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CHARACTERIZATION OF DYNAMICAL PROPERTIES OF NON-MARKOVIAN OPEN QUANTUM SYSTEMS

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Abstract

In the present Thesis we study the behavior of multi-time correlation functions and of thermodynamical quantities such as heat in open quantum systems undergoing an evolution generally affected by the presence of memory effects, i.e. non-Markovian. In the last decade, a large part of the scientific community in this field has dedicated its efforts to the understanding, precise definition and quantification of non-Markovianity in the quantum realm and now we have at our disposal several benchmark results and a plethora of different estimators that allow to determine the degree of non-Markovianity of a given dynamics. It comes therefore natural to investigate how other different dynamical quantities relate to such estimators also in order to understand the physical implications of memory effects on the statistics of observable quantities.

In the first part of this work, a quantitative test of the violation of the so-called quantum regression theorem in presence of a non-Markovian dynamical regime is investigated. The quantum regression theorem represents a procedure that, whenever valid, allows to reconstruct two-time correlation functions of system's operators from the sole knowledge of the dynamics of mean values. It is worth stressing that two-time correlation functions are necessary in order to fully characterize the statistical properties of a quantum system, since they are able to catch aspects of the dynamics, such as fluorescence spectrum, in general not accessible looking at mean values. Despite their relevance however, obtaining two-time correlation functions often represents a formidable task, since the knowledge of the full "system+environment" dynamics is required, a generally too demanding request in the context of open quantum systems theory. The quantum regression theorem represents in this regard the easiest route to determine two-time correlation functions, this highlighting its importance. In this work we show that, in a pure-dephasing spin-boson model, the quantum regression theorem represents a stronger condition than non-Markovianity, in the sense that any presence of memory effects in the reduced dynamics inevitably results in violations to the former. These results have been published in [1].

The second part of the Thesis is devoted to the characterization of heat flow at the microscopic level in open quantum systems, both finite and infinite dimensional. In particular we begin by studying the time behavior of its mean value in a non-Markovian dynamical regime, showing that, at variance with what happens in the Born-Markov semigroup limiting case, heat can backflow from the environment to the system. After providing a condition for the occurrence of such phenomenon and a measure for its amount for a given dynamics, the relationship with suitable non-Markovianity estimators is sought in two paradigmatic models, namely the spin-boson and the quantum brownian motion. The results, collected in [2, 3], on the one hand allow for the identification of parameter-regions where the heat backflow is absent or maximum. On the other hand they show that the occurrence of heat backflow represents a stricter condition than non-Markovianity, in the sense that non-Markovianity allows for the observation of heat flowing back from the environment to the system and, vice versa, a Markovian dynamics prevents its occurrence. This Thesis concludes with the formulation of a new family of lower bounds to the mean dissipated heat in an environmental-assisted erasure-protocol scenario where Landauer's principle applies. As originally conceived for classical systems, this principle states that every irreversible erasure of information stored in a system inevitably carries along an amount of heat dissipated into the environment which is expended to perform the action. Within the framework recently put forward in [4], which guarantees the validity of Landauer's principle in an open quantum systems scenario, we provide an asymptotically tight family of lower bounds to the dissipated heat which are also valid in the non-equilibrium setting. This construction is applied to an open system consisting of a three-level V-system, in which one transition is externally pumped by a laser field while the other is coupled through an XX-interaction to an environment consisting of a spin chain. Beside calculating all these quantities, an exact solution for the dynamics of such system is also provided. These results are collected in [5].

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Giacomo

Contents

To my Beloved Family

1 Introduction

Quantum mechanics provides a description of statistical experiments at the microscopic level. The standard under-graduate course in quantum mechanics deals with closed systems and with their evolution, which are dictated by a one-parameter group of unitary operators.

Every concrete physical system has however to be considered as *open* for two fundamental reasons.

The first one is the unavoidable (mutual) interaction with an environment. Since the description of the compound "system+environment" (which again would be closed in its overall) is almost never feasible due to the complexity of the environment, one has to restrict the attention on the system, keeping track of the effects of the interaction with the environment on the dynamics. The solution of this problem is precisely what the theory of open quantum systems deals with.

The second reason is that quantum mechanics is, as mentioned at the beginning, an intrinsic statistical theory where, following the modern formulation developed by Ludwig [6], Holevo [7] and Kraus [8], the experimental quantities which can be compared with the predictions of the theory are the relative frequencies that a preparation apparatus, representing an ensemble of identically prepared quantum systems, triggers a macroscopic measurement apparatus. This coupling between a quantum system and a measurement device however does actually represent a paradigmatic example of open quantum system interacting with an environment. For this reason, many concepts and tools introduced within the statistical formulation of quantum mechanics for composite systems lie now at the basis of the description of open quantum systems.

The interaction between system and environment generally entails the loss of those typical quantum properties, such as coherence or entanglement, a phenomenon which generally goes under the name of *decoherence* [9]. The preservation of such properties has however been proven to be an essential feature in countless physical situations such as quantum computation, quantum information and even quantum biology, in which the "quantumness" of concrete physical systems (in unavoidable contact with an environment) was to be taken into account. In the last few decades therefore, an increasing effort

has been put into developing the theory of open quantum systems, the reason being thus both practical and fundamental.

Whenever we move from a closed to an open quantum system, its dynamics gets immediately more involved than just unitary evolution, and is given in terms of a so-called *master equation*. Though a general structure for the latter in the case of completely generic initial conditions, couplings and Hamiltonians is still nowadays not known, a cornerstone result in this direction was given by Gorini, Kossakowski, Sudarshan and Lindblad, who determined the form of the generator of a completely positive quantum dynamical semigroup. Starting from a microscopic description of the physical model under consideration, the set of assumptions and approximations involved to obtain a master equation of this form are however proven to be very restrictive and thus this approach very often fails to apply to concrete situations. The key assumption to obtain an effective dynamics described in terms of a quantum dynamical semigroup, usually considered as the closest quantum counterpart of classical time-homogeneous Markov process, is that memory effects are taken to be negligible, due to a separation of the much faster time scale of the environment with respect to that of the open system.

It is usually the case that violations of this time-scales separation occur, for example, in situations of strong coupling regime between system and environment, structured or finite-dimensional environment or low bath temperatures. Even if this is not the case, the huge and fast development of quantum technologies has opened the possibility to access time-scales of the order of femtoseconds, allowing to resolve the dynamics of open quantum systems at very short time scales, comparable to those of the environment. Within all these situations, memory effects, generically referred to as *non-Markovian effects*, play a fundamental role in the correct determination of the statistical properties of open quantum systems. As a consequence, lots of efforts have been devoted in the last decades to the characterization of memory effects in quantum systems, meanwhile addressed both to actually define what is meant by a non-Markovian dynamics in the quantum realm and to quantitatively estimate the degree of non-Markovianity of a given reduced dynamics. Several benchmark results have been obtained in this regard [10–20] and now we have at our disposal a plethora of quantifier of non-Markovianity, each of which shedding light upon this property of the dynamics from a slightly different angle. It is therefore very natural to ask how the presence or absence of memory effects in the reduced dynamics affects other statistically relevant properties, such as multi-time correlation functions or thermodynamical quantities e.g. energy, heat and work. This is the leitmotif of the present Thesis, in which we will consider several of these properties and quantities in order to investigate their behavior in presence of a non-Markovian dynamics, searching for a connection between them.

1.1 Thesis Outline

This Thesis is organized as follows.

Chapter 2 provides an introduction to the main notions of open quantum systems theory which will be useful throughout the remaining of the work. In the first Section we introduce the notions of composite quantum systems, which stand at the very basis of open quantum systems' theory. In particular the concepts of statistical operators, POVMs, trace and partial trace, linear maps and complete positivity are presented here. In the following Section we apply them to the framework of open quantum systems, where the definitions and properties of quantum dynamical maps and master equations are discussed in detail. The connection between the dynamical descriptions provided by full unitary evolutions, dynamical maps and master equations is drawn, together with explicit indications of how to obtain one from another. Finally, the constraints on the structure of the master equations imposed by the properties of the associated dynamical map are presented. In particular in Subsection 2.2.4.1 we show how trace and hermiticity preservation reflect upon the structure of time-local master equations, and in Subsection 2.2.4.2 we conclude the Chapter by discussing the role of complete positivity on the latter, presenting the well-known Gorini-Kossakowski-Sudarshan-Lindblad generator.

Chapter 3 is devoted to clarify the notion of non-Markovianity. In order to make the exposition of the concepts as clear as possible, we first introduce this concept in Section 3.1 within the classical theory of stochastic processes. Building upon this, we then move to speak about quantum non-Markovianity in Section 3.2, showing the analogies and the differences with the classical case and making a detailed survey of all the main criteria and measures of non-Markovianity so far introduced.

In Chapter 4 we discuss the relationship between non-Markovianity and the quantum regression theorem, an useful theoretical tool which, whenever valid, allows to reconstruct, from the bare knowledge of the mean values of system's observables, the two-time (multi-time) correlation functions. The latter quantities contain significant information about the system which are not contained in the mean values; a well known example of this is represented by resonance fluorescence spectrum [21, 22]. In general, accessing them can prove a formidable task; the quantum regression theorem is arguably the most simple way to accomplish it. In this Chapter we will investigate how the assumptions and approximations which guarantee the validity of this procedure relate with the conditions under which the dynamics describing the evolution of an open quantum system is Markovian or non-Markovian. A suitable figure of merit for the violations of the quantum regression theorem, that can be interpreted as the relative error between the two-time correlation functions obtained exactly and by applying this procedure, is also introduced in order to make the connection with the non-Markovianity more quantitative. This analysis is then carried out explicitly in a specific system, the so-called pure dephasing spin-boson model, where the estimator of the violations to the quantum regression theorem is analytically evaluated and related to two well-known measures of non-Markovianity, one based on the time-behavior of the trace distance between two reduced states of the system [11] and the other based on violation of completely-positive divisibility [13].

In Chapters 5 and 6, discussion is centred on the characterization of the change in the environmental energy, i.e. *heat*, in non-driven open quantum systems undergoing a non-Markovian evolution.

In particular, Chapter 5 is devoted to investigate how the mean heat flow between an open system and its environment behaves in presence of memory effects in the reduced dynamics. This task is accomplished by means of the so-called full-counting statistics formalism which allows to reconstruct in principle all the cumulants of the probability distribution for the change in a generic observable of a quantum system. This investigation tool, widely employed in quantum thermodynamics community to characterize, for example, the energy flow in quantum thermal machines, is presented in Section 5.2. By making use of it, we reconstruct the heat flow which occurs in a non-Markovian dynamical regime, both for finite and Gaussian open quantum systems. At variance with what happens in the Born-Markov semigroup approximation, where a steady heat flow from the hotter to the colder subsystem takes place, a backflow of heat from the environment to the system can originate, even in absence of initial temperature gradient, when the dynamics is non-Markovian. A suitable condition for the occurrence of this phenomenon and a measure for its amount as property of the dynamical map determining the reduced dynamics is given in Section 5.3 and related with suitable quantifiers of non-Markovianity in two paradigmatic and important models: the spin-boson system in Subsection 5.3.2 and the quantum brownian motion in Section 5.3.3.

In Chapter 6 we will finally deal with the formulation of a new family of lower bounds for the mean dissipated heat in a general environmental-assisted erasure-protocol scenario, where Landauer's principle applies [4, 23]. After discussing the second principle of quantum thermodynamics in Section 6.1 and its equivalent formulation in terms of Landauer's principle in Section 6.2, we derive, again by means of a full-counting statistics approach, the above-mentioned family of lower bounds, which have the properties to be always asymptotically tight and also valid in a non-equilibrium scenario. Their explicit evaluations are carried out in a novel interesting quantum system consisting of a three-level V-system, externally pumped by a laser, and coupled to an environment made of a two-level system through an XX interaction. Analytic exact solutions for the dynamics of such system are also provided and discussed in Section 6.4.

Conclusions are finally drawn in Chapter 7.

2

Open quantum systems

2.1 Composite quantum systems

At the very root of open quantum systems theory lies the concept of composite quantum system, of which we will then now present the main notions that will be useful for our purposes.

As the name suggests, a composite quantum system is made of two (or more) quantum systems, generally interacting with each other, regarded as subsystems of the former. Without lack of generality, let us assume to deal with a composite quantum system made of two subsystems, which we label as S and E for future convenience.

Quantum mechanics associates to every physical system a separable Hilbert space $\mathscr{H}$, equipped with the scalar product $\langle\phi|\psi\rangle$, with $|\phi\rangle, |\psi\rangle \in \mathscr{H}$, and with the induced norm $\| \, |\psi\rangle \, \| = \sqrt{\langle\psi|\psi\rangle}$. Denoted with $\mathscr{H}_S$ and $\mathscr{H}_E$ the Hilbert spaces associated to the subsystems S and E respectively, the structure of the Hilbert space of the composite system SE is simply given by the tensor product $\mathscr{H}_{SE} = \mathscr{H}_S \otimes \mathscr{H}_E$. Given a generic Hilbert space $\mathscr{H}$, we will denote with $\mathcal{B}(\mathscr{H})$ the set of all linear and bounded operators O on the Hilbert space; such set is itself a Banach space with respect to the $\| \cdot \|_\infty$ norm defined as

$$\| \, O \, \|_\infty = \sup_{\||\psi\rangle\|=1} \| \, O \, |\psi\rangle \, \| \, . \tag{2.1}$$

In case of a composite system, given two linear operators $O_S \in \mathscr{B}(\mathscr{H}_S)$ and $O_E \in \mathscr{B}(\mathscr{H}_E)$, we can define the linear operator acting on $\mathscr{H}_{SE}$ by taking their tensor product $O_S \otimes O_E$ and any operator $O_{SE} \in \mathscr{B}(\mathscr{H}_{SE})$ can be written as

$$O_{SE} = \sum_k O_{S,k} \otimes O_{E,k}. \tag{2.2}$$

In particular, operators of one particular subsystem of a composite system, say S for convenience, take the form $O_S \otimes \mathbb{1}_E$, and are said to be *local* operators of S (or equivalently, to act locally on $\mathscr{H}_S$).

Moreover, given a positive operator $O \in \mathcal{B}(\mathscr{H})$ acting on a generic Hilbert space, i.e. such that

$$\langle\psi|O|\psi\rangle \geq 0 \qquad \forall\, |\psi\rangle \in \mathscr{H}, \tag{2.3}$$

its *trace*, given a complete orthonormal basis orthonormal basis $\{u_k\}_{k=1,2,\ldots} \in \mathscr{H}$, is defined as

$$\mathrm{Tr}\,[O] \equiv \sum_k \langle u_k|O|u_k\rangle\,. \tag{2.4}$$

If the trace is finite, i.e. if the series in Equation (2.4) converges, then the result is independent on the choice of the basis; the set of all operators $O \in \mathcal{B}(\mathscr{H})$ whose trace is finite, which will be denoted with $\mathcal{T}(\mathscr{H})$ and referred to as *the set of trace-class operators*, is a Banach space with respect to the so-called *trace norm* defined as

$$\parallel O \parallel_1 = \mathrm{Tr}\,[|O|] \qquad O \in \mathcal{T}(\mathscr{H}) \tag{2.5}$$

Whenever composite systems are taken into account, the trace can be carried out also on a particular subsystem S/E of the composite systems, thus producing an operator acting on the complementary Hilbert space one associated with the subsystem S/E (thus on E/S respectively). This operation, called *partial trace*, will be denoted with a pedex corresponding to the subsystem over which the operation is being performed, i.e.

$$O_{S/E} = \mathrm{Tr}_{E/S}\,[O_{SE}]\,, \tag{2.6}$$

which describes an average performed over the degrees of freedom of the system over which the trace is performed. From a physical point of view, the partial trace over a system corresponds to averaging out that contribution in favour of focusing the attention on the remaining subsystem.

A remarkable property of the trace is that it gives the following form of duality between $\mathcal{T}(\mathscr{H})$ and $\mathcal{B}(\mathscr{H})$

$$\begin{aligned} Tr :&\mathcal{B}(\mathscr{H}) \times \mathcal{T}(\mathscr{H}) \to \mathbb{C} \\ &(O, A) \mapsto \mathrm{Tr}\left[O^\dagger A\right] \end{aligned}\,, \tag{2.7}$$

which is well defined since the product of a trace class operator and of a bounded operator is still a trace class operator. Equation (2.7) defines a scalar product on $\mathcal{T}(\mathscr{H})$ [1] ,

[1] $\mathcal{T}(\mathscr{H})$ is a bilateral ideal of $\mathcal{B}(\mathscr{H})$, which means that $\forall O \in \mathcal{T}(\mathscr{H})$ and $\forall B \in \mathcal{B}(\mathscr{H})$, we have that the products OB, BO still belong to $\mathcal{T}(\mathscr{H})$ and in particular

$$\parallel BO \parallel_1 \leq \parallel B \parallel_\infty \parallel O \parallel_1\,. \tag{2.8}$$

Another important bilateral ideal of $\mathcal{B}(\mathscr{H})$ is represented by the set $\mathcal{HS}(\mathscr{H})$ made of linear operators on $\mathscr{H}$ such that

$$\mathrm{Tr}\left[O^\dagger O\right] < +\infty. \tag{2.9}$$

$\mathcal{HS}(\mathscr{H})$ is both a Hilbert space with respect to the Hilbert-Schmidt scalar product (2.13) and a Banach space with respect to the Hilbert-Schmidt norm

$$\parallel A \parallel_2 = \sqrt{\mathrm{Tr}\,[O^\dagger O]}, \qquad O \in \mathcal{HS}(\mathscr{H}). \tag{2.10}$$

known as *Hilbert-Schmidt* scalar product, defined as

$$\langle O, B\rangle = \mathrm{Tr}\left[O^\dagger B\right]. \tag{2.13}$$

According to the modern statistical formulation of quantum mechanics [6–8], a generic system's *state*, i.e. the representative of an equivalence class of preparation procedures, is represented by a trace class, semi-positive and with trace equal to 1 operator, called *statistical operator*, i.e. an element of

$$\mathcal{S}(\mathscr{H}) = \{\rho \in \mathcal{T}(\mathscr{H}) | \rho \geq 0, \parallel \rho \parallel_1 = 1\}, \tag{2.14}$$

which is a convex subset of $\mathcal{T}(\mathscr{H})$. The latter property physically traduces the possibility to consider a statistical mixture of states as a state itself. In particular, the extremal points of $\mathcal{S}(\mathscr{H})$, i.e. one dimensional projectors

$$\rho = |\Psi\rangle \langle\Psi|, \qquad |\Psi\rangle \in \mathscr{H}, \tag{2.15}$$

are referred to as *pure states* and correspond to the highest control in the preparation procedure since their Von-Neumann entropy

$$S(\rho) \equiv -\mathrm{Tr}\left[\rho \ln \rho\right] \tag{2.16}$$

is zero. In contrast, any state which can be written as a convex combination of pure states is said to be *mixed*

$$\rho = \sum_k \lambda_k |\Psi_k\rangle \langle\Psi_k|, \quad \lambda_k \geq 0, \sum_k \lambda_k = 1, \quad \langle\Psi_k|\Psi_l\rangle = \delta_{k,l}. \tag{2.17}$$

In the case of a composite quantum system, given a generic statistical operator $\rho_{SE} \in \mathcal{S}(\mathscr{H}_{SE})$ describing its state, one can introduce the statistical operators representing the states of the subsystems S and E, often called *marginals*, respectively by means of the partial trace (2.6)

$$\begin{aligned} \rho_S &\equiv \mathrm{Tr}_E\left[\rho_{SE}\right], \quad \rho_S \in \mathcal{S}(\mathscr{H}_S) \\ \rho_E &\equiv \mathrm{Tr}_S\left[\rho_{SE}\right], \quad \rho_E \in \mathcal{S}(\mathscr{H}_E). \end{aligned} \tag{2.18}$$

In the simplest case where the subsystems S and E do not interact with each other and thus are *uncorrelated*, the state of the composite system ρ_{SE} is given by a *factorized (or product) state* of the form

$$\rho_{SE} = \rho_S \otimes \rho_E. \tag{2.19}$$

Since the following chain of inequalities holds

$$\parallel B \parallel_\infty \leq \parallel B \parallel_2 \leq \parallel B \parallel_1, \tag{2.11}$$

it follows that

$$\mathcal{T}(\mathscr{H}) \subseteq \mathcal{HS}(\mathscr{H}) \subseteq \mathcal{B}(\mathscr{H}). \tag{2.12}$$

Note that, even though $O \in \mathcal{B}(\mathscr{H})$ is not positive, its Hilbert-Schmidt norm is well defined by virtue of the fact that the operator $|O| \equiv \sqrt{O^\dagger O}$ is positive by construction.

Another class of states describing a composite system are those of the form

$$\rho_{SE} = \sum_k p_k \rho_{S,k} \otimes \rho_{E,k}, \quad p_k \geq 0 \forall k, \sum_k p_k = 1, \tag{2.20}$$

with $\rho_{S/E,k} \in \mathcal{S}(\mathscr{H}_{S/E})$. These statistical operators physically correspond to states, referred to as *separable*, which have been prepared by means of local operations performed independently on the two subsystems plus a classical communication; correlations built up this way between S and E are only classical.

There is one other class of states of the composite system SE, i.e. the collection of all the statistical operators which cannot be represented as separable state. Such states are called *entangled*. The entanglement is a genuinely quantum feature and has a central role in many fields of application, such as for example quantum information theory and theoretical foundations problems. Since an extended exposition and discussion of the entanglement and its witnesses in a general framework are beyond the scopes of this Thesis, we refer the interested reader to [24].

Alongside with states, regarded as preparation procedures, in the statistical interpretation of quantum mechanics one associates to registration procedures, operated by suitable macroscopic devices, the *observables* of the system. Their mathematical representatives are given in terms of *positive operator-valued measures* (POVMs) which, provided Ω denotes the set of the possible outcomes of a measurement performed on a given observable and $\Sigma(\Omega)$ its $\sigma-$algebra, are linear and convex-preserving maps of the form

$$\begin{aligned} \mathcal{F} \,:\, \Sigma(\Omega) &\longrightarrow \mathcal{B}(\mathscr{H}) \\ M &\longrightarrow \mathcal{F}(M), \end{aligned} \tag{2.21}$$

where $\mathcal{F}(M) \in \mathcal{B}(\mathscr{H})$ is called *effect* and has the following properties:

$$0 \leq F(M) \leq \mathbb{1}, \tag{2.22}$$

$$F(\Omega) = \mathbb{1}, \tag{2.23}$$

$$F(\cup_k M_k) = \sum_k F(M_k) \quad \text{if } M_k \cap M_l = \emptyset \ \text{ for } k \neq l. \tag{2.24}$$

The effect $\mathcal{F}(M)$ is in general not idempotent, i.e. $\mathcal{F}^2(M) \neq \mathcal{F}(M)$; when it does, $\mathcal{F}(M)$ corresponds to a projection operator and we speak of *projection-valued measure* (PVM).

The final and key ingredient which combines together states and observables to give statistical predictions, which can then be compared with experimental quantities, is provided precisely by the above-introduced duality form (2.7), induced by the trace, between $\mathcal{T}(\mathscr{H})$ and $\mathcal{B}(\mathscr{H})$. Given a generic quantum system prepared in a state $\rho \in \mathcal{S}(\mathscr{H})$, the probability that a certain observable described by a POVM $\mathcal{F}$ takes value in a Borel set M is given by the so-called *Born rule*

$$\mu_\rho^F(M) = \mathrm{Tr}\left[\rho\, F(M)\right]. \tag{2.25}$$

This expression represents the deep core of the statistical formulation of quantum mechanics. [2]

2.1.1 Linear transformations

Let's now describe a general one-step transformation of the operators considered above without connecting them, for the moment, to any specific evolution process, as it is not necessary at this level of the discussion.

For convenience we will restrict our attention to the finite-dimensional case $\mathscr{H} \cong \mathbb{C}^N$. This also implies that

$$\mathcal{T}(\mathscr{H}) \cong \mathcal{B}(\mathscr{H}) \cong \mathcal{L}(\mathbb{C}^N), \tag{2.27}$$

with $\mathcal{L}(\mathbb{C}^N)$ being the space of linear operators on $\mathbb{C}^N$. It is worth noticing that $\mathcal{L}(\mathbb{C}^N)$ is a Hilbert space with respect to the Hilbert-Schmidt scalar product (2.13) $\langle \cdot, \cdot \rangle : \mathcal{L}(\mathbb{C}^N) \times \mathcal{L}(\mathbb{C}^N) \to \mathbb{C}$. By making use of it it, it is easy to introduce for every linear map $\Lambda \in \mathcal{L}(\mathbb{C}^N)$ the adjoint map $\Lambda^\dagger$ such that

$$\langle \Lambda^\dagger[\omega], \sigma \rangle = \langle \omega, \Lambda[\sigma] \rangle, \quad \forall \omega, \sigma \in \mathcal{L}(\mathbb{C}^N). \tag{2.28}$$

Moreover, a map Λ is said to be *positive* if

$$\langle \omega, \Lambda[\sigma] \rangle \geq 0, \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N). \tag{2.29}$$

Let's now consider a basis $\{\sigma_\alpha\}_{\alpha=1,\ldots,N^2}$ which is orthonormal in $\mathcal{L}(\mathbb{C}^N)$ with respect to the Hilbert-Schmidt scalar product (2.13), i.e.

$$\langle \sigma_\alpha, \sigma_\beta \rangle = \delta_{\alpha,\beta}. \tag{2.30}$$

Every linear map Λ which acts on $\mathcal{L}(\mathbb{C}^N)$, often also referred to as *superoperator*, can be expanded on this basis as

$$\Lambda[\omega] = \sum_{\alpha,\beta} \Lambda_{\alpha\beta} \mathrm{Tr}\left[\sigma_\beta^\dagger \, \omega\right] \sigma_\alpha, \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.31}$$

where

$$\Lambda_{\alpha\beta} = \langle \sigma_\alpha, \Lambda[\sigma_\beta] \rangle = \mathrm{Tr}\left[\sigma_\alpha^\dagger \, \Lambda[\sigma_\beta]\right]. \tag{2.32}$$

This representation is usually called *Hilbert-Schmidt* representation and, in what follows, we will denote with a boldface typeface the Hilbert-Schmidt matrix $\mathbf{\Lambda}$, with entries given by $\Lambda_{\alpha\beta}$, associated with Λ .

[2] Note that the properties of POVMs and of statistical operators guarantee that $\mu_\rho^F(M)$ is a real number between 0 and 1 and that the map

$$\begin{aligned} \mu_\rho^F \; : \; \Sigma(\Omega) \; &\longrightarrow [0,1] \\ M \; &\longrightarrow \mu_\rho^F(M) = \mathrm{Tr}\left[\rho \, F(M)\right] \end{aligned} \tag{2.26}$$

is a classical probability measure.

Moreover, the set of linear maps on $\mathcal{L}(\mathbb{C}^N)$ is itself a Hilbert space, denoted as $\mathcal{L}\left(\mathcal{L}(\mathbb{C}^N)\right)$, which can be identified with the algebra of the $N^2 \times N^2$ complex matrices and is equipped with respect a scalar product given by

$$(\Lambda_1, \Lambda_2) = \sum_\alpha \langle \Lambda_1[\sigma_\alpha], \Lambda_2[\sigma_\alpha] \rangle, \qquad \Lambda_1, \Lambda_2 \in \mathcal{L}\left(\mathcal{L}(\mathbb{C}^N)\right). \tag{2.33}$$

Two different sets of orthonormal bases for the set of linear transformations can thus be introduced, each one with reference to the scalar product defined on the respective Hilbert space. These two sets, which will be denoted as $\{E_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ and $\{F_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$, read

$$E_{\alpha\beta}[\omega] = \sigma_\alpha \mathrm{Tr}\left[\sigma_\beta^\dagger, \omega\right], \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.34}$$

$$F_{\alpha\beta}[\omega] = \sigma_\alpha \omega \sigma_\beta, \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.35}$$

and give rise to two representations of any generic superoperator that are equivalent but that allow to access some relevant properties in a more/less convenient way.

Given a generic superoperator Λ as considered before, its expansion on the basis $\{E_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ reads

$$\Lambda[\omega] = \sum_{\alpha\beta} \Lambda_{\alpha\beta} E_{\alpha\beta} = \sum_{\alpha,\beta} \Lambda_{\alpha\beta} \mathrm{Tr}\left[\sigma_\beta^\dagger \omega\right] \sigma_\alpha, \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.36}$$

with

$$\Lambda_{\alpha\beta} = (E_{\alpha\beta}, \Lambda) = \mathrm{Tr}\left[\sigma_\alpha^\dagger \Lambda[\sigma_\beta]\right]. \tag{2.37}$$

By direct confrontation with (2.31), it is straightforward to realize that this is equivalent to the Hilbert-Schmidt representation, this in turn meaning that the expansion on the first basis $\{E_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ corresponds to the interpretation of viewing the map Λ as a linear operator that acts on the Hilbert space $\mathcal{L}(\mathbb{C}^N)$. This representation is well suited for studying compositions of maps: if $\mathbf{\Lambda}_{1,2}$ denote in fact the two Hilbert-Schmidt matrices associated with the linear maps $\mathbf{\Lambda}_{1,2}$, the matrix associated with $\Xi = \Lambda_1 \circ \Lambda_2$ is simply given by the matrix product $\mathbf{\Xi} = \mathbf{\Lambda}_1 \mathbf{\Lambda}_2$. This will turn out to be useful in Section 2.2.3, when time-local expressions for the master equations will be derived.

Expansion of the superoperator Λ on the second basis $\{F_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ on the other hand leads to

$$\Lambda[\omega] = \sum_{\alpha\beta} \Lambda'_{\alpha\beta} F_{\alpha\beta} = \sum_{\alpha\beta} \Lambda'_{\alpha\beta} \sigma_\alpha \omega \sigma_\beta, \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.38}$$

where

$$\Lambda'_{\alpha\beta} = (F_{\alpha\beta}, \Lambda) = \sum_\gamma \mathrm{Tr}\left[\sigma_\beta \sigma_\gamma^\dagger \sigma_\alpha^\dagger \Lambda[\sigma_\gamma]\right]. \tag{2.39}$$

Even in this situation, the set of coefficients $\{\Lambda'_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ can be rearranged as the entries of a matrix which will denoted with $\mathbf{\Lambda}'$. This representation will be useful to check a very important property of linear maps, which is *complete positivity*. As we will discuss more thoroughly in Subsection 2.1.2, the complete positivity of Λ will in fact correspond to the positivity of the associated matrix $\mathbf{\Lambda}'$.

It is of course possible, finally, to move from one representation to the other simply as

$$\Lambda'_{\alpha'\beta'} = \sum_{\alpha\beta} \Lambda_{\alpha\beta}(F_{\alpha'\beta'}, E_{\alpha\beta}) = \sum_{\alpha\beta} \Lambda_{\alpha\beta} \mathrm{Tr}\left[\sigma_{\beta'}\sigma_{\beta}^{\dagger}\sigma_{\alpha'}^{\dagger}\sigma_{\alpha}\right] \tag{2.40}$$

and viceversa.

2.1.2 Complete positivity

The notion of *complete positivity* has a long history tracing back to Stinespring [25], Choi [26, 27] and Kraus [28]. Its enormous relevance in quantum mechanics is due to the fact that, together with the requirement of being trace-preserving, this property characterizes those linear maps which, among those introduced in the previous Subsection, properly describe well-defined and physically implementable quantum states transformations.

Definition 2.1. A linear map $\Lambda : \mathcal{T}(\mathscr{H}) \to \mathcal{T}(\mathscr{H})$, with $\mathscr{H} \cong \mathbb{C}^N$, is completely positive if and only if the map [3]

$$\Lambda \otimes \mathbb{1}_N : \mathcal{T}(\mathscr{H} \otimes \mathbb{C}^N) \to \mathcal{T}(\mathscr{H} \otimes \mathbb{C}^N) \tag{2.41}$$

is positive.

This property is evidently much more demanding than just positivity (see Equation (2.29)); a well-known example of a positive map which is not completely positive is represented by the transposition map, which thus does not represent either a physical evolution nor an implementable measurement procedure.

Physically, complete positivity traduces the following idea: if, alongside the quantum system of interest, whose evolution we assume to be given in terms of a map Λ, we consider an uncoupled ancillary system undergoing trivial evolution $\mathbb{1}_N$, the extended dynamics, described by $\Lambda \otimes \mathbb{1}_N$, is still positivity-preserving. Borrowing the notions from composite quantum systems above introduced, the combined map $\Lambda \otimes \mathbb{1}_N$ can thus be viewed as an operation which acts locally on one of the two subsystems without affecting the other one.

Completely positive maps, at variance with the positive ones, can be given an important representation provided by the well-known *Kraus decomposition*. It can be proven [27, 28] that a linear map $\Lambda \in \mathcal{L}(\mathbb{C}^N)$ is completely positive if and only if it can be written as

$$\Lambda[\omega] = \sum_{\alpha=1}^{N^2} \Omega_\alpha \omega \Omega_\alpha^{\dagger}, \tag{2.42}$$

where the operators $\Omega_\alpha \in \mathcal{L}(\mathbb{C}^N)$ are called *Kraus operators*.

[3] As stated above, for convenience we have restricted our attention to finite-dimensional quantum systems. The definition of complete positivity of a map in the infinite-dimensional case is that the extended map $\Lambda \otimes \mathbb{1}_n$ must be positive for any $n \in \mathbb{N}$.

Kraus decomposition has a direct connection with the representation of linear maps given by Equation (2.38). Suppose in fact that the $N^2 \times N^2$ matrix $\mathbf{\Lambda}'$ associated with the map Λ is positive definite (which means hermitian and with positive eigenvalues $\{\lambda'_\alpha\}_{\alpha=1,\dots,N^2}$); this implies that it can be diagonalized through a unitary matrix $\mathbf{U}$, i.e. $\mathbf{\Lambda}' = \mathbf{U}\mathbf{D}\mathbf{U}^\dagger$, where $\mathbf{D} = \mathrm{diag}\left(\lambda'_1, \dots, \lambda'_{N^2}\right)$ and where the columns of $\mathbf{U}$ are made by eigenvectors of $\mathbf{\Lambda}'$. If we now define the operators $\tilde{\boldsymbol{\sigma}} = \mathbf{U}\boldsymbol{\sigma}$, we immediately obtain that Equations (2.38) and (2.42) coincide upon the identification

$$\Omega_\alpha = \sqrt{\lambda'_\alpha}\tilde{\sigma}_\alpha. \tag{2.43}$$

As anticipated before, the complete positivity of a linear map Λ can be conveniently checked by looking at the positivity of the associated matrix $\mathbf{\Lambda}'$.

Finally, it is important for future purposes to introduce the more familiar *Choi matrix* Λ_{Choi} associated with a linear map Λ and to prove that it coincides with the representation of the map given by $\mathbf{\Lambda}'$, so that it can be exploited as well in order to study the complete positivity of Λ. First of all, consider the orthonormal basis $\{|u_k\rangle\}_{k=1,\dots,N}$ in $\mathscr{H} \cong \mathbb{C}^N$ and denote with $e_{kl} = |u_k\rangle\langle u_l|$ the induced orthonormal basis on $\mathcal{L}(\mathbb{C}^N)$. The Choi matrix associated with a linear map Λ is the matrix

$$\Lambda_{Choi} = \begin{pmatrix} \Lambda[e_{11}] & \Lambda[e_{12}] & \cdots & \Lambda[e_{1N}] \\ \Lambda[e_{21}] & \Lambda[e_{22}] & \cdots & \Lambda[e_{2N}] \\ \vdots & \vdots & \ddots & \vdots \\ \Lambda[e_{N1}] & \Lambda[e_{N2}] & \cdots & \Lambda[e_{NN}] \end{pmatrix}. \tag{2.44}$$

It is easy to see that the last expression can be equivalently re-expressed as

$$\Lambda_{Choi} = \sum_{kl} \Lambda[e_{kl}] \otimes e_{kl} = N\left(\Lambda \otimes \mathbb{1}_N\right)\left[|\phi\rangle_{ME}\langle\phi|_{ME}\right], \tag{2.45}$$

where the last equality has been obtained by introducing the maximally entangled state in $\mathscr{H} \otimes \mathscr{H} \cong \mathbb{C}^N \otimes \mathbb{C}^N$

$$|\phi\rangle_{ME} = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} |u_k\rangle \otimes |u_k\rangle. \tag{2.46}$$

Equation (2.45) represents a well-known and important theoretical result known as *Choi-Jamiołkowski* isomorphism between completely positive maps on $\mathcal{L}(\mathbb{C}^N)$ and states in $\mathbb{C}^N \otimes \mathbb{C}^N$. The property of Λ_{Choi} to be positive definite and its partial trace gives Id is then translated into the fact that the output state $\left(\Lambda \otimes \mathbb{1}_N\right)\left[|\phi\rangle_{ME}\langle\phi|_{ME}\right]$ is still a well-defined statistical operator in $\mathbb{C}^N \otimes \mathbb{C}^N$. Moreover it is immediate to see the positivity of Λ_{Choi} implies the positivity of $\Lambda \otimes \mathbb{1}_N$ and thus, in light of Definition 2.1, the complete positivity of Λ. We finally explicitly show the equivalence between the Choi matrix and the representation provided by Equation (2.38), i.e. $\mathbf{\Lambda}'$. On the one hand, the coefficients of the Choi matrix on the basis $|u_k, u_l\rangle \in \mathscr{H} \otimes \mathscr{H} \cong \mathbb{C}^N \otimes \mathbb{C}^N$ read

$$\begin{aligned} \langle u_k, u_l|\,\Lambda_{Choi}\,|u_{k'}, u_{l'}\rangle &= N\langle u_k, u_l|\left(\Lambda \otimes \mathbb{1}_N\right)\left[|\phi\rangle_{ME}\langle\phi|_{ME}\right]|u_{k'}, u_{l'}\rangle \\ &= \langle u_{k'}|\,\Lambda[|u_l\rangle\langle u_{l'}|]\,|u_{k'}\rangle. \end{aligned} \tag{2.47}$$

On the other hand, we have that the matrix elements $\Lambda'_{\alpha\beta}$ defined in Equation (2.39) on the basis e_{kl}, provided $\alpha \leftrightarrow (k,l)$, $\beta \leftrightarrow (k',l')$ and $\gamma \leftrightarrow (k'',l'')$, reads

$$\begin{aligned}\Lambda'_{\alpha\beta} &= \sum_{k'',l''} \mathrm{Tr}\left[|u_{k'}\rangle\langle u_{l'}| \, |u_{l''}\rangle\langle u_{k''}| \, |u_l\rangle\langle u_k| \; \Lambda[|u_{k''}\rangle\langle u_{l''}|]\right] \\ &= \langle u_{k'}| \; \Lambda[|u_l\rangle\langle u_{l'}|] \, |u_{k'}\rangle \, . \end{aligned} \tag{2.48}$$

which coincides with Equation (2.47).

