):** We consider different preparations of the initial global state, by choosing different values of parameter  $g$ , while taking  $s = 2$ ,  $d = 0$ , and  $\lambda = 1$ . In the inset, we plot the logarithmic negativity for the same choice of the parameters. **Panel (b):** Entropy production rates corresponding to different values of  $d$  and  $g = 2d + 1$  in the parametrisation of the initial state (we have taken  $s = 4$  and  $\lambda = 1$ ). As in the previous case, the inset shows the behaviour of the logarithmic negativity.

with the trends observed in Figure 5.4b. Indeed, a bias in the local energies would make the reduced state of one of the two oscillators more mixed, and thus less prone to preserve the entanglement that is initially set in the joint harmonic state. Such imbalance would give different weights to the two local dissipation processes, thus establishing an effective preferred local channel for dissipation. In turn, this would result in a lesser weight to the contribution given by correlations.

We conclude our analysis in this Section by exploring the parameter space in a more systematic way by fixing the global energy  $s$  and randomly choosing the three parameters left, provided that the constraints in Equation (5.106) are fulfilled. For our numerical study, we resort to the uniform distribution, in the way specified in the caption of Figure 5.5. In the same picture, we see that the curve for  $\dot{\Sigma}(t)$  comprising all the others is the one corresponding to unit global purity, i.e.,  $g = 1$ , and  $d = 0$ ,  $\lambda = 1$  (dashed line). The globally pure state is indeed the furthest possible from a diagonal one: the rate at which entropy production varies is increased in order to reach the final diagonal state  $\sigma_\infty$ .

#### 5.4.4 Dependence on the initial entanglement

We now compare the trends corresponding to different choices of the parameters characterising the initial state. As non-Markovian effects are reflected in oscillating behaviour of the entropy production, we can contrast cases corresponding to different initial preparations by looking



**Figure 5.5:** Entropy production rates  $\dot{\Sigma}(t)$  (absolute value) as a function of time. The initial CM is parametrised by fixing  $s$  ( $s = 10$  in the figure) and randomly choosing  $d, g, \lambda$  such that they are uniformly distributed in the intervals  $[0, s - 1]$ ,  $[2d + 1, d + 10]$  and  $[-1, 1]$  respectively. The figure reports  $N_R = 1000$  different realisations of the initial state. The dashed line corresponds to the globally pure state ( $g = 1$ ) with  $d = 0$ ,  $\lambda = 1$ . All the plots are obtained considering an Ohmic SD with a Lorentz-Drude cut-off and  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ .

at the maximum and the minimum values  $\dot{\Sigma}_{\max}$  and  $\dot{\Sigma}_{\min}$  that the entropy production rate assumes for each choice of the parameters. Taking into account the evidence previously gathered, in the simulations reported in this Section we fix the minimum value for  $g$ , i.e.,  $g = 2d + 1$ , and  $\lambda = +1$  as significant for the points that we want to put forward. In fact, with such choices we are able to parametrise the initial state with a minimum number of variables, while retaining the significant features that we aim at stressing. We can further assume, without loss of generality,  $d \geq 0$ : this is simply equivalent to assuming that the first oscillator is initially prepared in a state with a larger degree of mixedness than the second one, i.e.,  $\mu_1 \leq \mu_2$ . In this case, we can express  $d$  in terms of the smallest symplectic eigenvalue of the partially transposed CM  $\tilde{\nu}_-$ . Therefore, taking into account the constraints given by Equation (5.106), one has that  $d = -\frac{1}{2}(\tilde{\nu}_-^2 - 2s\tilde{\nu}_- + 1)$ . We already mentioned in Section 5.4.1 that, for the system at hand, we are able to derive a closed expression for the CM at any time  $t$ , given by Equation (5.94). We can further notice that the positive and negative peaks in the entropy production rate are attained at short times. We can thus perform a Taylor expansion of  $\Delta(t)$  in Equation (5.95) to obtain

$$\Delta_\Gamma(t) = [1 - \Gamma(t)] \int_0^t d\tau \Delta(\tau) + \int_0^t d\tau \Gamma(\tau) \Delta(\tau) + \mathcal{O}(\alpha^4). \quad (5.108)$$

As  $\Delta(t) \propto \alpha^2$  and  $\Gamma(t) \propto \alpha^2$ , we can retain only the first term consistently with the weak coupling approximation we are resorting to. Therefore, we can recast Equation (5.94) in a form that is more suitable for numerical evaluations, namely

$$\boldsymbol{\sigma}(t) = [1 - \Gamma(t)] \boldsymbol{\sigma}(0) + \left[ 2 \int_0^t d\tau \Delta(\tau) \right] \mathbb{I}. \quad (5.109)$$

By substituting [Equation \(5.109\)](#) into [Equation \(5.86\)](#), we get the analytic expression for the entropy production rate, that we report here for the sake of completeness:

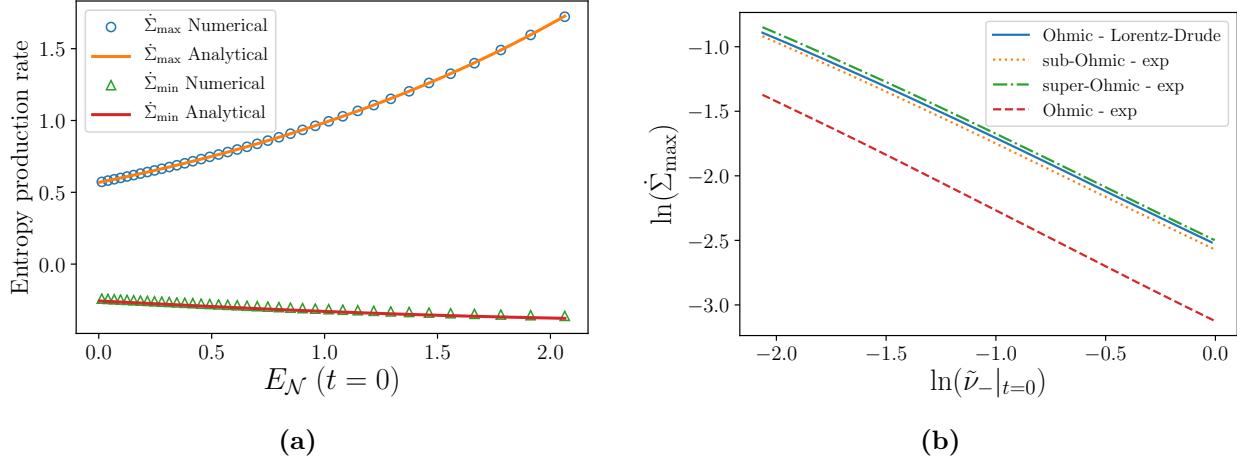
$$\begin{aligned}\dot{\Sigma}(t) = -8\gamma(t) + \frac{4\gamma^2(t)(s - 2s\Gamma(t) + \bar{\Delta}(t))}{\Delta(t)} \\ + \frac{4\Delta(t)(s - 2s\Gamma(t) + \bar{\Delta}(t))}{\tilde{\nu}_-(2s - \tilde{\nu}_-)(1 - \Gamma(t))^2 + 2s\bar{\Delta}(t)(1 - \Gamma(t)) + \bar{\Delta}^2(t)},\end{aligned}\quad (5.110)$$

where  $\bar{\Delta}(t) = 2 \int_0^t \Delta(\tau) d\tau$ . In this way, all the information about the initial state is encoded in the value of  $\tilde{\nu}_-$  while  $s$  is fixed. Note that this expression holds for any SD: once we choose the latter, we can determine the time-dependent coefficients  $\Delta(t)$  and  $\gamma(t)$  and thus the entropy production rate  $\dot{\Sigma}(t)$ . We can then compute the maximum of the entropy production rate and study the behaviour of  $\dot{\Sigma}_{\max}$  and  $\dot{\Sigma}_{\min}$  as functions of the entanglement negativity  $E_N$  at  $t = 0$ . In [Figure 5.6a](#) we compare numerical results to the curve obtained by considering the analytical solution discussed above and reported in [Equation \(5.110\)](#). Remarkably, we observe a monotonic behaviour of our chosen figure of merit with the initial entanglement negativity: the more entanglement we input at  $t = 0$  the higher the maximum of the entropy production rate is. We can get to the same conclusion (in absolute value) when we consider the negative peak  $\dot{\Sigma}_{\min}$ . The monotonic behavior highlighted above holds regardless of the specific form of the spectral density. In [Figure 5.6b](#) we study  $\dot{\Sigma}_{\max}$  against the smallest symplectic eigenvalue  $\tilde{\nu}_-$  of the partially transposed CM, obtaining different curves according to the reservoir's spectral properties. We find evidence of a power law of the form  $\dot{\Sigma}_{\max} \propto \tilde{\nu}_-^\delta$ .

### 5.4.5 Markovian Limit

We are now interested in assessing whether the analytical and numerical results gathered so far bear dependence on the non-Markovian character of the dynamics. With this in mind, we explore the Markovian limit, in which the problem is fully amenable to an analytical solution, that can also be used to validate our numerical results. Such limit is obtained by simply choosing an Ohmic SD with a Lorentz-Drude regularisation – [Equation \(5.107\)](#) – and taking the long time and high temperature limits, i.e.,  $\omega_0 t \gg 1$  and  $\beta^{-1} \gg \omega_0$ , as discussed in the [Example 4.6.1](#). Therefore, [Equation \(5.93\)](#) reduces to a master equation describing the dynamics of two uncoupled harmonic oscillators undergoing Markovian dynamics, for which we take  $\mathbf{A} = -\gamma_M \mathbb{I}$  and  $\mathbf{D} = \gamma_M(2\bar{n} + 1)\mathbb{I}$  in [Equation \(5.87\)](#), with  $\bar{n} = (e^{\beta\omega_0} - 1)^{-1}$ , and  $\gamma_M \equiv 4\alpha^2\omega_c^2\omega_0/(\omega_c^2 + \omega_0^2)$ .

Working along the same lines as in the non-Markovian case, we study the behaviour of  $\dot{\Sigma}(t)$  by suitably choosing the parameters encoding the preparation of the initial state. For example, in [Figure 5.7a](#) we plot the entropy production rate as a function of time for different values of  $g$ . The limiting procedure gives back a coarse-grained dynamics monotonically decreasing towards the thermal state, to which it corresponds a non-negative entropy production rate, asymptotically vanishing in the limit  $t \rightarrow \infty$ . Moreover, the memoryless dynamics leads to a monotonic decrease of the entanglement negativity, as shown in the inset of [Figure 5.7a](#). In



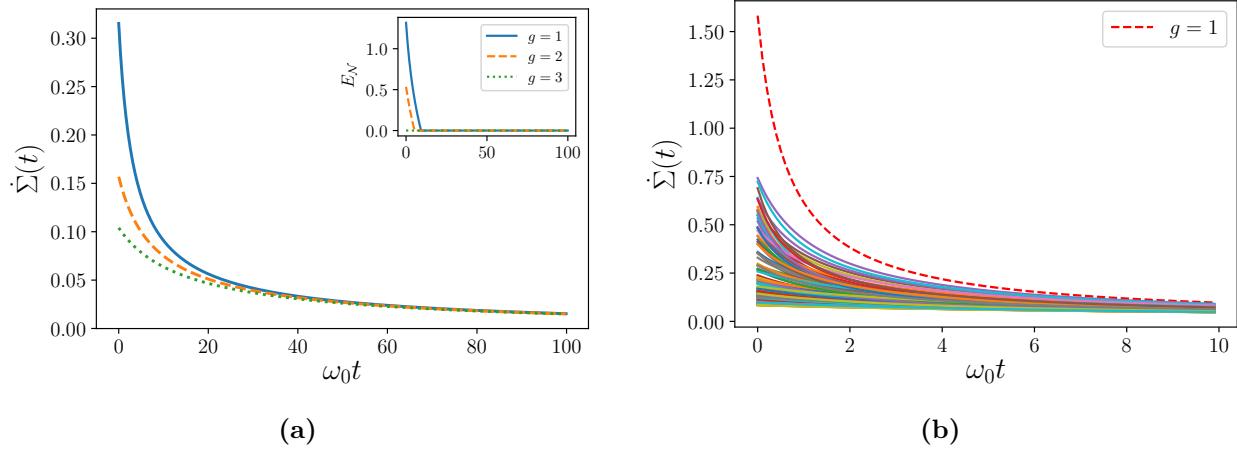
**Figure 5.6:** Entropy production rate in a system of two non-interacting oscillators undergoing the non-Markovian dynamics described in Section 5.4.1. In the parametrisation (5.104) and (5.105), we take  $s = 4$ ,  $g = 2d + 1$ ,  $\lambda = 1$ , while  $0 \leq d \leq 3$ . **Panel (a):** Maximum and minimum of the entropy production rate  $\dot{\Sigma}_{\max}$  and  $\dot{\Sigma}_{\min}$  as functions of the entanglement negativity at  $t = 0$ . We compare the numerical results (triangles and circles) to the analytical solution in Equation (5.110) (solid line). We have used an Ohmic SD with a Lorentz-Drude cut-off and  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.01\omega_0^{-1}$ . **Panel (b):** Plot of  $\dot{\Sigma}_{\max}$  against the smallest symplectic eigenvalue of the partially transposed CM at  $t = 0$  (logarithmic scale) for different SDs (as stated in the legend). In this plot,  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ .

this case, the globally pure state ( $g = 1$ , dashed line in Figure 5.7b) still plays a special role: all the curves corresponding to value of  $g$  smaller than the unity remain below it.

The Markovian limit provides a useful comparison in terms of integrated quantities. In this respect, we can study what happens to the entropy production  $\Sigma = \int_0^{+\infty} \dot{\Sigma}(t)dt$ . Although the non-Markovian dynamics entails the negativity of the entropy production rate in certain intervals of time, the overall entropy production is larger than the quantity we would get in the corresponding Markovian case, as can be noticed in Figure 5.8a. We can eventually study the dependence of the Markovian entropy production rate on the initial entanglement. Note that, in this limit, Equation (5.86) yields an analytic expression for the entropy production rate at a generic time  $t$ , that explicitly reads as

$$\begin{aligned} \dot{\Sigma}(t) = & -8\gamma_M + 4\gamma_M \left[ 1 + e^{-2\gamma_M t} s \tanh \left( \frac{\beta\omega_0}{2} \right) \right] \\ & + \frac{4\gamma_M \coth \left( \frac{\beta\omega_0}{2} \right) e^{2\gamma_M t} [s + (e^{2\gamma_M t} - 1) \coth \left( \frac{\beta\omega_0}{2} \right)]}{[2s - \tilde{\nu}_- + (e^{2\gamma_M t} - 1) \coth \left( \frac{\beta\omega_0}{2} \right)] [\tilde{\nu}_- + (e^{2\gamma_M t} - 1) \coth \left( \frac{\beta\omega_0}{2} \right)]}. \end{aligned} \quad (5.111)$$

From our numerical inspection, we have seen that the entropy production rate is maximum



**Figure 5.7:** Entropy production rates corresponding to different preparations of the initial global state in the Markovian limit. The initial state is parametrised through Equations (5.104) and (5.105), whereas, for the dynamics, we have taken  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.01\omega_0^{-1}$ . **Panel (a):** Entropy production rate obtained taking different values of  $g$  (thus varying the global purity of the state of the system) with  $s = 2$ ,  $d = 0$ ,  $\lambda = 1$ . **Panel (b):** The initial CM is parametrised by setting  $s = 10$  and randomly sampling (in a uniform manner)  $d, g, \lambda$  from the intervals  $[0, s - 1]$ ,  $[2d + 1, d + 10]$  and  $[-1, 1]$ , respectively. We present  $N_R = 100$  different realisations of the initial state. The dashed line represents the state with unit global purity ( $g = 1$ ) and  $d = 0$ ,  $\lambda = 1$ .

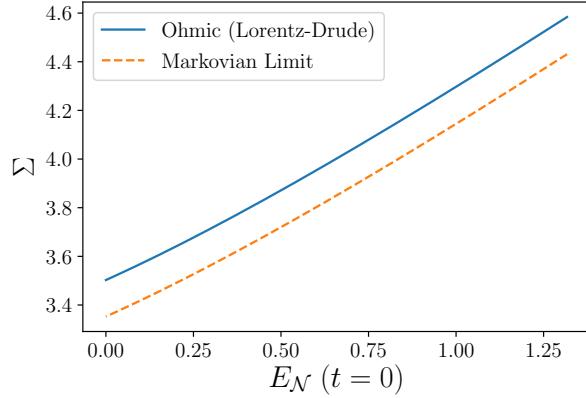
at  $t = 0$ , so that

$$\dot{\Sigma}_{\max} \equiv \dot{\Sigma}(0) = -8\gamma_M + 4s\gamma_M \tanh\left(\frac{\beta\omega_0}{2}\right) + \frac{4s\gamma_M \coth\left(\frac{\beta\omega_0}{2}\right)}{(2s - \tilde{\nu}_-)\tilde{\nu}_-}. \quad (5.112)$$

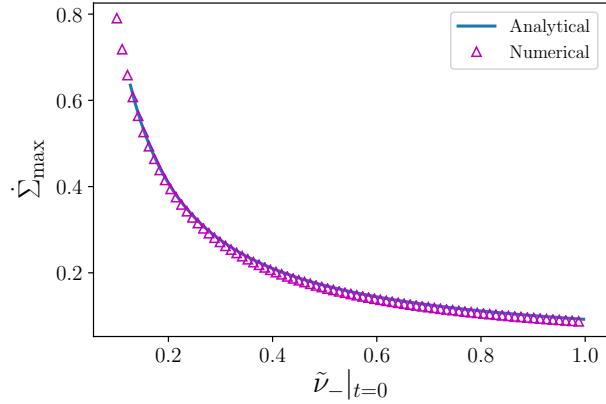
If we fix the parameter  $s$  and plot  $\dot{\Sigma}_{\max}$  against  $\tilde{\nu}_-$ , we can contrast analytical and numerical results [cf. Figure 5.8b]. We can draw the same conclusion as in the non-Markovian case: the more entanglement we input, the higher the entropy production rate.