2.2 Reduced dynamics: dynamical maps and master equations

In this Section it is shown how the concepts introduced above apply to the framework of open quantum systems. As we stated at the beginning of this Chapter, the notion of composite quantum systems stands at the basis of open quantum systems. A bipartite structure like the one considered in Section 2.1 in fact arises very naturally whenever our quantum system of interest interacts with an external environment, often also referred to as bath or reservoir to stress that it is usually considered having much more degrees of freedom than the system. The overall system is assumed to be closed, so that its dynamics is given in terms of a unitary evolution. It is however often the case that the description of this overall dynamics is too complicated by the presence of the environment and thus unfeasible even by means of numerical simulations. In any case, even in the rare situations where this approach turns out to be attainable, one would get from it a huge amount of unnecessary information for a sufficiently complete description of the system and of its dynamics. Last but not least, in practical situations it may often be the case that an experimental control is achievable only on a small part of the full system.

For all these reasons one is naturally led to consider a reduced description given in terms of a restricted set of relevant dynamical variables while performing an average over the remaining degrees of freedom. It is immediately clear then that we can apply the whole construction put forward in Section 2.1 with S denoting the reduced system we focus on and E denoting the environment, whose presence modifies the dynamics of the former (that is why we used the labels S and E from the beginning).

2.2.1 Dynamical maps

Let $\mathscr{H}_S$ and $\mathscr{H}_E$ be respectively the Hilbert spaces associated with the system, often simply called *open system*, and the environment (degrees of freedom of the composite system we are not interested in, which will be therefore averaged off). The reduced system is represented by the reduced state obtained from the total state through Equation (2.18)

$$\rho_S = \mathrm{Tr}_E\left[\rho_{SE}\right], \tag{2.49}$$

where $\mathrm{Tr}_E\left[\cdot\right]$ denotes the partial trace over $\mathscr{H}_E$.

Since the overall system is assumed closed, its dynamics is governed by a total Hamiltonian which can be written as

$$\mathcal{H}_{Tot}(t) = \mathcal{H}_S(t) \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \mathcal{H}_E(t) + \mathcal{H}_{SE}(t), \tag{2.50}$$

where every interaction between the reduced system and the environment is contained in the interaction Hamiltonian term $\mathcal{H}_{SE}(t)$. The evolution operator thus becomes

$$\mathcal{U}(t, t_0) = \overleftarrow{T} \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} ds\, \mathcal{H}_{Tot}(s)\right] \tag{2.51}$$

where $\overleftarrow{T}$ is the chronological time-ordering operator, whose action is to order products of time-dependent operators such that their time-arguments increase from right to left. The total state of the composite system is then formally given by

$$\rho_{SE}(t) = \mathcal{U}(t, t_0)\rho_{SE}(t_0)\mathcal{U}^\dagger(t, t_0) \tag{2.52}$$

and the latter, by means of the partial trace over the environmental degrees of freedom, gives the reduced state at time t

$$\rho_S(t) = \mathrm{Tr}_E\left[\mathcal{U}(t, t_0)\rho_{SE}(t_0)\mathcal{U}^\dagger(t, t_0)\right]. \tag{2.53}$$

This way one establishes a family of linear maps $\Xi : \mathcal{S}(\mathscr{H}_S \otimes \mathscr{H}_E) \to \mathcal{S}(\mathscr{H}_S)$ such that

$$\rho_{SE}(t_0) \mapsto \rho_S(t) = \Upsilon(t, t_0)\rho_{SE}(t_0) = \mathrm{Tr}_E\left[\mathcal{U}(t, t_0)\rho_{SE}(t_0)\mathcal{U}^\dagger(t, t_0)\right] \tag{2.54}$$

which are completely positive and trace preserving (CPTP), since any unitary map is CPTP, the partial trace is CPTP and any composition of two CPTP map is again a CPTP map.

However, in order to give a self-consistent description of the reduced dynamics which is solely based on the open quantum system, an endomorphism of the set $\mathcal{S}(\mathscr{H}_S)$ has however to be introduced, which thus associates to any reduced state $\rho_S(t_0)$ its corresponding evolved state $\rho_S(t)$ at a subsequent time t. This can be done if we assume that the initial total state is a factorized state, i.e. of the form

$$\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0). \tag{2.55}$$

The definition of a linear map $\Lambda(t, t_0) : \mathcal{S}(\mathscr{H}_S) \to \mathcal{S}(\mathscr{H}_S)$ such that

$$\rho_S(t_0) \mapsto \rho_S(t) = \Lambda(t, t_0)\rho_S(t_0) = \mathrm{Tr}_E\left[\mathcal{U}(t, t_0)(\rho_S(t_0) \otimes \rho_E(t_0))\mathcal{U}^\dagger(t, t_0)\right] \tag{2.56}$$

can then be properly introduced. $\Lambda(t, t_0)$ is in this case called *quantum dynamical map*. The latter is CPTP by construction, which can be easily seen by considering a spectral decomposition of the environmental state $\rho_E(t_0) = \sum_k p_k |\phi_k\rangle \langle\phi_k|$ and elaborating as

follows

$$\begin{aligned}\rho_S(t) &= \mathrm{Tr}_E\left[U(t,t_0)\ (\rho_S(t_0)\otimes\rho_E(t_0))\ U^\dagger(t,t_0)\right]\\ &= \sum_j \langle\phi_j|\, U(t,t_0)\ \left[\rho_S(0)\otimes\left(\sum_k p_k\,|\phi_k\rangle\,\langle\phi_k|\right)\right] U^\dagger(t,t_0)\,|\phi_j\rangle\\ &= \sum_{jk}\left(\sqrt{p_k}\,\langle\phi_j|\, U(t,t_0)\,|\phi_k\rangle\right)\ \rho_S(0)\ \left(\sqrt{p_k}\,\langle\phi_k|\, U^\dagger(t,t_0)\,|\phi_j\rangle\right)\\ &= \sum_{jk}\Omega_{jk}(t,t_0)\rho_S(0)\Omega^\dagger_{jk}(t,t_0),\end{aligned} \tag{2.57}$$

where $\Omega_{jk}(t,t_0)\equiv\sqrt{p_k}\,\langle\phi_j|\, U(t,t_0)\,|\phi_k\rangle$. It is evident that this expression corresponds to a Kraus decomposition (2.42), thus guaranteeing the complete positivity of the map $\Lambda(t,t_0)$. Finally, the trace-preserving character is an immediate consequence of the unitarity of the operator $U(t,t_0)$.

2.2.2 Master equations

In the previous Section it has been shown how the evolution of open quantum systems can be consistently given in terms of the so-called family of quantum dynamical maps, which act at the level of the reduced system, obtained by partial trace over the environment of the total unitary evolution operator. Nevertheless it is often the situation in physics that one has to deal with equations of motion rather than with evolution maps, which are instead usually obtained by solving the former. When such equations of motion are relative to the reduced system only we speak of *master equations*, which represent the topic of the present Section. In particular we will show how the latter can be obtained from the unitary evolution or from the dynamical map and, viceversa, how to reconstruct the dynamical maps from the knowledge of the master equations. Moreover, we will investigate which constraints can be imposed on the structure of the master equations such that to lead to physically implementable dynamics, i.e. giving rise to CPTP dynamical maps. The latter problem is in fact of great relevance, since master equations are usually introduced either through several approximations, either on a phenomenological basis, thus losing a priori the equivalence with the full unitary dynamics.

2.2.2.1 Projection operator approach to the description of the reduced system's dynamics

Starting from the unitary time evolution of the composite system it is possible to derive by means of the *projection operator technique*, the master equation for the reduced statistical operator. This technique, on which more extensive presentations can be found in the literature (see for example [21]), stems from the general idea that, when we have to deal with a composite system made of a relevant subsystem and a (possibly complex) environment, a way to try to obtain a manageable dynamics is to get rid of the unimportant degrees of freedom by means of some projection operator.

A projection operator is defined as a linear map $\mathcal{P}$ which sends states into states, thus being completely positive and trace-preserving, and which is in addition idempotent $\mathcal{P}^2 = \mathcal{P}$. Consider the generic situation described many times above where a system S is coupled to an environment E such that the dynamics of the overall system is dictated by an Hamiltonian of the form $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \lambda\mathcal{H}_{SE}$, with λ being a constant denoting the coupling strength between S and E. Within this generic framework, one can introduce two projection operators $\mathcal{P}$ and $\mathcal{Q}$ whose actions on a generic element $\rho_{SE} \in \mathcal{S}(\mathscr{H}_S \otimes \mathscr{H}_E)$ is defined as

$$\begin{aligned} \mathcal{P}\rho_{SE} &\equiv \mathrm{Tr}_E\left[\rho_{SE}\right] \otimes \rho_E \equiv \rho_S \otimes \rho_E, \\ \mathcal{Q}\rho_{SE} &= \left(\mathbb{1} - \mathcal{P}\right)\rho_{SE}, \end{aligned} \tag{2.58}$$

with ρ_E being a *fixed* state of the environment, usually taken to be the stationary Gibbs state $\rho_\beta = e^{-\beta\mathcal{H}_E}/\mathrm{Tr}_E\left[e^{-\beta\mathcal{H}_E}\right]$. These two maps have the properties to be idempotent, i.e. $\mathcal{P}^2 = \mathcal{P}$ and same for $\mathcal{Q}$, and to satisfy $\mathcal{P} + \mathcal{Q} = \mathbb{1}$ and $\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$).

The state $\mathcal{P}\rho_{SE}$ is often called *relevant part* of the statistical operator ρ_{SE}, due to the possibility to reconstruct the reduced statistical operator simply by means of the partial trace over the environment

$$\rho_S = \mathrm{Tr}_E\left[\mathcal{P}\rho_{SE}\right]. \tag{2.59}$$

Correspondingly, the state $\mathcal{Q}\rho_{SE}$ is referred to as *irrelevant part*.

Starting from the the Liouville-Von Neumann master equation for ρ_{SE} in the interaction picture (denoted by a " $\sim$ " over the quantities)

$$\frac{d}{dt}\tilde{\rho}_{SE}(t) = -i\lambda\left[\tilde{\mathcal{H}}_{SE}(t), \tilde{\rho}_{SE}(t)\right] = \lambda\tilde{\mathcal{L}}(t)\tilde{\rho}_{SE}(t), \tag{2.60}$$

one obtains the corresponding two equations of motion

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}_{SE}(t) = \mathcal{P}\frac{d}{dt}\tilde{\rho}_{SE}(t) = \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\rho}_{SE}(t) = \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}_{SE}(t), \tag{2.61}$$

$$\frac{d}{dt}\mathcal{Q}\tilde{\rho}_{SE}(t) = \mathcal{Q}\frac{d}{dt}\tilde{\rho}_{SE}(t) = \lambda\mathcal{Q}\tilde{\mathcal{L}}(t)\tilde{\rho}_{SE}(t) = \lambda\mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \lambda\mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}_{SE}(t). \tag{2.62}$$

The aim being to obtain a closed equation of motion for the relevant part of $\tilde{\rho}_{SE}$, we first formally solve the second equation to get

$$\mathcal{Q}\tilde{\rho}_{SE}(t) = \mathcal{G}(t, t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \lambda\int_{t_0}^{t} ds\mathcal{G}(t, s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\rho}_{SE}(s), \tag{2.63}$$

with

$$\mathcal{G}(t, s) \equiv \overleftarrow{T}\exp\left[\lambda\int_s^t d\tau\mathcal{Q}\tilde{\mathcal{L}}(\tau)\right] \tag{2.64}$$

being the forward-time propagator.and $\overleftarrow{T}$ being the time-ordering operator defined in Equation (2.51), and we substitute it into the first one, obtaining

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}_{SE}(t) = \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{G}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \lambda^2\int_{t_0}^{t} ds\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{G}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\rho}_{SE}(s). \quad (2.65)$$

This result has been obtained without any assumption or approximation. A great simplification can be obtained by considering that the total initial state is factorized, which implies $\mathcal{Q}\tilde{\rho}_{SE}(0) = 0$, and furthermore assuming that $\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P} = 0$ (which can always be set upon a shift in the interaction Hamiltonian), under which Equation (2.65) reduces to the following *time non-local* equation, often called *Nakajima-Zwanzig* equation,

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}_{SE}(t) = \int_{t_0}^{t} ds\,\mathcal{K}_{NZ}(t,s)\mathcal{P}\tilde{\rho}_{SE}(s), \quad (2.66)$$

with $\mathcal{K}_{NZ}(t,s) = \lambda^2\mathcal{P}\tilde{\mathcal{L}}(t)D(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}$. In light of its form $\mathcal{K}_{NZ}(t,\tau)$ is commonly called *memory kernel*. Equation (2.63) can be cast into an equivalent but local in time equation by introducing the backward-time propagator

$$\mathscr{G}(t,s) \equiv \overrightarrow{T}\exp\left[-\lambda\int_{s}^{t} d\tau\tilde{\mathcal{L}}(\tau)\right], \quad (2.67)$$

with $\overrightarrow{T}$ being the anti-chronological ordering operator, and inserting it into the expression for the formal solution of the irrelevant part of the statistical operator

$$\mathcal{Q}\tilde{\rho}_{SE}(t) = \mathcal{G}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \lambda\int_{t_0}^{t} ds\mathcal{G}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\mathscr{G}(t,t_0)\left(\mathcal{P}+\mathcal{Q}\right)\tilde{\rho}_{SE}(t). \quad (2.68)$$

Upon defining the operator

$$\Sigma(t) = \lambda\int_{t_0}^{t} ds\mathcal{G}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\mathscr{G}(t,t_0), \quad (2.69)$$

expression (2.68) reads

$$\left(1-\Sigma(t)\right)\mathcal{Q}\tilde{\rho}_{SE}(t) = \mathcal{G}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \Sigma(t)\mathcal{P}\tilde{\rho}_{SE}(t). \quad (2.70)$$

Solving with respect to $\mathcal{Q}\tilde{\rho}_{SE}(t)$ and inserting the result into the equation of motion for the relevant part leaves with

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}_{SE}(t) = \mathcal{K}_{TCL}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \mathcal{I}(t)\mathcal{Q}\tilde{\rho}_{SE}(t), \quad (2.71)$$

where

$$\mathcal{K}_{TCL}(t) \equiv \lambda\mathcal{P}\tilde{\mathcal{L}}(t)\left(1-\Sigma(t)\right)^{-1}\mathcal{P} \quad (2.72)$$

is the *time-local generator* and

$$\mathcal{I}(t) \equiv \lambda\mathcal{P}\tilde{L}(t)\left(1-\Sigma(t)\right)^{-1}\mathcal{G}(t,t_0)\mathcal{Q} \quad (2.73)$$

denotes the inhomogenous contribution. Though we will return on this in Chapter 4, we note that the inhomogeneous term vanishes in the case system and environment are uncorrelated to each other. While this condition is assumed to be true at the initial time $t = t_0$, it is almost certainly not met at generic time t, since the coupled evolution between system and environment leads to the onset of correlations between S and E. This fact thus play a role in the determination of two-time correlation functions, as will be made explicit in the following Chapter.

2.2.2.2 Perturbation expansion of the time-local generator

Both the forms of the time-local generator $\mathcal{K}_{TCL}(t)$ and of the inhomogeneity $\mathcal{I}(t)$ are in general very difficult to be accessed in an exact way and, even in the case of an initially factorized total state (so that $\mathcal{I}(t) = 0$), it is very rare to be able to write down an exact evolution equation for the relevant part $\mathcal{P}\tilde{\rho}_{SE}$ and thus, by means of the partial trace over the environment, an exact closed master equation for $\tilde{\rho}_S(t)$. It is often the case that a set of physically sensible approximations is performed on the specific model under consideration, which allows to obtain simplified forms for $\mathcal{K}_{TCL}(t)$. The most common systematic approach is to expand the time-local generator in powers of the coupling strength λ and then truncate the series to the first lowest terms, thus invoking a weak coupling approximation. Since this method will be largely employed in this work of Thesis too, we will briefly recall this method and the respective results.

First of all, we notice that the term $(1 - \Sigma(t))^{-1}$ appearing in Equation (2.72) can be expanded in geometric series [4] as

$$(1 - \Sigma(t))^{-1} = \sum_{n=0}^{+\infty} [\Sigma(t)]^n \,. \tag{2.74}$$

The time-local generator then reads

$$\mathcal{K}_{TCL}(t) = \lambda \sum_{n=0}^{+\infty} \mathcal{P}\tilde{\mathcal{L}}(t) \, [\Sigma(t)]^n \, \mathcal{P}. \tag{2.75}$$

Now, by expanding both $\Sigma(t)$ and $\mathcal{K}_{TCL}(t)$ in powers of λ as

$$\Sigma(t) = \sum_{m=1}^{+\infty} \lambda^m \Sigma^{(m)}(t), \quad \mathcal{K}_{TCL}(t) = \sum_{m=1}^{+\infty} \lambda^m \mathcal{K}_{TCL}^{(m)}(t), \tag{2.76}$$

and comparing terms relative to the same power of λ, we get that

$$\mathcal{K}_{TCL}^{(1)}(t) = \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}, \quad \mathcal{K}_{TCL}^{(2)}(t) = \mathcal{P}\tilde{\mathcal{L}}(t)\Sigma^{(1)}(t)\mathcal{P}, \tag{2.77}$$

where

$$\Sigma^{(1)}(t) = \int_0^t ds \mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{P}. \tag{2.78}$$

[4] Since Equation (2.72) we are assuming that $(1 - \Sigma(t))^{-1}$ exists, which is the case for small times t or for not too large values of the coupling λ.

Further terms proportional to higher powers of λ can be considered; the interested reader is referred to [21]. By making use of the above-mentioned condition $\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P} = 0$, the master equation for the statistical operator $\tilde{\rho}_S(t)$ at second order in λ is therefore given by

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\lambda^2 \int_0^t ds \mathrm{Tr}_E \left\{ \left[\tilde{\mathcal{H}}_{SE}(t), \left[\tilde{\mathcal{H}}_{SE}(s), \tilde{\rho}_S(t) \right] \right] \right\}. \tag{2.79}$$

This form of the master equation will be considered many times in this Thesis.

It is finally worth noticing that even the inhomogeneity $\mathcal{I}(t)$ can be in principle expanded in series of power of λ in the exact same way; since we were considering, as previously stated, that $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$, this term has been neglected since vanishing but it will play an important role in the determination of the validity of the so-called quantum regression theorem (see Chapter 4), when it will be applied to a state at time t, not necessarily in factorized form any more.

2.2.3 From dynamical maps to master equations and vice-versa

In Subsection 2.2.2.1 we have seen how to derive a master equation for the reduced statistical operator starting from the microscopic knowledge of the model under examination, i.e. the Hamiltonian of the composite system, by means of projection operators. It is often the case that this amount of information on the overall system is not accessible, and instead only the evolution of the reduced system is known in terms of a family of CPTP dynamical maps. In this Subsection we explicitly show how a master equation can be derived from the knowledge of $\Lambda(t, t_0)$. In particular, we will focus our attention to those in time-local form, which are often more manageable and in particular will turn out to be more useful in order to access dynamical properties such as non-Markovianity. It is important to stress that this does not entail any loss of generality. In Subsection 2.2.2.1, the time non-local and the time-local master equations obtained by taking the trace over the environment of Eqs. (2.66) and (2.72) respectively, were by construction formally equivalent to each other.

Consider a one-parameter family of quantum dynamical maps $\{\Lambda(t, t_0)\}_{t \geq t_0}$, where every $\Lambda(t, t_0)$ is a CPTP linear map on $\mathcal{L}(\mathbb{C}^N)$. Its action on a generic state of the system $\rho_S(t_0)$ is to output another state $\rho_S(t)$ at time t, i.e.

$$\rho_S(t) = \Lambda(t, t_0)\rho_S(t_0). \tag{2.80}$$

Under the rather mild assumption of differentiability with respect to time and invertibility of $\Lambda(t, t_0)$, it is immediate to construct a time-local master equation

$$\frac{d}{dt}\rho_S(t) = \left[\frac{d}{dt}\Lambda(t, t_0) \right] \Lambda^{-1}(t, t_0)\rho_S(t) \equiv \mathcal{K}_{TCL}(t)\rho_S(t), \tag{2.81}$$

with $\mathcal{K}_{TCL}(t)$ being the time-local generator defined in Equation (2.72). Since the latter is then given by the composition of two linear maps, the representation of the three superoperators on the basis $\{E_{\alpha\beta}\}_{\alpha,\beta=0}^{N^2-1}$ given by Equation (2.36) is the most suited since,

as stated in Subsec 2.1.1, the composition of maps is translated into the product of the associated matrices, i.e.

$$\mathbf{K}^{TCL}(t) = \left[\frac{d}{dt}\mathbf{\Lambda}(t,t_0)\right]\mathbf{\Lambda}^{-1}(t,t_0). \tag{2.82}$$

In Subsection 2.2.4 we will put constraints on the structure of the master equation (2.82) in light of the properties of the dynamical map $\Lambda(t,t_0)$.

Finally, starting instead from the knowledge of the time-local generator $\mathcal{K}_{TCL}(t)$, the dynamical map $\Lambda(t,t_0)$ can be reconstructed by making use of the Dyson series expansion

$$\Lambda(t,0) = \overleftarrow{T}\exp\left[\int_0^t d\tau\,\mathcal{K}_{TCL}(\tau)\right], \tag{2.83}$$

where again $\overleftarrow{T}$ denotes the chronological time-ordering operator and the convergence of the series is guaranteed by the boundedness of $\mathcal{K}_{TCL}(t)$ due to the finite-dimensionality of the Hilbert space we are focusing on.

2.2.4 Structure of time-local master equations

As already stressed above, it is often the case that open system's dynamics are investigated through equations of motion, being local as well as non-local in time, not obtained from the full unitary evolution, but rather introduced on the basis of phenomenological approximations and ansatz that ultimately depend on the model considered. Since the equivalence with the full unitary evolution is therefore lost, it is not *a priori* guaranteed that they lead to a well-defined time evolution: it still represents an open problem to determine in full generality which is the operatorial structure of those master equations which lead to proper well-defined reduced evolutions. The aim of the three following Subsections is to tackle this topic by showing which properties of the dynamical map describing the reduced dynamics reflect in determine constraints on the structure of the associated master equation and, viceversa, which features of the latter can guarantee a proper and physically implementable dynamical map.

2.2.4.1 Trace and hermiticity preservation

Consider as our starting point a time-local master equation with a time-local generator $\mathcal{K}_{TCL}(t)$ given by Equation (2.72), either obtained from the unitary evolution through the projection-operator method, either from the knowledge of the dynamical map $\Lambda(t,t_0)$ through Equation (2.82). It is very important to notice that, by construction, $\mathcal{K}_{TCL}(t)$ satisfies the two following conditions

$$\mathrm{Tr}\left[K_{TCL}(t)\,\omega\right] = 0, \qquad \forall\omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.84}$$

$$\left(K_{TCL}\,\omega\right)^\dagger = K_{TCL}\,\omega^\dagger, \qquad \forall\omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.85}$$

which respectively reflects trace and hermiticity preservation of the evolution map.

Notice that we are not taking into account, the role that complete positivity has on fixing constraints on the structure of the associated time-local master equation, posticipating it to the two following, and conclusive, Subsections.

Consider now a basis $\{\sigma_\alpha\}_{\alpha=0,\dots N^2-1}$ on $\mathcal{L}(\mathbb{C}^N)$ such that it is orthonormal with respect to the Hilbert-Schmidt scalar product and moreover satisfies the following constraints

$$\sigma_0 = \frac{\mathbb{1}}{\sqrt{N}}, \tag{2.86}$$

$$\mathrm{Tr}\left[\sigma_\alpha\right] = 0, \quad \text{for}\, \alpha \neq 0, \tag{2.87}$$

it is possible to prove [29] that any trace and hermiticity preserving linear map Ξ on $\mathcal{L}(\mathbb{C}^N)$ can be expressed on this basis as

$$\Xi\,\omega = -i\left[\mathcal{H},\omega\right] + \sum_{\alpha\beta=1}^{N^2-1} \Xi'_{\alpha\beta}\left(\sigma_\alpha\omega\sigma_\beta^\dagger - \frac{1}{2}\{\sigma_\beta^\dagger\sigma_\alpha,\omega\}\right), \quad \forall\omega\in\mathcal{L}(\mathbb{C}^N), \tag{2.88}$$

where $\{\Xi'_{\alpha\beta}\}_{\alpha,\beta=0,\dots,N^2-1}$ are the coefficients of the matrix $\boldsymbol{\Xi}'$ associated to the map through the representation (2.38) and

$$\mathcal{H} = \frac{1}{2i}\left(\sigma^\dagger - \sigma\right) \tag{2.89}$$

denotes an effective Hamiltonian with

$$\sigma = \frac{1}{\sqrt{N}}\sum_{\alpha=1}^{N^2-1}\Xi'_{\alpha0}\sigma_\alpha. \tag{2.90}$$

The matrix $\boldsymbol{\Xi}'$ is hermitian, i.e.

$$\Xi'_{\alpha\beta} = \Xi'^*_{\beta\alpha}, \qquad \forall\alpha,\beta = 0,\dots,N^2-1 \tag{2.91}$$

due to the request of hermiticity preservation.

The application, by virtue of Eqs. (2.84), of this procedure to the time-local generator allows to express it as

$$\frac{d}{dt}\rho_S(t) = \mathcal{K}_{TCL}(t)\rho_S(t) = -i\left[\mathcal{H}(t),\rho_S(t)\right] + \sum_{\alpha\beta=1}^{N^2-1} K'^{TCL}_{\alpha\beta}(t)\left(\sigma_\alpha\rho_S(t)\sigma_\beta^\dagger - \frac{1}{2}\{\sigma_\beta^\dagger\sigma_\alpha,\rho_S(t)\}\right), \tag{2.92}$$

with

$$\begin{aligned}\mathcal{H} &= \frac{1}{2i}\left(\sigma^\dagger(t) - \sigma(t)\right),\\ \sigma(t) &= \frac{1}{\sqrt{N}}\sum_{\alpha=1}^{N^2-1}\left[\mathcal{K}'_{TCL}\right]_{\alpha0}(t)\sigma_\alpha,\end{aligned} \tag{2.93}$$

where the coefficients $\left(\left[\mathcal{K}'_{TCL}\right]_{\alpha\beta}(t)\right)^* = \left[\mathcal{K}'_{TCL}\right]_{\beta\alpha}(t)$ are the entries of the matrix $\mathbf{K}'_{TCL}(t)$ relative to the expansion of the time-local generator $\mathcal{K}_{TCL}$ on the basis $\{F_{\alpha\beta}\}_{\alpha,\beta=0}^{N^2-1}$, see Equation (2.38). The first term of equation (2.92) consists of an unitary contribution due

to the effective Hamiltonian $\mathcal{H}$, while the remaining part takes into account for the dissipative and decoherent effects due to the interaction with the environment. The submatrix made of the entries $\{\mathcal{K}_{TCL}(t)\}_{\alpha\beta=1,\dots,N^2-1}$ obtained from $\mathbf{K_{TCL}(t)}$ by removing the first row and column is still hermitian and thus there exist for any time t unitary matrices $\mathbf{V}(t)$ which diagonalize it

$$\mathbf{K_{TCL}}(t) = \mathbf{V}(t)\mathbf{\Gamma}(t)\mathbf{V}^*(t), \tag{2.94}$$

with $\mathbf{\Gamma}(t) = \mathrm{diag}\left(\gamma_1(t), \dots, \gamma_{N^2-1}(t)\right)$ and $\gamma_k(t)$ real functions of time $\forall k = 1, \dots, N^2-1$. It is then possible to write the master equation in diagonal form

$$\frac{d}{dt}\rho_S(t) = -i\left[\mathcal{H}(t), \rho_S(t)\right] + \sum_{k=1}^{N^2-1} \gamma_k(t)\left(\tilde{\sigma}_k(t)\rho_S(t)\tilde{\sigma}_k^\dagger(t) - \frac{1}{2}\{\tilde{\sigma}_k^\dagger(t)\tilde{\sigma}_k(t), \rho_S(t)\}\right), \tag{2.95}$$

where

$$\tilde{\sigma}_k(t) = \sum_{\alpha=1}^{N^2-1} V_{k\alpha}(t)\sigma_\alpha. \tag{2.96}$$

2.2.4.2 Complete positivity and time-local master equations: Quantum dynamical semigroups and the Gorini-Kossakowski-Sudarshan-Lindblad master equation

In the previous Subsection we have seen how the properties of a dynamical map to be trace and hermiticity preserving traduces into a set of constraints on the structure of the associated time-local master equation. In this and the following Subsections we will focus on another important property which characterizes, as stressed above, physically well-defined dynamical maps: complete positivity. The first benchmark result in this direction was provided by Gorini, Kossakowski, Sudarshan and Lindblad in 1976 [29], who found the most general form of time-local generators describing a sub-class of dynamics called *completely-positive quantum dynamical semigroups*.

First of all, a one-parameter family of quantum dynamical maps $\{\Lambda(t, t_0)\}_{t\geq t_0}$ is said to be a *completely positive quantum dynamical semigroup* [30] if it satisfies the following conditions

$$\begin{aligned} &\Lambda(t_0, t_0) = \mathbb{1}, \\ &\Lambda(t, t_0) = \Lambda(t, s)\Lambda(s, t_0)., \quad \forall t, s \geq t_0, \end{aligned} \tag{2.97}$$

with $\Lambda(t, s)$ being time-homogeneous, i.e. $\Lambda(t, s) = \Lambda(t - s)$.

For such a family of dynamical maps the well known Gorini-Kossakowski-Sudarshan-Lindblad theorem provides a complete characterization of the generator of the semigroup dynamics: in the finite dimensional case $\mathscr{H} \simeq \mathbb{C}^N$ and choosing $t_0 = 0$ for simplicity of notation it reads [29]

Theorem 2.2 (**Gorini-Kossakowski-Sudarshan-Lindblad** (GKSL)). *A linear operator $L \in \mathcal{L}(\mathbb{C}^N)$ is the generator of a completely positive quantum dynamical semigroup $\{\Lambda(t, 0)\}_{t\geq 0}$,*

with

$$\Lambda(t,0) = e^{t\,L}, \tag{2.98}$$

or equivalently

$$L = \lim_{t\to 0^+} \frac{\Lambda(t,0) - \mathbb{1}}{t}, \tag{2.99}$$

if and only if *it can be expressed as*

$$L\,\omega = -i\,[\mathcal{H},\omega] + \sum_{k=1}^{N^2-1} \gamma_k \left(\sigma_k \omega \sigma_k^\dagger - \frac{1}{2}\{\sigma_k^\dagger \sigma_k, \omega\}\right), \quad \forall \omega \in \mathcal{L}(\mathbb{C}^N), \tag{2.100}$$

with $\gamma_k \geq 0 \quad \forall k = 1,\ldots,N^2-1$, $\mathcal{H}^\dagger = \mathcal{H}$ *and* $\sigma_k \in \mathcal{L}(\mathbb{C}^N)$.

A generalization of the validity of this theorem to the case of infinite dimensional Hilbert spaces can be found in [31].

It directly follows from this Theorem that if the evolution of a reduced system $\rho_S(t)$ is given by the following master equation

$$\frac{d}{dt}\rho_S(t) = L\rho_S(t) = -i\,[\mathcal{H},\rho_S(t)] + \sum_{k=1}^{N^2-1} \gamma_k \left(\sigma_k \rho_S(t) \sigma_k^\dagger - \frac{1}{2}\{\sigma_k^\dagger \sigma_k, \rho_S(t)\}\right) \tag{2.101}$$

with $\gamma_k \geq 0$, $\mathcal{H}^\dagger = \mathcal{H}$ and $\sigma_k \in \mathcal{L}(\mathbb{C}^N)$, then the dynamical map $\Lambda(t,t_0)$ described a completely positive quantum dynamical semigroup and viceversa.

Few considerations deserve to be made. First of all, if we compare the structure of the GKSL generator (2.100) and the time-local generator $\mathcal{K}_{TCL}(t)$ given in Equation (2.95), it is immediately evident that the differences lie in the fact that the Lindblad operators as well as the coefficients γ_k do not depend on time and the latter are forced to be *positive* by the request of complete positivity of $\Lambda(t,0)$. The trace and hermiticity preservation in fact did not allow to put any constraint on the sign on the various $\gamma_k(t)$ beside them being real functions of time. We will see in Chapter 3 that this fact plays a crucial role in the characterization of quantum non-Markovianity.

Another important feature of the structure of the generator given by (2.100) is its invariance under unitary transformations of the set of operators

$$\sqrt{\gamma_k}\sigma_k \mapsto \sqrt{\tilde{\gamma}_k}\tilde{\sigma}_k = \sum_{l=1}^{N^2-1} u_{kl}\sqrt{\gamma_l}\sigma_l, \quad \{u_{kl}\} \in \mathcal{L}(\mathbb{C}^{N^2-1}), \tag{2.102}$$

and also under inhomogeneous transformations

$$\begin{aligned} &\sigma_k \mapsto \tilde{\tilde{\sigma}}_k = \sigma_k + a_k, \\ &\mathcal{H} \mapsto \tilde{\tilde{\mathcal{H}}} = \mathcal{H} + \frac{1}{2i}\sum_l \gamma_l \left(a_l^* \sigma_l - a_l \sigma_l^\dagger\right) + b, \end{aligned} \tag{2.103}$$

where the a_k are complex numbers and b is real.

It is natural to investigate which is the set of physical approximations that allows to describe the dynamics of a reduced system in terms of a completely-positive quantum dynamical semigroup. An example of derivation can be found in [21], where it is shown that, starting from the overall unitary evolution and under suitable conditions and approximations such as weak coupling, secular and Born-Markov approximations, a GKSL master equation is obtained. For the present purposes it is sufficient to remind that the latter consists in assuming that the environmental correlation functions decay on a time scale which is negligible compared to the time scale characterizing the evolution of the reduced system. If we denote with τ_S the relaxation time of the system and with τ_E the time-scale over which the environmental excitations induced by the interaction decay, then the Markov condition is expressed as

$$\tau_E \ll \tau_S. \tag{2.104}$$

Equation (2.104) means that the description of the dynamics is being given on a temporally coarse-grained scale. Any information that flows from the system to the environment cannot effect back the system, since the environment quickly forgets it and returns the same. Naively speaking, the reduced system is therefore interacting with the same environment. Under this assumption any memory effect is therefore neglected and it becomes thus clear why this class of dynamics is conceived to be as the quantum counterpart of classical stochastic Markovian processes, i.e. processes without memory (see for example [32, 33]). We will extensively come back on the notion of non-Markovianity in Chapter 3, where we will provide precise definitions both in the classical and in the quantum setting.

We conclude the present Subsection to present and discuss a straightforward generalization of the Gorini-Kossakowski-Sudarshan-Lindblad equation (2.100) to the time-dependent case. We will see examples of this master equation throughout the remaining of this Thesis.

This generalization consists in allowing the Lindblad operators σ_k as well as the coefficients γ_k to be time-dependent, provided the positivity constraint on the latter is maintained. The master equation this way obtained, called *time-dependent Lindblad equation*, becomes then of the form

$$\frac{d}{dt}\rho_S(t) = L(t)\rho_S(t) = -i\,[\mathcal{H}(t), \rho_S(t)] + \sum_{k=1}^{N^2-1} \gamma_k(t)\left(\sigma_k(t)\rho_S(t)\sigma_k^\dagger(t) - \frac{1}{2}\{\sigma_k^\dagger(t)\sigma_k(t), \rho_S(t)\}\right), \tag{2.105}$$

with $\gamma_k(t) \geq 0$, $\mathcal{H}^\dagger(t) = \mathcal{H}(t)$ and $\sigma_k(t) \in \mathcal{L}(\mathbb{C}^N)$ for any $t \geq 0$. In light of Equation (2.83), the corresponding quantum dynamical map is given by

$$\Lambda(t,0) = \overleftarrow{T} \exp\left[\int_0^t d\tau\, L(\tau)\right], \tag{2.106}$$

which is now completely positive by construction thanks to the positivity of the coefficients $\gamma_k(t)$. Another property of the quantum dynamical map obtained from a time-dependent Lindblad equation is that it is *completely-positive divisible* (CP-divisible). The

relevance of CP-divisible maps will be made evident in the following Chapter, in connection with the notion of quantum non-Markovianity.

Definition 2.3 (CP-divisibility)**.** A family of dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$ is CP-divisible, if, for any $t_0 \leq s \leq t$ the CPTP map $\Lambda(t,t_0)$ can be expressed as the composition of two other CPTP maps

$$\Lambda(t,t_0) = \Lambda(t,s)\Lambda(s,t_0). \tag{2.107}$$

Note that, given a one-parameter family of quantum dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$, one can always formally construct a two-parameters family of linear maps, known as transition maps, as

$$\Lambda(t,s) = \Lambda(t,t_0)\Lambda^{-1}(s,t_0) \quad t \geq s \geq t_0, \tag{2.108}$$

for those times s such that the inverse map $\Lambda^{-1}(s,t_0)$ exists. The crucial point is that the maps $\Lambda(t,s)$ this way obtained are *not* in general completely positive maps, nor even positive, since the inverse of a completely positive map is not completely positive. For this reason, these maps can be formally expressed as

$$\Lambda(t,s) = \overleftarrow{T} \exp\left[\int_s^t d\tau\, \mathcal{K}_{TCL}(\tau)\right], \tag{2.109}$$

where the time-local generator has the structure given in Equation (2.95) with $\gamma_k(t)$ that are not restricted to take on positive values due to the lack of complete positivity.

It is finally important to observe that if a family of CP-divisible dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$ is also *time-homogeneous*, i.e. if the transition map $\Lambda(t,s)$ depends only on the difference of times $t-s$, (2.107) reduces to the semigroup property (2.97).

This is reflected in the temporal homogeneity of the relative master equation, and in turn in the fact that the infinitesimal generator does not depend on time. In this situation we therefore recover the GKSL master equation.

3

Non-Markovianity of open quantum systems

3.1 Classical Markov processes

3.1.1 Formal definition and properties

A stochastic process $\{X_t, t \in [t_0, T] \subset \mathbb{R}\}$, is a family of measurable maps, called *random variables*,

$$X \,:\, \Omega \times [t_0, T] \longrightarrow \mathbb{R}, \tag{3.1}$$

that associates with every elementary event ω belonging to a common probability space $(\Omega, \Sigma, \mathbb{P})$ (with Ω denoting the sample space, Σ the $\sigma-$algebra of subsets of Ω and $\mathbb{P}$ the probability measure with $\mathbb{P}(\Omega) = 1$) and with every $t \in [t_0, T]$ a real number $X(\omega, t)$. For every fixed $\omega \in \Omega$, the assignment map $t \mapsto X(\omega, t)$ is called *realization* or *trajectory* of the stochastic process. From now on, for the purposes of this Thesis, t can be interpreted as time and our attention will be restricted to stochastic process which take value on a finite set $\Omega_n = \{x_0, \ldots, x_n\}$.

A family of joint probability distribution for every $n \in \mathbb{N}$ and all events $x_n \in \Omega_n$ which satisfies the following consistency conditions

$$\sum_{x_i} \mathbb{P}_1 (x_i, t) = 1, \tag{3.2}$$

$$\mathbb{P}_n (x_{n-1}, t_{n-1}; \ldots; x_0, t_0) > 0, \qquad \forall n \in \mathbb{N}, \tag{3.3}$$

$$\sum_{x_m} \mathbb{P}_n (x_{n-1}, t_{n-1}; \ldots; x_{m+1}, t_{m+1}; x_m, t_m; x_{m-1}, t_{m-1}; x_0, t_0) = \mathbb{P}_{n-1} (x_{n-1}, t_{n-1}; \ldots; x_{m+1}, t_{m+1}; x_{m-1}, t_{m-1}; x_0, t_0), \tag{3.4}$$

$$\mathbb{P}_n \left(x_{\pi(n-1)}, t_{\pi(n-1)}; \ldots; x_{\pi(0)}, t_{\pi(0)}\right) = \mathbb{P} (x_{n-1}, t_{n-1}; \ldots; x_0, t_0) \quad \text{for any permutation of the indexes } \pi(i), \tag{3.5}$$

uniquely determines a stochastic process. In fact, according to Kolmogorov's consistency theorem, for any family of joint probability distribution which satisfies the conditions (3.2), there exists a probability space and an associated stochastic process on it. In this framework, a stochastic process is classified as Markovian according to the following definition.

Definition 3.1. A stochastic process $\{X_t, t \in [t_0, T] \subset \mathbb{R}\}$ is *Markovian* if, for every $n \in \mathbb{N}$, for every ordered set of times $t_0 < t_1 < \ldots < t_n \in [t_0, T]$ and for every discrete set of events $x_0, x_1, \ldots, x_n$, the conditional probability, defined as

$$\mathbb{P}_{1|n}\left(x_n, t_n | x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right) = \frac{\mathbb{P}_{n+1}\left(x_n, t_n; x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right)}{\mathbb{P}_n\left(x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right)}, \tag{3.6}$$

satisfies the relation

$$\mathbb{P}_{1|n}\left(x_n, t_n | x_n, t_n; \ldots; x_0, t_0\right) = \mathbb{P}_{1|1}\left(x_n, t_n | x_{n-1}, t_{n-1}\right), \quad \forall n \in \mathbb{N}. \tag{3.7}$$

The Markov condition expresses the fact that the probability for the event $X(t_n) = x_n$ conditional to the whole history of previous events $X(t_0) = x_0, \ldots, X(t_{n-1}) = x_{n-1}$ actually depends only on the latest. In this sense a Markov process is said to characterize a 'memory-less' process. An immediate consequence of the condition (3.7) is that the whole hierarchy of joint probability distributions, and therefore the stochastic process itself, can be reconstructed by means of only two quantities, namely the initial probability density $\mathbb{P}_1(x_0, t_0)$ and the conditional probability $\mathbb{P}_{1|1}(x, t; x_0, t_0)$. In fact, it can be proven that

$$\mathbb{P}_n\left(x_{n-1}, t_{n-1}; \ldots; x_0, t_0\right) = \mathbb{P}_1\left(x_1, t_1\right) \prod_{k=0}^{n-2} \mathbb{P}_{1|1}\left(x_{k+1}, t_{k+1} | x_k, t_k\right). \tag{3.8}$$

3.1.2 The Chapmann-Kolmogorov equation

The condition (3.7) and the expression (3.8) naturally point the focus on the so-called *conditional transition probability* $\mathbb{P}_{1|1}\left(x, t | x_0, t_0\right)$. From its definition, it follows that it satisfies the conditions

$$\sum_x \mathbb{P}_{1|1}(x, t | x_0, t_0) = 1, \tag{3.9}$$

$$\lim_{t \to t_0} \mathbb{P}_{1|1}(x, t | x_0, t_0) = \delta_{x, x_0}. \tag{3.10}$$

The conditional transition probability is also often referred to as *propagator* due to the following relation

$$\mathbb{P}_1(x, t) = \sum_{x_0} \mathbb{P}_{1|1}(x, t | x_0, t_0) \mathbb{P}_1(x_0, t_0), \tag{3.11}$$

which means that it connects the one-time probability density at a generic time t to that at the initial time t_0. Moreover, another remarkable property is satisfied by the conditional

transition probability in the case of a Markov process, which is

$$\mathbb{P}_{1|1}\left(x,t|x_0,t_0\right)=\sum_{x_1}\mathbb{P}_{1|1}\left(x,t|x_1,t_1\right)\mathbb{P}_{1|1}\left(x_1,t_1|x_0,t_0\right),\qquad\forall t_0<t_1<t, \tag{3.12}$$

known as *Chapmann-Kolmogorov equation*.

Provided $\mathbb{P}_{1|1}(x,t|x_0,t_0)$ is differentiable with respect to time, the differential form of Eq.(3.12) can be also considered: by making use of Eq.(3.9), one has

$$\frac{\partial}{\partial t}\mathbb{P}_{1|1}(x,t|x_0,t_0)=L(t)\mathbb{P}_{1|1}(x,t|x_0,t_0), \tag{3.13}$$

where the linear generator $L(t)$ is defined through its action on a generic test function $\phi(x)$

$$L(t)\phi(x)\equiv\lim_{\Delta t\to 0^+}\frac{1}{\Delta t}\sum_y\left[\mathbb{P}_{1|1}(x,t+\Delta t|y,t)-\delta_{x,y}\right]\phi(y). \tag{3.14}$$

Such differential Chapmann-Kolmogorov equation is often referred to simply as *master equation*. If the process is in particular *time-homogeneous*, i.e. if the propagator $\mathbb{P}_{1|1}(x,t|x_0,t_0)$ depends only on the difference of times $\tau\equiv t-t_0$, then the generator $L(t)$ does not depend on time any more, this leading to a solution which satisfies a *semigroup* composition law (it is not a group because of the constraint $t-s\geq 0$), this fact being the expression of the irreversibility of the stochastic processes. It is immediate to see that this represents the classical counterpart of the quantum dynamical semigroup introduced in Chapter (2) Section 2.2.4.2.

In light of Eq.(3.11), the structure of the master equation (3.13) for $\mathbb{P}_{1|1}(x,t|x_0,t_0)$ is also shared by the single-time probability density $\mathbb{P}_1(x,t)$, i.e.

$$\frac{\partial}{\partial t}\mathbb{P}_1(x,t)=L(t)\mathbb{P}_1(x,t). \tag{3.15}$$

In the particular case of a stochastic jump process with an instantaneous jump rate $W(x|x_0,t)\Delta t\geq 0$ from the value x_0 to x within the time interval $[t,t+\Delta t]$, Eq. (3.15) takes the familiar form

$$\frac{\partial}{\partial t}\mathbb{P}_1(x,t)=\sum_{x_0}\left[W(x|x_0,t)\mathbb{P}_1(x_0,t)-W(x_0|x,t)\mathbb{P}_1(x,t)\right], \tag{3.16}$$

commonly known as *Pauli master equation* [21].

It is worth stressing however that no necessary condition that guarantees the non-Markovianity of the underlying process can be found involving the single-time probability density $\mathbb{P}_1(x,t)$. Eq. (3.7) in fact involves the entire family of joint probability distribution and in particular the conditional transition probability $\mathbb{P}_{1|1}(x,t|x_0,t_0)$ and thus, as we will see in the following Subsections, only sufficient conditions of non-Markovianity concerning $\mathbb{P}_1(x,t)$ can be introduced. Ultimately, the Chapman-Kolmogorov equation has then to be understood as an equation for the latter quantity, rather than as an equation for the single-time probability density. Stochastic processes, in fact, for which the single-time probability distribution $\mathbb{P}_1(x,t)$ satisfies a Chapmann-Kolmogorov equation

while the conditional transition probability distribution does not can be constructed [34]. Actually, strictly speaking not even the validity of the Chapmann-Kolmogorov equation for the conditional transition probability $\mathbb{P}_{1|1}(x,t|x_0,t_0)$ is in general equivalent to the Markov condition Eq.(3.7) and some processes for which the former holds but that are still non-Markovian can be found [35, 36]; however, in what follows we will overlook upon this fact since it goes beyond the scopes of the present work.

3.1.3 Divisibility and non-Markovianity

In view of the Section on the quantum counterpart non-Markovianity, we now focus on single-time probabilities $\mathbb{P}_1(x,t)$ and give two sufficient conditions for which a stochastic process is non-Markovian.

Consider for simplicity a $N-$dimensional classical system, so that the one-point probability distribution at time t is a probability vector $\mathbf{P}(t)$, whose elements $\{P_j(t)\}_{j=1,\dots,N}$ satisfy the conditions $P_j(t) \equiv \mathbb{P}_1(j,t) \geq 0 \ \forall j = 1,\dots,N$ and $\sum_j P_j(t) = 1$. In analogy with the quantum case presented in Chapter 2, the time evolution of $\mathbf{P}(t)$ can be in general described in terms of a family of linear maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$, called dynamical maps, according to which

$$\mathbf{P}(t) = \Lambda(t,t_0)\mathbf{P}(t_0). \tag{3.17}$$

Definition 3.2. If the matrix Λ preserves positivity and normalization, i.e.

$$\sum_j \Lambda_{jk} = 1, \qquad \forall k = 1,\dots,N \tag{3.18}$$

$$\Lambda_{jk} \geq 0, \quad \forall j,k = 1,\dots,N, \tag{3.19}$$

then it is called *stochastic matrix*.

In light of Eqs. (3.17) and (3.11), one is immediately led to identify the dynamical map $\Lambda_{ij}(t,t_0)$ with the conditional transition probability $\mathbb{P}_{1|1}(i,t|j,t_0)$. This equivalence however holds true in general only if t_0 is the initial time, while for a generic intermediate time $t_1 > t_0$, $\Lambda_{ij}(t,t_1) \neq \mathbb{P}_{1|1}(i,t|j,t_1)$. The reason is that $\mathbb{P}_{1|1}(i,t|j,t_1)$ is not uniquely defined for a general stochastic process, since it can be obtained through Eq. (3.6) from two different initial conditions $k \neq k'$, e.g. from two quantities $\mathbb{P}_{1|2}(i,t|j,t_1;k,t_0)$ and $\mathbb{P}_{1|2}(i,t|j,t_1;k',t_0)$.

On the other hand, provided $\Lambda(t,t_0)$ is invertible for every $t > t_0$, we can always construct the dynamical map $\Lambda(t,t_1)$ for $t_1 > t_0$ as:

$$\Lambda(t,t_1) = \Lambda(t,t_0)\Lambda^{-1}(t_1,t_0). \tag{3.20}$$

The point however is that $\Lambda(t,t_1)$ this way constructed may not be a *stochastic matrix* itself, i.e. fulfil the second condition in Eqs. (3.18).

These considerations, whose importance will become clear in a moment, lead, in the same spirit of Chapter 2 for the quantum case, to the introduction of the following definition:

Definition 3.3. A family of classical dynamical maps $\{\Lambda(t,t_0)\}_{t\geq 0}$ is *(P-)divisible*, if, for any $t \geq t_1 \geq t_0$,

$$\Lambda(t,t_0) = \Lambda(t,t_1)\Lambda(t_1,t_0), \tag{3.21}$$

with $\Lambda(t,t_1)$ being itself a stochastic matrix.

The crucial point is the relationship between P-divisible dynamical maps and Markov processes, which can be deduced from the above considerations and the Chapmann - Kolmogorov equation (3.12). It is in fact immediate to realize that, if $\Lambda_{ij}(t,t_1) = \mathbb{P}_{1|1}(i, t|j,t_1)$, then the dynamics of the classical system is Markovian. The latter identification holds when $\Lambda(t,t_1)$ is a stochastic matrix and therefore whenever the dynamical map is P-divisible. The violation of the P-divisibility condition then clearly poses itself as a sufficient indication of non-Markovianity.

3.1.4 The l_1-norm

Another sufficient condition for a classical stochastic process to be Markovian which is accessible by looking at probability vectors $\mathbf{P}(t)$ is related to the time-behavior of the l_1-*norm*, which induces a metric on the space of probability distributions and is defined in general as

$$\| \mathbf{P}(t) \|_1 \equiv \sum_j |P_j(t)|. \tag{3.22}$$

This norm has two very remarkable properties. The first one is that it naturally arises in an hypothesis-testing scenario. Consider in fact a random variable X distributed with *a priori* probabilities q and $1-q$ according to two probability vectors $\mathbf{P}^1(t)$ or $\mathbf{P}^2(t)$ respectively. Our goal is to infer, by means of a single sampling of X, the correct probability distribution of our random variable. The maximum probability to give the correct answer can be shown to be given by

$$\mathbb{P}^{MAX}(t) = \frac{1+ \| q\mathbf{P}^1(t) - (1-q)\mathbf{P}^2(t) \|_1}{2}. \tag{3.23}$$

The l_1-norm between two probability distribution is therefore the bias in favour of the correct discrimination between the two probability distributions $\mathbf{P}^{1,2}(t)$. A particular case which will be of relevance also in the quantum case, see Section (3.2.2), is the a-priori unbiased case, i.e. $q = 1/2$. In this case the l_1-norm

$$\| q\mathbf{P}^1(t) - (1-q)\mathbf{P}^2(t) \|_1 = \frac{1}{2} \| \mathbf{P}^1(t) - \mathbf{P}^2(t) \|_1 \tag{3.24}$$

is known as *Kolmogorov norm* [37].

The second crucial property of the l_1-norm is connected to its relationship with P-divisibile dynamical maps $\Lambda(t,t_0)$, which is contained in the following Theorem (see for example [38] for the proof)

Theorem 3.4. *A family of classical dynamical maps $\{\Lambda(t|t_0)\}_{t\geq 0}$ is (P-)divisible, if the l_1-norm is a monotonic contraction with time, i.e. $\forall t \geq t_1 \geq t_0$ and every pair of random vectors $\mathbf{P}^{1,2}(t)$*

and a priori probabilities q *and* $1-q$*,*

$$\begin{aligned} \| \, q\mathbf{P}^1(t) - (1-q)\mathbf{P}^2(t) \, \|_1 \equiv & \| \, \Lambda(t,t_1) \left(q\mathbf{P}^1(t_1) - (1-q)\mathbf{P}^2(t_1) \right) \, \|_1 \\ \leq & \| \, q\mathbf{P}^1(t_1) - (1-q)\mathbf{P}^2(t_1) \, \|_1, \end{aligned} \tag{3.25}$$

with $\Lambda(t,t_1)$ *in general given by Eq.*(3.20)*.*

An important corollary of this Theorem is obtained when we identify t_1 in Eq.(3.25) with the initial time t_0 of the stochastic process. In this case in fact the dynamical map $\Lambda(t, t_0)$ is, as already stressed before, a stochastic matrix by construction and therefore the l_1-norm between two probability distributions is a contraction, i.e.

$$\| \, q\mathbf{P}^1(t) - (1-q)\mathbf{P}^2(t) \, \|_1 \leq \| \, q\mathbf{P}^1(t_0) - (1-q)\mathbf{P}^2(t_0) \, \|_1 \, . \tag{3.26}$$

This inequality physically means that the ability to discriminate between two different probability distributions in the single-shot sampling hypothesis-testing scenario $\mathbb{P}^{MAX}(t)$ can only decrease with respect to its initial value.

As a consequence of Theorem (3.4) however, if the process is P-divisible and therefore Markovian, the decrease of $\mathbb{P}^{MAX}(t)$ is monotonic in time, i.e. $\frac{d}{dt}\mathbb{P}^{MAX}(t) < 0 \; \forall t > t_0$. If we bestow an information-oriented interpretation to the ability of discriminating between $\mathbb{P}_1^{1,2}(x,t)$, then we can interpret this situation as a monotonic loss of information during the stochastic evolution.

On the other hand, if the process is not P-divisible and thus non-Markovian, the decrease of $\mathbb{P}^{MAX}(t)$ can temporarily invert its trend (though the regrowth can never exceed its initial value because of the corollary mentioned above), which means that there exist intermediate times t such that $\frac{d}{dt}\mathbb{P}^{MAX}(t) > 0$. In the same framework of hypothesis-testing problem, a temporary regrowth ability to discriminate between the two possible probability distributions after some initial loss is a signature of an underlying memory in the process.

To summarize, the correct and proper definition of classical stochastic Markov process is given by Eq.(3.7) which involves all the family of joint probability distributions. Some sufficient conditions of non-Markovianity based on the time-behaviour of the single-time probability distributions can however be formulated in terms of the P-divisibility of the dynamical maps and of the contractivity property of the l_1-norm. In the next Section we will see how these concepts can (or cannot) have a natural counterpart in the quantum realm, thus providing the criteria and guidelines employed in the last decade to characterize quantum non-Markovian processes.

3.2 Quantum non-Markovianity

In the previous Section we made a very brief review of the concept of Markovianity in classical stochastic processes; in the present Section our aim is to transpose those concepts to the quantum realm, by this meaning that the system under consideration is a

quantum system. In the last decade, much efforts have been devoted by the scientific community in order to find a clear definition of a quantum Markovian process in the closest analogy possible with the classical framework. One of the main difficulties immediately encountered in this endeavour is that Eq. (3.7) has no immediate parallel in quantum mechanics, the main reason being that measurements, which are a necessary ingredient in the definition of every joint probability distribution according to the Born rule, perturb the state of the system affecting the subsequent outcomes. Consequently, no family of joint probability distributions satisfying the Kolmogorov consistency relations (3.2) can be constructed. To explicitly see this, consider a generic observable $A \in \mathcal{B}(\mathscr{H})$ which is measured at n discrete times. Assuming A to have a non-degenerate spectrum, i.e. $A = \sum_a a \left|a\right\rangle \left\langle a\right|$, and denoting with $U(t,0)$ the unitary evolution operator governing the evolution of the quantum system, the joint probability distribution to have obtained the set of outcomes $a_1, \ldots, a_n$ at times $t_0 \leq t_1 \leq \ldots \leq t_n$ is given by

$$\mathbb{P}\left(a_n, t_n; \ldots; a_1, t_1\right) = \mathrm{Tr}\left[\pi_{a_n} U(t_n, t_{n-1}) \pi_{a_{n-1}} \ldots \pi_{a_1} U(t_1, t_0)\ \rho(0) \right. \\ \left. U^\dagger(t_1, t_0) \pi_{a_1} \ldots \pi_{a_{n-1}} U^\dagger(t_n, t_{n-1}) \pi_{a_n}\right], \quad (3.27)$$

with $\pi_{a_i} = \left|a_i\right\rangle \left\langle a_i\right|$. It is immediate to realize that this joint probability distribution, though being valid for every n, does not fulfil the Kolmogorov consistency condition (3.2)

$$\sum_{a_{n-1}} \mathbb{P}\left(a_n, t_n; a_{n-1}, t_{n-1}; \ldots; a_1, t_1; a_0, t_0\right) \neq \mathbb{P}\left(a_{n-1}, t_{n-1}; \ldots; a_1, t_1; a_0, t_0\right) \quad (3.28)$$

since the orthogonal measurement of the observable A generally destroys every quantum interference as well as, when applied to open quantum systems, every correlations between system and environment, thus influencing the subsequent dynamics. For all these reasons, a proper definition of (non-)Markovianity in the quantum realm, which should be independent of any particular measurement scheme, is more subtle than in the classical framework.

Though still nowadays representing a debated topic, many benchmark results have been obtained in the last years that pave the way of a proper definition and quantification of quantum non-Markovianity and its relation with the presence of memory effects in open quantum systems dynamics. Almost all of these approaches characterize the non-Markovianity in terms of properties of the family of the quantum dynamical maps which govern the evolution of the quantum system and cope with the time-behaviour of the statistical operator $\rho(t)$. In the following Subsections we will present a number of them which will be useful and employed in the rest of the present work. It will become immediately clear the parallelism between these approaches and their classical counterparts presented in the previous Section. The first one in fact relates the non-Markovianity of an open system's dynamics to the violation of the CP-divisibility of the quantum dynamical map [13], which represents the natural quantum analogue of the P-divisibility in the classical context. The second approach defines the non-Markovianity through the contractivity property of some norm defined on $\mathcal{S}(\mathscr{H}_S)$ [11, 38–40].

Alongside with these definitions, two measures have been introduced in [11, 13, 40] in order to quantify the degree of non-Markovianity in terms of suitable (and possibly measurable in experiments) estimators. Inspired by the general criteria underlying these two measures, several others figures of merit have been introduced in recent years, all sharing the property to represent monotone contractions under the action of completely positive and trace-preserving maps. Depending on the case considered, i.e. finite dimensional systems versus continuous variable systems *et cetera*, or on the type of interaction, one of non-Markovianity witness can be more convenient, easy to be calculated or sensitive than the others and in general they will not coincide. For this reason, and due to the fact that we will use some of them in the remainder of the work, we will make a brief survey of some of them in the last Subsection of this Chapter.

3.2.1 CP-divisibility based criterion of quantum non-Markovianity

In the present Subsection we introduce and discuss the definition and measure of quantum non - Markovianity introduced by Rivas, Huelga and Plenio in [13]. Such approach, as we will see in a moment, copes with the notion of CP-divisibility of a family of quantum dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$, see Definition 2.3 introduced in Chapter 2 Subsection 2.2.4.2.

Definition 3.5 (RHP non-Markovianity)**.** The time-evolution of a quantum system described in terms of a family of dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$ is *Markovian* if the latter is CP-divisible.

It is then immediate to see that, since the complete positivity poses itself as the quantum counterpart of the classical notion of positivity, this definition can be seen as the quantum counterpart of the condition discussed in Subsection 3.1.3. A CP-divisible family of dynamical maps physically expresses the fact that the evolution of the open quantum system can be stopped and restarted at any intermediate time obtaining the same result as if with a one-step evolution. In light of this and of the analogies with the Chapmann-Kolmogorov equation which holds true in the case of Markov processes, one is led to interpret this with a lack of memory effects.

It is important to stress that, in order to check CP-divisibility of the time evolution, one can look at either the quantum dynamical map or at the associated time-local generator. In particular, given the knowledge of the transition map $\Lambda(t,s)$ (2.108), one can determine its complete-positivity (which expresses the CP-divisibility property (2.3), see Section (2.2.4.2)) by studying the positivity of the associated Choi matrix Eq. (2.44)

$$\Lambda_{Choi}(t,s) \equiv [\Lambda(t,s)\otimes \mathbb{1}_N]\left(|\phi\rangle_{ME}\langle\phi|_{ME}\right), \tag{3.29}$$

with $|\phi\rangle_{ME} = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}|k\rangle\otimes|k\rangle$ being the maximally entangled state between two copies of the quantum system under consideration ($\{|k\rangle\}_{k=1,\dots,N}$ denoting an orthonormal basis in $\mathscr{H}_S$, here considered of dimension N), see Section 2.1.2. Given instead the time-local generator $\mathcal{K}_{TCL}(t)$ in its time-dependent Lindblad form (2.105), CP-divisibility is granted

provided that

$$\gamma_k(t) > 0, \qquad \forall t > t_0. \tag{3.30}$$

Building on these considerations, Rivas, Huelga and Plenio in [13] proposed to quantify the degree of non-Markovianity of a quantum process by

$$\mathcal{I}(\Lambda) = \int_{\mathbb{R}^+} dt\, \mathfrak{g}(t), \tag{3.31}$$

where the quantity $\mathfrak{g}(t)$ denotes the right derivative of the trace norm of the Choi matrix Λ_{Choi} (3.29) associated to the quantum dynamical map Λ:

$$\mathfrak{g}(t) = \lim_{\epsilon \to 0^+} \frac{\| \Lambda_{Choi}(t, t+\epsilon) \|_1 - 1}{\epsilon}. \tag{3.32}$$

Note that $\mathfrak{g}(t)$ is different from zero if and only if the CP-divisibility of the map Λ is broken. In fact, when $\Lambda_{Choi}(t, t+\epsilon)$ is positive, the transition map $\Lambda(t, t+\epsilon)$ is completely-positive, which means that the image of the maximally entangled state through Eq. (3.29) is again a state and therefore its trace-norm is equal to 1, this fact finally implying that $\mathfrak{g}(t) = 0$. It is worth to emphasize that the evaluation of $\mathfrak{g}(t)$, and thus in turn this non-Markovianity measure, requires the knowledge of the quantum dynamical map, which can be accessed only by means of full process tomography. This is of course a much demanding task especially from the experimental point of view.

Finally, in a recent paper [41], Definition 3.5 has been employed to characterize the non-Markovianity in Gaussian channels and a contextual measure has been proposed. Gaussian channels are represented in terms of a family of completely positive and trace preserving maps generated by a quadratic bosonic Hamiltonian, which thus has the property to preserve the Gaussian nature of quantum states during evolution. The importance of presenting such approach relies in the fact that, in general, addressing the characterization of CP-divisibility in infinite-dimensional quantum system is highly complex. Though for Gaussian channels, a generalization of the Choi-Jamiolkowski isomorphism (which allows to construct the Choi matrix associated to the dynamical map and thus to access the complete positivity of the transition map by studying the positivity of the latter) has been recently formulated [42], a much simpler way to access the complete positivity of the transition map $\Lambda(t, s)$ for Gaussian channels can be given in terms of the so-called covariance matrix of the quantum Gaussian state. For these reasons and also because we will employ this criterion in Chapter 5, we very briefly recall the basic notions and notations concerning Gaussian states. For more detailed treatments of the vast literature on this very important class of quantum states, the reader is referred to [43, 44].

3.2.1.1 Continuous-variable systems and Gaussian states

A continuous-variable (CV) system, is a system whose degrees of freedom are associated to operators with a continuous spectrum. Here we consider CV systems made of a discrete number n of bosonic modes so they are associated to a Hilbert space $\mathscr{H} =$

$\otimes_{k=1}^{n}\mathscr{H}_k$, where $\mathscr{H}_k$ is the Fock space relative to the $k-$th mode spanned by the family $\{a_k^{(\dagger)}\}_{k=1,\dots,n}$ of creation (annihilation) operators satisfying the bosonic commutation relations $\left[a_k, a_j^\dagger\right] = \delta_k j$. Such commutation relations are equivalently rewritten in terms of the *canonical coordinates* of this system, given by $\mathbf{R} = (q_1, p_1, \dots, q_n, p_n)^T$ with $q_k = (a_k + a_k^\dagger)/\sqrt{2}$ and $p_k = i(a_k^\dagger - a_k)/\sqrt{2}$, as

$$[R_k, R_j] = i\Omega_{kj}, \quad \boldsymbol{\Omega} = \oplus_{k=1}^{n}\boldsymbol{\omega}, \quad \boldsymbol{\omega} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{3.33}$$

and impose the following important condition on the states involving their *covariance matrices*

$$\boldsymbol{\sigma} + \frac{i}{2}\boldsymbol{\Omega} \geq 0, \tag{3.34}$$

where $\boldsymbol{\sigma}$ is a $2n \times 2n$ matrix with entries

$$\sigma_{jk} = \frac{1}{2}\langle\{R_j, R_k\}\rangle - \langle R_j\rangle\langle R_k\rangle, \tag{3.35}$$

with $\langle\cdot\rangle \equiv \mathrm{Tr}\,[\rho\cdot]$ and $\{O_1, O_2\} = O_1O_2 + O_2O_1$. It is worth stressing that Eq.(3.34) traduces the condition $\rho > 0$.

A very important operator in this framework is the so-called *Weyl (or displacement) operator* defined as

$$W(\boldsymbol{\lambda}) = \otimes_{k=1}^{n} W(\lambda_k) = \otimes_{k=1}^{n} \exp\left[\lambda_k a_k^\dagger - \lambda_k^* a_k\right], \tag{3.36}$$

with $\lambda_k = \lambda_{k,r} + i\lambda_{k,i}$. The vector $(\lambda_{1,r}, \lambda_{1,i} \dots, \lambda_{n,r}, \lambda_{n,i})^T$ belongs to the real $2n-$dimensional space equipped with the symplectic form $\boldsymbol{\Omega}$ which is called *quantum phase space* in analogy with the classical Liouville space. The set of $W(\boldsymbol{\lambda})$ is complete and thus any operator $O \in \mathscr{H}$ can be expressed according to the *Glauber form*

$$O = \int_{\mathbb{C}^n} \frac{d^n\boldsymbol{\lambda}}{\pi^n} \mathrm{Tr}\left[O\, W(\boldsymbol{\lambda})\right] W^\dagger(\boldsymbol{\lambda}), \tag{3.37}$$

where

$$\chi\left[O\right](\boldsymbol{\lambda}) \equiv \mathrm{Tr}\left[O\, W(\boldsymbol{\lambda})\right] \tag{3.38}$$

is the so-called *characteristic function* of the operator O. It is clear that the characteristic function of a statistical operator $\rho \in \mathcal{S}(\mathscr{H})$ can be used to provide an equivalent unique description of the quantum system. For the sake of completeness, it is worth mentioning that taking the complex Fourier transform of the characteristic function leads to the so-called Wigner function, which has many remarkable properties and is widely employed in quantum optics and quantum information processing with continuous variables [43–46].

Definition 3.6. A CV system's state with n degrees of freedom is called Gaussian if its characteristic function, defined in Eq.(3.38) is Gaussian, i.e.

$$\chi\left[\rho\right](\boldsymbol{\lambda}) = \exp\left[i\langle\mathbf{R}\rangle^T\lambda - \frac{1}{2}\boldsymbol{\lambda}^T\boldsymbol{\sigma}\boldsymbol{\lambda}\right]. \tag{3.39}$$

A Gaussian state is therefore uniquely determined by first and second statistical moments of the quadrature vector, i.e. by the vector of mean values $\langle \mathbf{R} \rangle$ and by the covariance matrix $\boldsymbol{\sigma}$.

The quantum evolutions which preserve the Gaussian character of a quantum state are said to be Gaussian channels [47–49]. The action of a Gaussian channel on a generic Gaussian state can be written as [41, 42, 50]

$$\boldsymbol{\sigma}(t_0) \mapsto \boldsymbol{\sigma}(t) = \mathbf{X}(t,t_0)\boldsymbol{\sigma}(t_0)\mathbf{X}(t,t_0)^T + \mathbf{Y}(t,t_0), \quad \langle \mathbf{R} \rangle^T(t_0) \mapsto \langle \mathbf{R} \rangle^T(t) = \mathbf{X}(t,t_0)\langle \mathbf{R} \rangle^T(t_0), \tag{3.40}$$

with $\mathbf{X}(t,t_0)$, $\mathbf{Y}(t,t_0)$ being $2n \times 2n$ real matrices. Naively speaking, the contribution $\mathbf{Y}(t,t_0)$ of a Gaussian channel uniquely determined by the couple $(\mathbf{X}(t,t_0), \mathbf{Y}(t,t_0))$, can be regarded as a noise term which has to be non-negative, i.e. $\mathbf{Y}(t,t_0) \geq 0$; the $\mathbf{X}(t, t_0)$ contribution instead corresponds to a symplectic transformation which can be even negative provided $\mathbf{Y}(t,t_0)$ is large enough. The requirement of complete positivity poses a constraint on these two matrices, which represents the key brick to characterize the CP-divisibility and ultimately the non-Markovianity in the case of a Gaussian channel.

Theorem 3.7 (Demoen 1977)**.** *A Gaussian channel is completely positive iff the following condition holds*

$$\mathbf{Y}(t,t_0) + \frac{i}{2}\boldsymbol{\Omega} - \frac{i}{2}\mathbf{X}(t,t_0)\boldsymbol{\Omega}\mathbf{X}^T(t,t_0) > 0. \tag{3.41}$$

Note that, for $\mathbf{X}(t,t_0) = \mathbf{0}$ this relation reduces to (3.34).

Considering that the composition of two Gaussian channels $(\mathbf{X}(t_1,t_0), \mathbf{Y}(t_1,t_0))$ and $(\mathbf{X}(t_2,t_1), \mathbf{Y}(t_2,t_1))$ is again a Gaussian channel ($t_2 > t_1 > t_0$), the set of Gaussian channels forms a semigroup (which however must not be confused with the one - parameter semigroup introduced in Chapter 2 Section (2.2.4.2)), with product given by [51]

$$\begin{aligned}(\mathbf{X}(t_1,t_0), \mathbf{Y}(t_1,t_0)) \cdot (\mathbf{X}(t_2,t_1), \mathbf{Y}(t_2,t_1)) \\ = (\mathbf{X}(t_1,t_0)\mathbf{X}(t_2,t_1), \mathbf{X}(t_1,t_0)\mathbf{Y}(t_2,t_1)\mathbf{X}(t_1,t_0)^T + \mathbf{Y}(t_1,t_0)).\end{aligned} \tag{3.42}$$

Exploiting this result to write the transition Gaussian channel $(\mathbf{X}(t,s), \mathbf{Y}(t,s))$, in [41] Torre, Roga and Illuminati showed that

Theorem 3.8 (TRI 2015)**.** *A Gaussian channel is CP-divisible iff the following condition holds*

$$\mathbf{Y}(t+\epsilon,t) - \frac{i}{2}\boldsymbol{\Omega} + \frac{i}{2}\mathbf{X}(t+\epsilon,t)\boldsymbol{\Omega}\mathbf{X}^T(t+\epsilon,t) > 0, \tag{3.43}$$

According to the RHP criterion of non-Markovianity (3.5) introduced above, if and only if the quantity (3.43) is negative the process is non-Markovian.

Contextually, the authors have proposed also to measure the degree of non-Markovianity of the Gaussian channel as

$$\mathcal{I}_G = \int_{\mathbb{R}^+} dt\, \mathfrak{G}(t), \quad \mathfrak{G}(t) \equiv \frac{1}{2}\lim_{\epsilon \to 0^+} \sum_k \left[|\nu_k(t+\epsilon,t)| - \nu_k(t+\epsilon,t) \right], \tag{3.44}$$

where $\nu_k(t+\epsilon,t)$ are the eigenvalues of the (symmetric) matrix at the l.h.s. of Eq.(3.43).

3.2.2 Trace-norm based criterion of quantum non-Markovianity

Here we discuss in detail the definition and measure of non-Markovianity dynamics of an open quantum system based on the time-behaviour of the trace norm under the action of CP-divisible dynamical maps. This idea, pioneered by the work by Breuer, Laine and Piilo [11], has been subsequently developed in [38–40] to a more general framework which better highlights the relationship both with the RHP definition and with the classical notion of Markovianity. For this reason we will follow this line of exposition in the present Subsection. From the very first work in this direction [11], this definition had a clear-cut physical interpretation in terms of information flow between an open quantum system and its environment, thus allowing for a more immediate interpretation in terms of memory effects. The main idea behind it is to characterize and quantify the presence (or absence) of memory effects by means of an ensemble-discrimination scenario, in full analogy with the classical case presented in Section 3.1.4.