## 5.5 Conclusions

In this Chapter we have formulated a theory of the entropy production for nonequilibrium open quantum systems based on phase-space methods. We have seen that the latter allows us to consistently explore limits that would be otherwise inaccessible though the traditional formulation in terms of the von Neumann entropy. This formalism has been employed to study – both numerically and analytically – the dependence of the entropy production rate on the initial correlations between the components of a harmonic composite system. We have established that correlations play an important role in the rate at which entropy is intrinsically produced during the process. Indeed, we have shown that, when the system is prepared in a globally pure state, we should expect a higher entropy production rate. This is the case – regardless of the spectral density chosen – for initial entangled states of the



(a)



(b)

**Figure 5.8:** Panel (a): Entropy production in the non-Markovian case (solid line) as a function  $E_N(t = 0)$ , compared with its counterpart achieved in the corresponding Markovian limit (dashed line). We have taken  $s = 2$ ,  $d = 0$ ,  $\lambda = 1$ ,  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.01\omega_0^{-1}$ . Panel (b): Markovian limit: maximum entropy production rate as a function of the minimum symplectic eigenvalue of the partially transposed CM at  $t = 0$ . We have taken  $s = 4$ ,  $g = 2d + 1$ ,  $\lambda = 1$ ,  $0 \leq d \leq 3$ ,  $\alpha = 0.1\omega_0$ ,  $\omega_c = 0.1\omega_0$ ,  $\beta = 0.1\omega_0^{-1}$ . We compare the curve obtained numerically (triangles) to the analytical trend (solid line) found through Equation (5.112).

oscillators: larger initial entanglement is associated with higher rates of entropy production, which turns out to be a monotonic function of the initial degree of entanglement.

# Chapter 6

## Reaction Coordinate Mapping

In the previous Chapters, we have seen that the coupling of a quantum system to an environment embodies a challenge, both conceptually and practically. In general, these difficulties arise because the number of environmental degrees of freedom is so large that we are not able to explicitly track the complex dynamical evolution of such a many-body system. In [Chapters 3 and 4](#), we have seen that the open quantum system paradigm offers a set of effective tools to treat this problem, just by studying the effects on the reduced system, while we eliminate all the information about the environment. The usual approach – described in full detail in [Chapter 4](#) – relies on a set of assumptions – usually the so-called Born-Markov approximation – to obtain a tractable master equation ([Breuer, 2002](#)). Furthermore, in the last decades, the rapid technological advance has made possible to experimentally realise scenarios in which the standard Born-Markov approximation breaks down: persistent memory effects and strong system-environment coupling are commonly encountered in a variety of situations. For all these reasons, a great deal of effort has been devoted to studying open quantum systems dynamics with nonperturbative and non-Markovian system-bath interactions. Particularly, one of these methods is the Reaction Coordinate (RC) mapping approach ([Garg, 1985; Thoss, 2001](#)), which we will introduce in [Section 6.1](#), considering the paradigmatic case of the spin-boson model. We will then use this results in [Section 6.2](#) to show that a spin-boson model can serve as a quantum simulator of non-Markovian multiphoton Jaynes-Cummings models.

### 6.1 General features of the mapping

In this Section, we introduce the general features of the reaction coordinate mapping. Considering the paradigmatic case of a spin-boson model, we will show that an orthogonal transformation on the bath modes can be performed so as to incorporate a collective coordinate of the environment into an effective system Hamiltonian. This allows to explore a wider range of regimes, provided that the coupling with the system and the residual environment allows us to rely on the Born-Markov approximation.

### 6.1.1 Application to the spin-boson model

The spin-boson model describes a two-level system interacting with a large, typically infinite, number of bosonic modes, which embodies the environment. This model has been acknowledged as a paradigm for the exploration of quantum dissipation and quantum-to-classical transition (Leggett, 1987; Weiss, 2012). As many physical systems can be well approximated as a two-level system for sufficient low temperature, the spin-boson model has become a cornerstone in the description of quantum effects in diverse physical realizations, ranging from quantum-based setups (Leggett, 1987; Weiss, 2012) to biological complexes (Huelga, 2013). In addition, this model has played a key role in the development of the theory of open quantum systems (Breuer, 2002), providing a suitable test-bed to benchmark distinct approximations and tools aimed to efficiently deal with the large number of environmental degrees of freedom. Hence, the spin-boson model exhibits rich physics and it is of fundamental relevance in many different areas of research. The Hamiltonian of the spin-boson model can be written as

$$H_{\text{SB}} = H_{\text{S}} + H_{\text{E}} + H_{\text{SE}}, \quad (6.1)$$

where each term reads as

$$H_{\text{S}} = \frac{\epsilon_0}{2} \sigma_z + \frac{\Delta_0}{2} \sigma_x, \quad (6.2)$$

$$H_{\text{E}} = \sum_k \omega_k c_k^\dagger c_k, \quad (6.3)$$

$$H_{\text{SE}} = \sigma_x \sum_k f_k (c_k + c_k^\dagger). \quad (6.4)$$

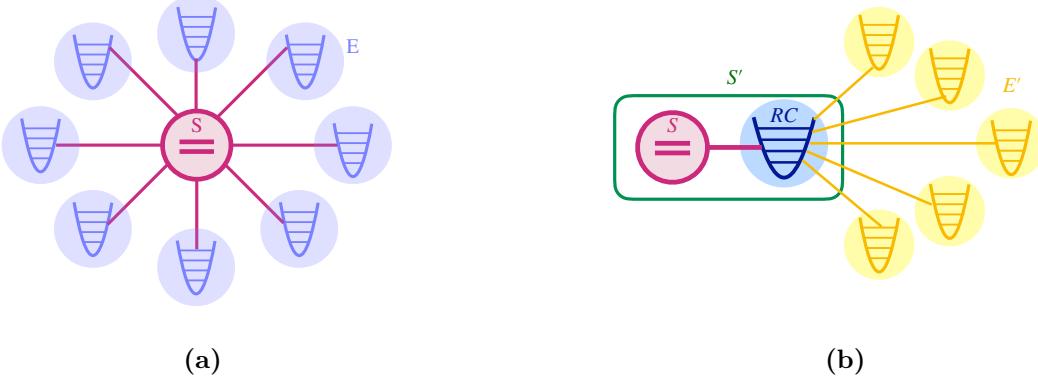
The first two terms represent the free Hamiltonians of the spin and environment, respectively, while the last one describes the interaction between them. Here we consider that the frequency splitting of the spin is given by  $\Delta_0$ , while  $\epsilon_0$  accounts for the bias between the eigenstates of the two-level system  $|\pm\rangle$ , and  $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  is the usual vector of spin- $\frac{1}{2}$  Pauli matrices — see [Figure 6.1a](#). Hence,  $\sigma_x |\pm\rangle = \pm |\pm\rangle$ ,  $\sigma_z |e\rangle = |e\rangle$  and  $\sigma_z |g\rangle = -|g\rangle$ . The interaction with the environment is dictated by  $H_{\text{SE}}$ , where the  $k^{\text{th}}$  mode with energy  $\omega_k$  is coupled to the spin with a strength  $f_k$ . These bosonic modes fulfill the usual commutation relation  $[c_k, c_{k'}^\dagger] = \delta_{k,k'}$ . Remarkably, the system-environment interaction can be completely characterized in terms of the spectral density, given by

$$J_{\text{SB}}(\omega) = \sum_k f_k^2 \delta(\omega - \omega_k), \quad (6.5)$$

which we assume to be known. We should stress that, unlike the case discussed in [Section 4.1](#), this version of the spin-boson model is not exactly solvable due to the presence of the term  $\frac{\epsilon_0}{2} \sigma_z$  in the system Hamiltonian.

### 6.1.2 Normal transformation of the bath variables

We now apply a transformation to [Equation \(6.1\)](#) that would help us incorporate the most important degrees of freedom into a new effective Hamiltonian (Iles-Smith, 2014). The idea



**Figure 6.1:** Panel (a): *Spin-boson model in the typical star configuration, where the environment is made of infinitely many harmonic oscillators, each of them with frequency  $\omega_k$ , interacting with the spin through  $\sigma_x f_k(c_k + c_k^\dagger)$ .* Panel (b): *Spin-boson model after the application of the reaction coordinate mapping: the system interacts with the residual harmonic environment through a collective mode, i.e., the reaction coordinate.*

is straightforward: we introduce a suitable collective coordinate of the environment, the so-called *reaction coordinate*, which couples directly to the spin, and, in turn, is coupled to a residual harmonic environment — see Figure 5.3b. For the sake of definiteness, let us suppose that the environment is made of  $N$  harmonic oscillators (we will then take the limit  $N \rightarrow \infty$ ), whose position and momentum operators are given by

$$x_k = \sqrt{\frac{1}{2\omega_k}}(c_k + c_k^\dagger), \quad p_k = i\sqrt{\frac{\omega_k}{2}}(c_k^\dagger - c_k), \quad (6.6)$$

and satisfy the canonical commutations laws  $[x_k, p_{k'}] = i\delta_{k,k'}$ . We can define two  $N$ -dimensional vectors  $\mathbf{x} = (x_k)_{1 \leq k \leq N}$  and  $\mathbf{p} = (p_k)_{1 \leq k \leq N}$ . We obtain a new set of bath coordinates by applying a transformation  $\Lambda$  (represented as a  $N \times N$  matrix) such that (Strasberg, 2016)

$$\mathbf{X} = \Lambda \mathbf{x}, \quad \mathbf{P} = \Lambda \mathbf{p}. \quad (6.7)$$

The latter can be equivalently expressed as

$$X_k = \sum_l \Lambda_{kl} x_l, \quad P_{k'} = \sum_{l'} \Lambda_{k'l'} p_{l'}. \quad (6.8)$$

First, we require that the transformation  $\Lambda$  preserves the commutation relations, i.e., that  $[x_k, p_{k'}] = i\delta_{k,k'}$  yields  $[X_k, P_{k'}] = i\delta_{k,k'}$ . By using Equation (6.8), one easily gets that  $\Lambda$  must be represented by an orthogonal matrix, i.e.,  $\Lambda \Lambda^T = \Lambda^T \Lambda = \mathbb{I}$ . The first column of the transformation  $\Lambda$  is defined by introducing a collective coordinate  $X \equiv X_1$  thought the relation

$$\tilde{\lambda}X = \sum_k \tilde{f}_k x_k, \quad (6.9)$$

where we have rescaled the coupling constants, i.e.,  $\tilde{f}_k = f_k \sqrt{2\omega_k}$ . Hence, since  $X_1 = \sum_k \Lambda_{1k} x_k$ , we get  $\Lambda_{1k} = \tilde{f}_k / \tilde{\lambda}$ . From the commutation relation  $[X_1, P_1] = i$ , we get the condition

$$\tilde{\lambda}^2 = \sum_k \tilde{f}_k^2. \quad (6.10)$$

Second, the aforementioned orthogonal transformation is uniquely fixed by requiring that the residual bath is in normal form. Let us notice that the Hamiltonian of the initial environment can be expressed in terms of the position and momentum operators  $x_k$  and  $p_k$  as

$$H_E = \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 x_k^2). \quad (6.11)$$

Hence we can focus our attention on the following term:

$$\sum_k \omega_k^2 x_k^2 = \sum_k \sum_{l,l'} \Lambda_{lk} \Lambda_{l'k} X_l X_{l'} \omega_k^2 \quad (6.12)$$

$$= X_1^2 \sum_k \Lambda_{1k} \Lambda_{1k} \omega_k^2 + 2X_1 \sum_{l'} X_{l'} \sum_k \Lambda_{1k} \Lambda_{l'k} \omega_k^2 + \sum_{l,l'} X_l X_{l'} \sum_k \Lambda_{lk} \Lambda_{l'k} \omega_k^2, \quad (6.13)$$

where, in the last line, we have explicitly separated the contribution of the first coordinate  $X_1$  of the new set of bath variables, namely the RC  $X$ . Furthermore, we should notice that the last term contains non-diagonal contributions, i.e.,  $X_l X_{l'}$ , with  $l \neq l'$ , thus the Hamiltonian cannot be written in a normal form without additional requirements. Therefore, we assume that  $\Lambda$  is an orthogonal matrix whose coefficients satisfy

$$\sum_k \Lambda_{lk} \Lambda_{l'k} \omega_k^2 = \delta_{ll'} \Omega_l^2, \quad (6.14)$$

where  $\Omega_l$  are the eigenfrequencies of the residual bath. In particular, if we take  $l = l' = 1$ , we get  $\sum_k \Lambda_{1k}^2 \omega_k^2 = \Omega_1^2$ , whence, as  $\Lambda_{1k} = \tilde{f}_k / \tilde{\lambda}$ , we obtain the RC frequency

$$\Omega^2 \equiv \Omega_1^2 = \frac{\sum_k \omega_k^2 f_k^2}{\lambda^2}. \quad (6.15)$$

Hence, with this constraint, Equation (6.12) becomes

$$\sum_k \omega_k^2 x_k^2 = \Omega^2 X^2 + 2X \sum_{l>1} \tilde{g}_l X_l + \sum_{l>1} \Omega_l^2 X_l^2, \quad (6.16)$$

where we have introduced new coupling constants  $\tilde{g}_l = \sum_k \Lambda_{1k} \Lambda_{lk} \omega_k^2$ . On the other hand, we readily obtain

$$\sum_k p_k^2 = P^2 + \sum_{l>1} P_l^2, \quad (6.17)$$

where  $P_1 \equiv P$ . Hence, the transformed total Hamiltonian becomes

$$H_{\text{SB}} = H_{\text{S+RC}} + H_{\text{RC-E}'} + H_{\text{E}'} + H_{\text{C}}, \quad (6.18)$$

where

$$H_{\text{S+RC}} = H_{\text{S}} + \tilde{\lambda}\sigma_x X + \frac{1}{2}(P^2 + \Omega^2 X^2), \quad (6.19)$$

$$H_{\text{RC-E}'} = X \sum_{k>1} \tilde{g}_k X_k, \quad (6.20)$$

$$H_{\text{E}'} = \frac{1}{2} \sum_{k>1} (P_k^2 + \Omega_k^2 X_k^2), \quad (6.21)$$

$$H_{\text{C}} = \frac{X^2}{2} \delta\Omega_0^2. \quad (6.22)$$

Note that  $H_{\text{S+RC}}$  is the Hamiltonian of the augmented system;  $H_{\text{RC-E}'}$  accounts for the interaction between the reaction coordinate and the residual bath, the latter modelled through the Hamiltonian  $H_{\text{E}'}$ . The last term  $H_{\text{C}}$  has been introduced *ad hoc* and represents the so-called counter-term involving the renormalisation frequency  $\delta\Omega_0^2 \equiv \sum_k \frac{\tilde{g}_k^2}{\Omega_k^2}$  (Martinazzo, 2011). Note that, if we rescale the coupling coefficients, i.e.,  $\tilde{f}_k \rightarrow \alpha \tilde{f}_k$  with a suitable choice of  $\alpha \in \mathbb{R}$ , the coupling constant  $\lambda$  would be affected [cf. Equation (6.10)], while the coupling coefficients  $\tilde{g}_k$  would not, as they turn out to be independent of  $\alpha$ . This means that this approach is intrinsically nonperturbative.

Furthermore, Equation (6.18) can be alternatively rewritten as

$$\begin{aligned} H_{\text{SB}} = & H_{\text{S}} + \Omega a^\dagger a + \sum_k \Omega_k b_k^\dagger b_k \\ & + (a + a^\dagger) \left[ \lambda \sigma_x + \sum_k g_k (b_k + b_k^\dagger) + (a + a^\dagger) \sum_k \frac{g_k^2}{\Omega_k} \right], \end{aligned} \quad (6.23)$$

where  $a, a^\dagger$  are respectively the creation and annihilation operators associated to the RC;  $b_k, b_k^\dagger$  are the bosonic operators describing the residual bath, and we have rescaled the coupling constants as  $\lambda = \tilde{\lambda}/\sqrt{2\Omega}$ ,  $g_k = \tilde{g}_k/(2\sqrt{\Omega\Omega_k})$ .

The procedure outlined above can be summarised as follows: we have redrawn the boundary between the system and environment by introducing a collective mode, namely the RC, that couples directly to the system. In this picture, the system interacts with the residual environment through the RC. Therefore, this justifies the introduction of the following spectral density

$$J_{\text{RC}}(\omega) = \sum_k g_k^2 \delta(\omega - \Omega_k). \quad (6.24)$$

We should stress that we do not need to determine the orthogonal transformation  $\Lambda$  explicitly, as the normal mode transformation – in the limit of  $N \rightarrow \infty$  harmonic oscillators – is fully determined by the SD  $J_{\text{SB}}(\omega)$  only (Strasberg, 2016).

### 6.1.3 Relation between the SB and RC spectral densities

The complete specification of the RC mapping requires an explicit relation between the SB and the RC spectral densities. This relation can be obtained following a procedure that was first put forward by Garg *et al.* (Garg, 1985), which consists in deriving the spectral densities both before and after the mapping through the corresponding classical equation of motion. Indeed, the SD encodes only the information about the interaction between the system and the environment, therefore we can momentarily regard the spin as a continuous coordinate  $q$  subject to a potential  $U(q)$ . Therefore, we can rewrite the Hamiltonian of the SB model [cf. Equation (6.1)] in the form

$$H_q = \frac{P_q^2}{2} + U(q) + q \sum_k \tilde{f}_k x_k + q^2 \sum_k \frac{\tilde{f}_k^2}{2\omega_k^2} + \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 x_k^2), \quad (6.25)$$

where we have added the counter-term that are quadratic in the coordinate  $q$ . This Hamiltonian yields the following equations of motion

$$\ddot{q}(t) = -\frac{\partial H_q}{\partial q} = -U'(q) - \sum_k \tilde{f}_k x_k(t) - q(t) \sum_k \frac{\tilde{f}_k^2}{\omega_k^2}, \quad (6.26)$$

$$\ddot{x}_k(t) = -\frac{\partial H_q}{\partial x_k} = -\tilde{f}_k q(t) - \omega_k^2 x_k(t). \quad (6.27)$$

We can eliminate the bath variables from the set of coupled differential equations by Fourier transforming both sides of Equations (6.26) and (6.27)<sup>1</sup>, obtaining a set of coupled algebraic equations

$$-z^2 \hat{q}(z) = -\hat{U}'(q) - \sum_k \tilde{f}_k \hat{x}_k(z) - \hat{q}(z) \sum_k \frac{\tilde{f}_k^2}{\omega_k^2}, \quad (6.28)$$

$$-z^2 \hat{x}_k(z) = -\tilde{f}_k \hat{q}(z) - \omega_k^2 \hat{x}_k(z). \quad (6.29)$$

We can derive a closed expression for  $\hat{x}_k(z)$  from Equation (6.29) and insert it into Equation (6.28) to eventually get an evolution equation of the form

$$\hat{L}_{\text{SB}}(z) \hat{q}(z) = -\hat{U}'(z), \quad (6.30)$$

where we have introduced the Fourier space propagator

$$\hat{L}_{\text{SB}}(z) = -z^2 \left( 1 + \sum_k \frac{\tilde{f}_k^2}{\omega_k^2(\omega_k^2 - z^2)} \right). \quad (6.31)$$

---

<sup>1</sup>The Fourier transform of a function  $h(t)$  is defined as

$$\hat{h}(z) = \int_{-\infty}^{+\infty} h(t) e^{-izt}, \quad \text{Im}(z) > 0.$$

If we recall that  $\tilde{f}_k = f_k \sqrt{2\omega_k}$  and we take the continuum limit, we obtain

$$\hat{L}_{\text{SB}}(z) = -z^2 \left( 1 + 2 \int_0^{+\infty} d\omega \frac{J_{\text{SB}}(\omega)}{\omega(\omega^2 - z^2)} \right) \quad (6.32)$$