Let us consider the following conceptual experiment: an experimenter, Alice, prepares at the initial time t_0 a quantum system in either $\rho_S^1(t_0)$ or $\rho_S^2(t_0)$ with probabilities q and $1-q$ respectively and then sends it to Bob which receive them at time t. Bob's task is to infer which state has been prepared by Alice by means of a single measurement on the system. Let $\{\Pi_1, \Pi_2 = \mathbb{1}_S - \Pi_1\}$ be a two-valued POVM associated with Bob's measurement: if the outcome of the measurement is 1, then the state is inferred to be in $\rho_S^1(t)$, otherwise if the outcome is 2 to be in $\rho_S^2(t)$. The probability of success of this discrimination protocol is then given by

$$\mathbb{P}_{succ}(t) = \left(q\mathrm{Tr}_S\Pi_1\rho_S^1(t) + (1-q)\mathrm{Tr}_S\Pi_2\rho_S^2(t)\right) = 1 + \mathrm{Tr}_S\Pi_1\left(q\rho_S^1(t) - (1-q)\rho_S^2(t)\right). \tag{3.45}$$

If Bob is clever and thus selects the best measurement scheme, he can achieve the maximum success probability which is given by [52]

$$\mathbb{P}_{succ}^{MAX}(t) = \frac{1}{2}\left(1 + \parallel \Delta_S(t) \parallel_1\right), \tag{3.46}$$

where $\Delta_S(t) \equiv q\rho_S^1(t) - (1-q)\rho_S^2(t)$ is called *Helstrom matrix*. This expression shows how the trace-norm of the Helstrom matrix represents the bias in favour of the correct ensemble identification in the single-shot experiment. It is moreover evident that the trace norm poses itself as the quantum counterpart of the l_1-norm introduced in Subsection 3.1.4.

Depending on the dynamics, given in terms of $\Lambda(t, t_0)$, which connects the initial states $\rho_S^{1,2}(t_0)$ prepared by Alice with the final states $\rho_S^{1,2}(t)$ received by Bob, $\mathbb{P}_{succ}^{MAX}(t)$ can vary with time. A first general answer in this direction is provided by the following Theorem by Kossakowski [53, 54]

Theorem 3.9. *A trace-preserving and hermiticity-preserving linear map Λ is positive iff the following condition holds*

$$\parallel \Lambda(t, t_0)A \parallel_1 \leq \parallel A \parallel_1, \qquad \forall A = A^\dagger \in \mathcal{T}(\mathscr{H}). \tag{3.47}$$

The equality sign holds if and only if Λ is a unitary transformation.

It follows from this Theorem that $\mathbb{P}_{succ}^{MAX}(t) \leq \mathbb{P}_{succ}^{MAX}(t_0)$, namely that the discrimination ability at any later time t that Bob can achieve is never greater than the value at the initial time.

An immediate consequence of this is that, if a family of quantum dynamical maps is P-divisible, which means that the transition map $\Lambda(t,s)$ (with $s > t_0$) defined in Eq.(2.109) is positive for any $s < t$, then Theorem (3.9) applies at any time and $\mathbb{P}_{succ}^{MAX}(t)$ decreases monotonically with time. On the other hand, if the map is not P-divisible, then at some intermediate time and for some couple of states $\rho^{1,2}$ the non-positive transition map $\Lambda(t,s)$ may lead to a temporary regrowth of the trace norm and thus of the discrimination ability. All these considerations, as well as the close similarity with the discussion made in the classical framework for the L_1-norm, leads to the following definition:

Definition 3.10. A process represented by a family of quantum dynamical maps $\{\Lambda(t,t_0)\}_{t\geq t_0}$ is said to be *Markovian* if, for every couple of initial states $\rho^{1,2}$ and for every $0 \leq q \leq 1$, the trace norm of the Helstrom matrix $\Delta \equiv q\rho_S^1(t) - (1-q)\rho_S^2(t)$ is a monotonic contraction of time (or equivalently, thanks to Theorem (3.9) if the process is P-divisible).

According to this definition, in a non-Markovian process the ability to discriminate between two ensembles $\rho^1(t)$ and $\rho^2(t)$, after being initially decremented due to Theorem (3.9), can temporarily regrowths, this fact being a signature of memory effects. In order to substantiate this interpretation, let us assume that the dynamics, described by the family of quantum dynamical maps Λ, correspond to an evolution of the system (prepared by Alice in the scenario depicted above) with an environment, so that the overall system is closed. Then let us consider the following quantities

$$I_{int}(t) = \| \, q\rho_S^1(t) - (1-q)\rho_S^2(t) \, \|_1, \tag{3.48}$$

denoting the amount of information inside the open system, and

$$I_{ext}(t) = \| \, q\rho_{SE}^1(t) - (1-q)\rho_{SE}^2(t) \, \|_1 - I_{int}(t), \tag{3.49}$$

denoting the information outside the open system (i.e. not accessible by Bob when measurements on the open system only are performed), where $\rho_{SE}^{1,2}(t) = U(t,t_0)(\rho_S^{1,2}(t_0) \otimes \rho_E)U^\dagger(t,t_0)$ and where we stress that the initial state of the composite system has been taken to be in factorized form in order for the quantum dynamical map to be well-defined. This last assumptions also implies that $I_{ext}(t_0) = 0$. Note that, in light of the considerations made above, $I_{int}(t)$ is a measure of the distinguishability between $\rho_S^1(t)$ and $\rho_S^2(t)$. Since at the level of the composite system the dynamics is unitary, there is no flow of information outside it, i.e.

$$I_{int}(t) + I_{ext}(t) \equiv \| \, q\rho_{SE}^1(t) - (1-q)\rho_{SE}^2(t) \, \|_1 = I_{int}(t_0), \tag{3.50}$$

and therefore any decrease in $I_{int}(t)$ due to Theorem (3.9) must correspond to an increment in $I_{ext}(t)$. Definition 3.10 therefore means that, during a Markov process, the system unidirectionally loses information either to the environment or to the correlations between them [34, 55] If however, for some intermediate time $s \in [t_0, t]$ and for at least

one pair of initial states of the system $\rho_S^{1,2}(t_0)$ it happens that

$$\sigma(t) = \frac{d}{dt} I_{int}(t) > 0, \tag{3.51}$$

then some of the information which was previously lost by the system flows back into it, i.e. a memory effect occurs.

Finally, we remind that the P-divisibility of the quantum process map can be checked either at the level of the dynamical map by looking at the positivity of the transition map $\Lambda(t,s)$ or at the level of the associated master equation. In particular, if we consider the time-local generator $\mathcal{K}_{TCL}(t)$ in the time-dependent Lindblad form (2.105)

$$\frac{d}{dt}\rho_S(t) = -i\left[\mathcal{H}(t), \rho_S(t)\right] + \sum_{k=1}^{N^2-1} \gamma_k(t)\left(\sigma_k(t)\rho_S(t)\sigma_k^\dagger(t) - \frac{1}{2}\{\sigma_k^\dagger(t)\sigma_k(t), \rho_S(t)\}\right), \tag{3.52}$$

the process is P-divisibile iff

$$\sum_k \gamma_k(t) |\langle m| L_k(t) |n\rangle|^2 > 0, \qquad \forall n \neq m, t \geq t_0, \tag{3.53}$$

$\{|n\rangle\}$ being a generic orthonormal basis of $\mathscr{H}_S$.

In their pioneering work [11], Breuer, Laine and Piilo studied the case of unbiased ensemble preparation by Alice, i.e. considered the particular case $q = 1/2$. In this particular case, the Helstrom matrix becomes traceless

$$\Delta_S(t) = \frac{1}{2}\left(\rho_S^1(t) - \rho_S^2(t)\right), \tag{3.54}$$

but every conclusion made above still holds.

Building on this definition, the following measure of non-Markovianity has been introduced in order to quantify the degree of non-Markovianity of a quantum process

$$\mathcal{N}(\Lambda) = \max_{\rho_S^{1,2}(t_0)} \frac{1}{2} \int_{\mathbb{R}^+} \left(|\sigma(t)| + \sigma(t)\right) dt, \tag{3.55}$$

where the maximization is performed over all pairs of initial states and the integration is extended over all the time regions where $\sigma(t)$, defined in Eq. (3.51), is positive.

$\mathcal{N}(\Lambda)$ is a positive functional of the family of dynamical maps and physically represents the extended sum of the information that flows back into the open system. The maximization involved in this measure, which is necessary to make it a property of the family of dynamical maps, is however an increasingly demanding task, both from theoretical and experimental point of view, as the dimension of the quantum system grows, despite a great simplification is provided by the properties of the functional $\mathcal{N}(\Lambda)$ and the convexity of $\mathcal{S}(\mathscr{H}_S)$. It can in fact be proven [40, 56] that the optimal couple of initial states $\rho_S^{1,2}(t_0)$, i.e. such that the maximum in (3.55) is achieved, is attained when they lie on the boundary of $\mathcal{S}(\mathscr{H}_S)$ and are mutually orthogonal. However, for systems of dimensions larger than 3, this procedure typically represents an overwhelming challenge (even from

the numerical point of view) and therefore either maximization over subclasses of initial states or the non-maximized version $\mathcal{N}_{\rho_S^{1,2}(t_0)}(\Lambda)$, which both represent lower bounds for the true measure $\mathcal{N}(\Lambda)$, are considered.

Finally, it is clear from the two definitions of quantum Markovianity (3.5) and (3.10), and in particular from a direct confrontation between Eqs. (3.30) and (3.53), that they coincide if there is only a single decay channel in the master equation. In general however the RHP condition for a quantum process to be Markovian is stricter with respect to trace-norm based condition, due to the fact that CP-divisible quantum dynamical maps are a subset of the P-divisible ones. This reflects also in the respective measures, in the sense that the following relation holds

$$\mathcal{I}(\Lambda) = 0 \implies \mathcal{N}(\Lambda) = 0, \tag{3.56}$$

but not the vice versa.

3.2.3 Other relevant non-Markovianity quantifiers

To conclude this Chapter, we review in the present Section some of the many other quantifiers of non-Markovianity that have been introduced in recent years. Every one of the witnesses which we will enumerate copes with different quantum dynamical properties and therefore, depending on the situation or the model considered, one can be more suitable than the others. Just to mention few examples: the trace-norm criterion introduced above does not witness non-Markovianity encoded in the non-unital part of the dynamics, which corresponds, in the finite dimensional case, to an affine transformation of the generalized Bloch vector [57]; the RHP non-Markovianity measure may not be accessed because the evolution of the quantum system can be approached only by fully numerical methods and therefore full process tomography would be infeasible; the dimension of the Hilbert space of the open quantum system is infinite and therefore the trace norm can prove a formidable (though in general not impossible) task to be evaluated analytically, maximization problem left aside. All of them however share one common leitmotif, which is that they are monotonic quantities under the action of completely positive and trace preserving maps.

3.2.3.1 Bloch Volume

A geometrical quantifier of non-Markovianity has been introduced in [16] by Lorenzo, Plastina and Paternostro, which is based on the change in the volume of the set of accessible states of the evolved open quantum system. Remarkably, this method applies well both in finite-dimensional systems and in quantum Gaussian systems.

In the case of a $N-$dimensional system, the statistical operator ρ can be equivalently expressed in terms of the generalized Bloch vector $r = (r_0, \mathbf{r})$, whose entries $\{r_j\}_{j=0}^{N^2-1}$ are given by the Hilbert-Schmidt scalar product of ρ with the orthonormal basis $\{G_j\}_{j=0}^{N^2-1}$,

with $G_0 = \mathbb{1}_S/\sqrt{N}$ and $\{G_j\}_{j=1}^{N^2-1} = \{u_{jk}, v_{jk}, w_l\}/\sqrt{2}$ being the traceless, hermitian generators of the Lie algebra $SU(N)$

$$u_{jk} = |j\rangle\langle k| + |k\rangle\langle j|, \qquad v_{jk} = -i\left(|j\rangle\langle k| - |k\rangle\langle j|\right),$$
$$w_l = \sqrt{\frac{2}{l(l+1)}}\sum_{j=1}^{l}\left(|j\rangle\langle j| - l\,|l+1\rangle\langle l+1|\right), \qquad 1 \le j < k \le N,\ 1 \le l \le N-1. \quad (3.57)$$

In agreement with Eq.(2.36), also any linear map Λ acting on the system can be represented as a $N^2 \times N^2$ matrix $\mathbf{\Lambda}(t, t_0)$ with entries

$$\Lambda_{jk}(t, t_0) = \mathrm{Tr}\left[G_j^\dagger\,\Lambda(t, t_0)\,[G_k]\right], \quad (3.58)$$

and physically represents an affine transformation of the Bloch vector

$$\mathbf{\Lambda}(t, t_0) = \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{c}(t, t_0) & \mathbf{A}(t, t_0) \end{pmatrix} \Rightarrow \mathbf{r}(t) = \mathbf{A}(t, t_0)\mathbf{r}(t_0) + \mathbf{c}(t, t_0)/\sqrt{N}, \quad (3.59)$$

where $\mathbf{A}(t, t_0)$ is responsible for rotations and shrinks while $\mathbf{c}(t, t_0)$ for translations. In particular, the determinant of the matrix $\mathbf{A}(t, t_0)$, i.e. $|\mathbf{A}(t, t_0)|$, describes the change in the volume of the set of dynamically accessible states.

In the case of Gaussian systems, a similar line of reasoning applies. Making reference to the notation introduced in Subsection 3.2.1.1, the covariance matrix $\boldsymbol{\sigma}$ relative to an $n-$mode bosonic system state evolves in a Gaussian channel according to Eq.(3.40). In full analogy with the treatment of $N-$dimensional quantum systems above discussed, this evolution equation can be written as an affine transformation on $\mathbb{R}^{4n^2}$

$$\mathbf{s}(t_0) \to \mathbf{s}(t) = \mathbf{M}(t, t_0)\mathbf{s}(t_0) + \mathbf{Z}(t, t_0), \quad (3.60)$$

where we have chosen a basis $\{G_j\}_{j=0}^{4N^2-1}$ and where $s_j(t) = \mathrm{Tr}\left[\boldsymbol{\sigma}(t)G_j\right]$, $M_{jk}(t, t_0) = \mathrm{Tr}[\mathbf{X}^T(t, t_0)G_j\mathbf{X}(t, t_0)G_k]$ and finally $Z_j(t, t_0) = \mathrm{Tr}\left[\mathbf{Y}(t, t_0)g_j\right]$. Upon the replacement $\mathbf{F}(t, t_0) \to \mathbf{M}(t, t_0)$, same physical considerations made above holds true for Gaussian states.

In both these cases, the main point is that the volume of the dynamically accessible states $|\mathbf{A}(t, t_0)|$ decreases monotonically with time as long as the quantum dynamical map is CP-divisible. Sticking to the definition (3.5) of non-Markovian quantum dynamics, any temporary regrowth in this determinant during the evolution is a signature of non-Markovianity. It is however worth stressing that this figure of merit, alongside with the trace-distance based one introduced by Breuer, Laine and Piilo in [11] is insensitive to any non-Markovianity due to translations, i.e. which are encoded in the vector $\mathbf{c}(t, t_0)$.

3.2.3.2 Relative Entropy and Quantum Mutual Information

Given two statistical operators $\rho^{1,2}$, their Von-Neumann relative entropy is defined as

$$S\left(\rho^1 \parallel \rho^2\right) \equiv \mathrm{Tr}\left[\rho^1 \log \rho^1\right] - \mathrm{Tr}\left[\rho^1 \log \rho^2\right]. \quad (3.61)$$

Though clearly not being symmetric in its arguments, this quantity has many interesting properties [21, 37] among which the so-called Klein's inequality $S\left(\rho^1 \parallel \rho^2\right) \geq 0$ (the equality sign holds iff $\rho^1 = \rho^2$), which allows to interpret it as a measure of the distinguishability between quantum states, and the contraction property under the action of completely positive and trace preserving maps $\Lambda(t, t_0)$ [50, 58], i.e.

$$S\left(\Lambda(t,t_0)\rho^1 \parallel \Lambda(t,t_0)\rho^2\right) \leq S\left(\rho^1 \parallel \rho^2\right). \tag{3.62}$$

In light of this, it is clear that the relative entropy becomes a monotonic contraction in the case of a quantum Markovian process according to CP-divisibility criterion (3.5) and, on the other hand, becomes a witness of non-Markovianity if, at some intermediate evolution time, it temporarily regrowths [59]. Other relative entropies than the Von Neumann's one, such as the Renyi entropy [60] or the Tsallis entropy [61], have also been proposed as they share the same contractivity property under completely positive and trace preserving maps.

Another witness of non-Markovianity is represented by the quantum mutual information defined as

$$\mathrm{I}(\rho_{SA}) \equiv S(\rho_S) + S(\rho_A) - S(\rho_{SA}), \tag{3.63}$$

$S(\rho) \equiv -\mathrm{Tr}\left[\rho \ln \rho\right]$ being the Von-Neumann entropy of state ρ. Here A is a label denoting an ancillary state which has been coupled to the quantum system of interest. This quantity, which can be equivalently rewritten as the relative entropy

$$\mathrm{I}(\rho_{SA}) = S(\rho_{SA}|\rho_S \otimes \rho_A), \tag{3.64}$$

measures the total amount of correlations between system and environment. It follows from the contractivity property of the relative entropy mentioned above that, if we apply a local quantum channel on the system which describes a decoherent evolution due to the coupling with an environment, we have

$$\begin{aligned} &\mathrm{I}(\rho_{SA}(t)) = \mathrm{I}((\Lambda(t,t_0)\otimes \mathbb{1}_A)\rho_{SA}) \\ &= S\left(\,(\Lambda(t,t_0)\otimes \mathbb{1}_A)\rho_{SA}\,|\,(\Lambda(t,t_0)\rho_S)\otimes\rho_A\right) \leq S\left(\rho_{SA}|\rho_S\otimes\rho_A\right) = \mathrm{I}(\rho_{SA}(t_0)). \end{aligned} \tag{3.65}$$

3.2.3.3 Entanglement

A different measure of non-Markovianity which shares the same perspective as the previous one is the entanglement-based one. The figure of merit in this case is given by an *entanglement monotone*, which is a measure for entanglement-type of correlations which onset between the open quantum system of interest and an ancilla and that cannot increase (nor be generated) under the action of local operations and classical communication (LOCC). Since quantum channels acting locally on the system $\Lambda(t, t_0) \otimes \mathbb{1}_A$ are particular examples of LOCC, any temporary regrowth in the time-behavior of the entanglement monotone E_{SA} is a signature of violation of the CP-divisibility and thus in turn, according to Def.(3.5), of non-Markovianity. Building on this considerations, in [13]

the following measure for the degree of non-Markovianity has been proposed

$$\mathfrak{I}_E = \Delta E + \int_{t_0}^{t_1} dt \left| \frac{dE_{SA}(t)}{dt} \right|, \tag{3.66}$$

, where $\Delta E \equiv E_{SA}(t_1) - E_{SA}(t_0)$. It is worth mentioning that a relationship between the amount of entanglement generated by a given non-Markovian dynamics (according to this definition) and the destruction of accessible information can be found in [62].

3.2.3.4 Fidelity and Bures distance

Especially in the context of continuous-variable systems, the computation of the previous measures, except the one by Torre, Roga and Illuminati and the one by Lorenzo, Plastina and Paternostro introduced above, proves a formidable task. It is mainly for this reason that the following witnesses, which are presented in these last paragraphs, have been introduced.

The first one relies on the so-called *Fidelity* between two quantum states ρ_S^1 and ρ_S^2, defined as

$$F(\rho_S^1, \rho_S^2) \equiv \left(\mathrm{Tr} \left[\sqrt{\sqrt{\rho_S^1}\rho_S^2\sqrt{\rho_S^1}} \right] \right)^2. \tag{3.67}$$

This quantity is directly related to a distance on the set of statistical operators $\mathcal{S}(\mathscr{H})$, known as *Bures distance* [63],

$$\mathcal{D}_B(\rho_S^1, \rho_S^2) \equiv \sqrt{2\left[1 - \sqrt{F(\rho_S^1, \rho_S^2)}\right]}, \tag{3.68}$$

interpreted by Uhlmann [58] as a generalization of transition probabilities for pure states to the case of statistical operators, which gives an estimate of the distance between two quantum states. Among the many important properties of the Fidelity (and of the Bures distance as well), the crucial one for the present purposes is, once again, its monotonicity under the action of completely positive and trace-preserving maps, i.e.

$$F(\Lambda(t, t_0)\rho_S^1(t_0), \Lambda(t, t_0)\rho_S^2(t_0)) \geq F(\rho_S^1(t_0), \rho_S^2(t_0)), \tag{3.69}$$

which traduces the condition that two states subject to the action of the same quantum channel can only decrease their mutual distinguishability. Remarkably, the expression of the fidelity for arbitrary quantum Gaussian states have been recently found [64, 65], which depends only on the vectors of mean values and on the covariance matrices.

The non-Markovianity measure based on the fidelity is consequently given by [66]

$$\mathcal{N}_F(\Lambda) = \max_{\mathbf{P}} \frac{1}{2} \int_{\mathbb{R}^+} \left(\left| \frac{d}{dt} F(\mathbf{P}, t) \right| - \frac{d}{dt} F(\mathbf{P}, t) \right), \tag{3.70}$$

where the maximization is performed on the full set of parameters $\mathbf{P}$ that characterize the pair of Gaussian quantum states.

3.2.3.5 Quantum Fisher Information and Quantum Interferometric Power

The last two related witnesses of non-Markovianity have been introduced in the context of local quantum estimation theory, where the aim is to infer the value $\lambda \in \Lambda$ that characterizes the system of interest (in the sense that it labels the quantum state, giving rise to a one-parameter family of statistical operators $\{\rho_\lambda\}$) but which cannot be measured directly. A measurement of a different but somehow related observable X is then carried out independently n times and a post - process of the outcomes, representing the experimental sample space $\Omega_n = \{x_1, \ldots, x_n\}$, is performed by means of the introduction of a suitable function, called *estimator*, $\hat{\lambda} : \Omega_n \to \Lambda$. In this framework, a result of capital importance is represented by the Cramér - Rao Theorem [67], according to which the variance $\mathrm{Var}(\hat{\lambda})$ of any such estimator $\hat{\lambda}$ is bounded from below

$$\mathrm{Var}(\hat{\lambda}) \geq \frac{1}{N\mathcal{F}(\Pi_x, \rho_\lambda)}, \tag{3.71}$$

with Π_x denoting the POVM representing the quantum measurement of the observable X and where

$$\mathcal{F}(\Pi_x, \rho_\lambda) = \int dx \frac{\left[\partial_\lambda \left(\mathrm{Tr}\left[\Pi_x \rho_\lambda\right]\right)\right]^2}{\mathrm{Tr}\left[\Pi_x \rho_\lambda\right]} \tag{3.72}$$

is the so-called *Fisher Information* (FI). The maximization over all possible measurement schemes Π_x of the FI leads to the so-called Quantum Fisher Information (QFI) [68–70]

$$\mathcal{J}(\rho_\theta) = \max_{\Pi_x} \mathcal{F}(\Pi_x, \rho_\lambda) = \mathrm{Tr}\left[L^2(\rho_\lambda)\,\rho_\lambda\right] = 4 \sum_{\substack{m,n \\ e_m + e_n > 0}} \frac{(e_m - e_n)^2}{e_m + e_n} \left|\langle \phi_m | \left(\mathbb{1}_S \otimes \mathcal{H}_A\right) |\phi_n\rangle\right|^2, \tag{3.73}$$

which represents the ultimate bound (at least in the case of parameter-independent measurement schemes [71]) to the precision in parameter estimation. In Eq. (3.73), the operator $L(\rho_\lambda)$ denotes the symmetric logarithmic derivative operator defined implicitly by the equation

$$\frac{d\rho_\lambda}{d\lambda} \equiv \frac{1}{2}\left(L(\rho_\lambda)\rho_\lambda + \rho_\lambda L(\rho_\lambda)\right). \tag{3.74}$$

The QFI is related to the concepts discussed in the previous paragraph since it can be shown that corresponds to the infinitesimal Bures distance between two quantum states ρ_λ and $\rho_{\lambda+\delta\lambda}$ belonging to the same one-parameter family $\{\rho_\lambda\}$, i.e.

$$\mathcal{J}(\rho_\lambda) = 4 \lim_{\delta\lambda \to 0} \left[\frac{\mathcal{D}_B(\rho_\lambda, \rho_{\lambda+\delta\lambda})}{\delta\lambda}\right]^2, \tag{3.75}$$

with $\rho_{SA} = \sum_n e_n |\phi_n\rangle \langle \phi_n|$. In other words, this quantity thus measures the sensitivity of the change in the states for infinitesimally small changes in the parameter λ [70]. From Eq. (3.73) it descends immediately that, since the Bures distance is a monotonic contraction under the action of completely positive and trace-preserving maps, also the QFI shares this behavior, therefore posing as a suitable candidate to witness the non-Markovianity of the reduced dynamics in the same fashion as Eq. (3.70). In other words, the time derivative of the QFI $\partial_t \mathcal{J}(\rho_\lambda(t))$ can be considered [72] and the regions where it

shows to be positive correspond to non-Markovian behavior according to Definition 3.5. The sum of these positive contributions can be also employed to give an estimate of the amount of non-Markovianity of the underlying dynamics. Finally we note that, interestingly, any eventual increment in the QFI immediately results, in light of Eq. (3.71), in a decrement in the variance (uncertainty) of the estimator $\hat{\lambda}$ and thus, equivalently, in an increment of the information about the parameter λ.

Another QFI - based witness of non-Markovianity is the one recently introduced in [73], based on another metrological figure of merit called *Quantum Interferometric Power* (QIP). The latter measures in a quantitative way the ability to estimate, according to black-box interferometry, a local phase shift in a worst case scenario with a bipartite system (system + ancilla) [73–75]. The Hamiltonian generating the evolution of the 'system + ancilla' compound is given by

$$\mathcal{H}_{SA} = \mathbb{1}_S \otimes \mathcal{H}_A, \tag{3.76}$$

whose spectrum is *a priori* unknown, so that a black-box operation $U_A^\lambda = e^{i\lambda\mathcal{H}_A}$ is imprinted in the ancilla after the transformation. While, as stated above, for any bipartite state ρ_{SA} and any local Hamiltonian $\mathcal{H}_A$ the variance of any estimator $\hat{\lambda}$ is bounded from below by the Quantum Fisher Information $\mathcal{J}(\rho_\lambda)$, the lack of information about the generator $\mathcal{H}_A$ implies that the most significant figure of merit is the QIP, defined as the minimum QFI over all possible local Hamiltonians $\mathcal{H}_A$ with non-degenerate spectrum [69]

$$\mathcal{Q}\left(\rho_{SA}\right) = \frac{1}{4}\inf_{\mathcal{H}_A} \mathcal{J}\left(\rho_{SA}^{\mathcal{H}_A}\right), \tag{3.77}$$

where the $1/4$ prefactor has been inserted for convenience to compensate the factor 4 in the expression of the QFI (3.75).

The QIP has many properties, among which it vanishes for zero-discord states from the perspective of the ancilla, is *invariant under local unitary operations* and reduces to an entanglement monotone for pure quantum states [69]. Most remarkably for the present aim is its monotonically decreasing behavior under completely positive and trace-preserving maps acting locally on the system. Moreover, analytic expressions for the QIP can be found both in the cases of the system being a qubit [69] or a Gaussian states undergoing a local Gaussian channel [76]. In the first case the result reads

$$\mathcal{Q}\left(\rho_{SA}\right) = \varsigma_{min}\left[M\right], \tag{3.78}$$

where $\varsigma_{min}\left[M\right]$ is the smallest eigenvalue of the 3×3 matrix of entries

$$M_{jk} = \frac{1}{2}\sum_{m,n:e_m+e_n>0} \frac{(e_m-e_n)^2}{e_m+e_n} \langle\phi_m|\left(\sigma_j\otimes\mathcal{H}_A\right)|\phi_n\rangle\langle\phi_n|\left(\sigma_k\otimes\mathcal{H}_A\right)|\phi_m\rangle, \tag{3.79}$$

with $\sigma_{1,2,3}\equiv\sigma_{x,y,z}$ being the Pauli matrices.

In the case of Gaussian states undergoing Gaussian evolutions, provided the two-mode covariance of the system + ancilla matrix in the standard form reads

$$\boldsymbol{\sigma}_{SA} = \begin{pmatrix} \boldsymbol{\alpha} & \boldsymbol{\gamma} \\ \boldsymbol{\gamma}^T & \boldsymbol{\beta} \end{pmatrix},$$
$$\boldsymbol{\alpha} = \mathrm{diag}(a,a),\ \boldsymbol{\beta} = \mathrm{diag}(b,b),\ \boldsymbol{\gamma} = \mathrm{diag}(c,d),\ a,b \geq 1, c \geq |d| \geq 0 \tag{3.80}$$

(every two-mode covariance matrix can be transformed to a standard form by means of local symplectic operations, i.e. change of basis), the QIP can be expressed as

$$\mathcal{Q}_G\left(\boldsymbol{\sigma}_{SA}\right) = \frac{C_x + \sqrt{C_x^2 + C_y C_z}}{2C_y}, \tag{3.81}$$

where

$$\begin{aligned} C_x &= (I_2 + I_3)(1 + I_1 + I_3 - I_4) - I_4^2, \\ C_y &= (I_4 - 1)(1 + I_1 + I_2 + 2I_3 + I_4), \\ C_z &= (I_2 + I_4)(I_1 I_2 - I_4) + I_3(1 + I_1)(2I_2 + I_3), \end{aligned} \tag{3.82}$$

with $I_{1,2,3,4}$ being the symplectic invariants of the covariance matrix

$$\begin{aligned} I_1 &= \det\boldsymbol{\alpha}, \quad I_2 = \det\boldsymbol{\beta}, \\ I_3 &= \det\boldsymbol{\gamma}, \quad I_4 = \det\boldsymbol{\sigma}_{SA}. \end{aligned} \tag{3.83}$$

In order to understand how to exploit the QIP in order to witness and quantify the non-Markovianity in the reduced dynamics of a quantum system S, consider that the latter, apart from being initially correlated to an ancilla A according with previous statements, is also coupled with an environment E (which does not interact with the ancilla), so that the total Hamiltonian is now of the form

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{SE} + \mathcal{H}_{SA}, \tag{3.84}$$

with the first three terms completely generic and the last one given by Eq. (3.76). More specifically, within this framework, the role of the ancilla is that of a measuring apparatus for the open system. The evolution of the system S is then determined by a CPT dynamical map $\Lambda(t,0)$ and thus the evolution of $\rho_{SA}(t)$ can be written as

$$\rho_{SA}(t) = \left(\Lambda(t,0) \otimes U_A^{\lambda}\right) \rho_{SA}(0). \tag{3.85}$$

Using this contractivity property of the QIP and its above - mentioned invariance under the action of local unitary operations, it is straightforward to see that, according to Def.(3.5), a dynamics is non-Markovian if there exists some intermediate time t and at least some initial state of the bipartite system such that

$$\frac{d}{dt}\mathcal{Q}\left(\rho_{SA}\right) > 0. \tag{3.86}$$

In the same fashion as [11, 13–16, 18, 77], the consequent measure is then given by

$$\mathcal{N}_{QIP} = \max_{\rho_{SA}(0)} \frac{1}{2} \int_{\mathbb{R}^+} dt \left(\left| \frac{d}{dt} \mathcal{Q}\left(\rho_{SA}\right) \right| + \frac{d}{dt} \mathcal{Q}\left(\rho_{SA}\right) \right), \tag{3.87}$$

where the maximization is carried out over all possible initial states for the bipartite system. We stress again that initial correlations (more specifically non-classical ones) are needed between the system and the ancilla in order for the QIP to not be zero.

4

Characterization of two-time correlation functions: the quantum regression theorem

The word 'regression' had his original meaning in the framework of classical stochastic processes, where, as stated at the beginning of Chapter 3, a process is uniquely determined by the infinite hierarchy of n-time joint probability distributions (3.2). In this context, the expression 'regression' indicated the possibility to reconstruct, starting from the first element of this hierarchy $\mathbb{P}_1(x_0, t_0)$, the 'successive' element, and consequently the entire family.

The first one that has introduced the so-called *regression hypothesis*, has been Lars Onsager in 1931 in his papers [78, 79], in the setting of classical statistical mechanics near equilibrium (linear response regime), where he stated (as a conjecture) that '*the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process*'. This means for example that the correlation in temperature fluctuations in a classical gas and the respective heat satisfy the same equation, which is a Fourier diffusive equation. Such conjecture has been successively demonstrated to hold, in the classical realm, exploiting the so-called *fluctuation-dissipation theorem* introduced by Callen and Welton in [80].

In 1968/1969, Melvin Lax showed how it was possible, for an atom weakly coupled to an electromagnetic field, to access two-time correlation functions of system operators having knowledge of the mean values (see articles [81]); this procedure, applied for the first time to a quantum system, had been named by Lax as 'quantum regression procedure', due to its analogy *in the final intention of the technique* with Onsager's work.

This lexicon lead however to misleading interpretations on the analogy between the works by Onsager and Lax which, going beyond the intents of the author as Lax himself stressed in [82], contributed to spread the impression among the scientific community that the procedure outlined by Lax was the quantum version of Onsager's regression procedure, although instead being only a prescription, valid under the physical

approximations characterizing the specific quantum model considered by him, to access multi-time correlation functions from the knowledge of single-time expectation values, i.e. mean values.

To clarify this puzzle Ford and O'Connell published a series of articles, some of which in a sort of repartee with Lax [83, 84], in which they showed, on the one hand, that the correct quantum version of Onsager regression procedure leads to the so-called quantum fluctuation-dissipation theorem [85–88], meanwhile identifying, on the other hand, with the specific assumptions and approximations involved in the specific model analyzed by Lax the intimate reason for the successful application of his quantum regression procedure.

Meanwhile, inspired by the results obtained by Lax with the use of his quantum regression theorem, several authors [21, 45, 89, 90], dealt with the problem to mathematically settle down the conditions under which such a regression procedure for obtaining multi-time correlation function for mean values was appropriate in the quantum setting; they called it *Quantum Regression Theorem*, maintaining, for the same motivations that induced Lax to call his procedure this way (see above), the terminology introduced in [81].

4.1 The quantum regression theorem

In Chapter 2 we introduced and discussed the concepts of quantum dynamical map and master equation, which allow to describe the dynamics of a reduced system's statistical operators and, consequently, to access the mean values of any system's observables O_S. In order to fully characterize the statistical properties of a quantum system, however, the sole knowledge of the latter is not sufficient and the expectation value of products of system's observables at different times is required. These quantities are known as *multi-time correlation functions*, and their relevance, beside being conceptual and fundamental, pours also into practical situations, since they are often related to measurable quantities. A very well-known example is in fact represented by the fluorescence spectrum of the electromagnetic field emitted by an atom which is the Fourier transform of a two-time correlation function of radiation modes operators [21, 22]

Despite their relevance however, multi-time correlation functions often represent a formidable task to be accomplished, due to the fact that the knowledge of the full system+environment dynamics is required, a generally too demanding request in the context of open quantum systems theory. The *quantum regression theorem* represents in this regard the easiest route to determine two-time correlation functions since it allows, whenever valid, to reconstruct two-time correlation functions from the knowledge of mean values. It is therefore important to clearly understand the conditions which guarantee the quantum regression theorem to apply, especially in relation to the concept of non-Markovianity.

4.1.1 Multi-time correlation functions

Here we will introduce the concept of multi-time correlation functions. A proper definition can be given, following [45], in terms of a multi-time sequence of generalized measurements performed on the quantum system under consideration. A two-step version of this multi-time measurement protocol for the special case of selective measurements will be also employed in Chapter 5 to obtain the full statistics of generic observables.

Definition 4.1. The most general form for a measurable multi-time correlation function is given by

$$\langle A_1(s_1)\dots A_m(s_m)B_n(t_n)\dots B_1(t_1)\rangle = \mathrm{Tr}\left[B_n(t_n)\dots B_1(t_1)\rho(t_0)A_1(s_1)\dots A_m(s_m)\right], \tag{4.1}$$

where ρ describes the initial state of a system of interest, $\{A_j(t_j)\}_{j=1,\dots,m}$ and $\{B_k(t_k)\}_{k=1,\dots,n}$ are arbitrary system's operators belonging to $\mathcal{B}(\mathscr{H})$ and evolved according to the Heisenberg picture with respect to the full Hamiltonian

$$A_j(t_j) = U^\dagger(t_j,t_0)A_jU(t_j,t_0), \tag{4.2}$$

and where $s_m > \dots > s_1 \geq 0$, $t_n > \dots > t_1 \geq 0$. The order between the sequences of the s_i and t_j is not specified at this level.

The demonstration that this is the most general form achievable can be found in Chapter 2.3 of [45]. Upon a further time-ordering of the combined set of times $\{s_1,\dots,s_m,t_1,\dots,t_n\}$ into a new sequence of $q \leq n+m$ elements [1] $\{r_1,\dots,r_q\}$, Equation (4.1) can be rewritten as [21, 22, 45]

$$\begin{aligned}\langle A_1(s_1)\dots A_m(s_m)B_n(t_n)\dots B_1(t_1)\rangle = \mathrm{Tr}\left[\Phi_qU(t_q,t_{q-1})\Phi_{q-1}U(t_{q-1},t_{q-2})\right.\\ \left.\Phi_{q-2}\cdots U(t_2,t_1)\Phi_1U(t_1,t_0)\rho(t_0)\right],\end{aligned} \tag{4.3}$$

where we have introduced the superoperator Φ_k through its action on a generic $\omega \in \mathcal{T}(\mathscr{H})$

$$\Phi_k[\omega] \equiv \begin{cases} A_i\omega, & \text{if } r_k = t_i \neq s_j \text{ for some i = 1, . . . , m and every j=1, . . . , n} \\ \omega B_j, & \text{if } r_k = s_j \neq t_i \text{ for some j = 1, . . . , n and every i=1, . . . , m} \\ A_i\omega B_j, & \text{if } r_k = t_i = s_j \text{ for some i = 1, . . . , m and some j=1, . . . , n} \end{cases}, \tag{4.4}$$

and where we have removed the square brackets, for easiness of notation, assuming that the super-operators always act on anything standing to their right.

In what follows we will deal, for the sake of simplicity, with two-time correlation functions, but in principle higher correlation functions can be considered (and reconstructed by means of the quantum regression theorem, if valid). Given a generic system initially described by a statistical operator ρ and evolving according to some unitary operator

[1] The number q of elements of the time-ordered set can be smaller than $n+m$ since, for some $i = 1,\dots,m$ and $j = 1,\dots,n$, one can have $s_i = t_j$.

$U(t, t_0)$, the two-time correlation function of generic operators $O_1, O_2 \in \mathcal{B}(\mathscr{H})$ is defined as

$$\langle O_1(t+\tau)O_2(t)\rangle \equiv \mathrm{Tr}\left[U^\dagger(t+\tau,t_0)O_1U(t+\tau,t_0)U^\dagger(t,t_0)O_2U(t,t_0)\rho(t_0)\right], \tag{4.5}$$

with $\tau \geq 0$. By exploiting the ciclicity property of the trace, Equation (4.5) can be re-expressed as

$$\langle O_1(t+\tau)O_2(t)\rangle = \mathrm{Tr}\left[O_1\,\chi(\tau,t)\right], \tag{4.6}$$

where

$$\chi(\tau,t) = U(t+\tau,t)\left(O_2\rho(t)\right)U^\dagger(t+\tau,t) \tag{4.7}$$

represents a trace-class operator sometimes referred to as *effective statistical operator* [91], even though it does not belong to $\mathcal{S}(\mathscr{H})$ since its trace is not equal to 1 any more.

4.1.2 Two-time correlation functions and the quantum regression theorem

Consider a quantum system of interest S interacting with an environment E such that the evolution of the composite system is given in terms of a unitary operator $U(t, t_0) = e^{-i\mathcal{H}(t-t_0)}$, with $\mathcal{H} = \mathcal{H}_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \mathcal{H}_E + \mathcal{H}_{SE}$. Moreover, assume that the initial state of the overall system is factorized

$$\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E, \tag{4.8}$$

with ρ_E fixed, and that the reduced dynamics can be described in terms of a collection of family of CPTP maps of the form

$$\Lambda(t,s) = \overrightarrow{T}\exp\left[\int_s^t d\tau\mathcal{L}(\tau)\right], \tag{4.9}$$

with $\overrightarrow{T}$ being the chronological time ordering operator and $\mathcal{L}(\tau)$ representing the infinitesimal generator in time-dependent Lindblad form (2.105), such that

$$\begin{cases} \frac{d}{dt}\Lambda(t,s) = \mathcal{L}(t)\Lambda(t,s), \\ \Lambda(s,s) = \mathbb{1}_S, \end{cases} \qquad t > s. \tag{4.10}$$

The mean value of a generic system's operator $A \in \mathcal{B}(\mathscr{H}_S)$ can thus be determined as

$$\langle A(t)\rangle = \mathrm{Tr}_S\left[A\,\Lambda(t,t_0)\rho_S(t_0)\right], \tag{4.11}$$

as well as its evolution equation, which reads

$$\begin{aligned}\frac{d}{dt}\langle A(t)\rangle &= \frac{d}{dt}\mathrm{Tr}_S A\,\rho_S(t)\\ &= \frac{d}{dt}\mathrm{Tr}_S\left[A\,\Lambda(t,t_0)\rho_S\right]\\ &= \mathrm{Tr}_S\left[A\,\left(\frac{d}{dt}\Lambda(t,t_0)\rho_S\right)\right]\\ &= \mathrm{Tr}_S\left[A\,\mathcal{L}(t)\Lambda(t,t_0)\rho_S\right]\\ &= \mathrm{Tr}_S\left[\mathcal{L}'(t)A\,\Lambda(t,t_0)\rho_S\right]\\ &= \mathrm{Tr}_S\left[\mathcal{L}'(t)A\,\rho_S(t)\right],\end{aligned} \tag{4.12}$$

where $\mathcal{L}'(t)$ is the adjoint map of $\mathcal{L}(t)$ as defined in Equation (2.28).

Given two open system's operators, $A\otimes\mathbb{1}_E$ and $B\otimes\mathbb{1}_E$, their two-time correlation function is then defined as

$$\begin{aligned}\langle A(t+\tau)B(t)\rangle &\equiv \mathrm{Tr}_{SE}\left[U^\dagger(t+\tau,t_0)\,(A\otimes\mathbb{1}_E)\,U(t+\tau,t_0)U^\dagger(t,t_0)\,(B\otimes\mathbb{1}_E)\,U(t,t_0)\rho_{SE}(t_0)\right]\\ &= \mathrm{Tr}_S\left[A\chi_S(\tau,t)\right],\end{aligned} \tag{4.13}$$

where we have introduced the reduced effective statistical operator

$$\chi_S(\tau,t) = \mathrm{Tr}_E\left[\chi(\tau,t)\right] = \mathrm{Tr}_E\left[U(t+\tau,t)\,(B\otimes\mathbb{1}_E\,\rho_{SE}(t))\,U^\dagger(t+\tau,t)\right]. \tag{4.14}$$

Now, suppose that we can describe the evolution of $\chi_S(\tau,t)$ *with respect to* τ with the same dynamical maps $\Lambda(t,s)$ which fix the evolution of the statistical operator, i.e.

$$\begin{cases}\chi_S(\tau,t) = \Lambda(t+\tau,t)\chi_S(0,t),\\ \chi_S(0,t) = B\rho_S(t).\end{cases} \tag{4.15}$$

If this is the case, then the two-time correlation function (4.13) can be written as

$$\langle A(t+\tau)B(t)\rangle = \mathrm{Tr}_S\left[A\,\Lambda(t+\tau,t)\chi_S(0,t)\right], \tag{4.16}$$

and its evolution equation becomes

$$\begin{aligned}\frac{d}{d\tau}\langle A(t+\tau)B(t)\rangle &= \frac{d}{d\tau}\mathrm{Tr}_S\left[A\,\chi_S(\tau,t)\right]\\ &= \frac{d}{d\tau}\mathrm{Tr}_S\left[A\,\Lambda(t+\tau,t)\chi_S(0,t)\right]\\ &= \mathrm{Tr}_S\left[A\,\left(\frac{d}{d\tau}\Lambda(t+\tau,t)\chi_S(0,t)\right)\right]\\ &= \mathrm{Tr}_S\left[A\,\mathcal{L}(\tau)\Lambda(t+\tau,t)\chi_S(0,t)\right]\\ &= \mathrm{Tr}_S\left[\mathcal{L}'(t)[A]\,\Lambda(t+\tau,t)\chi_S(0,t)\right]\\ &= \mathrm{Tr}_S\left[\mathcal{L}'(t)[A]\,\chi_S(\tau,t)\right].\end{aligned} \tag{4.17}$$

It is immediately evident a formal similarity between Equations (4.11) and (4.16) (or equivalently between Equations (4.12) and (4.17)), upon the substitution $\rho_S(0) \mapsto \chi_S(0, t)$. Under the above requirement, the two-time correlation functions can thus be fully determined by the sole knowledge of the dynamical map which determines the evolution of the statistical operator or equivalently of the mean values.

The validity of Equation (4.16) can be identified with the *validity of the quantum regression theorem* and, from now on, we will use the subscript qrt to denote the two-time correlation functions evaluated through Equation (4.16).

It is very important to stress that all the procedure relies on Equation (4.15), which requires that each and every assumption made in order to derive the dynamics of $\rho_S(t)$ can be legitimately made also to get the evolution of $\chi_S(\tau, t)$ with respect to τ [92]. In particular, the hypothesis of an initial total product state in Equation (4.8) is translated into the hypothesis of a product state at any intermediate time t,

$$\rho_{SE}(t) = \rho_S(t) \otimes \rho_E. \tag{4.18}$$

The physical idea is then that the quantum regression theorem holds whenever the system-environment correlations due to the interaction can be neglected [89].

Note that this condition will never be strictly satisfied as long as the system and the environment mutually interact, but it should be understood as a guideline to detect the regimes in which Equation (4.16) provides a satisfying description of the evolution of the two-time correlation functions. More precisely, Dümcke [93] demonstrated that the exact expression of the two-time (multi-time) correlation functions, see Equation (4.5), converges to the expression in Equation (4.16) in the weak coupling limit and in the singular coupling limit. As well-known, in these limits the reduced dynamics converges to a semigroup dynamics [29, 94]. Nevertheless, the correctness of a semigroup description of the reduced dynamics is not always enough to guarantee the accuracy of the quantum regression theorem [83, 95]. More in general, the investigation of a more precise link between a sharply defined notion of Markovianity of quantum dynamics and the quantum regression theorem represents the goal of the present Chapter.

It is worth stressing that the quantum regression theorem provided by Equation (4.16) can be equivalently formulated in terms of the differential equations satisfied by mean values and two-time correlation functions, as was originally done in [81]. For the sake of simplicity, let us focus on the finite dimensional case $\mathscr{H}_S \cong \mathbb{C}^N$ and consider a reduced dynamics fixed by the family of maps $\{\Lambda(t)\}_{t \geq t_0}$ and a basis $\{E_i\}_{1,\ldots,N^2}$ of linear operators on $\mathbb{C}^N$, such that the corresponding mean values fulfil the following coupled linear equations of motion [90]

$$\frac{d}{dt}\langle E_i(t)\rangle = \sum_j G_{ij}(t)\langle E_j(t)\rangle, \tag{4.19}$$

with the initial condition $\langle E_i(t)\rangle|_{t=0} = \langle E_i(0)\rangle$. In this case, the quantum regression theorem is said to hold if the two-time correlation functions satisfy [21, 92]

$$\frac{d}{d\tau}\langle E_i(t+\tau)E_k(t)\rangle_{qrt} = \sum_j G_{ij}(t+\tau)\langle E_j(t+\tau)E_k(t)\rangle_{qrt}\,, \tag{4.20}$$

with the initial condition

$$\langle E_i(t+\tau)E_k(t)\rangle_{qrt}|_{\tau=0} = \langle E_i(t)E_k(t)\rangle. \tag{4.21}$$

In the following Sections, we will consider two specific models of open quantum systems which allow the analytic evaluation of the exact two-time correlation functions obtained from the full unitary evolution $\langle E_i(t+\tau)E_k(t)\rangle$, see Equation (4.5). In such models we will compare these quantities with the same ones predicted by the quantum regression theorem $\langle E_i(t+\tau)E_k(t)\rangle_{qrt}$ and we will quantify the error made by using the latter procedure by computing the relative error

$$Z \equiv \left|1 - \frac{\langle A(t+\tau)B(t)\rangle_{qrt}}{\langle A(t+\tau)B(t)\rangle}\right|. \tag{4.22}$$

Note that, in general, this quantity is different for each couple of system's operators and thus one should calculate it for every couple of operators in the basis $\{E_i\}_{1,\dots,N^2}$ and perform a maximization over them. Nevertheless, in the following analyses it will be enough to deal with a single couple of system's operators, which fully encloses the violations of the quantum regression theorem for the models at hand.

4.2 The pure-dephasing spin-boson model

In this section, we take into account a model whose full unitary evolution can be exactly evaluated [21, 96], so as to obtain the exact expression of the two-time correlation functions, to be compared with the expression provided by the quantum regression theorem. This model is a pure-decoherence model, in which the decay of the coherences occurs without a decay of the corresponding populations. Indeed, this is due to the fact that the free Hamiltonian of the open system $H_S \otimes \mathbb{1}_E$ commutes with the total Hamiltonian H_T [21].

4.2.1 The model

Let us consider a two-level system linearly interacting with a bath of harmonic oscillators, so that the total Hamiltonian is

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{SE} = \frac{\omega_s}{2}\sigma_z \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \sum_k \omega_k b_k^\dagger b_k + \sum_k \sigma_z \otimes \left(g_k b_k^\dagger + g_k^* b_k\right), \tag{4.23}$$

with ω_s being the energy gap between the two levels of the system (in units of $\hbar$, which is henceforth set to 1 for convenience), σ_z being the z-Pauli matrix and k labels the environmental bosonic mode relative to the frequency ω_k and creation-annihilation operators $b_k^\dagger, b_k$.

Since we will be interested in evaluating expectation values of system's operators, we move to the more convenient interaction picture with respect to the free Hamiltonian $\mathcal{H}_S + \mathcal{H}_E$, according to which the interaction Hamiltonian reads

$$\tilde{\mathcal{H}}_{SE}(t) = e^{i(\mathcal{H}_S+\mathcal{H}_E)t}\,\mathcal{H}_{SE}\,e^{-i(\mathcal{H}_S+\mathcal{H}_E)t} = \sum_k \sigma_z \otimes \left(g_k b_k^\dagger(t) + g_k^* b_k(t)\right). \tag{4.24}$$

An analytic expression for the total evolution operator in the interaction picture

$$\tilde{U}(t) = \mathrm{T}_{\leftarrow} \exp\left[-i\int_0^t ds \tilde{\mathcal{H}}_{SE}(s)\right] \tag{4.25}$$

can be found by exploiting Magnus series expansion [97] and noticing that the commutator between the interaction Hamiltonian at two different times is a c-number function

$$\left[\tilde{\mathcal{H}}_{SE}(t), \tilde{\mathcal{H}}_{SE}(t)\right] = \sum_k \left[-2i|g_k|^2 \sin\left(\omega_k(t-t')\right)\right](\mathbb{1}_S \otimes \mathbb{1}_E) \equiv -2i\zeta(t-t'). \tag{4.26}$$

This allows to truncate Magnus expansion at second order (every higher order contribution in fact vanishes) thus giving

$$\begin{aligned}\tilde{U}(t) &= \exp\left[-\frac{1}{2}\int_0^t dt_1 \int_0^t dt_2 \Theta(t_1-t_2)\left[\tilde{\mathcal{H}}_{SE}(t_1), \tilde{\mathcal{H}}_{SE}(t_2)\right]\right] \cdot \exp\left[-i\int_0^t dt' \tilde{\mathcal{H}}_{SE}(t')\right] \\ &= \exp\left[i\int_0^t dt_1 \int_0^t dt_2 \Theta(t_1-t_2)\zeta(t_1-t_2)\right] \cdot \exp\left[-i\int_0^t dt' \tilde{\mathcal{H}}_{SE}(t')\right] \\ &= e^{i\Psi(t)} V(t),\end{aligned} \tag{4.27}$$

where the first factor is a global phase factor which is irrelevant to the forthcoming analysis and the second factor is the unitary operator

$$V(t) = \exp\left[\frac{1}{2}\sigma_z \otimes \sum_k \left(\alpha_k(t) b_k^\dagger - \alpha_k^*(t) b_k\right)\right], \tag{4.28}$$

with

$$\alpha_k(t) = 2g_k \frac{1-e^{i\omega_k t}}{\omega_k}. \tag{4.29}$$

Its action on a generic state of the composite system $|j\rangle \otimes |\phi\rangle$ (with $|\phi\rangle \in \mathscr{H}_E$ and $|j\rangle \in \mathscr{H}_S \quad j = 0, 1$) reads

$$V(t)\left(|j\rangle \otimes |\phi\rangle\right) = \exp\left[\sigma_z \otimes \sum_k \left(\alpha_k(t) b_k^\dagger - \alpha_k^*(t) b_k\right)\right](|j\rangle \otimes |\phi\rangle) = |j\rangle \otimes \bigtriangleup\left((-1)^j \frac{\boldsymbol{\alpha}_t}{2}\right)|\phi\rangle, \tag{4.30}$$

where we have introduced the *multi-mode displacement operator* [43]

$$\bigtriangleup(\boldsymbol{\beta}) = \prod_k D(\beta_k) = \prod_k \exp\left[\beta_k b_k^\dagger - \beta_k^* b_k\right], \tag{4.31}$$

where $\boldsymbol{\beta}$ denotes the infinite dimensional vector with components β_k. The single-mode displacement operator $D(\beta_k)$, widely employed especially in quantum optics due to its intimate relation with coherent states [43, 46, 98, 99], has, among others, the following properties which will be useful for forthcoming purposes

(i)
$$D^\dagger(\beta_k) = D(-\beta_k), \tag{4.32}$$

(ii)
$$D(\beta_k)\, D(\gamma_k) = D(\beta_k + \gamma_k)\, e^{i\, Im(\beta_k \gamma_k^*)}. \tag{4.33}$$

By making use of Equations (4.30), (4.32) and (4.33), it is easy to see that

$$\begin{aligned}
\tilde{\rho}_S(t) &= \mathrm{Tr}_E\left[\tilde{U}(t)\,(\rho_S(0)\otimes\rho_E)\,\tilde{U}^\dagger(t)\right] && (4.34)\\
&= \sum_{r,j=0}^{1} [\rho_S(0)]_{rj}\, \mathrm{Tr}_E\left[V(t)\,(|r\rangle\langle j|\otimes\rho_E)\,V^\dagger(t)\right]\\
&= \sum_{r,j=0}^{1} [\rho_S(0)]_{rj}\, |r\rangle\langle j|\, \mathrm{Tr}_E\left[\prod_k D\left((-1)^r\frac{\alpha_k(t)}{2}\right)\rho_E \prod_{k'} D^\dagger\left((-1)^j\frac{\alpha_{k'}(t)}{2}\right)\right]\\
&= \sum_{r,j=0}^{1} [\rho_S(0)]_{rj}\, |r\rangle\langle j|\, \mathrm{Tr}_E\left[\bigtriangleup\left((-1)^{j+1}\frac{\boldsymbol{\alpha}_t}{2}\right)\bigtriangleup\left((-1)^r\frac{\boldsymbol{\alpha}_t}{2}\right)\rho_E)\right]. && (4.35)
\end{aligned}$$

It is straightforward to show that, by virtue of property (4.33) of the displacement operator, the following relation holds

$$\bigtriangleup\left((-1)^{j+1}\frac{\boldsymbol{\alpha}_t}{2}\right)\bigtriangleup\left((-1)^r\frac{\boldsymbol{\alpha}_t}{2}\right) = \delta_{r,j}\cdot\mathbb{1} + (1-\delta_{r,j})\bigtriangleup((-1)^r\boldsymbol{\alpha}_t), \tag{4.36}$$

and, consequently, the quantity under the trace over the environment in Equation (4.34) can be written as

$$\begin{aligned}
\mathrm{Tr}_E\left[\bigtriangleup\left((-1)^{j+1}\frac{\boldsymbol{\alpha}_t}{2}\right)\bigtriangleup\left((-1)^r\frac{\boldsymbol{\alpha}_t}{2}\right)\rho_E)\right] &= \mathrm{Tr}_E\left[\left(\delta_{r,j}\cdot\mathbb{1} + (1-\delta_{r,j})\bigtriangleup((-1)^r\boldsymbol{\alpha}_t)\right)\rho_E)\right]\\
&= \delta_{r,j} + (1-\delta_{r,j})\,\mathrm{Tr}_E\left[\bigtriangleup((-1)^r\boldsymbol{\alpha}_t)\;\rho_E\right].
\end{aligned} \tag{4.37}$$

Substituting this expression into Equation (4.34) and moving back to Schrödinger picture finally leads to the expression of the reduced system's state

$$\rho_S(t) = \sum_{r,j=0}^{1} [\rho_S(0)]_{rj}\, |r\rangle\langle j|\, \left(\delta_{r,j} + (1-\delta_{r,j})\, e^{(-i)^j\omega_s t}\mathrm{Tr}_E\bigtriangleup((-1)^r\boldsymbol{\alpha}_t)\;\rho_E\right), \tag{4.38}$$

which can be conveniently visualized in matrix form as

$$\rho_S(t) = \Lambda(t,0)\rho_S(0) = \begin{pmatrix} \rho_{00} & \rho_{01}\gamma(t)e^{-i\omega_s t} \\ \rho_{10}\gamma^*(t)e^{i\omega_s t} & \rho_{11} \end{pmatrix}, \tag{4.39}$$

where the decoherence function $\gamma(t)$ is given by

$$\gamma(t) = \mathrm{Tr}_E\left[\bigtriangleup(\boldsymbol{\alpha}_t)\rho_E\right]. \tag{4.40}$$

4.2.2 The master equation

This Subsection is devoted to derive the time-local master equation governing the reduced system's dynamics

$$\frac{d\rho_S(t)}{dt} = \mathcal{K}_{TCL}(t)\,\rho_S(t). \tag{4.41}$$

To achieve this goal, we follow the construction discussed in Chapter 2 Subsection 2.2.3. The starting point is to find the representation of the dynamical map $\Lambda(t,0)$ on the basis $\{E_{\alpha\beta}\}_{\alpha,\beta=0}^{N^2-1}$ given by Equation (2.36), in order to be able to use Equation (2.82). The latter can be obtained with straightforward calculations from Equation (4.39) and reads

$$\mathbf{\Lambda}(t,0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & Re\left[\gamma(t)\right] & Im\left[\gamma(t)\right] & 0 \\ 0 & -Im\left[\gamma(t)\right] & Re\left[\gamma(t)\right] & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{4.42}$$

From Equation (4.42), through Equation (2.82) we then get the expression of the time-local generator $\mathcal{K}_{TCL}(t)$ on the same basis, i.e.

$$\mathbf{K}_{TCL}(t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & Re\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & Im\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & 0 \\ 0 & -Im\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & Re\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4.43}$$

Since the dynamical map $\Lambda(t,0)$ is trace and hermiticity preserving, we can moreover apply the construction put forward in Chapter 2 Subsection 2.2.4.1 to further specify the structure of the master equation. According to (2.86), we choose the following Hilbert-Schmidt basis

$$\frac{\mathbb{1}_S}{\sqrt{2}} \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \frac{\sigma_z}{\sqrt{2}} \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_+ \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{4.44}$$

and perform the change of basis (2.40) from $\{E_{\alpha\beta}\}_{\alpha,\beta=1,\dots,4}$ to $\{F_{\alpha\beta}\}_{\alpha,\beta=1,\dots,4}$, which leads to $\mathbf{K'}_{TCL}(t)$

$$\mathbf{K'}_{TCL}(t) = \begin{pmatrix} Re\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & 0 & 0 & -iIm\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ iIm\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] & 0 & 0 & -Re\left[\frac{\dot\gamma(t)}{\gamma(t)}\right] \end{pmatrix}. \tag{4.45}$$

Making use of Equations (2.88), (2.89) and (2.90), it is then straightforward to prove that the master equation can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t) = -i\frac{\epsilon(t)}{2}[\sigma_z, \rho_S(t)] + \frac{\mathcal{D}(t)}{2}\left(\sigma_z\rho_S(t)\sigma_z - \rho_S(t)\right), \tag{4.46}$$

where

$$\epsilon(t) = \omega_s - Im\left[\frac{\mathrm{d}\gamma(t)/\mathrm{d}t}{\gamma(t)}\right] \tag{4.47}$$

and the so-called dephasing function $\mathcal{D}(t)$ is

$$\mathcal{D}(t) = -Re\left[\frac{\mathrm{d}\gamma(t)/\mathrm{d}t}{\gamma(t)}\right] = -\frac{\mathrm{d}}{\mathrm{d}t}\ln|\gamma(t)|. \tag{4.48}$$

In the following, we will focus on the case of an initial thermal (Gibbs) state of the environment

$$\rho_E(0) \equiv \rho_\beta = \frac{e^{-\beta\mathcal{H}_E}}{Z_E}, \quad Z_E \equiv \mathrm{Tr}_E\left[e^{-\beta\mathcal{H}_E}\right], \tag{4.49}$$

relative to the inverse temperature β. Moreover, we will take the continuum limit of environmental modes: given a frequency distribution $f(\omega)$ of the bath modes, we introduce the spectral density $J(\omega) = 4f(\omega)|g(\omega)|^2$, so that one has [21]

$$\gamma(t) = \exp\left[-\int_0^\infty d\omega\, J(\omega)\coth\left(\frac{\beta\omega}{2}\right)\frac{1-\cos(\omega t)}{\omega^2}\right], \tag{4.50}$$

and hence $\epsilon(t) = \omega_s$ and

$$\mathcal{D}(t) = \int_0^\infty d\omega\, J(\omega)\coth\left(\frac{\beta\omega}{2}\right)\frac{\sin(\omega t)}{\omega}. \tag{4.51}$$

4.2.3 Measures of non-Markovianity

4.2.3.1 General expressions

For this specific model, all the definitions of Markovianity given in Chapter 3 are actually equivalent [100]. This is due to the fact that there is only one operator contribution in the time-local master equation (4.46), corresponding to the dephasing interaction.

For what concerns the estimators of the degree of non-Markovianity, we will explicitly calculate the one introduced by Breuer, Laine and Piilo (BLP, see Subsection 3.2.2) and the one by Rivas, Huelga and Plenio (RHP, see Subsection 3.2.1).) It is in fact interesting to

consider both of them since, as will be evident later, their numerical values are in general different and, more importantly, they depend in a different way on the parameters of the model.

Let us start by evaluating the BLP measure. The trace distance between two reduced states evolved through Equation (4.39) is given by

$$D(t,\rho_S^{1,2}) = \sqrt{\delta_p^2 + |\delta_c|^2|\gamma(t)|^2}, \tag{4.52}$$

where $\delta_p = \rho_{00}^1 - \rho_{00}^2$ and $\delta_c = \rho_{01}^1 - \rho_{01}^2$ are the differences between, respectively, the populations and the coherences of the two initial conditions ρ_S^1 and ρ_S^2. The couple of initial states that maximizes the growth of the trace distance is given by the pure orthogonal states $\rho_S^{1,2} = |\psi_\pm\rangle\langle\psi_\pm|$, where $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$, and the corresponding trace distance at time t is simply $|\gamma(t)|$. The BLP measure therefore reads

$$\mathscr{N} = \sum_m \left(|\gamma(b_m)| - |\gamma(a_m)|\right), \tag{4.53}$$

where $\Omega_+ = \bigcup_m (a_m, b_m)$ is the union of the time intervals in which $|\gamma(t)|$ increases. The BLP measure is different from zero if and only if $\mathrm{d}|\gamma(t)|/\mathrm{d}t > 0$ for some interval of time, which is equivalent to the requirement that the dephasing function $\mathcal{D}(t)$ in Equation (4.46) is not a positive function of time, i.e., that the CP-divisibility of the dynamics is broken, Sec. 3.2.1. As anticipated, for this model $\mathscr{N} > 0 \iff \mathscr{I} > 0$. Furthermore, given a pure dephasing master equation as in Equation (4.46), one has [13] $\mathfrak{g}(t) = 0$ if $\mathcal{D}(t) \geq 0$ and $\mathfrak{g}(t) = -\mathcal{D}(t)$ if $\mathcal{D}(t) < 0$, so that, see Equation (4.48),

$$\mathscr{I} = \sum_m \left(\ln|\gamma(b_m)| - \ln|\gamma(a_m)|\right), \tag{4.54}$$

where the a_m and b_m are defined as for the BLP measure.

4.2.3.2 Zero-temperature environment

In order to evaluate explicitly the non-Markovianity measures, we need to specify the spectral density $J(\omega)$. In the following, we assume a spectral density of the form

$$J(\omega) = \lambda \frac{\omega^s}{\Omega^{s-1}} e^{-\frac{\omega}{\Omega}}, \tag{4.55}$$

where λ is the coupling strength, the parameter s fixes the low frequency behaviour and Ω is a cut-off frequency. The non-Markovianity for the pure dephasing spin model with a spectral density as in Equation (4.55) has been considered in [101, 102] for the case $\lambda = 1$. We are now interested in the comparison between non-Markovianity and violations of the quantum regression theorem, so that, as will become clear in the next section, the dependence on λ plays a crucial role. In particular, we consider the case of low temperature, i.e., $\beta \gg 1$, so that $\coth\left(\frac{\beta\omega}{2}\right) \approx 1$. The dephasing function in this case

reads, see Equation (4.51),

$$\mathcal{D}_s(t) = \frac{\lambda\Omega\Gamma(s)}{(1+(\Omega t)^2)^{\frac{s}{2}}} \sin\left(s \arctan\left(\Omega t\right)\right), \tag{4.56}$$

with $\Gamma(s)$ the Euler gamma function. The latter can be expressed in a more elegant form by exploiting the identities

$$\sin\left(\arctan(x)\right) = \frac{x}{\sqrt{1+x^2}} \quad , \cos\left(\arctan(x)\right) = \frac{1}{\sqrt{1+x^2}} \tag{4.57}$$

together with

$$\sin\left(sx\right) = \sum_{k=0} \binom{s}{k} \left(\cos(x)\right)^k \left(\sin(x)\right)^{s-k} \sin\left(\frac{\pi}{2}(s-k)\right), \tag{4.58}$$

so that one is left with

$$\begin{aligned}
\mathcal{D}_s(t) &= \frac{\lambda\Omega\Gamma(s)}{2i\left(1+(\Omega t)^2\right)^s} \left[\sum_{k=0} \binom{s}{k} (\Omega t)^{s-k} (i^{s-k} - (-i)^{s-k})\right] \\
&= \frac{\lambda\Omega\Gamma(s)}{2i\left(1+(\Omega t)^2\right)^s} \left[(1+i\Omega t)^s - (1-i\Omega t)^s\right] \\
&= \lambda\Omega\Gamma(s) \frac{Im\left[(1+i\Omega t)^s\right]}{(1+(\Omega t)^2)^s}.
\end{aligned} \tag{4.59}$$

With analogous calculations, the decoherence function can be written as

$$\gamma_s(t) = \exp\left[-\lambda\Gamma(s-1)\left(1 - \frac{Re[(1+i\Omega t)^{s-1}]}{(1+(\Omega t)^2)^{s-1}}\right)\right]. \tag{4.60}$$

As before, let Ω_+ be the union of the time intervals for which $\mathcal{D}(t) < 0$, i.e., equivalently, $|\gamma(t)|$ increases. The number of solutions of the equation $\mathcal{D}(t) = 0$ grows with the parameter s: for $s = 1, 2$ the dephasing function is always strictly positive, while for $s = 3$ and $s = 4$ there is one zero at $t_3^* = \frac{\sqrt{3}}{\Omega}$ and $t_4^* = \frac{1}{\Omega}$ respectively. Indeed, if the number of zeros is odd, $\mathcal{D}(t)$ is negative from its last zero to infinity, while if the number of zeros is even, it approaches zero asymptotically from above. As a consequence, the two measures of non-Markovianity are equal to zero for $s = 1, 2$ and, to give an example, one has for $s = 3$

$$\begin{aligned}
\mathcal{N}_3(\lambda) &= \lim_{t\to\infty} |\gamma(t)| - |\gamma(t_3^*)| = e^{-\lambda} - e^{-\frac{9}{8}\lambda} \\
\mathcal{I}_3(\lambda) &= \lim_{t\to\infty} \ln|\gamma(t)| - \ln|\gamma(t_3^*)| = \frac{\lambda}{8},
\end{aligned} \tag{4.61}$$

and, analogously, for $s = 4$

$$\mathcal{N}_4(\lambda) = e^{-2\lambda} - e^{-\frac{5}{2}\lambda}, \qquad \mathcal{I}_4(\lambda) = \frac{\lambda}{2}. \tag{4.62}$$

In Fig. 4.1 **(a)** and **(b)**, we report, respectively, the BLP and the RHP measures of non-Markovianity as a function of λ, for different values of s.

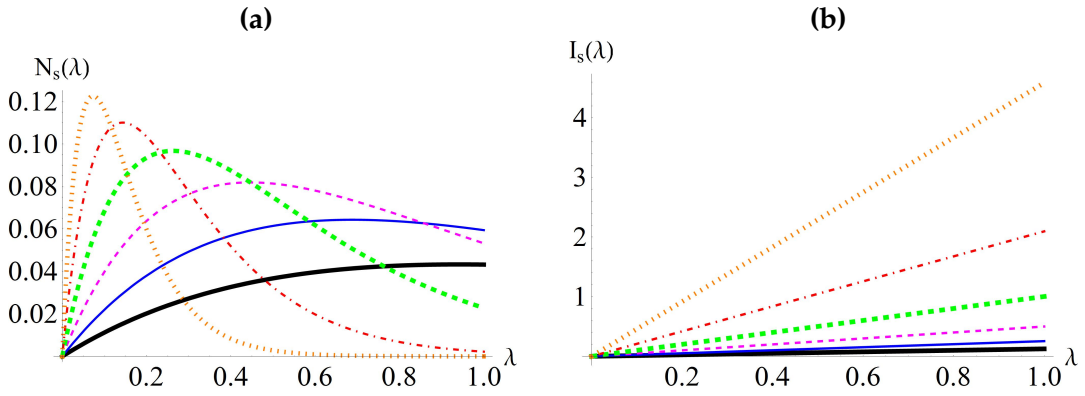

FIGURE 4.1: (Color online) **(a)** BLP measure of non-Markovianity $\mathcal{N}_s(\lambda)$, see Equation (4.53), and **(b)** RHP measure of non-Markovianity $\mathcal{I}_s(\lambda)$, see Equation (4.54), as a function of the coupling strength λ for increasing values of the parameter s. In both panels the curves are evaluated for $s = 3$ (black thick solid line), $s = 3.5$ (blue solid line), $s = 4$ (magenta dashed line), $s = 4.5$ (green dashed thick line), $s = 5$ (red dot-dashed line) and $s = 5.5$ (orange dotted line).

The behaviour of the two measures is clearly different. The RHP measure is a monotonically increasing function of both λ and s: the increase is linear with respect to the former parameter and exponential with respect to the latter. On the other hand, for every fixed s, there is a critical value of the coupling strength $\lambda^*(s)$, which is smaller for increasing s, that separates two different regimes of the BLP measure: for $\lambda < \lambda^*(s)$, the non-Markovianity measure increases with the increase of the system-environment coupling, while for $\lambda > \lambda^*(s)$ it decreases with the increase of the coupling. Analogously, there is a threshold value $s^*(\lambda)$ of the parameter s, which is higher for smaller values of λ, such that the BLP measure increases for $s < s^*(\lambda)$ and decreases for $s > s^*(\lambda)$, see also Fig. 4.2 **(a)**. Incidentally, the maximum value as a function of λ, $\max_\lambda \mathcal{N}_s(\lambda)$, is a monotonically increasing function of the parameter s. Indeed, the different behaviour of the non-Markovianity measures traces back to their different functional dependence of the decoherence function $\gamma_s(t)$, which is plotted in Fig. 4.2 **(b)** and **(c)** for different values of s and λ. One can see how $\gamma_s(t)$ takes on smaller values within $[0, 1]$ for growing values of λ, while its global minimum decreases with increasing s. Now, while the BLP measure is fixed by the difference between the values of $\gamma_s(t)$ at the edges of the time intervals $[a_m, b_m]$ in which $\gamma_s(t)$ increases, see Equation (4.53), the RHP measure is fixed by the ratio between the same values, see Equation (4.54). Hence, as the coupling strength grows over the threshold $\lambda^*(s)$ or the parameter s overcomes the threshold $s^*(\lambda)$, the difference between b_m and a_m is increasingly smaller, and therefore $\mathcal{N}_s(\lambda)$ is so. However, the ratio between b_m and a_m always increases with λ and s, as witnessed by the corresponding monotonic increase of $\mathcal{I}_s(\lambda)$.

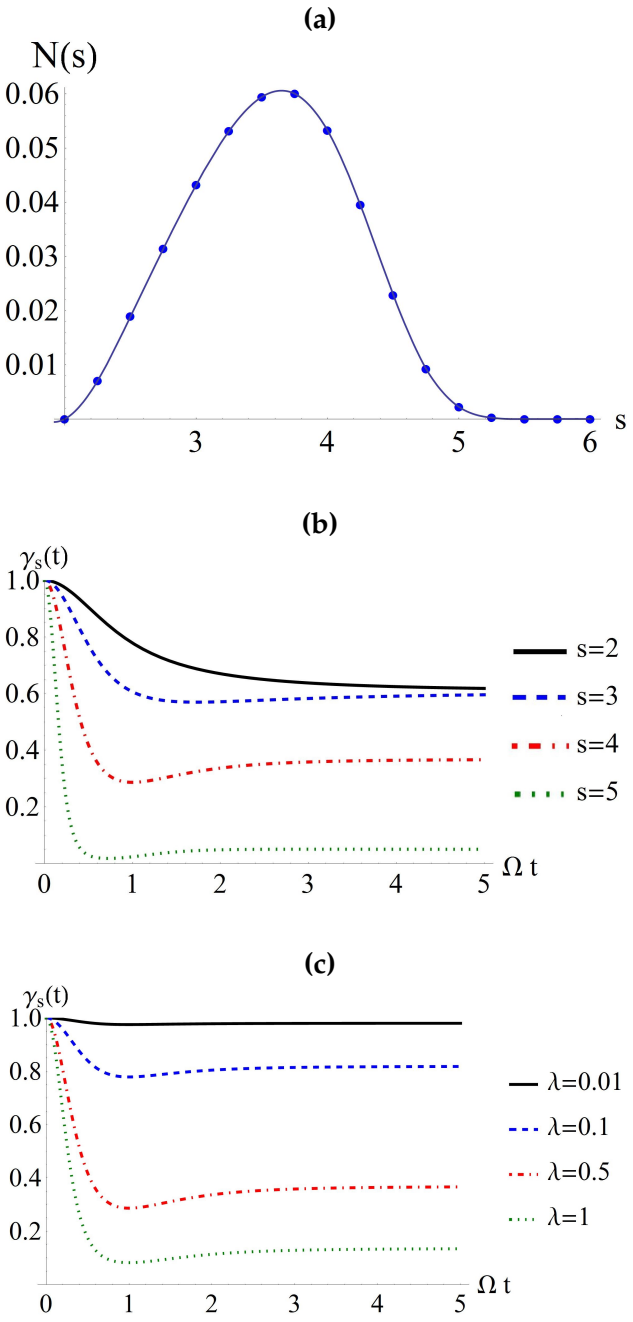

FIGURE 4.2: **(a)** BLP measure of non-Markovianity $\mathcal{N}_s(\lambda)$, see Equation (4.53), as a function of the parameter s, for $\lambda = 1$. **(b)** and **(c)** Decoherence function $\gamma_s(t)$ as a function of time for $\lambda = 0.5$ and different values of s **(b)**, and for $s = 4$ and different values of λ **(c)**.