If we solve the integral appearing in [Equation \(6.32\)](#) with the residue theorem, we get  $\hat{L}_{\text{SB}}(z) = -z^2 + \pi i J_{\text{SB}}(z)$ ; hence, the initial spectral density can be obtained by means of the so-called Leggett prescription ([Leggett, 1984](#))

$$J_{\text{SB}}(\omega) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \text{Im}[\hat{L}_{\text{SB}}(\omega - i\epsilon)]. \quad (6.33)$$

We can now use the same procedure to write the Fourier space propagator in terms of the RC spectral density. Let us consider the classical Hamiltonian

$$\begin{aligned} H'_q = & \frac{P_q^2}{2} + U(q) + \tilde{\lambda} q X + \frac{\tilde{\lambda}}{2\Omega^2} q^2 + \frac{1}{2} (P^2 + \Omega^2 X^2) \\ & + X \sum_k \tilde{g}_k X_k + X^2 \sum_k \frac{\tilde{g}_k^2}{2\Omega_k^2} + \frac{1}{2} \sum_k (P_k^2 + \Omega_k^2 X_k^2), \end{aligned} \quad (6.34)$$

which yields the following equations of motion:

$$\ddot{q} + \tilde{\lambda} X + \frac{\tilde{\lambda}^2}{\Omega^2} q = -U'(q) \quad (6.35)$$

$$\ddot{X} + \tilde{\lambda} q + \left( \Omega^2 + \sum_k \frac{\tilde{g}_k^2}{\Omega_k^2} \right) X + \sum_k \tilde{g}_k X_k = 0 \quad (6.36)$$

$$\ddot{X}_k + \tilde{g}_k X + \omega_k^2 X_k = 0. \quad (6.37)$$

Working along the same lines as before, we can move to the Fourier space and eliminate both the RC and the residual environment. Combining the [Equations \(6.36\)](#) and [\(6.37\)](#), we obtain

$$[\Omega^2 + \mathcal{L}(z)] \hat{X}(z) = -\tilde{\lambda} \hat{q}(z), \quad (6.38)$$

where

$$\mathcal{L}(z) \equiv -z^2 \left( 1 + \sum_k \frac{\tilde{g}_k^2}{\Omega_k^2(\Omega_k^2 - z^2)} \right), \quad (6.39)$$

or, in the continuum limit,

$$\mathcal{L}(z) \equiv -z^2 \left( 1 + 4\Omega \int_0^{+\infty} d\omega \frac{J_{\text{RC}}(\omega)}{\omega(\omega^2 - z^2)} \right), \quad (6.40)$$

where we have taken into account that  $\tilde{g}_k = 2\sqrt{\Omega\Omega_k} g_k$ . Substituting the latter into [Equation \(6.35\)](#), we eventually get an equation of the form

$$\hat{L}_{\text{RC}}(z)\hat{q}(z) = -\hat{U}'(q), \quad (6.41)$$

with

$$\hat{L}_{\text{RC}}(z) \equiv -z^2 + \frac{\tilde{\lambda}^2}{\Omega^2} \frac{\mathcal{L}(z)}{\Omega^2 + \mathcal{L}(z)}. \quad (6.42)$$

As the mapping, at this stage, is exact, the propagator will be identical before and after the transformation. This means that we can use  $\hat{L}_{\text{RC}}(z)$  in [Equation \(6.33\)](#) instead of  $\hat{L}_{\text{SB}}(z)$ . The way to obtain an initial underdamped or overdamped SD from an Ohmic SD for the RC is discussed in the [Example 6.1.1](#).

In this Section, we have explicitly considered the case in which the original coupling of the open system with the environment is absorbed by a single RC. In such case, one can derive the equations of motion, e.g, using the standard Born-Markov approximation, as we will discuss in [Section 6.1.4](#). However, this is not always the case: the coupling between the system and the surroundings can still hinder the derivation of the master equation in the aforementioned limit. If the coupling with the residual environment allows it, we can iteratively resort to the RC mapping in order to result into a Markovian description of the dynamics. The convergence properties of recursive RC mappings are thoroughly investigated in Refs. ([Martinazzo, 2011](#); [Woods, 2014](#)).

### Example 6.1.1: Underdamped and overdamped spectral densities

Let us suppose that the interaction between the RC and residual environment is modelled through an Ohmic SD of the form

$$J_{\text{RC}}(\omega) = \gamma\omega e^{-\omega/\Lambda}, \quad (6.43)$$

where  $\gamma > 0$ , and  $\Lambda$  is the cut-off frequency, such that  $\Lambda \rightarrow \infty$ . Using [Equation \(6.42\)](#) in [\(6.33\)](#), we obtain

$$J_{\text{SB}}(\omega) = \frac{4\gamma\Omega^2\lambda^2\omega}{(\Omega^2 - \omega^2)^2 + (2\pi\gamma\Omega\omega)^2}, \quad (6.44)$$

which we can compare the latter with an underdamped SD

$$J_{\text{UD}}(\omega) = \frac{\alpha\Gamma\omega_0^2\omega}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}. \quad (6.45)$$

It is easy to see that  $J_{\text{SB}}(\omega)$  recovers  $J_{\text{UD}}(\omega)$  if we take  $\Omega = \omega_0$ ,  $\lambda = \sqrt{\pi\alpha\omega_0/2}$ ,  $\gamma = \Gamma/(2\pi\omega_0)$ . This means that, for this instance, the RC mapping is exact, provided that  $\Lambda \rightarrow +\infty$ . Physically, this is readily understood: the underdamped SD displays

a sharp peak centered around the characteristic function  $\omega_0$ , hence it is natural to identify  $\omega_0$  as the frequency of the collective mode introduced by the RC mapping. Similarly, starting from [Equation \(6.44\)](#) we can obtain a overdamped SD, i.e.,

$$J_{\text{OD}}(\omega) = \frac{\alpha \omega_c \omega}{\omega_c^2 + \omega^2}, \quad (6.46)$$

as far as we take  $\Omega = 2\pi\gamma\omega_c$ ,  $\lambda = \sqrt{\pi\alpha\Omega/2}$ , and  $\gamma$  such that  $\omega_c \ll \Omega$ . However, in this case the mapping is not exact. Note that these SDs – or combination thereof – are frequently encountered in models of molecular systems ([Iles-Smith, 2016](#)).

#### 6.1.4 Master equation of the augmented system

Once the RC mapping has been carried out, one also needs to solve the dynamics. The guiding idea is to treat exactly the coupling between the spin and the RC, while the interaction between the latter and the residual environment is treated perturbatively up to the second order in the coupling strength. This allows us to rely on the standard Born-Markov approximation, provided that either the coupling between the augmented system and the residual environment is weak or the residual environment correlation time is short compared to the relevant timescale of the system. Within such approximation, one can work out a master equation that, in the Schrödinger picture, reads

$$\begin{aligned} \dot{\rho}(t) = & -i [H_{\text{S+RC}}, \rho(t)] \\ & - \int_0^\infty d\tau \int_0^\infty d\omega J_{\text{RC}}(\omega) \cos \omega \tau \coth \left( \frac{\beta \omega}{2} \right) [x, [x(-\tau), \rho(t)]] \\ & - \int_0^\infty d\tau \int_0^\infty d\omega J_{\text{RC}}(\omega) \frac{\cos \omega \tau}{\omega} [x, \{[x(-\tau), H_{\text{S+RC}}], \rho(t)\}], \end{aligned} \quad (6.47)$$

where  $\rho \equiv \rho_{\text{S+RC}}$ ,  $x = a + a^\dagger$  and the residual environment is assumed to be in a thermal state, i.e.  $\rho_{E'} = e^{-\beta H_{E'}} / \text{Tr}_{E'} \{e^{-\beta H_{E'}}\}$ .

In order to obtain an expression for the interaction picture operators, one can proceed by truncating the space of the augmented system up to  $n^{\text{th}}$  basis states, and numerically diagonalising the Hamiltonian  $H_{\text{S+RC}}$ . To this end, let  $|\phi_n\rangle$  be an eigenstate of  $H_{\text{S+RC}}$  such that  $H_{\text{S+RC}} |\phi_j\rangle = \varphi_j |\phi_j\rangle$ . The operator  $x$  can thus be expanded as  $x = \sum_{jk} x_{jk} |\phi_j\rangle \langle \phi_k|$ , while in the interaction picture one has

$$x(t) = \sum_{jk} x_{jk} e^{i\xi_{jk} t} |\phi_j\rangle \langle \phi_k|, \quad (6.48)$$

where  $x_{jk} = \langle \phi_j | x | \phi_k \rangle$  and  $\xi_{jk} = \varphi_j - \varphi_k$ . We can now introduce the following operators

$$\begin{aligned}\chi &= \int_0^{+\infty} d\tau \int_0^{+\infty} d\omega J_{\text{RC}}(\omega) \cos \omega \tau \coth \left( \frac{\beta \omega}{2} \right) x(-\tau) \\ &\approx \frac{\pi}{2} \sum_{jk} J_{\text{RC}}(\xi_{jk}) \coth \left( \frac{\beta \xi_{jk}}{2} \right) x_{jk} |\phi_j\rangle \langle \phi_k|,\end{aligned}\quad (6.49)$$

and

$$\Xi = \int_0^{+\infty} d\tau \int_0^{+\infty} d\omega J_{\text{RC}}(\omega) \frac{\cos \omega \tau}{\omega} [H_{\text{S+RC}}, x(-\tau)] \approx \frac{\pi}{2} \sum_{jk} J_{\text{RC}}(\xi_{jk}) x_{jk} |\phi_j\rangle \langle \phi_k|,\quad (6.50)$$

where we have assumed the imaginary parts to be negligible. These operators include the rates affecting the RC, and they appear in the final form of the master equation

$$\dot{\rho}_{\text{S+RC}}(t) = -i [H_{\text{S+RC}}, \rho_{\text{S+RC}}(t)] - [x, [\chi, \rho_{\text{S+RC}}(t)]] + [x, \{\Xi, \rho_{\text{S+RC}}(t)\}].\quad (6.51)$$

Equation (6.51) provides an accurate description of the system dynamics, as far as the system-environment SD enables to apply the Born-Markov approximation. In Refs. (Iles-Smith, 2014; Iles-Smith, 2016), the numerical results gathered using the RC mapping have been benchmarked against other simulation methods available for open system dynamics, such as a semiclassical approach based on Zusman equations, a set of drift-diffusion equations of motion often used to describe molecular systems (Thoss, 2001), or the hierarchical equations of motion (HEOM) technique (Tanimura, 1989; Tanimura, 2020). Specifically, the HEOM is a widely used method to simulate the dynamics of open quantum systems: historically introduced in the case of an Ohmic SD with a Lorentz-Drude cut-off (Tanimura, 1989), it has been extended to those cases in which the SD leads to bath correlation functions decomposable using a basis of exponentials (Tanimura, 2020). Conversely, the RC mapping is less restrictive in terms of spectral density, provided that the latter allows to ultimately resort to the Born-Markov approximation.

## 6.2 Spin-boson model as a simulator of multiphoton Jaynes-Cummings models

In this Section, we will follow the theoretical framework developed in (Casanova, 2018; Puebla, 2019), combining the ideas of the reaction-coordinate mapping, to show that the paradigmatic spin-boson model can serve as an analogue quantum simulator for the realisation of dissipative multiphoton Jaynes-Cummings models. The quantum Rabi model (QRM), as well as its simplified version known as Jaynes-Cummings model (JCM) (Jaynes, 1963), play a central role in the description of light-matter interacting systems and in quantum information science (Scully, 1997; Nielsen, 2010). In these models, the interaction mechanism

between the spin and bosonic degrees of freedom has a linear form, namely, the spin gets excited or deexcited by absorbing or emitting one bosonic excitation.

While this interaction is ubiquitous in quantum physics and has applications in various experimental platforms (Braak, 2016), other forms of a spin-boson exchange mechanism beyond this simple case are also of interest. One possible generalization of the QRM or JCM consists in considering a spin-multiphoton interaction, where the spin exchange  $n$  excitations simultaneously with the bosonic mode. Such a generalization is often regarded as  $n$ -photon QRM or JCM, (nQRM or nJCM), and it has recently attracted attention mainly in its  $n = 2$  form (Felicetti, 2015; Puebla, 2017; Felicetti, 2018; Xie, 2019), although models with  $n > 2$  have been also analyzed (Lo, 1998). From an experimental point of view, however, such multiphoton terms are typically hard to attain. Thus, its realisation may benefit from quantum simulation protocols, allowing for enough tunability and control over multiphoton interactions terms, as proposed using optical trapped ions (Felicetti, 2015; Puebla, 2017) or superconducting qubits (Felicetti, 2018). These latter schemes realize effective multiphoton exchange terms by exploiting the nonlinear fashion in which the spin and bosonic degrees of freedom couple. It is however still possible to realise such multiphoton models even when the setup comprises solely a linear, i.e., standard, interaction mechanism and thus, it is not suited for a direct simulation of these models, as shown in (Casanova, 2018).

In this Section, in particular, by considering a full spin-boson model we naturally extend the theoretical framework beyond the standard local master equation description of dissipation effects in the simulator, as considered in (Puebla, 2019). Furthermore, we show that the simulated multiphoton Jaynes-Cummings models may acquire a non-Markovian behaviour when the spin-boson model features a structured environment, and thus, highlighting the suitability of the proposed theoretical framework to explore aspects of non-Markovianity in distinct light-matter interacting systems.

### 6.2.1 Analogue simulation of multiphoton spin-boson interactions

The task now consists in bringing the spin-boson Hamiltonian  $H_{\text{SB}}$  into the form of a  $n$ -photon model, i.e, into a model containing interaction terms of the form  $\sigma^\pm a^n$  and  $\sigma^\pm (a^\dagger)^n$ . For that, one could perform the approximate mapping used in Ref. (Casanova, 2018; Puebla, 2019) directly onto  $H_{\text{SB}}$ . Specifically, in Ref. (Casanova, 2018), the authors present a framework for the emergence of multiphoton and nonlinear spin-boson coupling via spin rotations, while in Ref. (Puebla, 2019), the latter scheme is generalised to dissipative scenarios. Here we combine the latter with known techniques to simulate a spin-boson model. In principle, this could be achieved by selecting a particular bosonic mode out of the environment with frequency  $\omega_q$  to now play the role of  $a$  in the interaction with the spin ( $c_q \rightarrow a$ ), while treating the rest of  $c_{k \neq q}$  as a residual environment. Here, however, we resort to a more sophisticated procedure, based on the so-called reaction coordinate (RC) mapping, described in Section 6.1.

Let us consider a more general version of the spin-boson model introduced in Section 6.1.1, explicitly considering the application of  $n_d$  drivings onto the spin. As discussed in Ref. (Casanova,

2018; Puebla, 2019), under certain conditions, applying spin drivings enables the realisation of different multiphoton Jaynes-Cummings interaction terms. In this manner, while a multiphoton Jaynes-Cummings model can be attained without the need of any additional driving,  $n_d = 0$ , the realisation of a multiphoton quantum Rabi model requires the application of at least one driving  $n_d = 1$ . In general, the free-energy Hamiltonian of the spin under  $n_d$  drivings with amplitude  $\epsilon_j$  and detuning  $\Delta_j$  with respect to the spin frequency splitting  $\Delta_0$  reads as

$$H_{S,d} = \frac{\Delta_0}{2}\sigma_x + \sum_{j=0}^{n_d} \frac{\epsilon_j}{2} [\cos(\Delta_j - \Delta_0)t \sigma_z + \sin(\Delta_j - \Delta_0)t \sigma_y]. \quad (6.52)$$

Clearly, setting  $\epsilon_{j>0} = 0$  (or  $\Delta_j = \Delta_0$ ) we recover the form of the standard drivingless  $H_S$  given in [Equation \(6.2\)](#). For the sake of simplicity, here we will focus in cases with  $n_d = 0$ , i.e., aiming at realizing multiphoton Jaynes-Cummings models. However, we stress that the procedure explained in the following can be applied in a straightforward manner when  $n_d > 0$ .

For our purposes, we can now assume that  $H_{S,d} \equiv H_S$  in [Equations \(6.1\)](#) and [\(6.2\)](#), then apply the RC mapping, as described in [Section 6.1](#), leading to the following Hamiltonian for the augmented system:

$$H_{S+RC} = \frac{\Delta_0}{2}\sigma_x + \Omega a^\dagger a + \lambda\sigma_x(a + a^\dagger) + \sum_{j=0}^{n_d} \frac{\epsilon_j}{2} [\cos(\Delta_j - \Delta_0)t \sigma_z + \sin(\Delta_j - \Delta_0)t \sigma_y]. \quad (6.53)$$

Crucially, we have observed that, for certain cases, such mapping allows for an exact relation between the original and transformed parameters ([Nazir, 2018](#)). Indeed, considering an underdamped spin-boson spectral density in the initial spin-boson model [cf. [Example 6.1.1](#)],

$$J_{SB}(\omega) = \frac{\alpha\Gamma\omega_0^2\omega}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}, \quad (6.54)$$

one can show that the resulting spectral density for the residual environment interacting with the reaction coordinate reads as

$$J_{RC}(\omega) = \gamma\omega e^{-\omega/\Lambda}, \quad (6.55)$$

provided  $\Lambda/\omega \gg 1$ , and where the parameters are related according to  $\Omega = \omega_0, \gamma = \Gamma/(2\pi\omega_0)$ , and  $\lambda = \sqrt{\pi\alpha\omega_0/2}$ . Here, the frequency  $\omega_0$  in  $J_{SB}(\omega)$  denotes the position at which the spectral density features a maximum, while  $\Gamma$  and  $\alpha$  give account for its width and strength, respectively. For  $J_{RC}(\omega)$ , the coupling strength is given by  $\gamma$  instead. This coupling of the system with the environment allows to make use of the Born-Markov approximation, and obtain a master equation of the form [Equation \(6.51\)](#) for the enlarged system. Once obtained the reaction coordinate Hamiltonian, we undertake the transformation of  $H_{S+RC}$ , and thus, of the [Equation \(6.51\)](#), to achieve a model that comprises spin-multiphoton interaction terms.

For that purpose, we will introduce two auxiliary Hamiltonians  $H_a$  and  $H_b$  which will arise in the intermediate steps by moving into suitable interaction picture and transforming them accordingly.