4.2.4 Validity of regression hypothesis

4.2.4.1 Exact expression versus quantum regression theorem

The exact unitary evolution, Equation (4.27), directly provides us with the average values, as well as the two-time correlation functions of the observables of the system. In

view of the comparison with the description given by the quantum regression theorem, see Sec. 4.1.2, let us focus on the basis of linear operators on $\mathbb{C}^2$, orthonormal with respect to the Hilbert-Schmidt scalar product, given by $\left\{\mathbb{1}/\sqrt{2}, \sigma_-, \sigma_+, \sigma_z/\sqrt{2}\right\}$. Indeed, the first and the last element of the basis are constant of motion, see Equation (4.39), while the mean values of σ_- and σ_+ evolve according to, respectively,

$$\langle \sigma_-(t)\rangle = \gamma(t) e^{-i\omega_s t}\langle \sigma_-(0)\rangle \tag{4.63}$$

and the complex conjugate relation. In a similar way, all the two-time correlation functions involving $\mathbb{1}/\sqrt{2}$ or $\sigma_z/\sqrt{2}$ satisfy the condition of the quantum regression theorem in a trivial way, as at most one operator within the two-time correlation function actually does not evolve in time.

Setting, for convenience of notation, $t_2 \equiv t+\tau$ and $t_1 = t$, the only non-trivial expressions are thus the following:

$$\begin{aligned}
\langle \sigma_-(t_2)\sigma_+(t_1)\rangle &= e^{-i\omega_s(t_2-t_1)}\gamma(t_2,t_1)e^{i\phi(t_2,t_1)}\langle (\sigma_-\sigma_+)(t_1)\rangle,\\
\langle \sigma_+(t_2)\sigma_-(t_1)\rangle &= e^{i\omega_s(t_2-t_1)}\gamma^*(t_2,t_1)e^{i\phi(t_2,t_1)}\langle (\sigma_+\sigma_-)(t_1)\rangle,
\end{aligned} \tag{4.64}$$

where

$$\gamma(t_2,t_1) = \mathrm{Tr}_E\, \rho_E \prod_k \Delta(\alpha_k(t_2) - \alpha_k(t_1)) \tag{4.65}$$

and

$$\phi(t_2,t_1) = \sum_k Im\left[\alpha_k^*(t_2)\alpha_k(t_1)\right]. \tag{4.66}$$

Here, to derive (4.64) we used the properties of the displacement operator [103]

$$\Delta(\alpha)\Delta(\beta) = \Delta(\alpha+\beta)e^{iIm(\alpha\beta^*)}, \quad \Delta^\dagger(\alpha) = \Delta(-\alpha),$$

and the equality $\langle (\sigma_+\sigma_-)(t)\rangle = \langle \sigma_+\sigma_-\rangle$.

We can now obtain the corresponding two-time correlation functions as predicted by the quantum regression theorem. By Equation (4.63), one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \sigma_-(t)\rangle = \left(\frac{\mathrm{d}\gamma(t)/\mathrm{d}t}{\gamma(t)} - i\omega_s\right)\langle \sigma_-(t)\rangle \tag{4.67}$$

and the complex conjugate relation for $\langle \sigma_+(t)\rangle$. The specific choice of the operator basis has lead us to a diagonal matrix G in Equation (4.19). Hence, one has immediately

$$\begin{aligned}
\langle \sigma_-(t_2)\sigma_+(t_1)\rangle_{qrt} &= e^{-i\omega_s(t_2-t_1)}\frac{\gamma(t_2)}{\gamma(t_1)}\langle \sigma_-(t_1)\sigma_+(t_1)\rangle,\\
\langle \sigma_+(t_2)\sigma_-(t_1)\rangle_{qrt} &= e^{i\omega_s(t_2-t_1)}\frac{\gamma^*(t_2)}{\gamma^*(t_1)}\langle \sigma_+(t_1)\sigma_-(t_1)\rangle.
\end{aligned} \tag{4.68}$$

The quantum regression theorem will be generally violated within this model, compare Equation (4.64) and (4.68). We quantify such a violation by means of the figure of merit

introduced in Equation (4.22), which for the couple of operators σ_- and σ_+ reads

$$Z = \left| 1 - \frac{\langle \sigma_-(t_2)\sigma_+(t_1)\rangle_{qrt}}{\langle \sigma_-(t_2)\sigma_+(t_1)\rangle} \right| = \left| 1 - \frac{\gamma(t_2)}{\gamma(t_1)\gamma(t_2,t_1)e^{i\phi(t_2,t_1)}} \right|. \tag{4.69}$$

4.2.4.2 Quantitative analysis of the violations of the quantum regression theorem

The expressions of the previous paragraph hold for generic initial state of the bath and spectral density. Now, we come back to the specific choice of an initial thermal bath. The results in Equation (4.68) are in this case in agreement with those found in [104], where the two-time correlation functions have been evaluated focusing on a spectral density as in Equation (4.55) with $s = 1$, while keeping a generic temperature of the bath. Instead, we will focus on the case $T = 0$ and maintain a generic value of s in order to compare the behaviour of the two-time correlation functions with the measures of non-Markovianity.

First, note that by using the definition of the displacement operator as well as Equation (4.29), one can show the general identity

$$\Delta(\alpha_k(t_2) - \alpha_k(t_1)) = \Delta\left(\alpha_k(t_2 - t_1)e^{i\omega_k t_1}\right). \tag{4.70}$$

But then, since for a thermal state $\mathrm{Tr}_E\, \Delta(\alpha)\rho_E$ is a function of $|\alpha|$ only [21], Equation (4.70) implies

$$\gamma(t_2, t_1) = \gamma(t_2 - t_1), \tag{4.71}$$

see Eqs.(4.65) and (4.40). In addition we have in the continuum limit, see Equation (4.66),

$$\phi(t_2,t_1) = \int \mathrm{d}\omega \frac{J(\omega)}{\omega^2} \left[\sin(\omega t_2) - \sin(\omega t_1) - \sin(\omega(t_2 - t_1))\right], \tag{4.72}$$

so that, for $J(\omega)$ as in Equation (4.55) and using Equation (4.51) in the zero temperature limit, we get

$$\phi_s(t_2, t_1) = (\mathcal{D}_{s-1}(t_2) - \mathcal{D}_{s-1}(t_1) - \mathcal{D}_{s-1}(t_2 - t_1))/\Omega. \tag{4.73}$$

The identities in Eqs.(4.59) and (4.60), along with Eqs. (4.71) and (4.73), finally provide us with the explicit expression of the estimator for the violations of the quantum regression theorem, see Equation (4.69),

$$Z_s(\lambda) = \big|1 - \exp\big[\lambda\Gamma(s-1)\big[1 - (1 + i\Omega(t_2 - t_1))^{1-s} - (1 + i\Omega t_1)^{1-s} + (1 + i\Omega t_2)^{1-s}\big)\big]\big|\big|, \tag{4.74}$$

whose behaviour as a function of λ and s is shown in Fig. 4.3 **(a)** and **(b)**.

The violation of the quantum regression theorem monotonically increases with increasing values of both the coupling strength λ and the parameter s. This behaviour is clearly in agreement with that of the RHP measure of non-Markovianity, see Sec. 4.2.3.2 and in particular Fig. 4.1. From a quantitative point of view there is, however, some difference as the estimator $Z_s(\lambda)$, at variance with the RHP measure, grows linearly with λ only for small values of s, while it growths faster for $s > 3$; compare with Fig. 4.1 **(b)**.

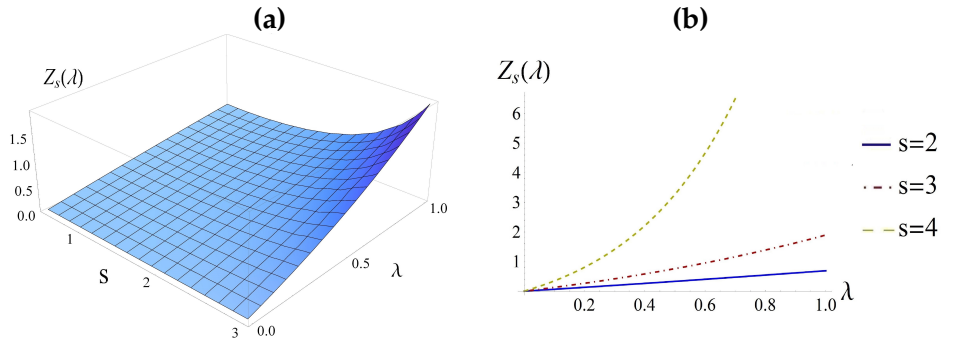

FIGURE 4.3: **(a)** $Z_s(\lambda)$ as a function of the parameter s and of the coupling strength λ, see Equation (4.74), for $\Omega t_1 = 1$ and $\Omega t_2 = 2$. **(b)** Sections of **(a)** for $s = 2, 3, 4$.

In any case, the RHP measure appears to be more directly related with the strength of the violation to the quantum regression theorem, as compared with the BLP measure. This can be traced back to the different influence of the system-environment correlations on the two measures. As we recalled in Subsection 4.1.2, the hypothesis that the state of the total system at any time t is well approximated by the product state between the state of the open system and the initial state of the environment, see Equation (4.18), lies at the basis of the quantum regression theorem. This hypothesis is expected to hold in the weak coupling regime, while for an increasing value of λ, the interaction will build stronger system-environment correlations, leading to a strong violation of the quantum regression theorem. The establishment of correlations between the system and the environment due to the interaction plays a significant role also in the subsequent presence of memory effects in the dynamics of the open system [59, 105, 106]. Indeed, different signatures of the memory effects can be affected by system-environment correlations in different ways. In particular, the CP-divisibility of the dynamical maps appears to be a more fragile property than the contractivity of the trace distance and therefore it is more sensitive to the violations of the quantum regression theorem. Furthermore, it is worth noting that the estimator $Z_s(\lambda)$ steadily increases with the coupling strength λ even for values of s such that the corresponding reduced dynamics is Markovian according to either definitions, see for example the blue solid line in Fig.4.3 **(b)**. The validity of the quantum regression theorem calls therefore for stricter conditions than the Markovianity of quantum dynamics.

4.3 Photonic realization of dephasing interaction

In the pure dephasing spin-boson model, there is no regime in which the quantum regression theorem is strictly satisfied, apart from the trivial case $\lambda = 0$. In addition, we have shown that the strength of the violations of this theorem has the same qualitative behaviour of the RHP non-Markovianity measure, as they increase with both λ and the parameter s. In this section, we take into account a different pure dephasing model, which allows us to deepen our analysis on the relationship between the quantum regression theorem and the Markovianity of the reduced-system dynamics. In particular, we

show that in general these two notions should be considered as different since the quantum regression theorem may be strongly violated, even if the open system's dynamics is Markovian, irrespective of the exploited definition.

4.3.1 The model

Let us deal with the pure-dephasing interaction considered in Ref. [107]. The open system here is represented by the polarization degrees of freedom of a photon generated by spontaneous parametric down conversion, while the environment consists in the corresponding frequency degrees of freedom. The overall unitary evolution, which is realized via a quartz plate that couples the polarization and frequency degrees of freedom, can be described as

$$U(t)\,|j,\omega\rangle = e^{in_j\omega t}\,|j,\omega\rangle \qquad j=0,1, \tag{4.75}$$

where $|0\rangle \equiv |H\rangle$ and $|1\rangle \equiv |V\rangle$ are the two polarization states (horizontal and vertical), with refractive indexes, respectively, $n_0 \equiv n_H$ and $n_1 \equiv n_V$, while $|\omega\rangle$ is the environmental state with frequency ω. If we consider an initial product state, see Equation (4.8), with a pure environmental state $\rho_E = |\Psi_E\rangle\langle\Psi_E|$, where

$$|\Psi_E\rangle = \int d\omega\, f(\omega)\,|\omega\rangle\,, \tag{4.76}$$

we readily obtain that the reduced dynamics is given by Equation (4.39). Again, we are in the presence of a pure dephasing dynamics, the only difference being the decoherence function, which now reads

$$\gamma(t) = \int d\omega\ |f(\omega)|^2\, e^{i\Delta n\omega t}, \tag{4.77}$$

with $\Delta n \equiv n_1 - n_0$. For the rest, the results of Secs. 4.2.1 and 4.2.3 directly apply also to this model: the master equation is given by Equation (4.46), with $\epsilon(t)$ and $\mathcal{D}(t)$ as in, respectively, Equation (4.47) (for $\omega_s = 0$) and Equation (4.48), while the non-Markovianity measures are as in Equation (4.53) and Equation (4.54). Analogously, the two-time correlation functions are given by Equation (4.64) with

$$\gamma(t_2,t_1) = \gamma(t_2-t_1), \qquad \phi(t_2,t_1) = 0, \tag{4.78}$$

while the application of the quantum regression theorem leads to the expressions in Equation (4.68) (with $\omega_s = 0$). Hence, the violations of the quantum regression theorem can be quantified by

$$Z = \left|1 - \frac{\langle\sigma_-(t_2)\sigma_+(t_1)\rangle_{qrt}}{\langle\sigma_-(t_2)\sigma_+(t_1)\rangle}\right| = \left|1 - \frac{\gamma(t_2)}{\gamma(t_1)\gamma(t_2-t_1)}\right|. \tag{4.79}$$

4.3.2 Lorentzian frequency distributions

4.3.2.1 Semigroup dynamics

Despite its great simplicity, this model allows to describe the transition between Markovian and non-Markovian dynamics in concrete experimental settings [107, 108]. Different dynamics are obtained for different choices of the initial environmental state, see Equation (4.8) and the related discussion, i.e., for different initial frequency distributions, see Equation (4.76). The latter can be experimentally set, e.g., by properly rotating a Fabry-Pérot cavity, through which a beam of photons generated by spontaneous parametric down conversion passes [107]. A natural benchmark is represented by the Lorentzian distribution

$$|f(\omega)|^2 = \frac{\delta\omega}{\pi\left[(\omega-\omega_0)^2+(\delta\omega)^2\right]}, \tag{4.80}$$

where $\delta\omega$ is the width of the distribution and ω_0 its central frequency, as this provides a reduced semigroup dynamics [106]. The decoherence function, which is given by the Fourier transform of the frequency distribution, see Equation (4.77), is in fact

$$\gamma(t) = e^{-\Delta n(\delta\omega - i\omega_0)t}. \tag{4.81}$$

Thus, replacing this expression in Eqs. (4.47) and (4.48), one obtains a Lindblad equation, given by Equation (4.46) with $\epsilon(t) = -\Delta n\,\omega_0$ and $\mathcal{D}(t) = \Delta n\,\delta\omega$. In addition, $\gamma(t_2 - t_1) = \gamma(t_2)/\gamma(t_1)$ and hence, as one can immediately see by Equation (4.79), $Z = 0$. For this model, as long as the reduced dynamics is determined by a completely positive semigroup, the quantum regression theorem is strictly valid. Let us emphasize, that this is the case even if the total state is not a product state at any time t. For example if the initial state of the open system is the pure state $|\psi_S\rangle = \alpha\,|H\rangle + \beta\,|V\rangle$, with $|\alpha|^2 + |\beta|^2 = 1$, the total state at time t is

$$|\psi_{SE}(t)\rangle = \int \mathrm{d}\omega f(\omega)(\alpha e^{in_H\omega t}\,|H,\omega\rangle + \beta e^{in_V\omega t}\,|V,\omega\rangle). \tag{4.82}$$

This is an entangled state, of course unless $\alpha = 0$ or $\beta = 0$; nevertheless, the quantum regression theorem does hold. This clearly shows that for the quantum regression theorem, as for the semigroup description of the dynamics [105, 106, 109], the approximation encoded in Equation (4.18) should be considered as an effective description of the total state, which can be very different from its actual form, even when the theorem is valid.

4.3.2.2 Time-inhomogeneous Markovian and non-Markovian dynamics

Now, we consider a more general class of frequency distributions; namely, the linear combination of two Lorentzian distributions,

$$|f(\omega)|^2 = \sum_{j=1,2} \frac{A_j\delta\omega_j}{\pi\left[(\omega-\omega_{0,j})^2+(\delta\omega_j)^2\right]}, \tag{4.83}$$

with $A_1 + A_2 = 1$. The decoherence function (4.77) is in this case

$$\gamma(t) = \frac{e^{-\Delta n(\delta\omega_1 - i\omega_{0,1})t} + re^{-\Delta n(\delta\omega_2 - i\omega_{0,2})t}}{1+r}, \tag{4.84}$$

with $r \equiv \frac{A_2}{A_1}$, while the estimator of the violations of the quantum regression theorem, see Equation (4.79), can be written as a function of the difference between the central frequencies, $\Delta\omega = \omega_{0,1} - \omega_{0,2}$, as well as of the difference between the corresponding widths, $\Delta\delta\omega = \delta\omega_1 - \delta\omega_2$. If we assume that the two central frequencies are equal, $\omega_{0,1} = \omega_{0,2} = \omega_0$, the evolution of the two-level statistical operator is fixed by a time-local master equation as in Equation (4.46), with $\epsilon(t) = -\Delta n\,\omega_0$ and

$$\mathcal{D}(t) = \Delta n \frac{\delta\omega_1 e^{-\Delta n\delta\omega_1 t} + r\,\delta\omega_2 e^{-\Delta n\delta\omega_2 t}}{e^{-\Delta n\delta\omega_1 t} + r\,e^{-\Delta n\delta\omega_2 t}}. \tag{4.85}$$

The latter is a positive function of time: the reduced dynamics is CP-divisible, see Section 3.2.1, and hence it is Markovian with respect to both the BLP and RHP definitions. Indeed, now we are in the presence of a time-inhomogeneous Markovian dynamics. Nevertheless, as $\gamma(t_2 - t_1) \neq \gamma(t_2)/\gamma(t_1)$ the quantum regression theorem is violated, see Equation (4.79). This is explicitly shown in Fig. 4.4 **(a)**, where Z is plotted as a function of $\Delta\delta\omega = \delta\omega_1 - \delta\omega_2$ and $\Delta n\tau$, with $\tau = t_2 - t_1$. With growing difference between the two widths, as well as the length of the time interval, the deviations from the quantum regression theorem are increasingly strong, up to a saturation value of the estimator Z. Contrary to the semigroup case, here, even if the dynamics is Markovian according to both definitions, the actual behaviour of the two-time correlation functions cannot be reconstructed by the evolution of the mean values.

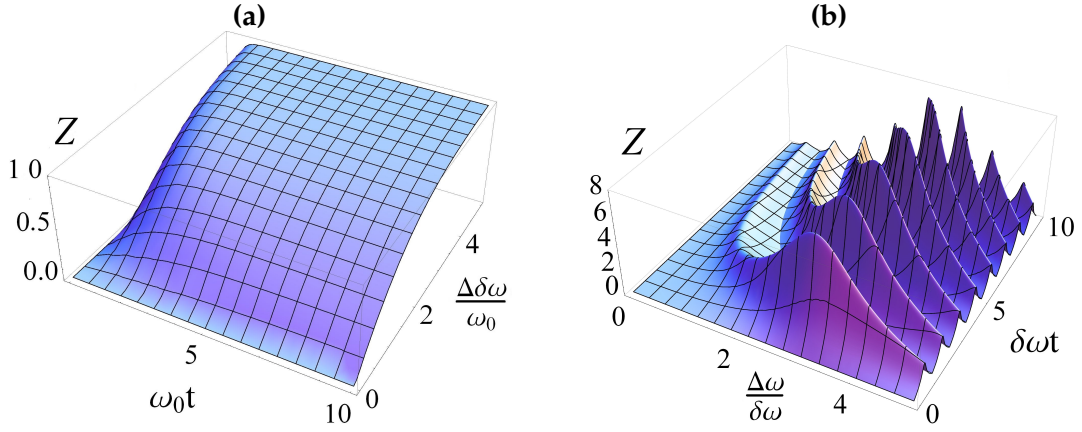

FIGURE 4.4: Violation of the quantum regression theorem, as quantified by the estimator Z in Equation (4.79) **(a)** in the time-inhomogeneous Markovian case, $\omega_{0,1} = \omega_{0,2} = \omega_0$, as a function of $\Delta\delta\omega = \delta\omega_1 - \delta\omega_2$ and $\omega_0\tau = \omega_0(t_2 - t_1)$, for $\omega_0 t_1 = 1$ and $r = 1$; **(b)** in the non-Markovian case, $\delta\omega_1 = \delta\omega_2 = \delta\omega$, as a function of $\Delta\omega_0 = \omega_{0,1} - \omega_{0,2}$ and $\delta\omega\,\tau$, for $\delta\omega\, t_1 = 1$ and $r = 2$; in all the panels $\Delta n = 1$.

Finally, let us consider a frequency distribution as in Equation (4.83), but now with $\delta\omega_1 = \delta\omega_2 = \delta\omega$ and $\omega_{0,1} \neq \omega_{0,2}$. This frequency distribution has two peaks and the resulting reduced dynamics is non-Markovian [106, 107]. In this case the BLP non-Markovianity measure (5.115) increases with the increasing of the distance between the

two peaks, while the estimator Z grows for small values of the distance and then it exhibits an oscillating behaviour, see Fig. 4.4 **(b)**. Indeed, for $\Delta\omega = 0$ one recovers the semigroup dynamics previously described and, accordingly, Z goes to zero. Summarizing, by varying the distance between the two peaks, one obtains a transition from a Markovian (semigroup) dynamics to a non-Markovian one and, correspondingly, the quantum regression theorem ceases to be satisfied and is even strongly violated. Nevertheless, the qualitative behaviour of, respectively, the non-Markovianity of the reduced dynamics and the violation of the quantum regression theorem appear to be different. In this Chapter, we explored the relationship between two criteria for Markovianity of a quantum dynamics, namely the CP-divisibility of the quantum dynamical map and the behaviour in time of the trace distance between two distinct initial states, and the validity of the quantum regression theorem, which is a statement relating the behaviour in time of the mean values and of the two-time correlation functions of system operators. The first open system considered is a two-level system affected by a bosonic environment through a dephasing interaction. For a class of spectral densities with exponential cut-off and power law behaviour at low frequencies we have studied the onset of non-Markovianity as a function of the coupling strength and of the power determining the low frequency behaviour, further giving an exact expression for the corresponding non-Markovianity measures. The deviation from the quantum regression theorem has been estimated evaluating the relative error made in replacing the exact two-time correlation function for the system operators with the expression reconstructed by the evolution of the corresponding mean values. It appears that the validity of the quantum regression theorem represents a stronger requirement than Markovianity, according to either criteria, which in this case coincide but quantify non-Markovianity in a different way and exhibit distinct performances in their dependence on strength of the coupling and low frequency behaviour. We have further considered an all-optical realization of a dephasing interaction, as recently exploited for the experimental investigation of non-Markovianity, obtaining also in this case, for different choices of the frequency distribution, significant violations to the quantum regression theorem even in the presence of a Markovian dynamics.

These results suggest that indeed the recently introduced new approaches to quantum non-Markovianity provide a weaker requirement with respect to the classical notion of Markovian classical process. Further and more stringent notion of Markovian quantum dynamics can therefore be introduced, e.g. relying on validity of the quantum regression theorem [110]. However, the usefulness of such criteria will heavily depend on the possibility to verify their satisfaction directly by means of experiments, as it is the case e.g. for the notion of Markovianity based on trace distance, without asking for an explicit exact knowledge of the dynamical equations.

5

Characterization of heat dynamics in non-Markovian open quantum systems

In Chapter 3 we explored in detail the notion of non-Markovianity in quantum systems, starting from its classical counterpart and discussing its relationship with the manifestation of memory effects in the dynamics. A wide variety of witnesses of quantum non-Markovianity have been presented, which, dealing with properties of the dynamical maps, allow to link the occurrence of non-Markovianity with specific time-behavior of physical quantities, such as, for example, distinguishability, interferometric power or correlations . It comes therefore natural to wonder how other relevant properties or observables of open quantum systems, maybe possibly endowed also with a thermodynamic meaning like energy, behave in presence of a dynamics which is non-Markovian according to the criteria set up above. This also goes in the long-term direction of trying to exploit non-Markovianity for practical purposes, an endeavour which is already giving results, for example, in quantum engines [111] or in quantum information [112].

Thermodynamics is one of the oldest physical theories and, up to now, has survived all major revolutions such as the advent of general relativity and quantum mechanics. Its systematic application to quantum systems is however a relatively recent field of study, and many of even fundamental notions are still subject of ongoing debates in the scientific community [113]. The leitmotif is again that to try to transpose to the quantum realm those concepts and theoretical techniques employed to access the thermodynamical properties of classical statistical ensembles, and supporting them with new theoretical tools typical of the quantum theory, in a similar fashion with the notion of non-Markovianity discussed in Chapter 3.

This Chapter will be conceptually divided in two parts, the former devoted to study of the first law of thermodynamics in non - Markovian open quantum systems and the latter to the investigation of the second law, with a particular focus on the so-called Landauer's principle, which connects the reign of thermodynamics with that of information theory.

In Section 5.1, we will then make a contextualization of the concepts of energy, heat and work, i.e. the quantities involved in the statement of the first law of thermodynamics. As

will be discussed in detail, the concepts of work and heat will become very subtle in the realm of quantum mechanics and, in fact, a general and universally accepted consensus on them still does not exist [113–117]. This is mainly due to the fact that, given a time-dependent Hamiltonian $\mathcal{H}(t)$, its operatorial form at a generic time t will not in general commute with its version at initial time $\mathcal{H}(0)$, making it hard, if not impossible, to associate an observable in the usual sense (i.e. a self-adjoint operator on the Hilbert space) with quantities such as work or heat. In order to properly introduce the latter, one common way is to rely on a different approach, known as *full counting statistics*, according to which the variation of these quantities are defined in terms of a two-time measurement protocol; this will be presented in detail in Section 5.2.

We will then move to the framework of non-Markovian open quantum systems and introduce in the following Section 5.3, both in the case of a finite - and infinite - dimensional system, the concept of *heat backflow* , defined roughly speaking as the fraction of energy which, during a coupled evolution that in a semigroup limiting case would result in a steady heat flow from the system S to the environment E, flows back from E to S. The very natural search for a connection between this idea and the notion of non-Markvianity as information backflow will be also carried out in two explicit models, the spin - boson for the finite-dimensional case and the quantum brownian motion for the infinite-dimensional case.

5.1 The first law of quantum thermodynamics: internal energy, work and heat

Thermodynamics is the discipline which deals with energy exchanges in physical systems, and separate them into heat and work contributions. Quantum thermodynamics makes reference to the type of systems under considerations, i.e. quantum systems. There is a vast literature in merit and several dedicated reviews can be found in the literature [116–121].

Consider a generic quantum system $\rho \in \mathcal{S}(\mathscr{H})$ whose evolution is generated by some possibly time-dependent Hamiltonian $\mathcal{H}(t)$. The variation of the (internal) energy of this system is simply given by

$$\Delta U(t) = \mathrm{Tr}\left[\mathcal{H}(t)\rho(t)\right] - \mathrm{Tr}\left[\mathcal{H}(0)\rho(0)\right]. \tag{5.1}$$

Following standard thermodynamics, Eq. (5.1) is split in two contributions

$$\begin{aligned}\Delta U(t) &= \int_0^t d\tau \, \frac{d}{d\tau}\left(\mathrm{Tr}\left[\mathcal{H}(\tau)\rho(\tau)\right]\right) \\ &= \int_0^t d\tau \, \left(\mathrm{Tr}\left[\frac{d\mathcal{H}(\tau)}{d\tau}\rho(\tau)\right] + \mathrm{Tr}\left[\mathcal{H}(\tau)\frac{d\rho(\tau)}{d\tau}\right]\right) \\ &\equiv \int_0^t d\tau \, \left[\delta W(\tau) + \delta Q(\tau)\right], \end{aligned} \tag{5.2}$$

where the two quantities

$$W(t) \equiv \int_{t_0}^{t} d\tau\, \delta W(\tau), \quad Q(t) \equiv \int_{t_0}^{t} d\tau\, \delta Q(\tau) \tag{5.3}$$

are respectively identified with *work* and *heat*. The former is in fact associated with an experimentally controllable time-variation of the Hamiltonian, while the second is associated with the uncontrollable evolution of the quantum system and brings along a variation in the Von - Neumann entropy of the quantum system. It is also conventional to consider as positive the work which is done on the system. Eq. (5.2) written as

$$\Delta U(t) = W(t) + Q(t) \tag{5.4}$$

is nothing but the expression of the first law of thermodynamics.

Note that in Eq. (5.2) the symbols 'δ' in front of the infinitesimal work and heat have been employed to emphasize that both these quantities are not exact differentials. It is in fact already clear at this level that, while the change in the internal energy only depends on the initial and final couples $(\rho, \mathcal{H})$, neither the work nor the heat in general do and, in fact, no observable for these two quantities can be found in the usual sense, i.e. no self-adjoint operators $\hat{O} \equiv \hat{W}, \hat{Q}$ can be found such that $\langle O(t) \rangle = \mathrm{Tr}\left[\hat{O}(t)\rho(t)\right]$.

In the context of open quantum systems, a system S interacts with an environment E, usually considered large, according to an Hamiltonian of the form $\mathcal{H}(t) = \mathcal{H}_S(t) + \mathcal{H}_E + \mathcal{H}_{SE}(t)$, where the time dependence takes into account for an eventual external driving field. Note that, since the dynamics of the total system is described by a unitary operator, we have that

$$\mathrm{Tr}_{SE}\left[\mathcal{H}(t)\frac{d\rho_{SE}(t)}{dt}\right] = -\frac{i}{\hbar}\mathrm{Tr}_{SE}\left\{\left[\mathcal{H}(t)\left[\mathcal{H}(t), \rho_{SE}(t)\right]\right)\right\} = 0 \tag{5.5}$$

and thus the the overall system, considered as a whole, satisfies the relations

$$Q_{SE}(t) = 0, \quad \Rightarrow W_{SE}(t) = \Delta U_{SE}(t). \tag{5.6}$$

The moment however we restrict our attention to the sub-parts of the total system, i.e. S or E, instead of the whole system SE, concepts such as work or heat immediately become incredibly subtle [114] and a debate on the most proper and meaningful definition is still ongoing. The main difficulties lie in the role of correlations between S and E, which do not belong to either of the bare subparts S or E but influence both of them, though in a very different way. One of such crucial differences lies in the action of the external force, which is assumed not act on the environment, in agreement both with conventional thermodynamics and open quantum systems theory points of view, where the environment is usually considered uncontrollable by an experimenter. It is precisely this the reason which has led many authors to define *heat* as the following quantity [4, 122]

$$Q_E(t) \equiv \mathrm{Tr}_E\left[\mathcal{H}_E\left(\rho_E(t) - \rho_E(0)\right)\right] = \int_0^t d\tau\, \mathrm{Tr}_E\left[\mathcal{H}_E\frac{d\rho_E(t)}{dt}\right], \tag{5.7}$$

i.e. the fraction of energy which is transferred to the environment. Accordingly, the work done (by an experimenter) on the environment is zero:

$$W_E(t) = \int_0^t d\tau \, \mathrm{Tr}_E \left[\frac{d\mathcal{H}_E}{dt} \rho_E(t) \right] = 0 \tag{5.8}$$

and, thanks to the first law, the transferred heat (5.7) also corresponds to the variation in the environmental internal energy $\Delta U_E(t) = Q_E(t)$.

Starting from this consideration, one can also define the concepts of work and heat for the reduced system in the following way. Exploiting in fact Eq. (5.5), we can elaborate on the expression of $Q_E(t)$ as follows

$$\begin{aligned} Q_E(t) &= -\int_0^t d\tau \, \mathrm{Tr}_{SE} \left[\mathcal{H}_E \frac{d\rho_{SE}(t)}{dt} \right] \\ &= -\int_0^t d\tau \, \mathrm{Tr}_{SE} \left[\left(\mathcal{H}_S(t) + \mathcal{H}_{SE}(t) \right) \frac{d\rho_{SE}(t)}{dt} \right] \end{aligned} \tag{5.9}$$

and define the heat $Q_S(t)$, in light of the relation $Q_{SE}(t) = 0$, as

$$Q_S(t) \equiv -Q_E(t) \tag{5.10}$$

The last equality leads immediately to the definitions of work and internal energy for the 'system + interaction' as

$$W_S(t) = \int_0^t d\tau \, \mathrm{Tr}_{SE} \left[\frac{d}{dt} \left(\mathcal{H}_S(t) + \mathcal{H}_{SE}(t) \right) \rho_{SE}(t) \right], \tag{5.11}$$

$$\Delta U_S(t) = \mathrm{Tr}_{SE} \left[\left(\mathcal{H}_S(t) + \mathcal{H}_{SE}(t) \right) \rho_{SE}(t) \right] - \mathrm{Tr}_{SE} \left[\left(\mathcal{H}_S(0) + \mathcal{H}_{SE}(0) \right) \rho_{SE}(0) \right]. \tag{5.12}$$

Note that also for the 'system + interaction' a balance equation in the form of the fist law applies, i.e.

$$\Delta U_S(t) = W_S(t) + Q_S(t). \tag{5.13}$$

It is important to stress that the correlations which onset during the evolution between the system and the environment have, in this construction [122], been incorporated into the system, in the spirit of the above mentioned scenario where the environment represents an uncontrolled system which only serves as a thermal bath. However, it is easy to verify that we could have exploited the linearity of the trace and of the derivative in Eq. (5.2) to split the first law in three parts, according to the terms of the Hamiltonian

$$(\Delta U_S(t) + \Delta U_E(t) + \Delta U_{SE}(t)) = (W_S(t) + W_E(t) + W_{SE}(t)) + (Q_S(t) + Q_E(t) + Q_{SE}(t)) \tag{5.14}$$

and consider the 'interactions' between S and E as a separate part of the overall system (thermodynamically speaking) to which a first law applies

$$\Delta U_j(t) = W_j(t) + Q_j(t), \qquad j \equiv S, E, SE. \tag{5.15}$$

The identification of the correlations as a third subpart of the overall system, external to the reduced system and to the environment, and the association of concepts such as

work and heat to it seem however less intuitive, and thus we will follow the construction made above in Eqs. (5.10) and (5.13).

Finally, it is worth mentioning that, as already stressed before, other different definitions of work and heat can be associated to the parts composing a composite quantum system; we will however not make a list of them here since it would lead us out of our purposes, but the interested reader is referred to [113–115] for discussions in merit.

5.2 Full-counting statistics and two-time measurement protocol

The present Section is devoted to the introduction of the so-called *full-counting statistics*, which is a very powerful theoretical tool mainly, but not exclusively, employed in the endeavour of characterizing the thermodynamical properties of quantum systems. As the name suggests, it allows to reconstruct, at least in principle, all the cumulants of the probability distribution of any generic observable of interest of a quantum system. More specifically, the full-counting statistics of a generic observable $\hat{A} \in \mathcal{B}(\mathscr{H})$ is identified with its variation over time with respect to its initial value, according to a two-time measurement protocol, and its main importance, as already stressed above, comes into stage whenever a thermodynamic quantity such as heat or work (which are not observables) are to be accessed (though of course it is not limited to these quantities but can be applied to any observable).

Consider then a quantum system described by a statistical operator $\rho \in \mathscr{H}$, whose evolution is determined in terms of a unitary operator $\hat{U}$. Consider moreover an observable $\hat{A} = \hat{A}^\dagger \in \mathcal{B}(\mathscr{H})$, whose eventual time dependence in the Shrödinger picture solely comes from the action of an external driving force (thus associated with an external work). We will denote with $\{a_t, |a_t\rangle\}$ the family of eigenvalues / eigenvectors of such observable at time t according to its spectral decomposition $\hat{A}(t) = \sum_{a_t} a_t \left|a_t\right\rangle \left\langle a_t\right| \equiv \sum_{a_t} a_t \hat{\Pi}_{a_t}$. The probability distribution $p_t(\Delta a)$ for a change $\Delta a \equiv a_t - a_0$ to occur between time t and initial time 0 can be formally defined in terms of the joint probability

$$\mathbb{P}_t\left[a_t; a_0\right] = \mathrm{Tr}\left[\hat{\Pi}_{a_t}\hat{U}(t,0)\hat{\Pi}_{a_0}\rho(0)\hat{\Pi}_{a_0}\hat{U}^\dagger(t,0)\hat{\Pi}_{a_t}\right] \tag{5.16}$$

as

$$p_t(\Delta a) = \sum_{a_t, a_0} \delta\left(\Delta a - (a_t - a_0)\right) \mathbb{P}_t\left[a_t; a_0\right], \tag{5.17}$$

where $\delta(\cdot)$ denotes the Dirac's delta function. Note that the variable Δa is now a classical random variable whose distribution at time t is described by $p_t(\Delta a)$. The joint probability (5.16), which can be formally regarded to as a two-time correlation function $\langle \hat{\Pi}_{a_t}\hat{\Pi}_{a_0}\rangle$, can be thought to be obtained by means of a *two-time measurement protocol* of the observable $\hat{A}(t)$. The latter is usually conceived as follows: at initial time $t = 0$ the selected observable whose statistics we want to reconstruct is measured and the outcome a_0 (belonging to the spectrum of $\hat{A}(0)$) is obtained as a result. The state of the system, initially

described by $\rho(0)$, then collapses in

$$\rho'(0) = \frac{\hat{\Pi}_{a_0}\rho(0)\hat{\Pi}_{a_0}}{\mathrm{Tr}_{SE}\left[\hat{\Pi}_{a_0}\rho(0)\right]}. \tag{5.18}$$

Immediately after the measurement, at time $t = 0^+$, the system is let undergo an evolution, dictated by the unitary $\hat{U}$, up to some generic time t, when another measurement of the observable $\hat{A}(t)$ is performed again. If this time a_t is obtained as an outcome, the final state describing the system is of the form

$$\rho''(t) = \frac{\hat{\Pi}_{a_t}U(t,0)\rho'(0)U^\dagger\hat{\Pi}_{a_t}}{\mathrm{Tr}_{SE}\left[\hat{\Pi}_{a_t}U(t,0)\rho'(0)U^\dagger\hat{\Pi}_{a_t}\right]}. \tag{5.19}$$

The joint probability to have obtained the two outcomes a_t at time t and a_0 at time 0 is then given by the Born rule and corresponds to (5.16).

In order to obtain all the cumulants of the probability distribution of Δa, thus fully characterizing the statistics of the change in the observable $\hat{A}(t)$, the cumulant generating function is introduced as the Fourier transform of the probability distribution, i.e.

$$\Theta(\eta, t) \equiv \ln\langle e^{i\eta\Delta a}\rangle_t = \ln\int d(\Delta a)\, p_t(\Delta a)e^{i\eta\Delta a}, \tag{5.20}$$

from which the $n^{th}-$order cumulant is simply obtained by derivation over the parameter η

$$\langle(\Delta a)^n\rangle_t = (-i)^n\frac{\partial^n}{\partial\eta^n}\Theta(\eta,t)|_{\eta=0}. \tag{5.21}$$

By substituting the expression of the probability distribution (5.17) in (5.20), we immediately have that

$$\Theta(\eta, t) = \ln\sum_{a_t,a_0} e^{i\eta(a_t-a_0)}P_t\left[a_t; a_0\right]. \tag{5.22}$$

It is important to stress that the cumulant generating function can be equivalently constructed as the real Laplace transform of $p_t(\Delta a)$, i.e.

$$\tilde{\Theta}(\eta, t) \equiv \ln\langle e^{-\eta\Delta a}\rangle_t = \ln\int d(\Delta a)\, p_t(\Delta a)e^{-\eta\Delta a}, \tag{5.23}$$

from which the cumulants are obtained through

$$\langle(\Delta a)^n\rangle_t = (-1)^n\frac{\partial^n}{\partial\eta^n}\Theta(\eta,t)|_{\eta=0}. \tag{5.24}$$

The introduction of $\Theta(\eta, t)$ carries along an important simplification. An important assumption is that the initial state commutes with the observable $\hat{A}(0)$, i.e.

$$\left[\hat{A}(0), \rho(0)\right] = 0. \tag{5.25}$$

This condition, though being widely assumed especially when the observable considered is the energy (as will be shown below in more detail) in which case it would correspond

to consider an initial state in Gibbs form, is however not strictly necessary, as shown in [117]. Using the spectral theorem

$$f(\hat{A}) = \sum_a f(a) \left|a\right\rangle \left\langle a\right|, \tag{5.26}$$

it is straightforward to prove that Eq. (5.22) can be re-expressed as

$$\Theta(\eta, t) = \ln \mathrm{Tr}\left[\rho(\eta, t)\right], \tag{5.27}$$

where the operator

$$\rho(\eta, t) = \hat{U}_{\eta/2}(t, 0)\rho(0)\hat{U}^{\dagger}_{-\eta/2}(t, 0) \tag{5.28}$$

is the initial statistical operator evolved according to the modified evolution operator

$$\hat{U}_{\eta}(t, 0) = e^{i\eta\hat{A}(t)}\hat{U}(t, 0)e^{-i\eta\hat{A}(0)}. \tag{5.29}$$

It is very important to note that the operator $\rho(\eta, t)$ is not a statistical operator since its trace is not normalized to 1, except than at the initial time where it coincides with $\rho(0)$. This fact plays a crucial role, since the full statistics constructed by derivation of the cumulant generating function $\Theta(\eta, t)$ stems, in light of Eq. (5.27), from the non-trace-preserving character of the modified evolution.

When the parameter η, usually referred to as *counting field parameter*, is set to zero $\eta = 0$, we retrieve the usual evolution operator and statistical operator

$$\hat{U}_{\eta}(t, 0)|_{\eta=0} = \hat{U}(t, 0), \qquad \rho(\eta, t)|_{\eta=0} = \rho(t). \tag{5.30}$$

Moreover, if the selected observable does not depend on time $\hat{A}(t) = \hat{A}(0) = \hat{A}$, provided $\hat{\mathcal{H}}$ denotes the Hamiltonian of the system such as $\hat{U}(t, 0) = e^{i\hat{\mathcal{H}}t}$, we can express the modified evolution operator equivalently as

$$\hat{U}_{\eta}(t, 0) = e^{i\eta\hat{A}}\hat{U}(t, 0)e^{-i\eta\hat{A}} = e^{-i\hat{\mathcal{H}}_{\eta}t}, \tag{5.31}$$

where

$$\hat{\mathcal{H}}_{\eta} = e^{i\eta\hat{A}}\hat{\mathcal{H}}e^{-i\eta\hat{A}}. \tag{5.32}$$

5.2.1 Generalized master equation

The FCS formalism illustrated above is particularly useful when applied to an open quantum system weakly coupled to an environment. In this scenario in fact, if the two-time measurement protocol is carried out on an observable *of the environment*, then we have that Eq. (5.27), which in this case reads

$$\Theta(\eta, t) = \ln \mathrm{Tr}_{SE}\left[\rho_{SE}(\eta, t)\right], \tag{5.33}$$

becomes

$$\Theta(\eta, t) = \ln \mathrm{Tr}_{S}\left[\rho_{S}(\eta, t)\right], \tag{5.34}$$

where we have defined the reduced modified density matrix

$$\rho_S(\eta,t) = \mathrm{Tr}_E\left[\hat{U}_{\eta/2}(t,0)\rho_{SE}(0)\hat{U}^\dagger_{-\eta/2}(t,0)\right]. \tag{5.35}$$

The meaning of Eq. (5.34) is the following: in order to reconstruct the full statistics of a single selected observable of the environment (which in the scenario of open quantum systems' theory is usually conceived to be not accessible) we can simply look at its effect on the evolution of the reduced system. This point of view shares also many similarities also with the quantum probe framework. The advantage brought by Eq. (5.34) is that, under the very same assumptions which lead to the expression of a master equation for the usual reduced statistical operator $\rho_S(t)$, e. g. weak coupling, Born-Markov, *et cetera*, a master equation for the modified operator $\rho_S(\eta,t)$ can be written as well, which is usually referred to as *generalized master equation* [117]. We stress however that the weak coupling assumption, in most cases needed for the master equation to be written in closed form, is not necessary for the previous results to hold true and in fact we will see in Section 6.4 an example where the cumulant generating function of the dissipated heat is reconstructed for a specific model without any assumption on the coupling.

To summarize, the powerfulness and usefulness of this method relies in the fact that, by solving (analytically or numerically) a master equation for an operator which has the same degree of complexity of that of the reduced system, we can access the statistics of an observable of the environment. It is important to notice that this is possible since we are looking at a single specific observable and not at the general statistical properties of the environment (i.e. we cannot infer properties of the dynamics of the environmental state by looking at the reduced system).

By means of the projection-operator technique and second-order time convolutionless expansion the dynamical generator (see Chapter 2 Section 2.2.2.1), a *generalized master equation* (GME) for $\rho_S(\eta,t)$ can be written for a generic microscopic Hamiltonian of the form $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{SE}$ [117], with $\mathcal{H}_0 = \mathcal{H}_S + \mathcal{H}_E$ being the free part and $\mathcal{H}_{SE}$ being the interaction term. Writing the latter in the following general form [21]

$$\mathcal{H}_{SE} = \sum_k C^k \otimes B^k, \qquad C^k \in \mathcal{B}(\mathscr{H}_S), B^k \in \mathcal{B}(\mathscr{H}_E), \tag{5.36}$$

and assuming that the initial state of the environment $\rho_E(0)$ commutes with the desired observable $A \in \mathcal{B}(\mathscr{H}_E)$ whose statistics we want to reconstruct, the GME reads

$$\begin{aligned}\frac{d}{dt}\rho_S(\eta,t) = &-i\left[\mathcal{H}_S, \rho_S(\eta,t)\right] \\ &- \sum_{jk}\int_0^t d\tau \Big[\Phi_{jk}(\tau)C^jC^k(-\tau)\rho_S(\eta,t) + \Phi_{jk}(-\tau)\rho_S(\eta,t)C^j(-\tau)C^k \\ &- \Phi_{kj}(-\eta,\tau)C^j\rho_S(\eta,t)C^k(-\tau) - \Phi_{kj}(-\eta,\tau)C^j(-\tau)\rho_S(\eta,t)C^k\Big],\end{aligned} \tag{5.37}$$

where

$$\Phi_{jk}(\eta,\tau) \equiv \mathrm{Tr}_E\left[B^j_{2\eta}(t)B^k\rho_E(0)\right] \tag{5.38}$$

is the *generalized environmental correlation function*, with

$$B_\eta^j(t) = e^{i(\eta/2)A} B^j(t) e^{-i(\eta/2)A} \tag{5.39}$$

and $B^j(t) = e^{i\mathcal{H}_0 t} B^j e^{-i\mathcal{H}_0 t}$. Note that in the above equations we have omitted the hat symbol over the operators in order to facilitate the readability. We will conform to this notation in what follows as well whenever there is no risk of confusion or otherwise stated. The quantity in Eq. (5.38) reduces to the familiar environmental correlation function for vanishing values of the counting field parameter η.

Since the aim of this Chapter is to reconstruct observables of the quantum system endowed with a thermodynamical significance, we will from now on identify the generic self-adjoint operator A of the above expressions with the energy of the environment $\mathcal{H}_E$, whose change in time gives the heat.

In this case, the generalized environmental correlation function constructed from the microscopic Hamiltonian $\mathcal{H}$ can be proven to satisfy the following symmetry

$$\Phi_{jk}(\eta, t) = \Phi_{kj}(-\eta - i\beta, -t), \tag{5.40}$$

with β being the inverse temperature ($k_B = 1$) of the initial bath, which reduces to the well-known Kubo-Martin-Schwinger (KMS) condition for the usual environmental correlation function [123]

$$\Phi_{jk}(t) = \Phi_{kj}(-t - i\beta). \tag{5.41}$$

The latter, which is often found in literature in its frequency-domain expression as

$$\Phi_{jk}(\omega) = e^{\beta\omega} \Phi_{kj}(-\omega), \tag{5.42}$$

with

$$\Phi_{jk}(\eta, \omega) = \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{i\omega t} \Phi_{jk}(\eta, t), \tag{5.43}$$

expresses the so called *detailed balance* condition.

It is worth to consider the form of the GME when the Born-Markov and the secular approximations are performed on Eq. (5.37). These approximations, are known to lead from an Hamiltonian microscopic evolution to an effective semigroup description of the dynamics in the case of the statistical operator of the reduced system [21]; the same implementation of all the passages and considerations that can be found in [21] to the modified operator $\rho_S(\eta, t)$ and its GME Eq. (5.37), imply that the dynamics of populations and coherences of $\rho_S(\eta, t)$ are decoupled and evolve according to [117]

$$\begin{aligned}
\frac{d}{dt}\rho_{nn}(\eta, t) &= -2\pi \sum_{jk} \sum_{m} \left[\Phi_{jk}(-\omega_{mn}) C_{nm}^j C_{mn}^k \rho_{nn}(\eta, t) - \Phi_{jk}(\eta, \omega_{mn}) C_{nm}^j C_{mn}^k \rho_{mm}(\eta, t) \right], \\
\frac{d}{dt}\rho_{nm}(\eta, t) &= -\left(\Gamma_{nm} + i\Omega_{nm}\right) \rho_{nm}(\eta, t),
\end{aligned} \tag{5.44}$$

where

$$\Gamma_{nm} = 2\pi \sum_{jk} \left[-\Phi_{jk}(0) C^j_{mm} C^k_{nn} + \frac{1}{2} \sum_l \left(\Phi_{jk}(-\omega_{nl}) C^j_{nl} C^k_{ln} + \Phi_{kj}(\omega_{ml}) C^j_{ml} C^k_{lm} \right) \right], \tag{5.45}$$

$$\Omega_{nm} = \omega_{nm} - \sum_{jk} \sum_l \left[\int_{-\infty}^{+\infty} d\omega \mathrm{P} \frac{\Phi_{jk}(\omega)}{\omega + \omega_{ln}} C^j_{nl} C^k_{ln} - \int_{-\infty}^{+\infty} d\omega \mathrm{P} \frac{\Phi_{jk}(\omega)}{\omega + \omega_{lm}} C^j_{ml} C^k_{lm} \right], \tag{5.46}$$

where $\omega_{nm} \equiv \omega_n - \omega_m$ is the energy difference (in units of $\hbar$) between the system's energies relative to eigenstates n and m. In order to derive Eq. (5.45), the SokhotskiPlemelj relation

$$\int_{-\infty}^{\infty} dt\, e^{\pm i\omega t} = \pi \delta(\omega) \pm \mathrm{P} \frac{1}{\omega} \tag{5.47}$$

has been used, with $\delta(\cdot)$ and P being the Dirac's delta function and the Cauchy Principal Value respectively. Note that the dependence on the counting field parameter η is only on the population dynamics, while the coherences undergo an exponentially damped evolution.

5.3 Heat backflow in weakly-coupled discrete- and continuous-variables systems

In the present Section our aim is to characterize the following quantity

$$\mathrm{Tr}_E \left[\mathcal{H}_E \left(\rho_E(t) - \rho_E(0) \right) \right] \tag{5.48}$$

in a non-driven open quantum system $\mathscr{H}_S$ weakly coupled to an environment $\mathscr{H}_E$ by means of FCS formalism. The inclusion of multiple environments attached to the same system, which forms a widely used model for quantum engines, will result trivial extension. The absence of an external driving, in light of the considerations made at the beginning of Subsection 5.2, implies that energy at the end of the two time measurement protocol commutes with the initial one, and therefore we can make use of Eq. (5.31) in the following calculations. Note that, in light of Eq. (5.7) and of the related considerations, we have that the quantity defined in Equation (5.48) is nothing but the heat $Q_E(t)$.

As stated at the beginning of this Section, we consider an open quantum system coupled to an environment, through an interaction Hamiltonian $\mathcal{H}_{SE}$ such that the total Hamiltonian governing the evolution of the composite system reads $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{SE}$, with $\mathcal{H}_0 = \mathcal{H}_S + \mathcal{H}_E$ being the free Hamiltonian. The coupling between S and E will be considered small such that it allows for a second-order expansion of the dynamical generator and thus for an closed expression of a time-local master equation for the statistical operator $\rho_S(t)$. In Subsection 5.3.2 we will first deal with finite dimensional systems $dim(\mathscr{H}_S) = N_S < +\infty$, and then we move to the infinite dimensional case in Subsection 5.3.3, with the restriction to Gaussian channels. In both cases we will not assume, at variance with existing literature, the Born-Markov and secular approximations which would lead, as already stressed, to a time-independent GKSL form of the generator (and

therefore to a semigroup dynamics), but instead we will take into account a generally non-Markovian reduced dynamics. This will allow for energy transfers, in the short and intermediate stages of the coupled evolution, even in the case of absent initial temperature gradient, in striking contrast with the mentioned limiting case previously studied in [124, 125], which however will be recovered in the long-time limit.

Since we are interested in accessing the statistics of energy, we identify the generic observable $A \in \mathcal{B}(\mathscr{H}_E)$ with the Hamiltonian $\mathcal{H}_E$ and, according to condition (5.25), we assume the initial state of the composite system to be of factorized form

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_\beta, \qquad \rho_\beta \equiv \frac{e^{-\beta \mathcal{H}_E}}{Z_E}, \tag{5.49}$$

with $Z_E = \mathrm{Tr}_E \left[e^{-\beta \mathcal{H}_E} \right]$. In particular, our attention will be concentrated on the first moment of the probability distribution of energy, i.e. $\langle Q_E(t) \rangle_t$. The same treatment of higher - order cumulants of this probability distribution will provide an interesting subject for future studies.

According to the two-time measurement protocol described above, the statistics of energy can be reconstructed through the cumulant generating function Eq. (5.34), with $\rho_S(\eta, t)$ given as the solution of the GME

$$\frac{d}{dt} \rho_S(\eta, t) = \Xi^\eta(t) \rho_S(\eta, t), \tag{5.50}$$

where the time-dependent superoperator $\Xi^\eta(t)$ in the second-order approximation has the form

$$\Xi^\eta(t)\,[\omega] = -i\,[\mathcal{H}_S, \omega] - \int_0^t d\tau\, \mathrm{Tr}_E \left\{ \left[\mathcal{H}_{int},\, [\mathcal{H}_{int}(-\tau),\, \omega \otimes \rho_E(0)]_\eta \right]_\eta \right\}, \tag{5.51}$$

where $[\mathcal{H}_{int}(t)\,,\, B]_\eta \equiv \mathcal{H}^\eta_{int}(t) B - B \mathcal{H}^{-\eta}_{int}(t)$, with $\mathcal{H}^\eta_{int}(t) = e^{(i/2)\eta \mathcal{H}_E} \mathcal{H}_{int}(t) e^{-(i/2)\eta \mathcal{H}_E}$ and $\mathcal{H}_{int}(t) = e^{i\mathcal{H}_0 t} \mathcal{H}_{int} e^{-i\mathcal{H}_0 t}$. In the expressions above and in the remainder of the thesis, we remind that we set $\hbar = 1$ and $k_B = 1$ for simplicity.

The formal solution of (5.51) has the form

$$\rho_S(\eta, t) = T_+ \exp \left[\int_0^t d\tau \Xi^\eta(\tau) \right] \rho_S(0), \tag{5.52}$$

with T_+ indicating the chronological time ordering operator.

In the case of a discrete system described by means of a finite-dimensional Hilbert space, the Hilbert-Schmidt representation of operators and superoperators (see Chapter 2 Section 2.1.1) allows for the following matrix representation of Eq. (5.51)

$$|\rho_S(\eta, t)\rangle = T_+ \exp \left[\int_0^t d\tau \boldsymbol{\Xi}^\eta(\tau) \right] |\rho_S(0)\rangle \equiv \boldsymbol{\Lambda}^\eta(t, 0)\, |\rho_S(0)\rangle\,, \tag{5.53}$$

where $|\rho_S(\eta,t)\rangle$, $\boldsymbol{\Xi}^\eta(t)$ and $\boldsymbol{\Lambda}^\eta(t,0)$ denoting, respectively, the vector and matrix forms in the Hilbert-Schmidt space of the operator $\rho_S(\eta,t)$, of the dynamical generator $\Xi^\eta(t)$ and of the dynamical map $\Lambda^\eta(t,0)$. We also recall that $\rho_S(\eta,0)=\rho_S(0)$.

The time-dependent first moment of the energy transfer is then given by

$$\langle\Delta q\rangle_t = \langle\mathbb{1}|\,\frac{\partial}{\partial(i\eta)}\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\,, \tag{5.54}$$

where $\langle\mathbb{1}|$ denotes the trace operation in Hilbert-Schmidt space. The above expression can be rewritten as follows:

$$\begin{aligned}\langle\Delta q\rangle_t &= \langle\mathbb{1}|\,\frac{\partial}{\partial(i\eta)}\,(\boldsymbol{\Lambda}^\eta(t,0)\,|\rho_S(0)\rangle\rangle)_{|\eta=0}\\ &= \langle\mathbb{1}|\,\frac{\partial}{\partial(i\eta)}\,(\boldsymbol{\Lambda}^\eta(t,0))\,|\rho_S(0)\rangle\rangle_{|\eta=0} + \langle\mathbb{1}|\,\boldsymbol{\Lambda}^\eta(t,0)\frac{\partial}{\partial(i\eta)}\,(|\rho_S(0)\rangle\rangle)_{|\eta=0}\,.\end{aligned} \tag{5.55}$$

Note however that

$$\langle\mathbb{1}|\,\boldsymbol{\Lambda}^\eta(t,0)\,|\rho_S(0)\rangle\rangle_{|\eta=0}\equiv \mathrm{Tr}_S\left[(\boldsymbol{\Lambda}^\eta(t,0)\,|\rho_S(0)\rangle\rangle]_{|\eta=0}\right]=\mathrm{Tr}_S\left[\rho_S(\eta,t)_{|\eta=0}\right]\equiv\mathrm{Tr}_S\left[\rho_S(t)\right]=1, \tag{5.56}$$

and also

$$\langle\mathbb{1}|\,|\rho_S(0)\rangle\rangle_{|\eta=0}\equiv\mathrm{Tr}_S\left[\rho_S(\eta,0)_{|\eta=0}\right]=\mathrm{Tr}_S\left[\rho_S(0)\right]=1, \tag{5.57}$$

from which it follows that $\langle\mathbb{1}|$ is a left eigenvector of $\boldsymbol{\Lambda}^\eta(t,0)$, i.e. $\langle\mathbb{1}|=\langle\mathbb{1}|\,\boldsymbol{\Lambda}^\eta(t,0)$. Consequently the state $\langle\mathbb{1}|$ is itself an eigenvector of the dynamical generator $\boldsymbol{\Xi}^\eta(t)$ relative to the eigenvalue 0. Using this fact, the second term in the last line of Eq. (5.55) can be further elaborated into

$$\langle\mathbb{1}|\,\boldsymbol{\Lambda}^\eta(t,0)\frac{\partial}{\partial(i\eta)}\,(|\rho_S(0)\rangle\rangle)_{|\eta=0}=\langle\mathbb{1}|\,\frac{\partial}{\partial(i\eta)}\,|\rho_S(0)\rangle=\frac{\partial}{\partial(i\eta)}\,(\langle\mathbb{1}|\,|\rho_S(0)\rangle\rangle)=0, \tag{5.58}$$

while the first term can be written as

$$\begin{aligned}&\langle\mathbb{1}|\,\frac{\partial}{\partial(i\eta)}\,(\boldsymbol{\Lambda}^\eta(t,0))\,|\rho_S(0)\rangle\rangle_{|\eta=0}=\langle\mathbb{1}|\int_0^t d\tau\,\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\boldsymbol{\Lambda}^\eta(t,0)\,|\rho_S(0)\rangle\rangle_{|\eta=0}\\ &=\langle\mathbb{1}|\int_0^t d\tau\,\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\,.\end{aligned} \tag{5.59}$$

Upon integration by parts, and using the relations $\left[\left(\int_0^t d\tau\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\right),\,\boldsymbol{\Xi}^\eta(t,)\right]=0$ we obtain that Eq. (5.59) simplifies into

$$\begin{aligned}&\langle\mathbb{1}|\int_0^t d\tau\,\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\\ &=\langle\mathbb{1}|\int_0^t d\tau\,\left(\int_0^\tau ds\frac{\partial\boldsymbol{\Xi}^\eta(s)}{\partial(i\eta)}\right)\boldsymbol{\Xi}^\eta(\tau)\boldsymbol{\Lambda}^\eta(\tau,0)\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\\ &\qquad\qquad+\langle\mathbb{1}|\int_0^t d\tau\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\boldsymbol{\Lambda}^\eta(\tau,0)\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\\ &=\langle\mathbb{1}|\int_0^t d\tau\frac{\partial\boldsymbol{\Xi}^\eta(\tau)}{\partial(i\eta)}\boldsymbol{\Lambda}^\eta(\tau,0)\,|\rho_S(\eta,t)\rangle\rangle_{|\eta=0}\,.\end{aligned} \tag{5.60}$$

Putting the pieces together, we have that the mean value of the energy of the environment can be expressed in a compact form as

$$\langle \Delta q \rangle_t = \int_0^t d\tau \theta(\tau), \tag{5.61}$$

where the function

$$\theta(t) \equiv \langle \mathbb{1} | \frac{\partial \Xi^{\eta}(t)_{|\eta=0}}{\partial(i\eta)} | \rho_S(t) \rangle , \tag{5.62}$$

provides the rate by which the system and its environment exchange energy and, more specifically, $\theta(t) > (<) 0$ indicates an increment (decrement) in the environmental energy, i.e. an heat flow from the reduced system (environment) to the environment (reduced system).

In the case of continuous variable (CV) systems (see Chapter 3 Section 3.2.1.1) however, it proves useful to consider the *characteristic function* (3.38) associated to the operator $\rho_S(\eta, t)$ [43, 46]

$$\chi \left[\rho_S(\eta, t) \right] (\lambda, \lambda^*) \equiv \chi^{(\eta)}(\lambda, \lambda^*, t) = \mathrm{Tr}_S \left[\rho_S(\eta, t) e^{\lambda a^\dagger - \lambda^* a} \right] , \tag{5.63}$$

with $a, a^\dagger$ denoting the annihilation and creation operators relative to the system. From (5.63) it follows immediately that the cumulant-generating function can be written as

$$\Theta(\eta, t) = \ln \mathrm{Tr}_S \left[\rho_S(\eta, t) \right] = \ln \chi^{(\eta)}(0, 0, t). \tag{5.64}$$

The time-dependent first moment of the energy transfer is thus given by

$$\langle \Delta q \rangle_t = \frac{\partial \chi^{(\eta)}(0, 0, t)}{\partial(i\eta)} |_{\eta=0}, \tag{5.65}$$

and the heat flow per unit of time $\theta(t)$ reads

$$\theta(t) = \frac{\partial \dot{\chi}^{(\eta)}(0, 0, t)}{\partial(i\eta)} |_{\eta=0}, \tag{5.66}$$

where the $\cdot$ sign denotes the time derivative.

It can be noticed that the cumulant generating function $\Theta(\eta, t) = \ln \mathrm{Tr}_S \left[\rho_S(\eta, t) \right]$ reduces to the large deviation function [126] according to $\vartheta(\eta) = lim_{t \to +\infty} \Theta(\eta, t)/t$, which is not time - dependent any more. This in turn means that, whenever well-defined, the cumulants of the probability distribution in the long - time limit tend to become linear with time [117, 127], and therefore in particular

$$\langle \Delta q \rangle_t \approx \langle \Delta q \rangle t. \tag{5.67}$$

This relation, which we will explicitly check in the models considered below, gives a neat indication of the behavior of the heat flow per unit of time in the long time limit of the dynamics, as well as in a coarse - grained description of the latter (in any cases, whenever a GKSL generalized master equation is suitable): the quantity $\theta(t)$ introduced

in Eq. (5.62) (or (5.66)) becomes a constant function with time, thus physically indicating a steady heat flow. The latter is achieved by applying a temperature gradient and, in accordance with the second law of thermodynamics (which we will discuss more thoroughly in Section 6.1, goes from the hotter subsystem to the colder one. It is worth of notice that this long-time analysis of the energy current has been successfully applied for example in [124, 125] to non-linear (anharmonic) junction systems, which have been shown to be central components in many quantum thermal machines [128, 129].

5.3.1 Definition and measure

Inspired by the considerations made above, we are naturally led to give the following definition:

Definition 5.1. Given a system S weakly coupled to an environment E, we speak of time regions of *heat backflow from E to S* whenever, considering dynamical situations which in the Born-Markov semigroup approximation would lead to a non-negative steady energy transfer from system to environment, we have that at some time t

$$\theta(t) < 0. \tag{5.68}$$

Building on this condition, a measure for the total amount of energy which has flown back from the environment to the system during the evolution is naturally introduced as

$$\langle \Delta q \rangle_{back} = \max_{\rho_S(0)} \frac{1}{2} \int_0^{+\infty} dt \, \left(|\theta(t)| - \theta(t) \right), \tag{5.69}$$

where the maximization procedure is performed to make it a property of the dynamical map, i.e. independent on the possible choices of initial states of the system. Note that the integrand of Eq. (5.69) is different from zero if and only if $\theta(t)$ assumes negative values and it represents, in principle, a measurable quantity.

Despite the formal similarity which may appear between this quantifier and some of non-Markovianity estimators introduced in Chapter 3 [11, 13, 130], it should not be confused with an alternative non-Markovianity measure, rather providing only an estimate of the heat backflow .

A final important comment about this definition of heat backflow deserves to be made. Since the latter is defined as, roughly speaking, the fraction of heat which, during the evolution, flows out of the environment, the 'system' we speak about when we write expressions such as 'heat backflow from E to S' is more precisely the open quantum system including the interaction term, as discussed in Section 5.1. In other words, we cannot know whether the energy which leaves the environment and which is witnessed by the negativity of $\theta(t)$ and estimated by Eq. (5.69), has gone to the bare reduced system or has been stored in the interaction term. In order to further distinguish which one of these two contributions is the effective receiver of the heat flowing from the environment, one should calculate explicitly the time behavior of the change in the free system's

Hamiltonian $\langle \Delta \mathcal{H}_S \rangle_t$ and of the change in the interaction Hamiltonian $\langle \Delta \mathcal{H}_{SE} \rangle_t$. The problem however is that the latter quantity is almost never accessible in the context of open quantum system's theory, since it involves the knowledge of the environment's evolution alongside as that of the system's. We will therefore restrict our attention to the weak coupling scenario which, beside allowing the calculation of the (modified) statistical operator as solution of a closed master equation, allows to consider the interaction term negligible with respect to the contributions of the free Hamiltonians and granting us the possibility to identify the bare system S with the receiver of the heat backflow contributions. In the second example which we will analyze in detail, the case of a quantum brownian particle, we will be able to reconstruct both these quantities thanks to a fully numerical - simulation approaChapter This will allow us to extend our analysis to the strong coupling regime while being still able to keep track of the separate contributions.

We will now proceed to study this quantity and its relationship with suitable estimators of non/Markovianity in the following Section, where we will explicitly see applications to two important and paradigmatic models: the spin boson model for the finite - dimensional case and the quantum brownian motion for the CV case.

5.3.2 The spin-boson model

The spin - boson model is one of the building blocks of open quantum systems' theory, and thus has been thoroughly studied in the literature [21, 131–134]. The difference with the pure-dephasing case already analyzed in detail in Chapter 4 lies in the interaction term, which is now of the form

$$\mathcal{H}_{SE} = \sigma_x \otimes B_E, \qquad B_E \equiv \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right), \tag{5.70}$$

which therefore does not commute any more with the free Hamiltonian

$$\mathcal{H}_0 = \mathcal{H}_S + \mathcal{H}_E = \frac{\omega_0}{2} \sigma_z \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \left(\sum_k \omega_k b_k^\dagger b_k \right). \tag{5.71}$$

At variance with the pure dephasing spin - boson model, where the dynamics was only on the coherences of the system's statistical operator and the populations were constants of motion, this interaction Hamiltonian provokes the evolution of both the coherences and the populations. Note that, at this level, we have not assumed the rotating-wave approximation and consequently the counter-rotating terms $\sum_k \sigma_+ \otimes b_k^\dagger$ and $\sum_k \sigma_- \otimes b_k$ are still present.

Having assumed weak coupling between the two - level system and the bosonic bath, a closed generalized master equation of the form (5.37) can be written for this model

at second order perturbation expansion [117, 125], whose analytical solution can be approached, due to the finite dimensionality of the quantum system, moving to the Hilbert-Schmidt representation. In this space, the conditional density operator $\rho_S(\eta,t)$ is represented by the vector $|\rho_S(\eta,t)\rangle = (\rho^\eta_{00}(t),\rho^\eta_{01}(t),\rho^\eta_{10}(t),\rho^\eta_{11}(t))^T$, where

$$\rho^\eta_\alpha(t) = \mathrm{Tr}_S\left\{\sigma^\dagger_\alpha \rho_S(\eta,t)\right\}, \tag{5.72}$$

and $\{\sigma_\alpha\}_{\alpha=0,1,2,3} = \{|0\rangle\langle 0|, |0\rangle\langle 1|, |1\rangle\langle 0|, |1\rangle\langle 1|\}$ (note that the subscript 'S' has been dropped to the components of the Hilbert - Schmidt vector for readability). Concretely, if $\partial_t\rho_S(\eta,t) = \Xi^\eta(t)\rho_S(\eta,t)$, the dynamical generator, regarded as a linear map on the space of linear operators on $\mathbb{C}^2$, is represented by a 4×4 matrix $\boldsymbol{\Xi}^\eta(t)$, whose entries are given by [125]

$$\boldsymbol{\Xi}^\eta(t) = -\int_0^t d\tau \begin{pmatrix} V_+(\tau) & 0 & 0 & W^\eta_+(\tau) \\ 0 & Y_+(\tau) & Z^\eta_+(\tau) & 0 \\ 0 & Z^\eta_-(\tau) & Y_-(\tau) & 0 \\ W^\eta_-(\tau) & 0 & 0 & V_-(\tau) \end{pmatrix}. \tag{5.73}$$

All the quantities appearing in (5.73), defined below, are nothing but linear combinations of the environmental correlation function Eq. (5.38)

$$\Phi(\tau) \equiv \mathrm{Tr}_E\left\{B_E B_E(-\tau)\rho_E\right\}, \tag{5.74}$$

and read

$$\begin{aligned} V_\pm(\tau) &= \Phi(\tau)e^{\mp i\omega_0\tau} + \Phi(-\tau)e^{\pm i\omega_0\tau}, \\ W^\chi_\pm(\tau) &= -\left[\Phi(\tau-\chi)e^{\pm i\omega_0\tau} + \Phi(-\tau-\chi)e^{\mp i\omega_0\tau}\right], \\ Y_\pm(\tau) &= 2Re\left[\Phi(\tau)\right]e^{\mp i\omega_0\tau}, \\ Z^\chi_\pm(\tau) &= -\left[\Phi(\tau-\chi) + \Phi(-\tau-\chi)\right]e^{\pm i\omega_0\tau}. \end{aligned} \tag{5.75}$$

We stress again that the familiar master equation describing the evolution of the statistical operator in the spin-boson model [21, 134, 135] can be obtained from Eq. (5.73) simply by setting the counting field parameter $\eta = 0$. Moreover, upon introducing the Bloch vector $\mathbf{v}(t)$ defined as

$$\rho_S(t) = \frac{1}{2}\left(\mathbb{1}_2 + \mathbf{v}(t)\cdot\boldsymbol{\sigma}\right), \quad v_j(t) = \mathrm{Tr}_S\left[\sigma_j\rho_S(t)\right], \quad \left(\boldsymbol{\sigma}\equiv(\sigma_x,\sigma_y,\sigma_z)^T\right), \tag{5.76}$$

the master equation for vanishing values of the counting field parameter η give rise to the following differential equations for the Bloch vector

$$\frac{d}{dt}\mathbf{v}(t) = \mathbf{A}(t)\mathbf{v}(t) + \mathbf{b}(t), \tag{5.77}$$

where

$$\mathbf{A}(t) = \begin{pmatrix} 0 & -\omega_0 & 0 \\ \omega_0 + a_{yx}(t) & a_{zz}(t) & 0 \\ 0 & 0 & a_{zz}(t) \end{pmatrix}, \qquad \mathbf{b}(t) = \begin{pmatrix} 0 \\ 0 \\ b_{zz}(t) \end{pmatrix}, \tag{5.78}$$

with

$$a_{yx}(t) = \frac{1}{2}\int_0^t d\tau\, D_1(\tau)\sin(\omega_0\tau), \quad a_{zz}(t) = -\frac{1}{2}\int_0^t d\tau\, D_1(\tau)\cos(\omega_0\tau), \tag{5.79}$$

and

$$b_z(t) = -2\int_0^t d\tau\, D_2(\tau)\sin(\omega_0\tau). \tag{5.80}$$

We note that a Bloch representation could have been introduced also for the modified operator $\rho_S(\eta, t)$ as

$$\rho_S(\eta, t) = \frac{1}{2}\left(v_0(t)\mathbb{1}_2 + \mathbf{v}(t)\cdot\boldsymbol{\sigma}\right), \tag{5.81}$$

where now a fourth component $v_0(t) = \mathrm{Tr}_S\left[\rho_S(\eta, t)\right]$ has to be taken into account due to the fact that the trace of $\rho_S(\eta, t)$ is not equal to 1 at every time any more.