The first step consists indeed in moving to a rotating frame in which  $H_{\text{S+RC}} \equiv H_{a,1}^I$  where  $H_a = H_{a,0} + H_{a,1}$ , with  $H_{a,0} = -(\Delta_0/2)\sigma_x$ . In this manner, we find

$$H_a = \Omega a^\dagger a + \lambda \sigma_x (a + a^\dagger) + \sum_{j=0}^{n_d} \frac{\epsilon_j}{2} [\cos(\Delta_j t) \sigma_z + \sin(\Delta_j t) \sigma_y],$$

while [Equation \(6.51\)](#) transforms into

$$\dot{\rho}_a(t) = -i [H_a, \rho_a(t)] - [x, [\hat{\chi}, \rho_a(t)]] + [x, \{\hat{\Xi}, \rho_a(t)\}], \quad (6.56)$$

where  $\hat{\chi} = U_{a,0}\chi U_{a,0}^\dagger$  and  $\hat{\Xi} = U_{a,0}\Xi U_{a,0}^\dagger$ , such that  $U_x = \mathcal{T}e^{-i \int_0^t ds H_x(s)}$  is the time-evolution operator of a generic Hamiltonian  $H_x$ .

Then, we perform a further transformation using the unitary operator  $T(\alpha)$ , defined as

$$T(\alpha) \equiv \frac{1}{\sqrt{2}} [D^\dagger(\alpha) (|e\rangle\langle e| - |g\rangle\langle g|) + D(\alpha) (|g\rangle\langle g| + |e\rangle\langle e|)] \quad (6.57)$$

with  $D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$  the standard displacement operator ([Cahill, 1969; Scully, 1997](#)). The following properties are satisfied

$$T^\dagger(\alpha) a^\dagger a T(\alpha) = a^\dagger a + |\alpha|^2 - \sigma_z(a\alpha^* + a^\dagger\alpha), \quad (6.58)$$

$$T^\dagger(\alpha) \sigma_y T(\alpha) = -i D(2\alpha) \sigma^+ + \text{H.c.}, \quad (6.59)$$

$$T^\dagger(\alpha) \sigma_z T(\alpha) = D(2\alpha) \sigma^+ + \text{H.c.}, \quad (6.60)$$

$$T^\dagger(\alpha) \sigma_x (a + a^\dagger) T(\alpha) = -\sigma_z(a + a^\dagger) + 2\text{Re}[\alpha]. \quad (6.61)$$

The latter can be used to explicitly determine the form of the the  $H_b = T^\dagger H_a T$ ; a direct computation yields

$$H_b = \Omega a^\dagger a - \Omega \sigma_z(a\alpha + a^\dagger\alpha^*) - \lambda \sigma_z(a + a^\dagger) + \sum_{j=0}^{n_d} \frac{\epsilon_j}{2} [\sigma^+ D(2\alpha) e^{-i\Delta_j t} + \text{H.c.}], \quad (6.62)$$

where we have neglected a constant energy shift. Therefore, by selecting  $\alpha = -\lambda/\Omega$  we obtain a simple Hamiltonian to pursue multiphoton interactions, namely

$$H_b = \Omega a^\dagger a + \sum_j \frac{\epsilon_j}{2} \left[ \sigma^+ e^{2\lambda/\Omega(a-a^\dagger)} e^{-i\Delta_j t} + \text{H.c.} \right]. \quad (6.63)$$

As a result, upon this unitary transformation, [Equation \(6.56\)](#) becomes

$$\dot{\rho}_b = -i [H_b, \rho_b] - [T^\dagger x T, [T^\dagger \hat{\chi} T, \rho_b(t)]] + [T^\dagger x T, \{T^\dagger \hat{\Xi} T, \rho_b(t)\}], \quad (6.64)$$

with  $\rho_b = T^\dagger \rho_a T$ . The dissipator acting on  $\rho_b$  has the same form as in [Equation \(6.56\)](#) but with transformed operators, namely  $T^\dagger xT$ ,  $T^\dagger \hat{\chi}T$  and  $T^\dagger \tilde{\Xi}T$ , where  $T \equiv T(-\lambda/\Omega)$ .

Moving now to an interaction picture with respect to the Hamiltonian  $H_{b,0} = (\Omega - \tilde{\nu})a^\dagger a - \tilde{\omega}\sigma_z/2$ , we obtain

$$H_{b,1}^I = \tilde{\nu}a^\dagger a + \frac{\tilde{\omega}}{2}\sigma_z + \sum_j \frac{\epsilon_j}{2} \left[ \sigma^+ e^{-i(\Delta_j + \tilde{\omega})t} e^{2\lambda/\Omega(a(t) - a^\dagger(t))} + \text{H.c.} \right], \quad (6.65)$$

with  $a(t) = ae^{-i(\Omega - \tilde{\nu})t}$ . We can then expand the exponential in [Equation \(6.63\)](#), provided that  $|2\lambda/\Omega| \sqrt{\langle (a + a^\dagger)^2 \rangle} \ll 1$ . The latter condition, known as Lamb-Dicke regime, allows us to truncate the exponential to a finite number of terms, arriving to a Hamiltonian containing multiphoton interaction terms. In addition, we consider the driving frequencies to be  $\Delta_j = \pm n_j(\tilde{\nu} - \Omega) - \tilde{\omega}$  with  $|\Omega - \tilde{\nu}| \gg \epsilon_j/2$  so that one can safely perform a rotating-wave approximation keeping only those terms that are resonant, i.e., time independent.

In this manner, we can approximate  $H_{b,1}^I \approx H_n$ , where  $H_n$  contains the aimed multiphoton interactions, i.e.,

$$H_n = \frac{\tilde{\omega}}{2}\sigma_z + \tilde{\nu}a^\dagger a + \sum_{j \in r} \frac{\epsilon_j(2\lambda)^{n_j}}{2\Omega^{n_j} n_j!} [\sigma^+ a^{n_j} + \text{H.c.}] + \sum_{j \in b} \frac{\epsilon_j(2\lambda)^{n_j}}{2\Omega^{n_j} n_j!} [\sigma^+ (-a^\dagger)^{n_j} + \text{H.c.}]. \quad (6.66)$$

Note that the sets  $r$  and  $b$  encompass the terms with amplitude  $\epsilon_j$  driving red- and blue-sidebands, that is, those terms in Eq. (6.52) with frequency  $\Delta_{j \in r} = +n_j(\tilde{\nu} - \Omega) - \tilde{\omega}$  and  $\Delta_{j \in b} = -n_j(\tilde{\nu} - \Omega) - \tilde{\omega}$ . Each of these drivings will contribute with a multiphoton interaction, either  $\sigma^+ a^{n_j} + \text{H.c.}$  for  $j \in r$  or  $\sigma^- a^{n_j} + \text{H.c.}$  for  $j \in b$ , which produce transitions between the states  $|m\rangle |g\rangle \leftrightarrow |m \mp n_j\rangle |e\rangle$ . Furthermore, it is worth mentioning that the largest error committed in the approximation that leads to [Equation \(6.66\)](#) stems from the zeroth order in the expansion of the exponential. These contributions are of the form  $\epsilon_j(\sigma^+ e^{i n_j(\Omega - \tilde{\nu})t} + \text{H.c.})/2$ , which will produce a significant effect after a time interval  $t \approx n_j(\Omega - \tilde{\nu})/\epsilon_j^2$ .

In order to show how the dissipative part transforms, we introduce the time-dependent unitary operator

$$\Phi = U_{b,0}^\dagger T^\dagger U_{a,0}. \quad (6.67)$$

Then, one can see that, by defining  $\tilde{\chi} = \Phi \chi \Phi^\dagger$ ,  $\tilde{\Xi} = \Phi \Xi \Phi^\dagger$  and  $\tilde{x} = \Phi(a + a^\dagger)\Phi^\dagger$ , the resulting master equation for  $\rho_n(t)$  is

$$\dot{\rho}_n(t) = -i[H_n, \rho_n(t)] - [\tilde{x}, [\tilde{\chi}, \rho_n(t)]] + [\tilde{x}, \{\tilde{\Xi}, \rho_n(t)\}], \quad (6.68)$$

where the state  $\rho_n(t)$  of the multiphoton model is related to the original spin-boson upon the reaction coordinate mapping,  $\rho_{S+RC}(t)$ , through a unitary transformation

$$\rho_n(t) \approx \Phi \rho_{S+RC}(t) \Phi^\dagger. \quad (6.69)$$

From the previous expression it follows that the purity of the total state  $\rho_{S+RC}$  and that of  $\rho_n$  are approximately equal. Moreover, the reduced spin state in the different frameworks are related according to  $\text{tr}_B[\rho_{SB}(t)] = \text{tr}_{RC}[\rho_{S+RC}(t)] \approx \text{tr}_{RC}[\Phi^\dagger \rho_n(t) \Phi]$ , where  $\text{tr}_B[\cdot]$  and  $\text{tr}_{RC}[\cdot]$  denote the trace over the environment degrees of freedom, and reaction coordinate, respectively. In this manner, having access to the spin degree of freedom one can have access to the dissipative spin dynamics dictated by the master equation (6.68) under a multiphoton Hamiltonian  $H_n$ , given in Equation (6.66), whose parameters can be tuned. In addition, we remark that the initial state at  $t_0 = 0$  in the multiphoton frame is related to that of the spin-boson model as  $\rho_n(0) = T^\dagger \rho_{S+RC}(0) T$ .

At this stage, a few comments regarding the validity of Equation (6.69) are in order. While the steps performed from  $H_{S+RC}$  to  $H_b$  are exact,  $H_n$  is attained in an approximate manner. The good functioning of the simulation depends on how these approximations are met. That is, Equation (6.69) holds within the Lamb-Dicke regime  $|2\lambda/\Omega| \sqrt{\langle (a + a^\dagger)^2 \rangle} \ll 1$  and for parameters satisfying  $|\Omega - \tilde{\nu}| \gg \epsilon_j/2 \forall j$ , so that one can perform a rotating-wave approximation. Note that, as the parameters  $\lambda$  and  $\Omega$  are directly related to the original spin-boson spectral density, these conditions set constraints onto the accessible parameters, as well as on the temperature of the environment. Furthermore, in order to observe coherent multiphoton dynamics the noise rates in Equation (6.68) must be small compared to parameters involved in  $H_n$ . For the considered shape of  $J_{SB}(\omega)$  this translates into  $\Gamma \ll \tilde{\nu}, \tilde{g}_n$  where  $\tilde{g}_n = \epsilon_0(2\lambda)^n / (2\Omega^n n!)$  for a  $n_d = 0$  and  $\Delta_0 = \pm n(\tilde{\nu} - \Omega) - \tilde{\omega}$  [cf. Equation (6.66)].

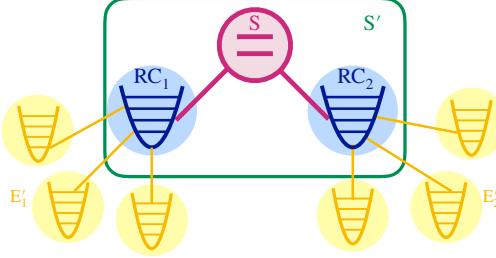
### 6.2.2 Structured environments

The simulation of multiphoton spin-boson interactions is not restricted to a specific form of  $J_{SB}(\omega)$ . Here we show the derivation of the procedure to obtain an effective multiphoton Hamiltonian when the initial spin-boson model features a more complicated interaction with the environment. For simplicity, we consider that  $J_{SB}(\omega)$  can be split in two parts,  $J_{SB}(\omega) = J_{SB,1}(\omega) + J_{SB,2}(\omega)$ , although its generalisation to more parts is straightforward. The first contribution,  $J_{SB,1}(\omega)$ , is considered here to be suitable for the realisation of multiphoton interactions as described in 6.2.1. In addition, we will work under the assumption that the environment degrees of freedom corresponding to  $J_{SB,2}(\omega)$  can be treated and simplified using again a collective or reaction coordinate, as sketched in Figure 6.2.

As discussed previously, we identify a collective coordinate for each of the contributions to the spectral density  $J_{SB}(\omega)$ . In this manner, we augment the system to include both reaction coordinates, denoted here by  $S' = S + RC_1 + RC_2$ . Hence, its Hamiltonian is given by

$$H_{S'} = H_{S,d} + \Omega_1 a_1^\dagger a_1 + \lambda_1 \sigma_x(a_1 + a_1^\dagger) + \Omega_2 a_2^\dagger a_2 + \lambda_2 \sigma_x(a_2 + a_2^\dagger), \quad (6.70)$$

where  $H_{S,d}$  is the original spin Hamiltonian which may contain spin rotations, introduced in Equation (6.52), while the subscripts denote the corresponding reaction coordinate. The parameters  $\lambda_i$  and  $\Omega_i$  are determined by the spectral density  $J_{SB,i}(\omega)$ . The dynamics of the



**Figure 6.2:** We show the implementation of the reaction coordinate mapping for structured environments. If the SD is expressed as  $J_{SB}(\omega) = J_{SB,1}(\omega) + J_{SB,2}(\omega)$ , we can introduce two reaction coordinates in parallel. See main text for further details.

augmented system  $S'$  is governed by the following master equation:

$$\begin{aligned}\dot{\rho}_{S'}(t) = & -i [H_{S'}, \rho_{S'}(t)] - [x_1, [\chi_1, \rho_{S'}(t)]] - [x_2, [\chi_2, \rho_{S'}(t)]] \\ & + [x_1, \{\Xi_1, \rho_{S'}(t)\}] + [x_2, \{\Xi_2, \rho_{S'}(t)\}],\end{aligned}\quad (6.71)$$

where  $x_i = a_i + a_i^\dagger$  for  $i = 1, 2$ , and  $\chi_i$  and  $\Xi_i$  are defined in analogy to Equations (6.49) and (6.50).

In order to find a suitable transformation to realise multiphoton interaction terms from  $H_{S'}$  we proceed in a similar manner as for a single reaction coordinate. That is, we first move to a rotating frame where  $H_{S'} \equiv H_{a,1}^I$ , with  $H_a = H_{a,0} + H_{a,1}$  and  $H_{a,0} = -\Delta_0/2\sigma_x$ . Therefore, the transformed Hamiltonian reads as

$$H_a = \sum_{k=1,2} \Omega_k a_k^\dagger a_k + \lambda_k \sigma_x (a_k + a_k^\dagger) + \sum_j \frac{\epsilon_j}{2} [\cos \Delta_j t \sigma_z + \sin \Delta_j t \sigma_y]. \quad (6.72)$$

The next step is to perform the transformation using the unitary operator  $T(\alpha)$ , defined in Equation (6.57)<sup>2</sup>. As aforementioned, we consider that the first reaction coordinate is suitable for the quantum simulation of multiphoton interaction terms, due to the form of its spectral density. This argument enables to choose  $\alpha \equiv -\lambda_1/\Omega_1$ , hence  $H_b \equiv T^\dagger(-\lambda_1/\Omega_1) H_a T(-\lambda_1/\Omega_1)$ . This transformation acts trivially on the second reaction coordinate, but it does affect the coupling between the latter and the spin. Finally, if we move to an interaction picture with respect to  $H_{b,0} = (\Omega_1 - \tilde{\nu}_1) a_1^\dagger a_1 - \tilde{\omega} \sigma_z / 2$ , we obtain the Hamiltonian  $H_{n,2} \approx H_{b,1}^I \equiv U_{b,0}^\dagger H_{b,1} U_{b,0}$ ,

$$\begin{aligned}H_{n,2} = & \frac{\tilde{\omega}}{2} \sigma_z + \tilde{\nu} a_1^\dagger a_1 + \Omega_2 a_2^\dagger a_2 - \lambda_2 \sigma_z (a_2 + a_2^\dagger) \\ & + \sum_{j \in r} \frac{\epsilon_j}{2n_j!} \left( \frac{2\lambda_1}{\Omega_1} \right)^{n_j} [\sigma^+ a_1^{n_j} + \text{H.c.}] + \sum_{j \in b} \frac{\epsilon_j}{2n_j!} \left( \frac{2\lambda_1}{\Omega_1} \right)^{n_j} [\sigma^+ (-a_1^\dagger)^{n_j} + \text{H.c.}],\end{aligned}\quad (6.73)$$

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<sup>2</sup>In this case, we need one more property of the operator  $T$ , namely  $T^\dagger(\alpha) \sigma_x T(\alpha) = -\sigma_z$ .

where we have considered  $\Delta_j = \pm n_j(\tilde{\nu} - \Omega_1) - \tilde{\omega}$ , and assumed the Lamb-Dicke regime  $|\lambda_1/\Omega_1| \sqrt{\langle (a_1 + a_1^\dagger)^2 \rangle} \ll 1$ , and  $|\Omega_1 - \tilde{\nu}| \gg \epsilon_j/2$  to perform a rotating-wave approximation. Note that, while the multiphoton terms are identical to those of  $H_n$  in [Equation \(6.66\)](#), the second reaction coordinate interacts with the spin degree of freedom. Indeed, depending on the parameters of  $H_{n,2}$ , the effect of such interaction may effectively turn into non-Markovian effects for the reduced state of the spin and first reaction coordinate,  $\rho_n = \text{Tr}_2[\rho_{n,2}]$ . The final master equation governing the dynamics of  $\rho_{n,2}$  is

$$\begin{aligned}\dot{\rho}_{n,2}(t) = & -i[H_{n,2}, \rho_{n,2}(t)] - [\tilde{x}_1, [\tilde{\chi}_1, \rho_{n,2}(t)]] - [\tilde{x}_2, [\tilde{\chi}_2, \rho_{n,2}(t)]] \\ & + \left[ \tilde{x}_1, \left\{ \tilde{\Xi}_1, \rho_{n,2}(t) \right\} \right] + \left[ \tilde{x}_2, \left\{ \tilde{\Xi}_2, \rho_{n,2}(t) \right\} \right],\end{aligned}\quad (6.74)$$

where the operators involved are defined as in the case involving a single reaction coordinate [cf. [Equation \(6.68\)](#)]. It is worth stressing that the relation between the states given in [Equation \(6.69\)](#) still holds. From the previous derivation one can conclude that the extension to more collective coordinates is straightforward.

### 6.2.3 Examples and numerical simulations

In this Section, we will provide examples of the previously explained general theoretical framework to investigate the performance of the quantum simulation of different multiphoton Hamiltonians  $H_n$ , as well as to discuss the limitation in the parameter regime for their realisation. First, we will consider the case in which the original spin-boson model interacts just with a discrete number of modes, which can be viewed as a limit of vanishing spectral broadening  $\Gamma \rightarrow 0$ . This scenario will allow us to examine the validity of the required approximations without the effect of dissipation. Then, we will consider  $\Gamma \neq 0$ , where the reaction-coordinate mapping appears as a key step to realise a desired multiphoton Jaynes-Cummings model.

In all the cases, we will assess the performance of the realisation of the targeted multiphoton Jaynes-Cummings models by means of the fidelity  $F(t)$  between two states, defined as

$$F(t) = \left[ \text{Tr} \sqrt{\sqrt{\rho_1(t)} \rho_2(t) \sqrt{\rho_1(t)}} \right]^2. \quad (6.75)$$

In particular, we will analyse to what extent is the relation given in [Equation \(6.69\)](#) satisfied. In other words, we will compare the aimed state of a multiphoton Jaynes-Cummings model  $\rho_n(t)$  with the one retrieved using the analogue simulator,  $\Phi \rho_{S+RC}(t) \Phi^\dagger$ . We remark that when two reaction coordinates are included, the state  $\rho_n(t)$  obeys the master equation given in [Equation \(6.74\)](#), whose Hamiltonian is  $H_{n,2}$ , [Equation \(6.73\)](#), while  $\rho_{S+RC}(t)$  must be replaced by  $\rho_{S'}$ , as explained in [Section 6.2.2](#).

In addition, we will show that the theoretical framework allows us to realise non-Markovian multiphoton Jaynes-Cummings models. As discussed in [Section 4.1.2](#), non-Markovian effects

can be witnessed through the trace distance, defined as

$$D(\rho_x, \rho_y) = \frac{1}{2} \text{Tr} \|\rho_x - \rho_y\|_1, \quad (6.76)$$

for a given pair of states  $\rho_x, \rho_y$ . For our purposes, we do not need to provide a measure, therefore we will consider that the non-Markovian character of the dynamics emerges when the time derivative of the trace distance is positive, i.e.,  $\sigma(t, \rho_{x,y}(0)) > 0$  for a certain pair of states. Specifically, we calculate  $\sigma(t, \rho_{x,y}(0))$  using two initial states  $\rho_{x,y}$  in the multiphoton Jaynes-Cummings model, and corroborate that  $\sigma(t, \rho_{x,y}(0))$  is obtained to a very good approximation when the states  $\rho_{x,y}$  are replaced by their simulated ones using the spin-boson model, namely  $\rho_x(t) \rightarrow \Phi \rho_{x,S+RC} \Phi^\dagger$  and  $\rho_y(t) \rightarrow \Phi \rho_{y,S+RC} \Phi^\dagger$ . In this manner, we offer a proof-of-principle that non-Markovian multiphoton models can be realised.

### Dissipationless multiphoton Jaynes-Cummings models

We start considering the simplest case, namely, when the spin-boson model simply involves the interaction with a discrete number of modes. This corresponds to either consider  $\Gamma \rightarrow 0$  in the underdamped spectral density  $J_{SB}(\omega)$ , or equivalently, assuming that dissipation effects are sufficiently small so that they can be discarded. Note that for a single bosonic mode with  $\Gamma = 0$ , the spin-boson model adopts the form of a generalized quantum Rabi model, which is indeed  $H_{S+RC}$  as given in [Equation \(6.53\)](#). Recall that in this particular case  $H_{SB} \equiv H_{S+RC}$  as there are no further modes in the system. In particular, we set  $n_d = 0$  in [Equation \(6.52\)](#) as we aim to realize a single multiphoton Jaynes-Cummings interaction. The Hamiltonian for a nJCM can be written in general as

$$H_{nJCM} = \frac{\tilde{\omega}}{2} \sigma_z + \tilde{\nu} a^\dagger a + \tilde{g}_n (\sigma^+ a^n + \sigma^- (a^\dagger)^n). \quad (6.77)$$

At resonant condition,  $\tilde{\omega} = n\tilde{\nu}$ , the coupling constant  $\tilde{g}_n$  fixes the time required to transfer population from the state  $|e\rangle|0\rangle$  to  $|g\rangle|n\rangle$ , denoted as  $\tau_n = \pi/(2\tilde{g}_n\sqrt{n!})$ . Both are related to the spin-boson parameters as [cf. [Equation \(6.66\)](#)]

$$\tilde{g}_n = \frac{\epsilon_0}{2 n!} \left( \frac{2\lambda}{\Omega} \right)^n, \quad (6.78)$$

$$\tau_n = \frac{\sqrt{n!}}{\epsilon_0} \left( \frac{\Omega}{2\lambda} \right)^n. \quad (6.79)$$

Clearly, as  $2\lambda/\Omega$  must be small to lie within the Lamb-Dicke regime, the coupling  $\tilde{g}_n$  decreases considerably for increasing  $n$ , requiring longer evolution times under the spin-boson Hamiltonian to observe a significant effect, that is, an evolution time of the order of  $\tau_n$ . Furthermore, if we recall what we have commented about [Equation \(6.66\)](#), we can obtain a rough estimate of a correct simulation of the desired Jaynes-Cummings model, i.e.,  $t = k\tau_n$ , where  $k \approx (2\lambda/\Omega)^n n(\Omega - \tilde{\nu})/(\epsilon_0\sqrt{n!})$ .

In Figure 6.3, we show the results for the realization of 2JCM and 3JCM models using a spin-boson model interacting with a single bosonic mode. In order to observe the paradigmatic Rabi oscillations between the states  $|e\rangle|0\rangle$  and  $|g\rangle|n\rangle$ , we choose  $\rho_{S+RC}(0) = |-\rangle\langle -| \otimes \rho_{RC}^{\text{th}}$  as an initial state for the spin-boson model, where  $\rho_{RC}^{\text{th}}$  is a thermal state at temperature  $\beta^{-1}$  for the reaction coordinate mode, containing  $n^{\text{th}} = (e^{\beta\Omega} - 1)^{-1}$  bosons. Recall that, as we consider here a single spectral density with  $\Gamma = 0$ , the reaction coordinate mode is simply the only mode which interacts with the spin degree of freedom. In this manner, the initial state for the simulated multiphoton models reads as  $\rho_{nJCM}(0) = T^\dagger \rho_{S+RC}(0) T$ , which approximately amounts to  $\rho_{nJCM}(0) \approx |e\rangle\langle e| \otimes |0\rangle\langle 0|$  for sufficiently low temperature and small  $2\lambda/\Omega$ . The chosen parameters for the simulation of the 2JCM, plotted in Figures 6.3a and 6.3b are  $\pi\alpha = \epsilon_0 = 0.02\omega_0$ , recalling that  $\Omega = \omega_0$  it results in  $2\lambda/\Omega = 0.2$ . Choosing  $\tilde{\nu} = 10^{-3}\Omega$  and  $\tilde{\omega} = 2\tilde{\nu}$ , the coupling in 2JCM amounts to  $\tilde{g}_2 = 0.2\tilde{\nu}$ . The initial reaction-coordinate thermal state,  $\rho_{RC}^{\text{th}}$ , contains  $n^{\text{th}} = 10^{-3}$  bosons. In Figure 6.3b we show how the quantum simulation of the 2JCM model deteriorates for increasing number of bosons, as a large  $n^{\text{th}}$  will eventually break down the Lamb-Dicke regime.

For the 3JCM we choose again  $\pi\alpha = 0.02\omega_0$ , which leads in  $2\lambda/\Omega = 0.2$ . Then, we select the aimed coupling strength of the multiphoton interaction to be  $\tilde{g}_3 = 0.1\tilde{\nu}$  with  $\tilde{\omega} = 3\tilde{\nu}$ , while we vary  $\epsilon_0/\omega_0$ . The temperature is set to  $\beta\Omega \approx 100$  so that  $\rho_{RC}^{\text{th}} \approx |0\rangle\langle 0|$ . As in the previous case, the dynamics are well retrieved, see Figure 6.3c, where we have set  $\epsilon_0/\omega_0 = 2 \cdot 10^{-3}$ . Note however that, as a consequence of the rotating-wave approximation performed to achieve a resonant third order, and due to the longer times required to simulate a 3JCM compared to the 2JCM, the condition  $|\Omega - \tilde{\nu}| \gg \epsilon_0$  must be better satisfied. Indeed, for  $\epsilon_0/\omega_0 = 10^{-2}$  we already see a clear departure from the targeted dynamics, as indicated by a large infidelity  $1 - F(t) \gtrsim 10^{-1}$ , shown in Figure 6.3d.

In the following, we consider a spin interacting with two bosonic modes, again with  $\Gamma_{1,2} = 0$ . As explained in Section 6.2.2, we perform the map onto the first bosonic mode to attain a multiphoton interaction. Upon suitable transformations and approximations, the spin-boson model will take the form of a multiphoton Jaynes-Cummings model  $H_{nJCM,2}$ , where the subscript 2 indicates the presence of a second reaction coordinate in the system. The Hamiltonian  $H_{nJCM,2}$  reads as

$$H_{nJCM,2} = \frac{\tilde{\omega}}{2}\sigma_z + \tilde{\nu}a_1^\dagger a_1 + \Omega_2 a_2^\dagger a_2 + \tilde{g}_n \left( \sigma^+ a_1^n + \sigma^- (a_1^\dagger)^n \right) - \lambda_2 \sigma_z (a_2 + a_2^\dagger). \quad (6.80)$$

In this manner, the spin exchanges  $n$  quanta with the first bosonic mode as in  $H_{nJCM}$ , while the last term effectively shifts the spin frequency depending on the state of the second mode. The reduced state for the spin and first bosonic mode is given then by  $\rho_{nJCM}(t) = \text{Tr}_2[\rho_{nJCM,2}(t)]$ . Indeed, due to the interaction with the second bosonic mode, the multiphoton Jaynes-Cummings model may exhibit non-Markovian features. For that, we consider the spin-boson Hamiltonian  $H_{S'}$  given in Equation (6.70), which then approximately realizes  $H_{nJCM,2}$ . In particular, we select  $\Delta_0 = -2\Omega_1$ , so that the simulated model involves two-photon interaction terms, i.e., a 2JCM. The results are plotted in Figure 6.4, while the parameters are  $\pi\alpha_i = 0.02\Omega_i$  such that  $2\lambda_i/\Omega_i = 0.2$  for  $i = 1, 2$ ,  $\epsilon_0/\Omega_1 = 10^{-2}$ . The

coupling strength in  $H_{2\text{JCM},2}$  is given by  $\tilde{g}_2 = 0.2\tilde{\nu}$  with  $\tilde{\nu} = \Omega_2$ . As in the single-mode case, Rabi oscillations will be clearly visible selecting  $\rho_{S'}(0) = |-\rangle\langle-| \otimes \rho_{\text{RC}_1}^{\text{th}} \otimes \rho_{\text{RC}_2}^{\text{th}}$ . After its transformation, this state corresponds approximately to an initial spin state  $|e\rangle$  in the nJCM frame. In the same manner, in order to analyse the emergence non-Markovian behavior we consider the initial states  $|g\rangle\langle g|$  and  $|e\rangle\langle e|$  for the spin in  $H_{S'}$ . This implies initial spin states  $|\pm\rangle$  in the nJCM frame, which for pure dephasing noise it has been shown to be the pair of states maximizing  $\sigma(t)$  (Breuer, 2009).

The results plotted in Figure 6.4 have been gathered considering a sufficiently low temperature such that  $\rho_{\text{RC}_{1,2}}^{\text{th}} \approx |0\rangle\langle 0|$ . We then compute the trace distance  $D(\rho_1, \rho_2)$  using the states upon tracing out the second mode,  $\rho_{2\text{JCM}}(t) = \text{Tr}_2[\rho_{2\text{JCM},2}]$ . As shown in Figure 6.4b, the time-derivative of the trace distance,  $\sigma(t)$ , becomes positive during certain intervals — a clear indication of the non-Markovian behaviour of the simulated multiphoton Jaynes-Cummings model. In addition, we also calculate the non-trivial evolution of the purity for the states  $\rho_{S+\text{RC}_1}(t)$  and  $\rho_S(t) = \text{Tr}_{\text{RC}_1}[\rho_{S+\text{RC}_1}(t)]$ , which is shown in Figure 6.4c. According to our theoretical framework, their purity is approximately equal to that of  $\rho_{2\text{JCM}}(t)$  and the reduced spin state upon tracing both bosonic degree of freedom in the 2JCM,  $\text{Tr}[\rho_{2\text{JCM}}(t)]$ , respectively. Finally, the infidelity  $1 - F(t)$  between the targeted state  $\rho_{2\text{JCM},2}(t)$  and its reconstructed one  $\Phi\rho_{S+\text{RC}_1+\text{RC}_2}(t)\Phi^\dagger$  in Figure 6.4d.

## Dissipative multiphoton Jaynes-Cummings models

We now consider a more realistic scenario in which the spin-boson model interacts with an environment whose spectral density has an underdamped shape, i.e.  $J_{\text{SB}}(\omega)$  has the form of Equation (6.45), with  $\Gamma \neq 0$ . In this manner, we extend the theoretical framework beyond the standard local master equation description (Puebla, 2019). As explained in Section 6.2.1, this situation can be mapped using a reaction coordinate, which now in turn interacts with a Markovian residual environment. The evolution of the state of the augmented system, spin and reaction coordinate, evolves according to the master equation given in Equation (6.51). Indeed, the effect of spectral broadening,  $\Gamma \neq 0$ , introduces dissipation into the simulated multiphoton Jaynes-Cummings model, whose state now obeys the master equation (6.68). We remark that the performance of the simulated dissipative model is not altered when the effect of dissipation is taken into account correctly. Nevertheless, whenever  $\Gamma \gg \tilde{\nu}$ , dissipation dominates the dynamics, and the paradigmatic Rabi oscillations will eventually fade away.

In Figure 6.5 we show the results of numerical simulations aimed to retrieve a 2JCM with different  $\Gamma/\tilde{\nu}$  values, and for different quantities. As for Figure 6.3, we used  $\pi\alpha = \epsilon_0 = 0.02\omega_0$ , so that  $2\lambda/\Omega = 0.2$ . We chose again  $\tilde{\nu} = 10^{-3}\Omega$  and  $\tilde{\omega} = 2\tilde{\nu}$ , and therefore the coupling in 2JCM amounts to  $\tilde{g}_2 = 0.2\tilde{\nu}$ , while the temperature is such that  $\rho_{\text{RC}}^{\text{th}}$  contains  $n^{\text{th}} = 10^{-3}$  bosons. The spin is initialised in the  $|-\rangle$  state, so that  $\rho_{S+\text{RC}}(0) = |-\rangle\langle-| \otimes \rho_{\text{RC}}^{\text{th}}$ . In particular, the value  $\Gamma/\tilde{\nu} = 2 \cdot 10^{-1}$  considered in Figure 6.5a already produces a significant departure from the Rabi oscillation between the states  $|e\rangle|0\rangle$  and  $|g\rangle|2\rangle$  in the dissipationless 2JCM [cf. Figure 6.3a for  $\Gamma = 0$ ]. Note that the results plotted in Figure 6.5a corresponds to a critically damped 2JCM since  $\Gamma = \tilde{g}_2$ . As plotted in Figure 6.5b, the effect of the dissipation

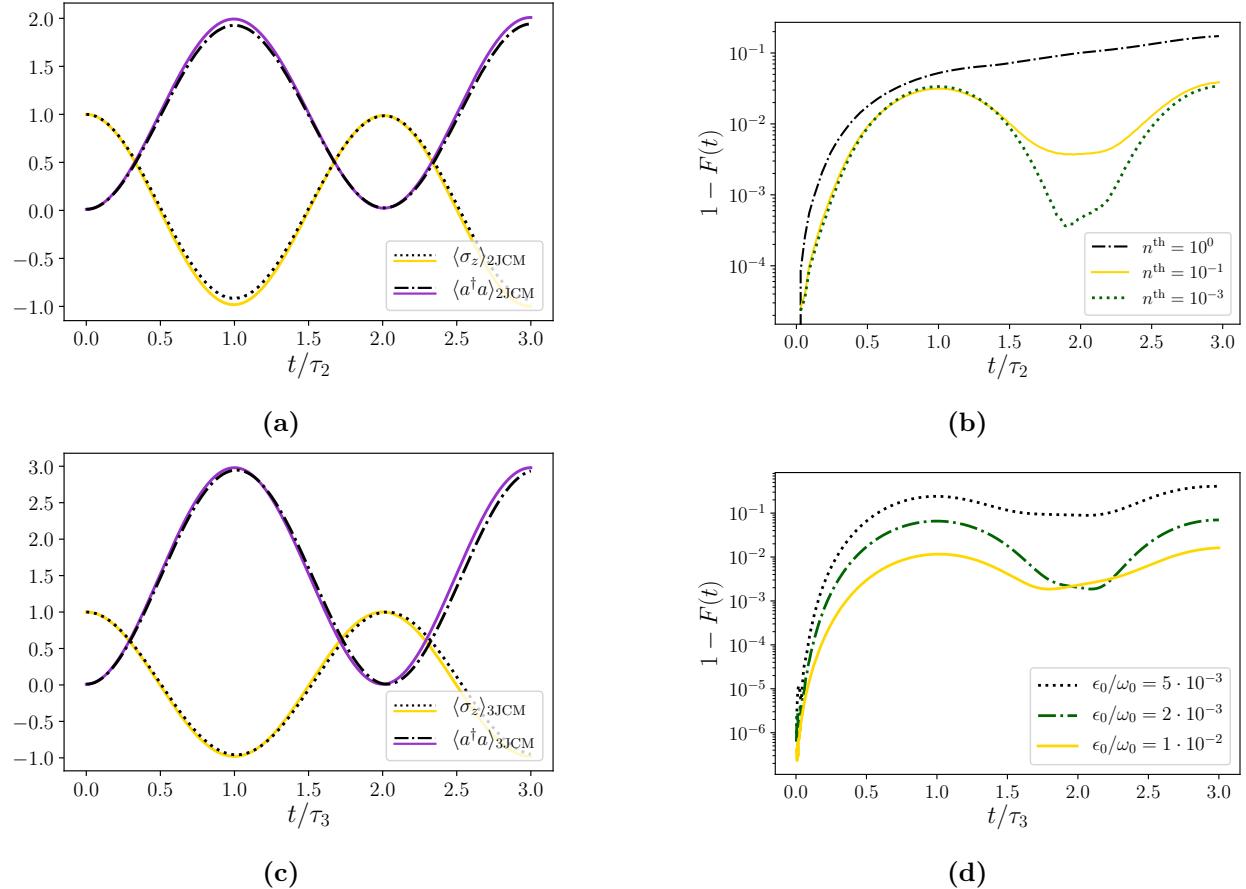
is clearly visible in the evolution of the purity for both the total state (spin plus bosonic mode) and the reduced spin state, namely,  $\text{Tr}[\rho_{S+RC}^2(t)]$  and  $\text{Tr}[\rho_S^2(t)]$ . As in previous cases, the purity of these states is directly related to those of the simulated model as a consequence of the relation  $\rho_{2JCM}(t) \approx \Phi \rho_{S+RC}(t) \Phi^\dagger$ . Furthermore, Rabi oscillations or population revivals appear in the evolution of von Neumann entropy<sup>3</sup>,  $S_{vN}(\rho) = -\rho \log_2 \rho$  for the reduced spin state. This is plotted in [Figure 6.5c](#) for different  $\Gamma/\tilde{\nu}$  values. Finally, we note that the performance of the quantum simulation is independent of the dissipation as demonstrated by the good fidelities attained in these cases [cf. [Figure 6.5d](#)], allowing for the simulation of different parameter regimes in a nJCM.

## 6.3 Conclusions

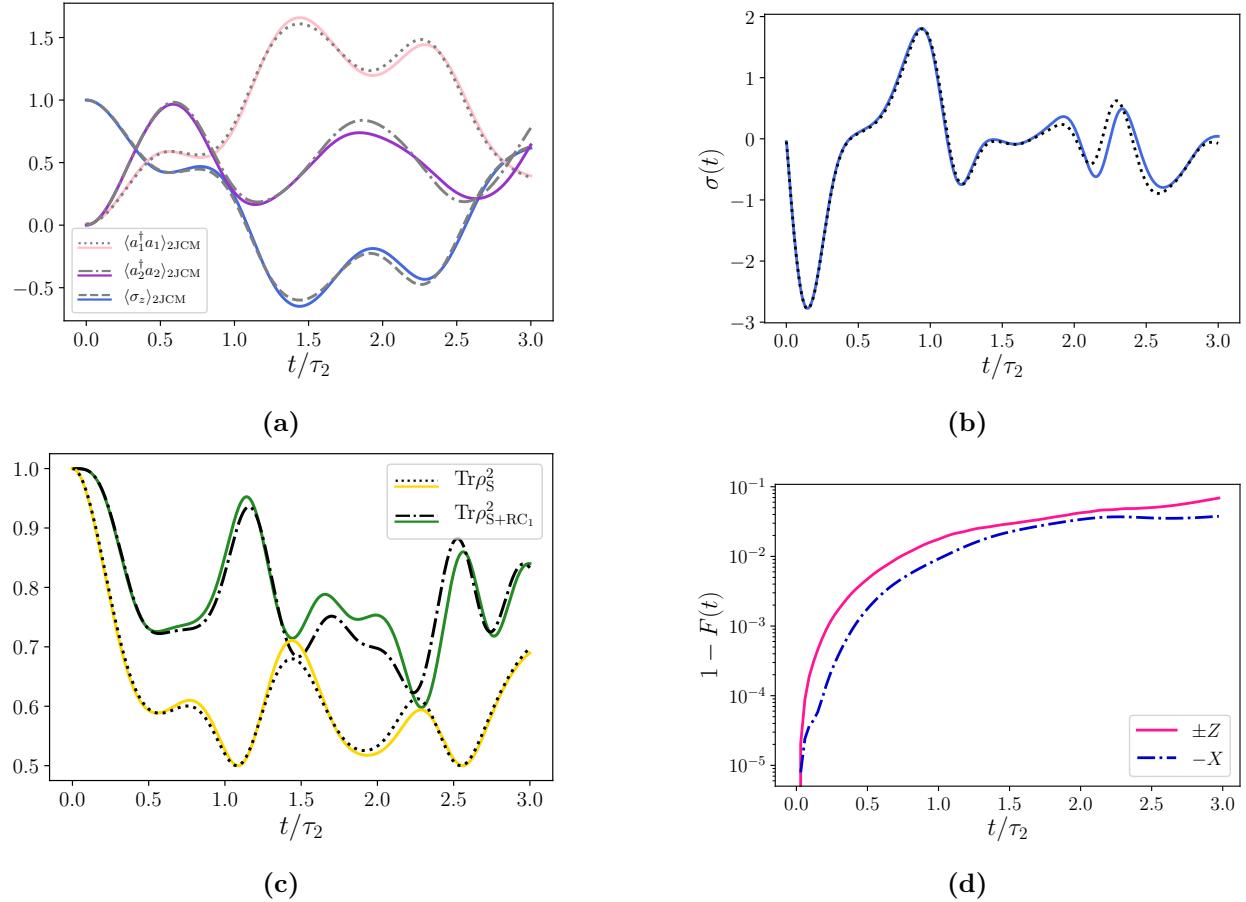
In this Chapter, we have shown that, under certain hypothesis, the coupling between the system and the environment can be analytically treated by means of the reaction coordinate mapping. For some spectral densities, this approach considerably reduces the complexity of simulating the dynamics of a spin-boson model. The resulting Hamiltonian has been used in [Section 6.2](#) to generate multiphoton interaction terms, while the dissipation effects must be transformed accordingly. We have thus obtained a theoretical scheme to realise multiphoton Jaynes-Cummings models using the paradigmatic spin-boson model as an analogue quantum simulator. We have performed numerical simulations starting from the spin plus reaction-coordinate Hamiltonians and aiming to realise different multiphoton Jaynes-Cummings. We first performed simulations considering one reaction coordinate without dissipation to better illustrate the performance of the required approximations to achieve two- and three-photon Jaynes-Cummings models. We have then shown that non-Markovian multiphoton Jaynes-Cummings can be indeed attained when a second reaction coordinate is included, as unveiled by the standard trace distance measure. Finally, we have provided numerical simulations investigating the interplay between spectral broadening, dissipation and the decoherence in the targeted multiphoton models.

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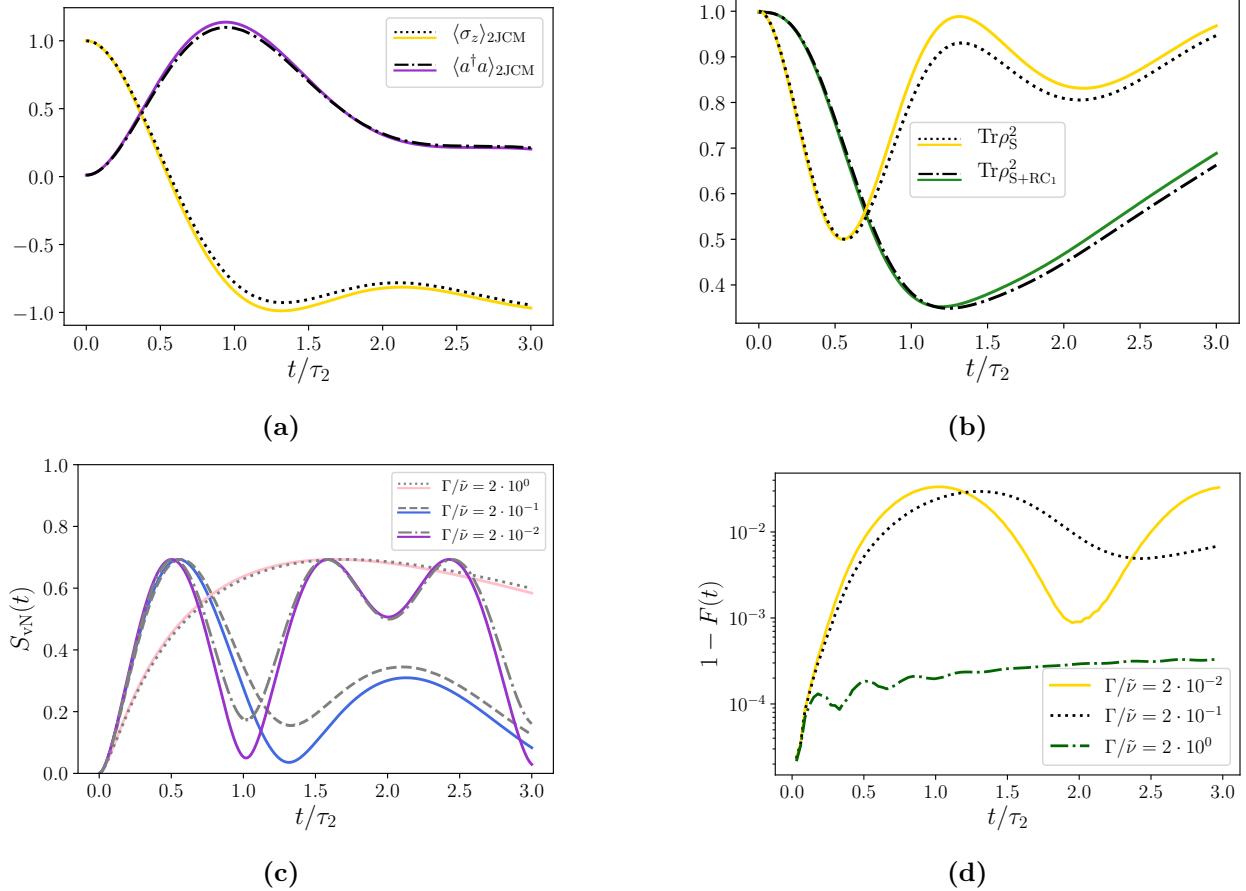
<sup>3</sup>Note that we in this Section we are defining the von Neumann entropy using the logarithm base 2.



**Figure 6.3:** Dynamics of the simulated multiphoton Jaynes-Cummings models,  $n = 2$  (top) and  $n = 3$  (bottom). In Panels (a) and (c) we show the targeted dynamics (solid lines) and the one obtained using the spin-boson Hamiltonian (either dotted or dashed lines) for  $\langle a^\dagger a \rangle$  and  $\langle \sigma_z \rangle$ , as indicated in the plots, and as a function of the time rescaled by  $\tau_n$  (Eq. (6.79)). In Panels (b) and (d) we plot the infidelity  $1 - F(t)$  between the ideal  $\rho_{n\text{JCM}}(t)$  state and its approximated one  $\Phi \rho_{\text{S+RC}}(t) \Phi^\dagger$  for different conditions, namely, in Panel (b) for different temperatures (or mean occupation number  $n^{\text{th}}$ ), and in Panel (d) for different values of  $\epsilon_0/\omega_0$ .



**Figure 6.4:** Non-Markovian dynamics for a 2JCM and its simulation using a spin-boson model  $H_{S'}$ . In **Panel (a)** we show the dynamics for the expectation values  $\langle a_i^\dagger a_i \rangle$  with  $i = 1, 2$  and  $\langle \sigma_z \rangle$  for the target 2JCM model (solid lines) and its reconstructed values using  $H_{S'}$  (discontinuous lines). The considered initial state reads as  $\rho_{S'}(0) = |-\rangle \langle -| \otimes \rho_{RC_1}^{\text{th}} \otimes \rho_{RC_2}^{\text{th}}$ , with  $\beta$  very large such that  $\rho^{\text{th}} \approx |\rangle \langle 0|$ . In **Panel (b)** we plot the time-derivative of the trace distance  $\sigma(t)$  after tracing out the second bosonic mode, and considering the initial states  $|e\rangle$  and  $|g\rangle$  for the spin in  $H_{S'}$ , while both reaction coordinates find themselves in their vacuum. Clearly,  $\sigma(t) > 0$  during certain intervals, revealing the non-Markovianity introduced due to the interaction with the second mode. **Panel (c)** shows the evolution of purity for the state upon tracing the second mode,  $\text{Tr}[\rho_{S+RC_1}^2(t)]$ , and for the reduced state of the spin,  $\text{Tr}[\rho_S^2(t)]$ , for the same case shown in **Panel (a)**. In **Panel (d)**, we compare the infidelity  $1 - F(t)$  between the ideal state and the simulated one using  $H_{S'}$  for the three different initial states employed here.



**Figure 6.5:** Dynamics of a dissipative 2JCM using a spin-boson model. In **Panel (a)** we show the dynamics of the expectation values of  $\langle a^\dagger a \rangle$  and  $\langle \sigma_z \rangle$ , as in [Figure 6.3](#), for the dissipative 2JCM (solid lines) and its simulation using the spin-boson model (points), for  $\Gamma/\tilde{\nu} = 2 \cdot 10^{-1}$  and  $\rho_{S+RC}(0) = |-\rangle \langle -| \otimes \rho_{RC}^{\text{th}}$  with  $n^{\text{th}} = 10^{-3}$ . For the same case, we also show in **Panel (b)** the evolution of the purities for the spin state  $\text{Tr}[\rho_S^2(t)]$  and for the total state  $\text{Tr}[\rho_{S+RC}^2(t)]$ . In **Panel (c)** we compare the different behavior as  $\Gamma/\tilde{\nu}$  varies for the von Neumann entropy of the reduced spin state,  $S_{\text{vN}}(\rho_S(t))$ . The values of  $\Gamma/\tilde{\nu}$  are indicated in the legend. Finally, the state infidelity  $1 - F(t)$  between the targeted  $\rho_{2\text{JCM}}$  and its approximate simulation,  $\Phi \rho_{S+RC}(t) \Phi^\dagger$ , is plotted in **Panel (d)** for different  $\Gamma/\tilde{\nu}$ . See main text for further details on the parameters employed for the simulation.

# Chapter 7

## Conclusions and outlook

In this Thesis we have studied issues pertaining to the simulation, characterisation, and control of the dynamics of open quantum systems. We have seen that recent theoretical and experimental progress has revealed new interesting physical scenarios that question the standard theoretical framework, which crucially hinges upon the mathematical notion of quantum dynamical semigroup and, physically, the Born-Markov approximation. We have introduced and discussed general tools to suitably explore those situations in which the system-environment interaction is responsible for strong coupling and non-Markovian effects. We have also discussed the main features and drawbacks of the traditional theory of irreversibility for open quantum systems. The latter, being formulated by means of the von-Neumann entropy, can be sometimes formally inconsistent or not particularly well suited to some interesting physical scenarios. We have shown that a re-formulation in terms of the Wigner – or, equivalently, Rényi-2 – entropy is indeed useful and insightful at the same time. For instance, it enables us to consistently explore the zero-temperature limit, and establish a closer connection with the theory of classical stochastic processes. The phase-space entropy production has been used to assess the impact of initial correlations shared by two non-interacting harmonic oscillators undergoing a non-Markovian dynamics. We have shown that, for such systems, the entropy production rate turns out to be a monotonic function of the initial degree of entanglement. It would be interesting, and indeed very important, to study how such conclusions are affected by the possible interaction between the constituents of our system, as well as non-Gaussian scenarios involving either non-quadratic Hamiltonians or spin-like systems (Santos, 2018). On a similar note, a systematic study concerning the role played by coherences in the entropy production rate would corroborate the splitting between classical and quantum contributions put forward in Ref. (Santos, 2019)

We have also seen that the system-environment interaction is sometimes modelled by a spectral density that enables to remap the initial configuration of the system into an equivalent setting. This can be achieved through the introduction of one or more effective modes, called reaction coordinates. In this Thesis, we have resorted to this approach to show that, starting from a non-trivial spin-boson model, one can obtain multiphoton interaction terms appearing in the

Hamiltonian of the celebrated Jaynes-Cummings model. We have numerically shown that a spin-boson model can – in a suitable range of parameters – serve as a simulator for two and three-photon models. This would be beneficial to experimental scenarios, where such multiphoton terms are typically hard to attain. On a general note, it would be interesting to ascertain how much progress can be made in the simulation, characterisation, and control of open quantum systems dynamics, possibly combining recent advances in the field [see, e.g., ([Tamascelli, 2018](#); [Mascherpa, 2020](#))] and numerical methods based on machine learning techniques, such those used, e.g., in Refs. ([Banchi, 2018](#); [Luchnikov, 2020](#)).

# Appendix A

## Correlation function for a bosonic thermal reservoir

In this Appendix, we explicitly derive the two-point correlation function when the environment interacting with an arbitrary system is made of infinitely many independent harmonic oscillators in a thermal state. Let us suppose, without loss of generality, that the interaction Hamiltonian between the system and the bosonic environment is in the form

$$H_I = X \otimes B, \quad (\text{A.1})$$

where  $X$  is an operator of the system, while  $B$  is an operator of the bath, given by

$$B = \sum_k \left( g_k b_k^\dagger + g_k^* b_k \right). \quad (\text{A.2})$$

Let us compute the correlations function defined as

$$\alpha_\beta(\tau) \equiv \langle B(\tau)B \rangle_E = \text{tr}_E (B(\tau)B\rho_E), \quad (\text{A.3})$$

where  $\rho_E$  is a canonical Gibbs state, i.e.,

$$\rho_E = \frac{e^{-\beta H_E}}{\mathcal{Z}_E}, \quad (\text{A.4})$$

with  $\mathcal{Z}_E = \text{tr}_E e^{-\beta H_E}$  the reservoir partition function. It is easy to see that, since the Hamitonian of the environment reads as

$$H_E = \sum_k \omega_k b_k^\dagger b_k, \quad (\text{A.5})$$

one can write down the following expression:

$$e^{-\beta H_E} = \exp \left( -\beta \sum_k \omega_k b_k^\dagger b_k \right) = \prod_k e^{-\beta \omega_k b_k^\dagger b_k}. \quad (\text{A.6})$$

Similarly, one has

$$\mathcal{Z}_E = \prod_{k=0}^{\infty} \mathcal{Z}_k. \quad (\text{A.7})$$

To sum up, the environmental state (A.4) can be rewritten as

$$\rho_E = \prod_{k=0}^{\infty} \frac{e^{-\beta\omega_k b_k^\dagger b_k}}{\mathcal{Z}_k} \equiv \prod_{k=0}^{\infty} \rho_k, \quad (\text{A.8})$$

where  $\mathcal{Z}_k$  and  $\rho_k$  are the partition function and the statistical operator associated with the  $k$ -th harmonic oscillator in thermal state at inverse temperature  $\beta$ . The partition function can be readily evaluated, yielding

$$\mathcal{Z}_k = \text{Tr}_{E_k} \left[ e^{-\beta\omega_k b_k^\dagger b_k} \right] = \sum_{n_k=0}^{\infty} e^{-\beta\omega_k n_k} = \frac{1}{1 - e^{-\beta\omega_k}}, \quad (\text{A.9})$$

where we have observed that  $b_k^\dagger b_k |n_k\rangle = n_k |n_k\rangle$  and summed the geometric series. Moreover, in the interaction picture, the bath operators read as

$$B(\tau) = \sum_k \left( g_k^* b_k e^{-i\omega_k \tau} + g_k b_k^\dagger e^{i\omega_k \tau} \right), \quad (\text{A.10})$$

$$B(0) = \sum_k \left( g_k^* b_k + g_k b_k^\dagger \right). \quad (\text{A.11})$$

We can also exploit the identity

$$B(\tau)B = \frac{1}{2} ([B(\tau), B(0)] + \{B(\tau), B(0)\}), \quad (\text{A.12})$$

to rewrite the two-point correlation function as

$$\alpha_\beta(\tau) = \frac{1}{2} (\langle [B(\tau), B(0)] \rangle_E + \langle \{B(\tau), B(0)\} \rangle_E). \quad (\text{A.13})$$

Therefore, using the well-known relations  $\{b_k, b_{k'}\} = 0 = \{b_k^\dagger, b_{k'}^\dagger\}$ , and the fact that the anticommutator  $\{b_k, b_{k'}^\dagger\}$  is non-null if and only if  $k = k'$ , we get

$$\langle \{B(\tau), B(0)\} \rangle = \sum_k |g_k|^2 \left( \langle \{b_k, b_k^\dagger\} \rangle_E e^{-i\omega_k \tau} + \langle \{b_k^\dagger, b_k\} \rangle_E e^{i\omega_k \tau} \right). \quad (\text{A.14})$$

We can now observe that

$$\begin{aligned} \langle \{b_k, b_k^\dagger\} \rangle_E &= \text{tr}_E \left( \{b_k, b_k^\dagger\} \rho_E \right) = 1 + \frac{2}{\mathcal{Z}_E} \text{tr}_E \left( b_k^\dagger b_k \prod_{k'} e^{-\beta\omega_{k'} b_{k'}^\dagger b_{k'}} \right) \\ &= 1 - \frac{2}{\omega_k} \frac{\partial}{\partial \beta} \ln \mathcal{Z}_k = \frac{1 + e^{-\beta\omega_k}}{1 - e^{-\beta\omega_k}} = \coth \left( \frac{\beta}{2} \omega_k \right), \end{aligned} \quad (\text{A.15})$$

whence we obtain

$$\langle \{B(\tau), B(0)\} \rangle = 2 \sum_k |g_k|^2 \cos \omega_k \tau \coth \left( \frac{\beta}{2} \omega_k \right). \quad (\text{A.16})$$

Analogously, one can show that

$$\langle [B(\tau), B(0)] \rangle = -2i \sum_k |g_k|^2 \sin \omega_k \tau. \quad (\text{A.17})$$

Therefore, assuming that the bath modes form a continuum, one obtains the following expression for the two point correlation function:

$$\alpha_\beta(\tau) \equiv \langle B(\tau)B \rangle_E = \text{tr}_E (B(\tau)B\rho_E) = \int_0^{+\infty} d\omega J(\omega) \left[ \cos \omega \tau \coth \left( \frac{\beta}{2} \omega \right) - i \sin \omega \tau \right], \quad (\text{A.18})$$

that coincides with [Equation \(4.15\)](#) of the main text.

# Appendix B

## Projector operators techniques

In this Appendix, following (Breuer, 2002), we review the projector operators techniques for deriving master equations from an underlying microscopic model.

### B.1 Projection operators

Let us consider the usual setting in which  $\mathcal{H}_S$  and  $\mathcal{H}_E$  are the Hilbert spaces of the system and the environment, respectively; therefore, the space of the composite system has a tensor product structure, i.e.,  $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$ . In the standard approach, one introduces the projector operator

$$\rho \mapsto \mathcal{P}\rho \equiv \text{tr}_E \rho \otimes \rho_E \equiv \rho_S \otimes \rho_E, \quad (\text{B.1})$$

where  $\rho_S \equiv \text{tr}_E \rho$  is the reduced density operator, whereas  $\rho_E$  is some fixed environmental state. Therefore, this operator projects the joint state  $\rho$  onto a smaller subspace, whose elements are in the uncorrelated form  $\rho_S \otimes \rho_E$ ; hence, in order to determine  $\rho_S$ , we do not need the full density matrix  $\rho$ , but just its relevant part  $\mathcal{P}\rho$ . By construction,  $\mathcal{P}$  meets the minimal requirement of being positive and trace preserving, thus it maps states into states. In addition to that, it sends separable states to separable states, meaning that this technique does not artificially create entanglement between the two subparties (Breuer, 2007).

Similarly, one can define a complementary operator  $\mathcal{Q}$ :

$$\mathcal{Q}\rho = \rho - \mathcal{P}\rho \quad (\text{B.2})$$

which projects on the irrelevant part of the dynamics. From the definitions above (and from the assumption that  $\text{tr}_E \rho_E = 1$ ), it is not difficult to conclude that the operators  $\mathcal{P}$  and  $\mathcal{Q}$  satisfy the following properties:  $\mathcal{P} + \mathcal{Q} = \mathbb{I}$ ,  $\mathcal{P}^2 = \mathcal{P}$ ,  $\mathcal{Q}^2 = \mathcal{Q}$ ,  $\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$ .

## B.2 Nakajima-Zwanzig equation

Let us consider the usual situation in which a system  $S$  interacts with its environment  $E$  according to a microscopic model, whose total Hamiltonian reads in the following way:

$$H = H_0 + \alpha H_I, \quad (\text{B.3})$$

where  $H_0 = H_S + H_E$  is the free Hamiltonian of the system and the environment, while  $H_I$  accounts for the interaction between them, whose strength is quantified by the coupling constant  $\alpha$ .

The whole system evolves unitarily, therefore the full density matrix satisfies the von Neumann equation, that, in the the Schrödinger picture, reads as

$$\dot{\rho}(t) = -i [H, \rho(t)]. \quad (\text{B.4})$$

It convenient to move to the interaction picture with respect to  $H_0$ , where we have<sup>1</sup>

$$\rho^I(t) = e^{iH_0 t} \rho(t) e^{-iH_0 t} \equiv \rho(t), \quad (\text{B.5})$$

$$H_I^I(t) = e^{iH_0 t} H_I e^{-iH_0 t} \equiv H_I(t). \quad (\text{B.6})$$

Inverting these relations and plugging them into [Equation \(B.4\)](#), we obtain the von Neumann equation in the aforementioned interaction picture:

$$\dot{\rho}(t) = -i\alpha [H_I(t), \rho(t)] \equiv \alpha \mathcal{L}_t[\rho(t)]. \quad (\text{B.7})$$

By applying the projection operators  $\mathcal{P}$  and  $\mathcal{Q}$  to [Equation \(B.7\)](#), we get the following set of coupled differential equations:

$$\partial_t \mathcal{P} \rho(t) = \mathcal{P} \partial_t \rho(t) = \alpha \mathcal{P} \mathcal{L}_t[\rho(t)], \quad (\text{B.8})$$

$$\partial_t \mathcal{Q} \rho(t) = \mathcal{Q} \partial_t \rho(t) = \alpha \mathcal{Q} \mathcal{L}_t[\rho(t)]. \quad (\text{B.9})$$

By inserting the identity  $\mathcal{P} + \mathcal{Q} = \mathbb{I}$  on the right-side of each equation, we get

$$\partial_t \mathcal{P} \rho(t) = \alpha \mathcal{P} \mathcal{L}_t[\mathcal{P} \rho(t)] + \alpha \mathcal{P} \mathcal{L}_t[\mathcal{Q} \rho(t)], \quad (\text{B.10})$$

$$\partial_t \mathcal{Q} \rho(t) = \alpha \mathcal{Q} \mathcal{L}_t[\mathcal{P} \rho(t)] + \alpha \mathcal{Q} \mathcal{L}_t[\mathcal{Q} \rho(t)]. \quad (\text{B.11})$$

The idea is to get a closed equation for the relevant part  $\mathcal{P} \rho(t)$  by solving [Equation \(B.11\)](#) and plugging the solution into [Equation \(B.10\)](#). The formal solution of [Equation \(B.11\)](#), corresponding to a given initial state  $\rho(t_0)$ , is obtained by using an operator generalisation of the Lagrange method for ordinary differential equations, yielding

$$\mathcal{Q} \rho(t) = \mathcal{G}(t, t_0) \mathcal{Q} \rho(t_0) + \alpha \int_{t_0}^t ds \mathcal{G}(t, s) \mathcal{Q} \mathcal{L}_s[\mathcal{P} \rho(s)], \quad (\text{B.12})$$

---

<sup>1</sup>Note that, to ease the notation, we will drop the superscript that refers to the interaction picture.

where we have introduced the propagator

$$\mathcal{G}(t, s) \equiv \mathcal{T}_{\leftarrow} \exp \left[ \alpha \int_s^t d\tau \mathcal{Q} \mathcal{L}_\tau \right], \quad (\text{B.13})$$

$\mathcal{T}_{\leftarrow}$  being the time-ordering operator. The propagator  $\mathcal{G}(t, s)$  satisfies the differential equation

$$\partial_t \mathcal{G}(t, s) = \alpha \mathcal{Q} \mathcal{L}_t [\mathcal{G}(t, s)] \quad (\text{B.14})$$

with the initial condition  $\mathcal{G}(s, s) = \mathbb{I}$ . Now, we can plug [Equation \(B.12\)](#) into [\(B.10\)](#), yielding the following exact equation for the time evolution of the relevant part of the density matrix:

$$\partial_t \mathcal{P} \rho(t) = \alpha \mathcal{P} \mathcal{L}_t [\mathcal{G}(t, t_0) \mathcal{Q} \rho(t_0)] + \alpha \mathcal{P} \mathcal{L}_t [\mathcal{P} \rho(t)] + \alpha^2 \int_{t_0}^t ds \mathcal{P} \mathcal{L}_t [\mathcal{G}(t, s) \mathcal{Q} \mathcal{L}_s [\mathcal{P} \rho(s)]] . \quad (\text{B.15})$$

This equation is sometimes referred to as *generalised Nakajima-Zwanzig (NZ) equation*. In the right hand side we have an inhomogeneous term  $\mathcal{P} \mathcal{L}_t [\mathcal{G}(t, t_0) \mathcal{Q} \rho(t_0)]$  depending on the initial state  $\rho(t_0)$ ; furthermore, this equation is not local in time because of the presence of an integral over the past history of the system in the interval  $[t_0, t]$ . This makes the NZ equation a potential candidate to describe memory effects of the reduced dynamics.

Furthermore, one also usually assumes that  $\mathcal{P} \mathcal{L}_t \mathcal{P} = 0$ ; more explicitly, one requires that  $\text{tr}_E (H_I(t) \rho_E) = 0$ , as

$$\mathcal{P} \mathcal{L}_t [\mathcal{P} \rho(t)] = -i \text{tr}_E [H_I(t), \rho_S(t) \otimes \rho_E] \otimes \rho_E = -i [\text{tr}_E (H_I(t) \rho_E), \rho_S] \otimes \rho_E = 0. \quad (\text{B.16})$$

Under this hypothesis, we obtain the *Nakajima-Zwanzig equation* for the relevant part of the dynamics

$$\partial_t \mathcal{P} \rho(t) = \int_{t_0}^t ds \mathcal{K}_{t,s}^{\text{NZ}} [\mathcal{P} \rho(s)] + \alpha \mathcal{P} \mathcal{L}_t [\mathcal{G}(t, t_0) \mathcal{Q} \rho(t_0)], \quad (\text{B.17})$$

where we have the *convolution (or memory) kernel*

$$\mathcal{K}_{t,s}^{\text{NZ}} \equiv \alpha^2 \mathcal{P} \mathcal{L}_t [\mathcal{G}(t, s) \mathcal{Q} \mathcal{L}_s [\mathcal{P}]], \quad (\text{B.18})$$

which, in general, is a highly singular object. We should note that we have not made any assumption about the form of the initial state so far. Now, if we also assume that at time  $t = t_0$  the system is in a product state, i.e.,

$$\rho(t_0) = \rho_S(t_0) \otimes \rho_E, \quad (\text{B.19})$$

it is immediate to see that  $\mathcal{P}\rho(t_0) = \rho(t_0)$ , whence  $\mathcal{Q}(t_0) = 0$ . This condition cancels the inhomogeneity out in [Equation \(B.17\)](#), thus NK equation reads as

$$\partial_t \mathcal{P}\rho(t) = \int_{t_0}^t ds \mathcal{K}_{t,s}^{\text{NZ}}[\mathcal{P}\rho(s)]. \quad (\text{B.20})$$

We have eventually got the Nakajima-Zwanzig equation, that exactly accounts for the time evolution of the relevant part of the density matrix. We should stress the fact that we have not done any approximation, except for a couple of assumptions (namely, [Equations \(B.16\)](#) and [\(B.19\)](#)), that in practical cases are not very restrictive.

### B.2.1 Perturbative expansion of the memory kernel

In order to overcome this issue, one can resort to a perturbative expansion of the memory kernel. More concretely, we need to expand the propagator  $\mathcal{G}(t, s)$  in such a way that we eventually get a dynamical equation that is of order  $\alpha^2$ . If we Taylor expand the right hand side of [Equation \(B.13\)](#), we will get the following expression:

$$\mathcal{G}(t, s) = \mathbb{I} + \alpha \mathcal{T}_\leftarrow \left[ \int_s^t d\tau \mathcal{Q}\mathcal{L}(\tau) \right] + \mathcal{O}(\alpha^2). \quad (\text{B.21})$$

Since the final goal is to rewrite a perturbative version of [Equation \(B.20\)](#) in the second order w.r.t. the coupling constant  $\alpha$ , we should stop the expansion of  $\mathcal{G}(t, s)$  at zeroth order, i.e.,  $\mathcal{G}(t, s) \approx \mathbb{I}$ , as [Equation \(B.20\)](#) is already of order  $\alpha^2$  — cf. [Equation \(B.18\)](#). Therefore, [Equation \(B.20\)](#) reads as

$$\partial_t \mathcal{P}\rho(t) = \alpha^2 \int_{t_0}^t ds \mathcal{P}\mathcal{L}_t [\mathcal{Q}\mathcal{L}_s[\mathcal{P}\rho(s)]]. \quad (\text{B.22})$$

We can rewrite [Equation \(B.22\)](#) in a more familiar way using the definition of the projector  $\mathcal{P}\rho$  given by [Equation \(B.1\)](#), the property  $\mathcal{Q} = 1 - \mathcal{P}$  and [Equation \(B.16\)](#); we get the a master equation in the form

$$\dot{\rho}_S(t) = -\alpha^2 \int_{t_0}^t ds \text{tr}_E [H_I(t), [H_I(s), \rho_S(s) \otimes \rho_E]]. \quad (\text{B.23})$$

However, the technique we have just shown has some drawbacks from a practical point of view: on one hand, this perturbative approach for the derivation of the equations of motion simplifies the expression of the memory kernel, on the other hand we end up with a integro-differential equation which is not easy to solve in the general case.

### B.3 Time-convolutionless master equations

In the previous Section, we have pointed out that it is difficult to treat the NZ equation, mainly because of the time convolution in the memory kernel  $\mathcal{K}_{t,s}^{\text{NZ}}$ . The motivation that informs the time-convolutionless projection operator technique is basically the following: we would like to get rid of the dependence of the future time evolution from the NZ equation, getting a time-local version of the former. To this end, we should first introduce an operator that, applied to our density matrix, goes backwards in time. The definition of this backward propagator is somehow similar to that of  $\mathcal{G}(t, s)$ , i.e.,

$$G(t, s) \equiv \mathcal{T}_\rightarrow \exp \left[ -\alpha \int_s^t d\tau \mathcal{L}_\tau \right]. \quad (\text{B.24})$$

with an extremely important difference: this object is the backward propagator of the total system ( $S + E$ ), that undergoes a unitary dynamics. Note that  $\mathcal{T}_\rightarrow$  denotes the anti-chronological time ordering. When it is applied to the full density matrix, this propagator works in the following way:

$$\rho(s) = G(t, s)\rho(t). \quad (\text{B.25})$$

Using the property  $\mathcal{P} + \mathcal{Q} = \mathbb{I}$ , one gets

$$\rho(s) = G(t, s)(\mathcal{P} + \mathcal{Q})\rho(t). \quad (\text{B.26})$$

We can plug [Equation \(B.26\)](#) into [Equation \(B.12\)](#), getting the following expression of the irrelevant part of the density matrix

$$\mathcal{Q}\rho(t) = \mathcal{G}(t, t_0)\mathcal{Q}\rho(t_0) + \alpha \int_{t_0}^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{L}_s [\mathcal{P}G(t, s)(\mathcal{P} + \mathcal{Q})\rho(t)]. \quad (\text{B.27})$$

Then we define the operator

$$\Sigma(t) \equiv \alpha \int_{t_0}^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{L}_s [\mathcal{P}G(t, s)]. \quad (\text{B.28})$$

Note that  $\Sigma(t)$  contains both propagators  $\mathcal{G}$  and  $G$ , therefore it does not specify a well-defined chronological order. Furthermore, the following properties are trivially satisfied:

$$\Sigma(t)|_{\alpha=0} = 0, \quad \Sigma(t_0) = 0. \quad (\text{B.29})$$

With the help of [Equation \(B.28\)](#), one gets

$$\mathcal{Q}\rho(t) = \mathcal{G}(t, t_0)\mathcal{Q}\rho(t_0) + \Sigma(t)\mathcal{P}\rho(t) + \Sigma(t)\mathcal{Q}\rho(t), \quad (\text{B.30})$$

whence

$$[\mathbb{I} - \Sigma(t)] \mathcal{Q}\rho(t) = \mathcal{G}(t, t_0) \mathcal{Q}\rho(t_0) + \Sigma(t) \mathcal{P}\rho(t). \quad (\text{B.31})$$

If we look at [Equation \(B.31\)](#), we conclude that, to get a closed expression for the irrelevant part  $\mathcal{Q}\rho(t)$ , we need to invert the operator  $[\mathbb{I} - \Sigma(t)]$ . This is not always possible, but, thanks to the properties [\(B.29\)](#), we can say that the inversion is mathematically justified if one works in the hypothesis of small couplings and for small  $t - t_0$ . In this limit, one has

$$[\mathbb{I} - \Sigma(t)] [\mathbb{I} - \Sigma(t)]^{-1} = [\mathbb{I} - \Sigma(t)]^{-1} [\mathbb{I} - \Sigma(t)] = \mathbb{I}. \quad (\text{B.32})$$

Therefore, from [Equation \(B.31\)](#), we get

$$\mathcal{Q}\rho(t) = [\mathbb{I} - \Sigma(t)]^{-1} \mathcal{G}(t, t_0) \mathcal{Q}\rho(t_0) + [\mathbb{I} - \Sigma(t)]^{-1} \Sigma(t) \mathcal{P}\rho(t), \quad (\text{B.33})$$

meaning that the irrelevant part of the dynamics  $\mathcal{Q}\rho(t)$  at a time  $t$  is determined once we know the relevant part  $\mathcal{P}\rho(t)$  at time  $t$  and the initial condition  $\mathcal{Q}\rho(t_0)$ . Therefore, the dependence on the history of the relevant part that makes the Nakajima-Zwanzig memory kernel non local in time has been removed though the introduction of the backward propagator  $G(t, s)$ .

If we plug [Equation \(B.33\)](#) into [Equation \(B.10\)](#), we finally get a closed form of the master equation governing the relevant part of the dynamics. This equation is known in literature as *time-convolutionless (TCL) master equation*

$$\partial_t \mathcal{P}\rho(t) = \mathcal{K}_t^{\text{TCL}} [\mathcal{P}\rho(t)] + \mathcal{I}_t [\mathcal{Q}\rho(t_0)], \quad (\text{B.34})$$

where we have introduced the *time-local generator*

$$\mathcal{K}_t^{\text{TCL}} \equiv \alpha \mathcal{P} \mathcal{L}_t [[\mathbb{I} - \Sigma(t)]^{-1} \mathcal{P}], \quad (\text{B.35})$$

and the inhomogeneity

$$\mathcal{I}_t \equiv \alpha \mathcal{P} \mathcal{L}_t [[\mathbb{I} - \Sigma(t)]^{-1} \mathcal{G}(t, t_0) \mathcal{Q}]. \quad (\text{B.36})$$

The master equation [\(B.34\)](#) is general; for instance, we have not assumed anything about the form of the initial state. It is exact, linear and local in time; unfortunately its practical use is limited by the fact that the operators  $\mathcal{K}_t^{\text{TCL}}$  and  $\mathcal{I}_t$  are, in general, very complicated objects. If we further assume that the initial state is in a tensor product form, i.e.,  $\rho(t_0) = \rho_S(t_0) \otimes \rho_E$ , one has  $\mathcal{I}_t = 0$ , therefore [Equation \(B.34\)](#) becomes

$$\partial_t \mathcal{P}\rho(t) = \mathcal{K}_t^{\text{TCL}} [\mathcal{P}\rho(t)]. \quad (\text{B.37})$$

### B.3.1 Perturbative expansion of the TCL generator

As we have already pointed out, the TCL generator  $\mathcal{K}^{\text{TCL}}$  can be quite hard to explicitly evaluate. Nonetheless, there exist a way to treat it perturbatively in a systematic way

(Chaturvedi, 1979). Let us assume that the quantity  $[\mathbb{I} - \Sigma(t)]^{-1}$  does exist and can be regarded as the formal sum of a geometric series

$$[\mathbb{I} - \Sigma(t)]^{-1} = \sum_{n=0}^{\infty} [\Sigma(t)]^n, \quad (\text{B.38})$$

therefore, [Equation \(B.35\)](#) reads as

$$\mathcal{K}_t^{\text{TCL}} = \alpha \sum_{n=0}^{\infty} \mathcal{P} \mathcal{L}_t [[\Sigma(t)]^n \mathcal{P}]. \quad (\text{B.39})$$

The idea is to write the TCL generator in powers of  $\alpha$ , i.e.,

$$\mathcal{K}_t^{\text{TCL}} = \sum_{n=1}^{\infty} \alpha^n \mathcal{K}_n(t). \quad (\text{B.40})$$

In order to get a closed expression for each term  $\mathcal{K}_n(t)$  of the expansion, we need to expand  $\Sigma(t)$  in powers of  $\alpha$  as well, i.e.,

$$\Sigma(t) = \sum_{n=1}^{\infty} \alpha^n \Sigma_n(t) \quad (\text{B.41})$$

If we plug [Equation \(B.41\)](#) into [Equation \(B.39\)](#), we obtain the following expansion:

$$\begin{aligned} \mathcal{K}_t^{\text{TCL}} &= \alpha (\mathcal{P} \mathcal{L}_t [\mathcal{P}] + \mathcal{P} \mathcal{L}_t [[\Sigma(t)] \mathcal{P}] + \dots) \\ &= \alpha \left( \mathcal{P} \mathcal{L}_t [\mathcal{P}] + \mathcal{P} \mathcal{L}_t [(\alpha \Sigma_1(t) + \alpha^2 \Sigma_2(t) + \dots) \mathcal{P}] \dots \right) \end{aligned} \quad (\text{B.42})$$

By comparing [Equations \(B.40\)](#) and [\(B.42\)](#), and sorting equal powers of  $\alpha$ , we can get the expression of each contribution  $\mathcal{K}_n(t)$ . For instance, collecting all the terms proportional to  $\alpha$ , we get

$$\mathcal{K}_1(t) = \mathcal{P} \mathcal{L}_t [\mathcal{P}], \quad (\text{B.43})$$

while, for those proportional to  $\alpha^2$ , we have

$$\mathcal{K}_2(t) = \mathcal{P} \mathcal{L}_t [\Sigma_1(t) \mathcal{P}], \quad (\text{B.44})$$

and so on. The following step is to determine a closed expression of each term  $\Sigma_n(t)$ ; this can be done starting from the definition of  $\Sigma(t)$  – cf. [Equation \(B.28\)](#) – and expanding the propagators  $\mathcal{G}(t, s)$  and  $G(t, s)$ , whose definition is given by [Equations \(B.13\)](#) and [\(B.24\)](#), respectively, in powers of  $\alpha$ . Let us determine explicitly the first two terms  $\Sigma_1(t)$  and  $\Sigma_2(t)$ . We first expand the two propagators

$$\mathcal{G}(t, t_1) = \mathbb{I} + \alpha \int_{t_1}^t dt_2 \mathcal{Q} \mathcal{L}_{t_2} + \mathcal{O}(\alpha^2), \quad (\text{B.45})$$

$$G(t, t_1) = \mathbb{I} - \alpha \int_{t_1}^t dt_2 \mathcal{L}_{t_2} + \mathcal{O}(\alpha^2). \quad (\text{B.46})$$

If we use these expansions in the definition (B.28) with  $t_0 = 0$ , we will get

$$\Sigma(t) = \alpha \int_0^t dt_1 \left[ \mathbb{I} + \alpha \int_{t_1}^t dt_2 \mathcal{Q}\mathcal{L}_{t_2} + \dots \right] \mathcal{Q}\mathcal{L}_s \mathcal{P} \left[ \mathbb{I} - \alpha \int_{t_1}^t dt_2 \mathcal{L}_{t_2} + \dots \right]. \quad (\text{B.47})$$

By comparing Equation (B.47) with the expansion (B.41) and collecting the terms proportional to the same power of  $\alpha$ , one easily finds that

$$\Sigma_1(t) = \int_0^t dt_1 \mathcal{Q}\mathcal{L}_{t_1}[\mathcal{P}]. \quad (\text{B.48})$$

We can also notice that  $[\Sigma_1(1)]^2 = 0$ , since  $\mathcal{P}\mathcal{Q} = 0$ . On the other hand, we get

$$\Sigma_2(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \{ \mathcal{Q}\mathcal{L}_{t_1} [\mathcal{Q}\mathcal{L}_{t_2}[\mathcal{P}]] - \mathcal{Q}\mathcal{L}_{t_2} [\mathcal{P}\mathcal{L}_{t_1}] \}. \quad (\text{B.49})$$

Therefore, we have:

$$\mathcal{K}_1(t) = \mathcal{P}\mathcal{L}_t[\mathcal{P}], \quad (\text{B.50})$$

$$\mathcal{K}_2(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}_t[\mathcal{Q}\mathcal{L}_{t_1}[\mathcal{P}]]. \quad (\text{B.51})$$

Usually a technical assumption is made, i.e.,

$$\mathcal{P}\mathcal{L}_{t_1}\mathcal{L}_{t_2} \dots \mathcal{L}_{t_{2n+1}}\mathcal{P} = 0 \quad (\text{B.52})$$

for  $n = 0, 1, 2, \dots$ . Now, for  $n = 0, 1, 2$ , the latter reads as follows:

$$\mathcal{P}\mathcal{L}_t\mathcal{P} = 0, \quad (\text{B.53})$$

$$\mathcal{P}\mathcal{L}_t\mathcal{L}_{t_1}\mathcal{P} = 0. \quad (\text{B.54})$$

By using these relations and  $\mathcal{Q} = 1 - \mathcal{P}$ , we eventually get

$$\mathcal{K}_1(t) = 0, \quad (\text{B.55})$$

$$\mathcal{K}_2(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}_t [\mathcal{L}_{t_1}[\mathcal{P}]]. \quad (\text{B.56})$$

Therefore, we have collected everything needed to write down a master equation up to the second order in the coupling strength  $\alpha$ ; in this limit, Equation (B.37) reads as

$$\partial_t \mathcal{P}\rho(t) = \int_0^t ds \mathcal{P}\mathcal{L}_t [\mathcal{L}_s[\mathcal{P}\rho(t)]] . \quad (\text{B.57})$$

More explicitly, one has:

$$\dot{\rho}_S(t) = -\alpha^2 \int_0^t ds \operatorname{tr} [H_I(t), [H_I(s), \rho_S(t) \otimes \rho_E]]. \quad (\text{B.58})$$

This equation should be contrasted to the corresponding equation we got using the Nakajima-Zwanzig technique, i.e., [Equation \(B.23\)](#): in principle, one can naively expect that the two master equations [\(B.23\)](#) and [\(B.58\)](#) approximate the exact reduced dynamics with the same accuracy, provided that both of them are based on a second order perturbative expansion. But this is not the case: the time convolutionless master equation [\(B.58\)](#) is local in time. This equation is not fully Markovian, as it retains some memory effects.

# Appendix C

## Time evolution of populations and coherences

In this Section, we explicitly derive Equations (4.81) and (4.82).

### C.1 Preliminary observations

In the hypothesis of Section 4.4.3, let us start from the identity

$$\langle m | A_\mu(\omega) | n \rangle = \sum_{\substack{j,k \\ E_j - E_k = \omega}} \underbrace{\langle m | j \rangle}_{\delta_{mj}} \underbrace{\langle j | A_\mu | k \rangle}_{\delta_{mk}} \underbrace{\langle k | n \rangle}_{\delta_{kn}} = \delta_{E_n - E_m, \omega} \langle m | A_\mu | n \rangle, \quad (\text{C.1})$$

that follows from Equation (4.52). Analogously, one has the identity

$$\langle m | A_\mu^\dagger(\omega) | n \rangle = (\langle n | A_\mu(\omega) | m \rangle)^* = \delta_{E_m - E_n, \omega} (\langle n | A_\mu | m \rangle)^* \quad (\text{C.2})$$

Now, we can consider the dissipator given by Equation (4.79), and evaluate the following quantity:

$$\begin{aligned} \langle m | \mathcal{D}[\rho_S(t)] | n \rangle &= \sum_{\omega} \sum_{\mu, \nu} \gamma_{\mu\nu}^t(\omega) \left[ \langle m | A_\nu(\omega) \rho_S(t) A_\mu^\dagger(\omega) | n \rangle \right. \\ &\quad \left. - \frac{1}{2} \langle m | A_\mu^\dagger(\omega) A_\nu(\omega) \rho_S(t) | n \rangle - \frac{1}{2} \langle m | \rho_S(t) A_\mu^\dagger(\omega) A_\nu(\omega) | n \rangle \right] \\ &= \sum_{\omega} \sum_{\mu, \nu} \sum_{j, k} \gamma_{\mu\nu}^t(\omega) \left[ \langle m | A_\nu(\omega) | j \rangle \langle j | \rho_S(t) | k \rangle \langle k | A_\mu^\dagger(\omega) | n \rangle \right. \\ &\quad \left. - \frac{1}{2} \langle m | A_\mu^\dagger(\omega) | j \rangle \langle j | A_\nu(\omega) | k \rangle \langle k | \rho_S(t) | n \rangle \right. \\ &\quad \left. - \frac{1}{2} \langle m | \rho_S(t) | j \rangle \langle j | A_\mu^\dagger(\omega) | k \rangle \langle k | A_\nu(\omega) | n \rangle \right], \end{aligned} \quad (\text{C.3})$$

whence

$$\begin{aligned} \langle m | \mathcal{D}[\rho_S(t)] | n \rangle &= \sum_{\omega} \sum_{\mu, \nu} \sum_{j, k} \gamma_{\mu\nu}^t(\omega) \delta_{\varepsilon_j - \varepsilon_m, \omega} \delta_{\varepsilon_k - \varepsilon_n, \omega} \langle m | A_\nu | j \rangle (\langle n | A_\mu | k \rangle)^* P_{jk}(t) \\ &\quad - \frac{1}{2} \sum_{\mu, \nu} \sum_j \gamma_{\mu\nu}^t(\varepsilon_m - \varepsilon_j) (\langle j | A_\mu | m \rangle)^* \langle j | A_\nu | m \rangle P_{mn}(t) \\ &\quad - \frac{1}{2} \sum_{\mu, \nu} \sum_k \gamma_{\mu\nu}^t(\varepsilon_n - \varepsilon_k) (\langle k | A_\mu | n \rangle)^* \langle k | A_\nu | n \rangle P_{mn}(t), \end{aligned} \quad (\text{C.4})$$

where we have used the properties (C.1) and (C.2) and observed that, due to the non-degeneracy of the spectrum, we have  $\delta_{\varepsilon_m - \varepsilon_j, \omega} \delta_{\varepsilon_k - \varepsilon_j, \omega} = \delta_{mk} \delta_{\varepsilon_m - \varepsilon_j, \omega}$ , and  $\delta_{\varepsilon_n - \varepsilon_k, \omega} \delta_{\varepsilon_j - \varepsilon_k, \omega} = \delta_{nj} \delta_{\varepsilon_n - \varepsilon_k, \omega}$ .

## C.2 Populations

Let us specialise our calculation to the diagonal elements, i.e., those for which the condition  $m = n$  holds. Equation (C.3) yields

$$\begin{aligned} \langle n | \mathcal{D}[\rho_S(t)] | n \rangle &= \sum_{\mu, \nu} \sum_k \gamma_{\mu\nu}^t(\varepsilon_k - \varepsilon_n) \langle n | A_\nu | k \rangle (\langle n | A_\mu | k \rangle)^* P_k(t) \\ &\quad - \sum_{\mu, \nu} \sum_k \gamma_{\mu\nu}^t(\varepsilon_n - \varepsilon_k) (\langle k | A_\mu | n \rangle)^* \langle k | A_\nu | n \rangle P_n(t). \end{aligned} \quad (\text{C.5})$$

We can define the following time-dependent transition rates:

$$W_t(n|k) \equiv \sum_{\mu, \nu} \gamma_{\mu\nu}^t(\varepsilon_k - \varepsilon_n) \langle k | A_\mu | n \rangle \langle n | A_\nu | k \rangle, \quad (\text{C.6})$$

where we have taken into account that  $A_\mu^\dagger = A_\mu$ . Furthermore, working along the same lines as in the previous calculation, one can easily check that

$$\langle n | [H_{\text{LS}}(t), \rho_S(t)] | n \rangle = 0. \quad (\text{C.7})$$

Therefore, the evolution equations for the populations reads as

$$\dot{P}_n = \sum_k [W_t(n|k)P_k(t) - W_t(k|n)P_n(t)]. \quad (\text{C.8})$$

## C.3 Coherences

On a similar note, we can derive the set of first order differential equations for the coherences. If we work in the interaction picture with respect to the renormalised Hamiltonian, from Equation (C.3)) we easily get

$$\dot{P}_{mn}(t) = -\frac{1}{2} \sum_k [W_t(k|n) + W_t(k|m)] P_{mn}(t). \quad (\text{C.9})$$

We can also write down the equations governing the coherences dynamics in the Schrödinger picture. Starting from Eq. (4.80), we easily obtain

$$\dot{P}_{mn}(t) = - \left\{ i\omega_{mn} + \frac{1}{2} \sum_k [W_t(k|n) + W_t(k|m)] \right\} P_{mn}(t), \quad (\text{C.10})$$

where  $\omega_{mn} = E_m - E_n$  are the renormalised Bohr frequencies of the system.

# Appendix D

## Positivity of the Kossakowski matrices

In this Appendix, we would like to explicitly show that the Kossakowski matrices  $\gamma_{\mu\nu}(\omega)$  given by [Equation \(4.104\)](#) are positive-definite for all values of  $\omega$ . This is crucial to prove that the derivation à la Davies discussed in [Chapter 4](#) leads to a generator of quantum dynamical semigroup, thus to a master equation describing a quantum Markovian process.

### D.1 Bochner's theorem

First, we need to introduce a theorem of Fourier analysis, known as Bochner's theorem ([Strichartz, 2003](#)). We know from linear algebra that we can associate to a generic  $N \times N$  matrix  $A = (a_{ij})$  with complex entries a quadratic form in  $\mathbb{C}^N$ , defined as

$$(\mathbf{v}, A\mathbf{v}) \equiv \sum_{i,j=1}^N a_{ij} v_i^* v_j, \quad (\text{D.1})$$

where  $\mathbf{v} = (v_1, \dots, v_N) \in \mathbb{C}^N$ .  $A$  is said to be positive definite if its quadratic form is non-negative, i.e.,  $(\mathbf{v}, A\mathbf{v}) \geq 0$ . The notion of postive-definiteness can be naturally extended to functions. A continuous function  $f : \mathbb{R}^N \rightarrow \mathbb{C}$  is said to be positive definite if and only if the matrix  $a_{ij} = f(t_i - t_j)$  is positive definite for any choice of points  $t_1, \dots, t_N$  in  $\mathbb{R}^N$  and for any  $N$ . More specifically, this means that

$$\sum_{i,j=1}^N v_i^* f(t_i - t_j) v_j \geq 0, \quad (\text{D.2})$$

for any choice of  $\mathbf{v} \in \mathbb{C}^N$ . Given these definitions, Bochner's theorem states that *the Fourier transform of a positive definite function is a positive quantity*.

## D.2 Proof of positive definiteness

In order to apply the results of the previous Section, let us first consider the following quantity:

$$\begin{aligned}
(\mathbf{v}, \gamma \mathbf{v}) &= \sum_{\mu\nu} v_\mu \gamma_{\mu\nu}(\omega) v_\nu = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \sum_{\mu\nu} v_\mu^* \langle B_\mu^\dagger(\tau) B_\nu(0) \rangle_E v_\nu \\
&= \int_{-\infty}^{+\infty} d\tau e^{i\tau\omega} \text{tr}_E \left\{ \left( \sum_\mu v_\mu^* B_\mu^*(\tau) \right) \left( \sum_\nu B_\nu v_\nu \right) \rho_E \right\} \\
&= \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \text{tr}_E (B^\dagger(\tau) B \rho_E), \tag{D.3}
\end{aligned}$$

where we have introduced:

$$B = \sum_\mu B_\mu v_\mu \tag{D.4}$$

and its Hermitian conjugate. Now, we need to prove that the function:

$$f(\tau) \equiv \text{tr}_E (B^\dagger(\tau) B \rho_E) \tag{D.5}$$

is positive definite. It is easy to check that

$$\begin{aligned}
\sum_{i,j=1}^N w_i^* f(t_i - t_j) w_j &= \sum_{i,j=1}^N w_i^* \text{tr}_E \{ B^\dagger(t_i - t_j) B \rho_E \} w_j \\
&= \sum_{i,j=1}^N w_i^* \text{tr}_E \{ e^{+iH_E(t_i-t_j)} B^\dagger e^{-iH_E(t_i-t_j)} B(0) \rho_E \} w_j \\
&= \text{tr}_E \left\{ \left( \sum_{i=1}^N e^{+iH_E t_i} B e^{-iH_E t_i} w_i \right)^\dagger \left( \sum_{j=1}^N e^{+iH_E t_j} B e^{-iH_E t_j} w_j \right) \rho_E \right\} \\
&= \text{tr} \{ (X^\dagger X \rho_E) \} = \langle X^\dagger X \rangle \geq 0. \tag{D.6}
\end{aligned}$$

Therefore, by virtue of Bochner's theorem, we can conclude that the Kossakowski matrices  $\gamma_{\mu\nu}(\omega)$  are positive definite.

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