A crucial role in the definition of the environmental correlation function $\Phi(t)$ is played by the spectral density

$$J(\omega) = \sum_k \frac{|g_k|^2}{2\omega_k}\delta(\omega - \omega_k), \tag{5.82}$$

which contains information about both the distribution of bath modes and their interaction strength with the system. In the limit of a continuous distribution of environmental modes, the spectral density can be given in terms of a smooth function $J(\omega)$, which is usually taken to have a power-law behavior for low-frequencies and a cut-off function for large values of ω. The environmental correlation function can be written in terms of the spectral density as

$$\begin{aligned}\Phi(\tau) &= \int_0^{+\infty} d\omega\, J(\omega)\left[\coth\left(\frac{\omega}{2T_E}\right)\cos(\omega\tau) - i\sin(\omega\tau)\right] \\ &\equiv \frac{1}{2}\left(D_1(\tau) - iD_2(\tau)\right),\end{aligned} \tag{5.83}$$

where T_E denotes the environmental temperature, the Boltzmann and Planck constants have been set equal to one $k_B = \hbar = 1$, and the functions $D_1(\tau)$ and $D_2(\tau)$, respectively known as *noise* and *dissipation* kernels [21], read

$$D_1(\tau) = 2\int_0^{+\infty} d\omega J_{eff}(\omega, \Omega, T_E)\cos(\omega\tau), \quad D_2(\tau) = 2\int_0^{+\infty} d\omega J(\omega)\sin(\omega\tau) \tag{5.84}$$

where, in the noise kernel expression, we have introduced the effective spectral density

$$J_{eff}(\omega, \Omega, T_E) \equiv J(\omega)\coth\left(\frac{\omega}{2T_E}\right). \tag{5.85}$$

The substitution of (5.73) in Eq. (5.62) leads to the following expression for the heat flow per unit of time

$$\theta(t) = \left[w_+(t) - w_-(t)\right]\rho_{00}(t) - w_+(t), \tag{5.86}$$

where we have used the fact that $\rho_{00}(t) + \rho_{11}(t) = 1$ and where we have defined the quantity

$$w_{\pm}(\tau) \equiv \frac{\partial}{\partial(i\chi)} \int_0^\tau ds\, W_{\pm}^{\chi}(s)\Big|_{\chi=0}. \tag{5.87}$$

In order to determine the full statistics of energy according to the two-time measurement protocol described above, it is clear from Eq. (5.86) that only the populations of the modified operator $\rho_S(\eta, t)$ are needed. Moreover, it is clear from (5.73) that the dynamics of the coherences is decoupled from the one of the populations.

It is therefore more convenient to introduce the vector $|\rho_d(t)\rangle = (\rho_{00}(t), \rho_{11}(t))^T$ and the 2×2 matrix $\Xi_d(t)$ obtained extracting the elements of $\Xi^{\eta=0}(t)$ relative to $|\rho_d^\eta\rangle$

$$\Xi_d(t) = \begin{pmatrix} a_+(t) & -a_-(t) \\ -a_+(t) & a_-(t) \end{pmatrix}, \tag{5.88}$$

where $a_\pm(t) = -\int_0^t d\tau V_\pm(\tau)$ and where we have used the relation

$$W_{\pm}^{\eta=0}(\tau) = -V_{\mp}(\tau). \tag{5.89}$$

The differential equation for the ground-state population $\rho_{00}(t)$ therefore reads

$$\frac{d}{dt}\rho_{00}(t) = (a_+(t) + a_-(t))\rho_{00}(t) - a_-(t), \tag{5.90}$$

whose formal solution has the form

$$\rho_{00}(t) = e^{\int_0^t d\tau a_{zz}(\tau)}\Big(\rho_{00}(0) - \int_0^t d\tau a_-(\tau) e^{-\int_0^\tau ds a_{zz}(s)}\Big), \tag{5.91}$$

with

$$a_{zz}(t) \equiv a_+(t) + a_-(t) \tag{5.92}$$

being one of the right eigenvalues of $\Xi_d(t)$. It is important to notice that, for reasons of computation-time advantages, it is better to express the quantity $a_-(t)$ as

$$a_-(t) = \frac{1}{2}\left(a_{zz}(t) + b_z(t)\right), \tag{5.93}$$

where $a_{zz}(t)$, given by Eq. (5.79), and

$$b_z(t) = -2\int_0^t d\tau\, D_2(\tau)\sin(\omega_0\tau), \tag{5.94}$$

have been usually employed in the treatment of the spin-boson model [21, 134]. In fact, while both $a_{zz}(t)$ and $a_-(t)$ can only be numerically accessed for a wide variety of spectral densities, the quantity $b_z(t)$ can be in those cases analytically solved. This splitting of the nonhomogeneous term $a_-(t)$ (5.90) into a numerical part $a_{zz}(t)$ and an analytic term $b_z(t)$ (5.93) thus allows for shorter computation times.

Before proceeding further with the calculation of the heat backflow measure, it is interesting to perform the Born-Markov and secular approximation and look at the long -

time limit semigroup resulting limit of the dynamics. The matrix (5.88) which governs the evolution of populations in this case takes the form

$$\Xi^{\eta}_{d,LT} = \begin{pmatrix} -\Gamma n(\omega_0) & \Gamma\left(1+n(\omega_0)\right) \\ \Gamma n(\omega_0) & -\Gamma\left(1+n(\omega_0)\right) \end{pmatrix}, \tag{5.95}$$

where $\Gamma \equiv 2\pi J(\omega_0)$. This expression can be immediately obtained by making use of the relation (5.47). As a consequence, the long-time limit version of the energy flux per unit of time $\theta_{LT}(t)$ can be found. In fact, since

$$w_{+,LT} = \left[\frac{\partial}{\partial(i\chi)}\int_0^{+\infty} d\tau W^{\chi}_{+}(\tau)\right]_{\chi=0} = -\omega_0\Gamma\left(1+n(\omega_0)\right) \tag{5.96}$$

and

$$w_{-,LT} = \left[\frac{\partial}{\partial(i\chi)}\int_0^{+\infty} d\tau W^{\chi}_{-}(\tau)\right]_{\chi=0} = \omega_0\Gamma n(\omega_0), \tag{5.97}$$

the expression for $\theta_{LT}(t)$ becomes

$$\begin{aligned}\theta_{LT}(t) &= \left[w_{+,LT}(\tau) - w_{-,LT}(\tau)\right]\rho_{00}(\tau) - w_{+,LT}(\tau) \\ &= -\omega_0\Gamma\left(1+2n(\omega_0)\right)\rho_{00,LT}(t) + \omega_0\Gamma\left(1+n(\omega_0)\right) = \omega_0\frac{d}{dt}\rho_{00,LT}(t).\end{aligned} \tag{5.98}$$

The integral form of this expression gives the following result

$$\langle\Delta q\rangle_{t,LT} = \omega_0\left(\rho_{00,LT}(t) - \rho_{00}(0)\right), \tag{5.99}$$

which expresses the fact that, under this approximated dynamical regime, the mean value of the variation in the environmental energy is just equal and opposite to the variation in the system's internal energy.

Interestingly, Eq.(5.99) is no longer true if we do not perform these approximations but we consider the dynamical generator as given by Eq. (5.73). First of all in fact, since

$$\left.\frac{\partial\Phi(\pm\tau-\chi)}{\partial(i\chi))}\right|_{\chi=0} = \pm i\frac{\partial\Phi(\pm\tau)}{\partial\tau}, \tag{5.100}$$

it becomes possible to re-express both the terms $w_+(t) - w_-(t)$ and $w_+(t)$ which appear in (5.86) in the following equivalent form:

$$\begin{aligned} w_+(t) - w_-(t) &= 2\int_0^t d\tau\ \left(\partial_\tau D_1(\tau)\right)\sin(\omega_0 t), \\ w_+(t) &= \int_0^t d\tau\left(\partial_\tau D_1(\tau)\right)\sin(\omega_0 t) - \int_0^t d\tau\left(\partial_\tau D_2(\tau)\right)\cos(\omega_0 t). \end{aligned} \tag{5.101}$$

An integration by parts of the quantities above, using both the boundary conditions $D_1(0)\sin(0) = 0$ and $D_2(0) = 0$ and Eqs. (5.90), (5.79), (5.93), and (5.80), then gives

$$\begin{aligned} w_+(t) - w_-(t) &= 2D_1(t)\sin(\omega_0 t) + \omega_0 a_{zz}(t), \\ w_+(t) &= D_1(t)\sin(\omega_0 t) - D_2(t)\cos(\omega_0 t) + \omega_0 a_-(t), \end{aligned} \tag{5.102}$$

from which immediately follows that

$$\theta(t) = \omega_0 \frac{d}{dt}\rho_{00}(t) + f(t), \tag{5.103}$$

where

$$f(t) \equiv -\delta p(t) D_1(t) \sin(\omega_0 t) + D_2(t) \cos(\omega_0 t), \tag{5.104}$$

Note that, for simplicity, we have denoted with $\delta p(t) \equiv \rho_{11}(t) - \rho_{00}(t)$ the difference in the system's populations. The first term on the right-hand side of Eq. (5.103) corresponds to the time derivative of the change in the free system's energy, since it is proportional through the fundamental system energy ω_0 (we remind that $\hbar = 1$) to the fraction of the system's population that moves to the ground state. The second term, $f(t)$, is instead a combination of elementary oscillating functions and environmental kernels: the first contribution is driven by the noise kernel $D_1(t)$ and also depends on the solution for the ground-state population of the system $\rho_{00}(t)$, at variance with the second which is proportional only to the dissipation kernel, therefore also being independent of the temperature of the bath.

The integral form of (5.103) can also be considered

$$\langle \Delta q \rangle_t = \omega_0 \left(\rho_{00}(t) - \rho_{00}(0)\right) + F(t), \tag{5.105}$$

where $F(t) = \int_0^t d\tau f(\tau)$. Equation (5.105) shows that the variation in the environmental energy, obtained in this case as the FCS mean $\langle \Delta q \rangle_t$, is given by the sum of two distinct contributions, at variance with its long-time semigroup limiting version (5.99). The first term on the right-hand side is in fact equal and opposite to the variation of the reduced system's energy, but there is an additional contribution which depends both on the detailed structure of the environment, and on the coupling between system and environment through the dissipation and noise kernels. As explicitly shown above, in the long-time semigroup limit this additional contribution vanishes since $f(t)$ goes to zero according to the behavior of both dissipation and noise kernel as given by (5.109), and will be responsible for energy exchanges also with subsystems at equal initial temperatures.

5.3.2.1 Numerical evaluation of the heat backflow measure

In this section we illustrate and discuss the results of the numerical evaluation of the measure of heat backflow (5.69) for the considered model as a function of the different parameters characterizing the dynamics.

In what follows, we will consider the initial state of the reduced system to be of the form

$$\rho_S(0) = Z^{-1}\left(|0\rangle\langle 0| + e^{-\omega_0/T_S}|1\rangle\langle 1|\right), \quad Z = 1 + e^{-\omega_0/T_S}, \tag{5.106}$$

which is a Gibbs state relative to an effective temperature T_S, here chosen to be greater than or equal to the environmental one. Eq. (5.106) is equivalent to ask that the initial state of the qubit is diagonal in the system's free Hamiltonian eigenbasis, i.e. $\rho_S(0) =$

$p_0 |0\rangle \langle 0| + p_1 |1\rangle \langle 1|$ with $|0\rangle, |1\rangle$ being the eigenstates of $\mathcal{H}_S = \omega_0 \sigma_z/2$. Since $p_0 + p_1 = 1$, any such state can be recast in Gibbs form (5.106) for a certain specific temperature T_S. The motivation behind this restriction of the possible choices of initial states is suggested by the structure of the equations of motion (5.73): since, in light of the latter, the evolution of the populations and of the coherences are decoupled from each other and since the coherences do not enter the expression of $\theta(t)$, any initial state with nonzero coherence is equivalent for the purpose to a diagonal state. The constraint

$$T_S \geq T_E \tag{5.107}$$

on the two initial temperatures instead traduces the condition, involved in the statement of the definition for the occurrence of heat backflow , that the temperature gradient would cause, in the semigroup limiting approximation, a steady and unidirectional heat flow from the system in favour of the environment. If Eq. (5.107) is dropped, then heat flows from the environment to the system would occur due to the temperature gradient, thus tampering its connection with the insurgence of memory effects in the dynamics and preventing to properly speak of *heat backflow* according to the definition we gave above.

Furthermore, we will consider the spectral density to assume the form

$$J(\omega) = \lambda \omega e^{-\frac{\omega}{\Omega}}, \tag{5.108}$$

which shows an Ohmic behavior at low frequencies, a linear dependence on the coupling strength λ, and finally an exponential cutoff part. Note that this functional form corresponds to the $s = 1$ case of the Ohmic-dependent spectral density considered in the analysis of the pure-dephasing spin-boson model studied in Chapter 4. An analytic form for the noise and dissipation kernels (5.109) can be found and reads (see Appendix A of [136] for a proof)

$$\begin{aligned} D_1(\tau) &= 2\lambda \left[\Omega^2 \frac{(\Omega\tau)^2 - 1}{(1 + (\Omega\tau)^2)^2} + 2T_E^2 \, Re \left[\psi' \left(\frac{T_E(1 + i\Omega\tau)}{\Omega} \right) \right] \right], \\ D_2(\tau) &= \frac{4\lambda\Omega^3\tau}{(1 + (\Omega\tau)^2)^2}, \end{aligned} \tag{5.109}$$

with $\psi'(z)$ being the derivative of the Euler digamma function $\psi(z) = \Gamma'(z)/\Gamma(z)$.

Figure 5.1 shows the time evolution of the ground-state population $\rho_{00}(t)$ **(a)** and the heat flow per unit of time $\theta(t)$ as given by (5.86) **(b)** in the weak-coupling limit $\lambda = 0.1$ and in units of ω_0, for $\Omega = 0.4\omega_0$, $T_S = 5\omega_0$, and different values of the environmental temperature $T_E/\omega_0 = 1, 3, 5$. Solid lines in Fig. 5.1 refer to the solutions obtained from the second-order time-convolutionless expansion of the generator, while the dashed lines denote the ones obtained in the Born-Markov approximation. It is clear from these plots that the time behavior of the solution of the ground-state population, $\rho_{00}(t)$, is related to the time behavior of the heat flow per unit of time $\theta(t)$: Both quantities, in fact, show a transition from oscillating to monotone behavior at almost the same time. We find that the oscillations of the exact solution (solid lines) of both quantities almost disappear

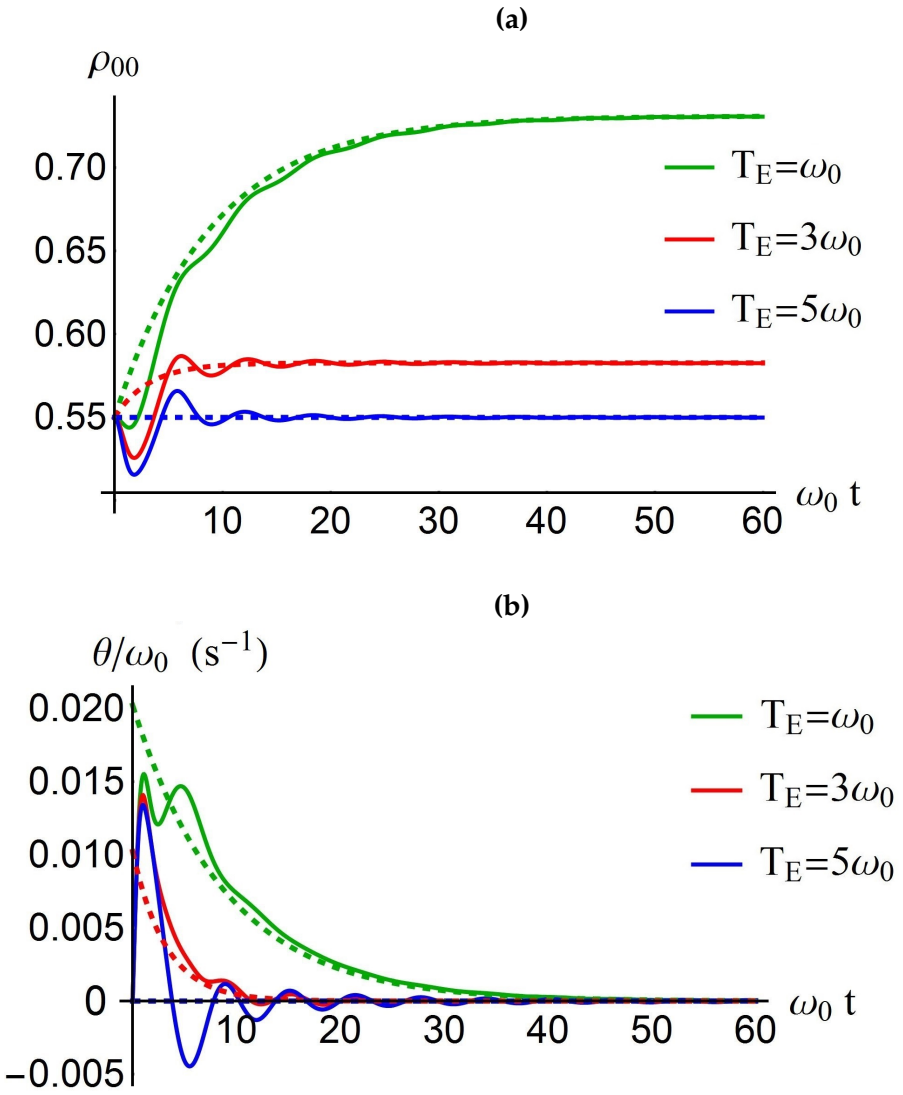

FIGURE 5.1: (Color online) **(a)** Time evolution of the ground-state population $\rho_{00}(t)$ for $\Omega = 0.4\omega_0$, $\lambda = 0.1$, and $T_S = 5\omega_0$, for different values of the environmental temperature $T_E/\omega_0 = 1, 3, 5$. The dashed lines refer to the Born-Markov approximation, while the solid lines refer to the time evolution obtained by the time-convolutioness GME. **(b)** Time evolution of $\theta(t)/\omega_0$ (s^{-1}) for the same parameters values and specific choice of initial Gibbs states. One can notice that above a certain temperature gradient between system and environment the heat backflow disappears.

in the long-time limit and superimpose the asymptotic value determined by the Born-Markov approximated solutions (dashed lines). The markedly different behaviors of solid and dashed lines in short and intermediate time, however, neatly show the inadequacy of Born-Markov approximation apart from the long-time limit case. An interesting property of the heat flow is represented by the first positive peak of $\theta(t)$, which can be observed even when the initial temperatures of the reduced system and of the environment are equal to each other; see Fig. 5.1**(b)**. Such peak is a general feature due to choice of the initial factorized state (5.106), which is essential in order to have a well-defined dynamical map [21], but represents a non-equilibrium preparation with respect to the

total system

$$\rho_{SE}(0) = \frac{e^{-\mathcal{H}_S/T}}{Z_S} \otimes \frac{e^{-\mathcal{H}_E/T}}{Z_E} \neq \frac{e^{-\mathcal{H}/T}}{Z}, \tag{5.110}$$

with Z_S and Z_E being the partition functions of the reduced system and environment respectively and Z being the partition function of the composite system $S + E$. This factorized non-equilibrium initial preparation is known to lead [137, 138] to an energy exchange between system and environment which takes place on short time scales due to the establishment of proper system-environment equilibrium correlations. Moreover, it can be noticed from Fig. 5.1 **(b)** how the value of the first local minimum of $\theta(t)$ decreases for decreasing values of the difference $T_E - T_S$, attaining its lowest value for $T_E = T_S$. Strong numerical evidences suggest that this trend is maintained for all values of the relevant parameters λ, Ω, T_E, thus making it possible to conclude that heat backflow (5.69) [i.e., the area of the negative region of $\theta(t)$] is maximized by the choice of having initial system and environment at the same temperature. This fact can be understood considering the fact that in this case there is no initial temperature gradient which favours an asymmetric flow of energy from the hotter subsystem, which considering Eq. (5.107) is the reduced system, to the colder one, in this case the environment, thus opposing the direction of the heat backflow from E to S.

We have thus evaluated the amount of heat backflow , as estimated by Eq. (5.69); the result $\langle \Delta q \rangle_{back}(\Omega, T_E)$ is given in Fig. 5.2, for the value of the coupling strength $\lambda = 0.1$ and for values of the parameters $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$. We remark that the values of the amount of heat backflow , given in units of ω_0, are represented on a color-bar scale for better visualization.

The calculation has been explicitly carried out by numerically evaluating the integral (5.69) over a fine grid of 2500 points, where the upper limit of time integration has been chosen to be equal to $100\omega_0^{-1}$. After such time interval, in fact, the heat flow per unit of time $\theta(t)$ superimposes, for this value of the coupling strength, the Born-Markov solution, i.e., oscillation of $\theta(t)$ as well as negativity regions are no longer significant. Finally, the maximization over the initial system state has been performed by setting the effective temperature T_S of the system to be equal to the environmental one T_E. Moreover, the upper limit in the integral (5.69) has been chosen to be equal to $100\omega_0^{-1}$:

In order to understand the behavior of the heat backflow shown in Fig. 5.2, one has to consider in some detail the dependence on the relevant parameters Ω and T_E of both the maximum and the correlation time of the noise and dissipation kernels $D_1(t)$ and $D_2(t)$, as given by (5.109). These behaviors are shown in Figs. 5.3 **(a)**, **(b)**, **(c)**, where the correlation time of noise kernel can be inferred from the width of the ratio $D_1(t)/D_1(0)$. More precisely the observed vertical gradient in Fig. 5.2 can be traced back to the varying amplitude of the noise kernel, whose maximum increases with growing temperature [see Fig. 5.3**(a)**], where one has to compare the initial value of the solid lines with the one of the dashed lines relative to the same Ω. Similarly, the observed horizontal gradient in Fig. 5.2 is mainly determined by the correlation time of the noise kernel, which decreases with growing cutoff frequencies; see Fig. 5.3**(b)**. For fixed temperature T_E, the correlation time of the noise kernel decreases for growing values of the cutoff frequency, so that for very large Ω the bath has a very short correlation time, which, in turn, is known to lead to

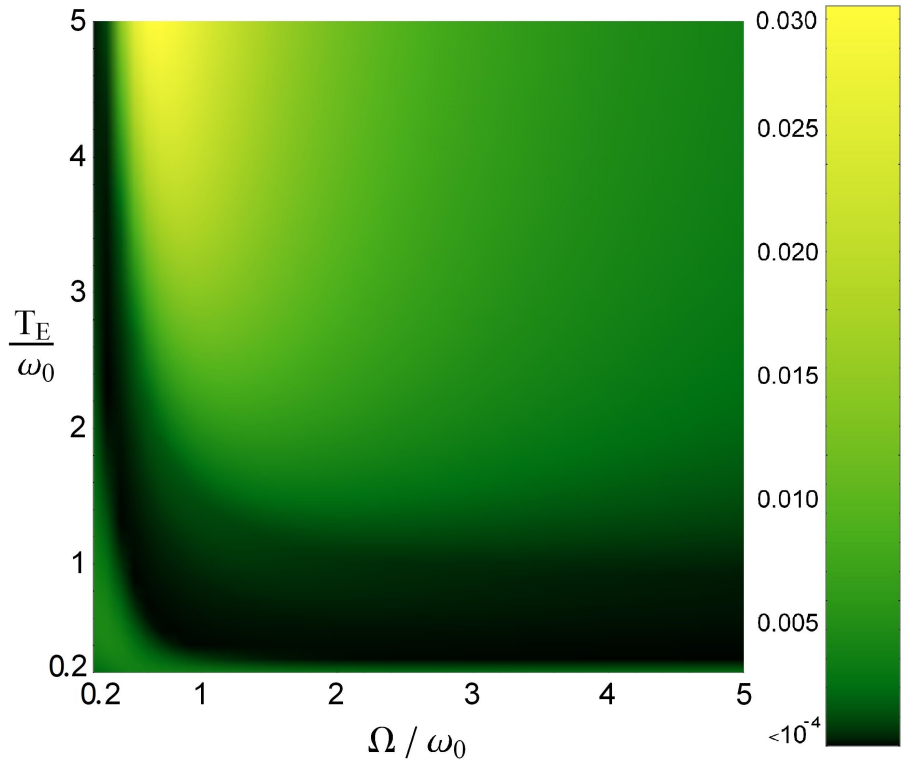

FIGURE 5.2: (Color online) Plot of the heat backflow $\langle \Delta q \rangle_{back}(\Omega, T_E)$ in units of ω_0 as given by Eq. (5.69), for values of the parameters $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$. The coupling constant is chosen to be $\lambda = 0.1$. The effective system temperature T_S has been chosen equal to T_E in order to maximize the oscillations of $\theta(t)$.

a semigroup dynamical regime. This last horizontal trend, however, is compensated in the low-temperature region by the opposite behavior of the amplitude of the dissipation kernel which increases with growing cutoff frequency; see Fig. 5.3**(c)**.

Finally, in order to explain the region of parameters where the heat backflow is suppressed (black region in Fig. 5.2), we have to consider the behavior of the effective spectral density. In particular $J_{eff}(\omega, \Omega, T_E)$ possesses one maximum ω_{max} with respect to its $\omega-$dependence, around which the dominant environmental modes are distributed. Following the discussion in [134], which is recovered more thoroughly in SubSection 5.3.2.2, if such maximum ω_{max}, identified by the condition $\partial_\omega J_{eff}(\omega, \Omega, T_E) = 0$, is equal to the system's transition frequency ω_0, then one has the resonance condition

$$\frac{\partial}{\partial \omega} J_{eff}(\omega, \Omega, T_E)_{|\omega=\omega_0} = 0. \tag{5.111}$$

Figure 5.4 displays the absolute value of $\partial_\omega J_{eff}(\omega, \Omega, T_E)_{|\omega=\omega_0}$ for all the values $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$, displayed on a colored scale, showing the deviation from the resonance condition (5.111), denoted by the white curve in the plot. It is immediate to see that heat backflow is almost suppressed (black region in Fig. 5.2) whenever these deviations are small, i.e., when the resonance condition approximately holds.

It is however fair to notice that this argument seems to fail for very small values of the

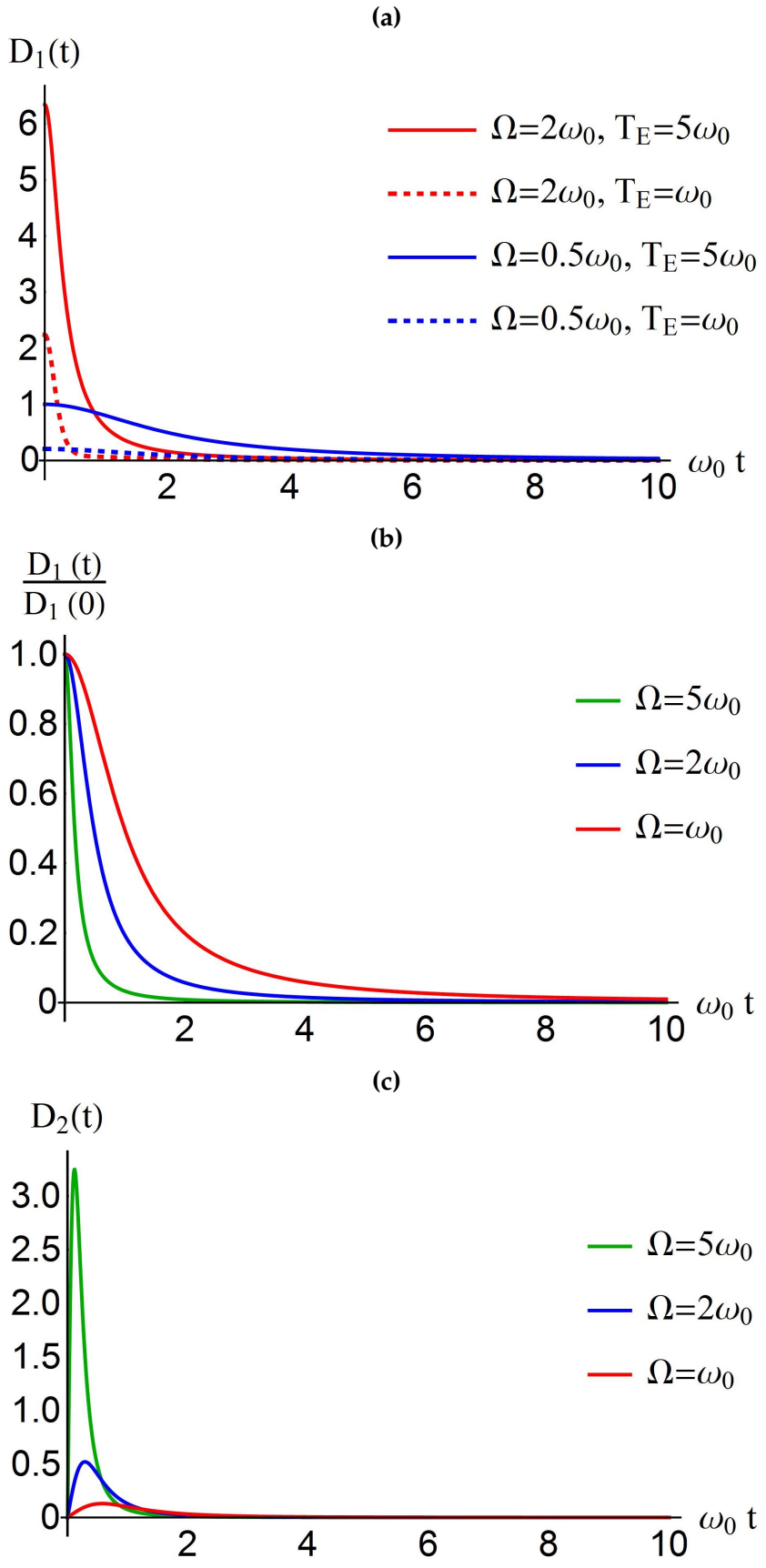

FIGURE 5.3: (Color online) **(a)** Time evolution of the noise kernel for different choices of the cutoff frequencies Ω and temperature T_E. **(b)** Time evolution of the environmental correlation function, inferred from the width of the noise kernel, normalized by its maximum value (attained at time $t = 0$) for $T_E = 5$ and different choices of cutoff frequency Ω. **(c)** Time evolution of the dissipation kernel for different choices of the cutoff frequencies Ω.

couple $(\Omega/\omega_0, T_E/\omega_0)$. In this tiny region of parameters however we may have encountered two sources of numerical issues, which might have led to a systematic error in the solution. The first one is that both the noise and dissipation kernels (and consequently all the derived quantities) oscillate very fast as these parameters enter this area; the second one is that the amount of heat backflow is very tiny because the change in the environmental energy, for these values of parameters, is increasingly small. The combination of these two effects might have been the cause for witnessing the small coloured area around the origin of Fig. 5.2. Similar considerations have been made in [135] for the calculation of the trace distance and the consequent measure of non-Markovianity. More refined numerical integration techniques (we employed Mathematica built-in functions and integration strategies) could be considered to improve the investigation of this region of dynamical parameters.

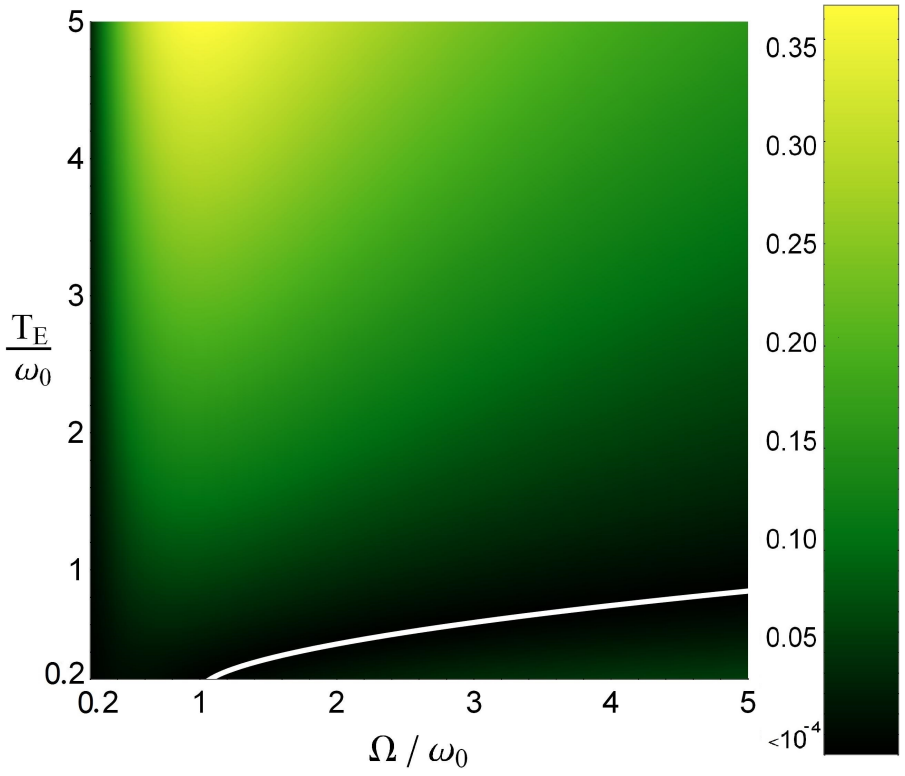

FIGURE 5.4: (Color online) Plot of the absolute value of $\partial_\omega J_{eff}(\omega, \Omega, T_E)|_{\omega=\omega_0}$, for $\lambda = 0.1$ and values of the cutoff frequency and environmental temperature $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$. The black region of this plot, which has to be compared with the one in Fig. 5.2, indicates those values of the parameters for which the resonance condition (5.111) approximately holds, while the white curve denotes those for which (5.111) strictly holds.

Our analysis further provides a tool to identify the parameters region in which the heat backflow shows a maximum value. From Fig. 5.2 it is, in fact, evident that this condition is reached for high values of the temperature T_E and for values of the cutoff frequency Ω around the system proper frequency ω_0.

5.3.2.2 Relationship with non-Markovianity of the reduced dynamics

In the present Section we discuss in detail the connection between the heat backflow measure between a reduced system and its environment, obtained in the FCS formalism, and the concept of non-Markovianity.

Among the different criteria and estimators of non-Markovianity listed in Chapter 3, we concentrate our attention on the trace-distance based one introduced by Breuer, Laine, and Piilo [11], due to its clear physical interpretation as occurrence (and measure) of *information backflow* from E to S. We recall that the latter corresponds to the case $q = 1/2$ of Eq. (3.55) and reads

$$\mathcal{N}_{BLP}(\Lambda) = \max_{\rho_S^{1,2}(t_0)} \frac{1}{2} \int_{\mathbb{R}^+} |\sigma_{BLP}(t)| + \sigma_{BLP}(t)\, dt, \tag{5.112}$$

where

$$\sigma_{BLP}(t) = \sigma_{|q=1/2}(t) = \frac{d}{dt} I_{int}(t)_{|q=1/2}(t) = \frac{1}{2}\frac{d}{dt} \parallel \rho_S^1(t) - \rho_S^2(t) \parallel_1 . \tag{5.113}$$

In the case of a two - level system, the quantity $I_{int}(t)_{|q=1/2}(t) = (1/2) \parallel \rho_S^1(t) - \rho_S^2(t) \parallel_1$ can be conveniently expressed in terms of the associated Bloch vector as

$$\begin{aligned} I_{int}(t)_{|q=1/2}(t) &= \frac{1}{4}\mathrm{Tr}_S \left[\left| \left(\mathbf{v}_S^1(t) - \mathbf{v}_S^2(t) \right) \cdot \boldsymbol{\sigma} \right| \right] \\ &= \frac{1}{2} \left| \mathbf{v}_S^1(t) - \mathbf{v}_S^2(t) \right| , \end{aligned} \tag{5.114}$$

where the fact that the two real eigenvalues of $\left(\mathbf{v}_S^1(t) - \mathbf{v}_S^2(t) \right) \cdot \boldsymbol{\sigma}$ were $\pm \left| \mathbf{v}_S^1(t) - \mathbf{v}_S^2(t) \right|$ was used in the last line. For the spin - boson model, following [134, 135], we will approximate the integral in Eq. (5.112) with the sum of the differences of the trace norm at various time steps upon introducing a suitable binning of the time axis and choosing an optimal couple of initial states (upon which we will comment hereafter for the case at hand)

$$\mathcal{N}_{BLP}(\Omega, T_E) \simeq \sum_i \left[I_{int}(t)_{|q=1/2}(t_{i+1}) - I_{int}(t)_{|q=1/2}(t_i) \right] , \tag{5.115}$$

with every term $I_{int}(t)_{|q=1/2}(t_i)$ explicitly evaluated by numerically solving the differential equations for the Bloch vector's components (5.77). Note that we have made substituted the abstract dependence of the non-Markovianity measure on the dynamical map Λ with the dynamical parameters (Ω, T_E) which characterize it for the model under consideration.

In order to compare the result with the above calculations made for the heat backflow measure, the same choice of spectral density (5.108) has been made and the result has been plotted for the same range of parameters as in Fig. 5.2, i.e. $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$ and $\lambda = 0.1$. We note that in [134], the authors employed a Lorentzian cutoff instead of an exponential one [see our Eq. (5.108) and their Eq. (19)]; after re - evaluating the non-Markovianity measure $\mathcal{N}(\Omega, T_E)$ with the current spectral density and comparing both results, it has turned out that no substantial changes have

occurred, thus confirming the conjecture that the information backflow does not significantly depend on the high-frequency part of the spectrum [102], at least in the case of a bosonic bath. The couple of initial states $\rho^1(0)$ and $\rho^2(0)$ used is the one that maximizes (5.112) which has been chosen in accordance with [134], namely those with associated Bloch vectors $v^1(0) = (0, 1, 0)^T$ and $v^2(0) = (0, -1, 0)^T$. Note that these couple of initial states are antipodal points of the Bloch sphere [56] with respect to the $z = 0$ - plane, meaning that their distinguishability is written in their coherences.

Figure 5.5 shows $\mathcal{N}(\Omega, T_E)$ for $\lambda = 0.1$ and for the above mentioned values of the parameters. Moreover, the upper limit in the integral (5.115) has been chosen equal to $t = 100\omega_0^{-1}$ as for calculating the quantity plotted in Fig. 5.2.

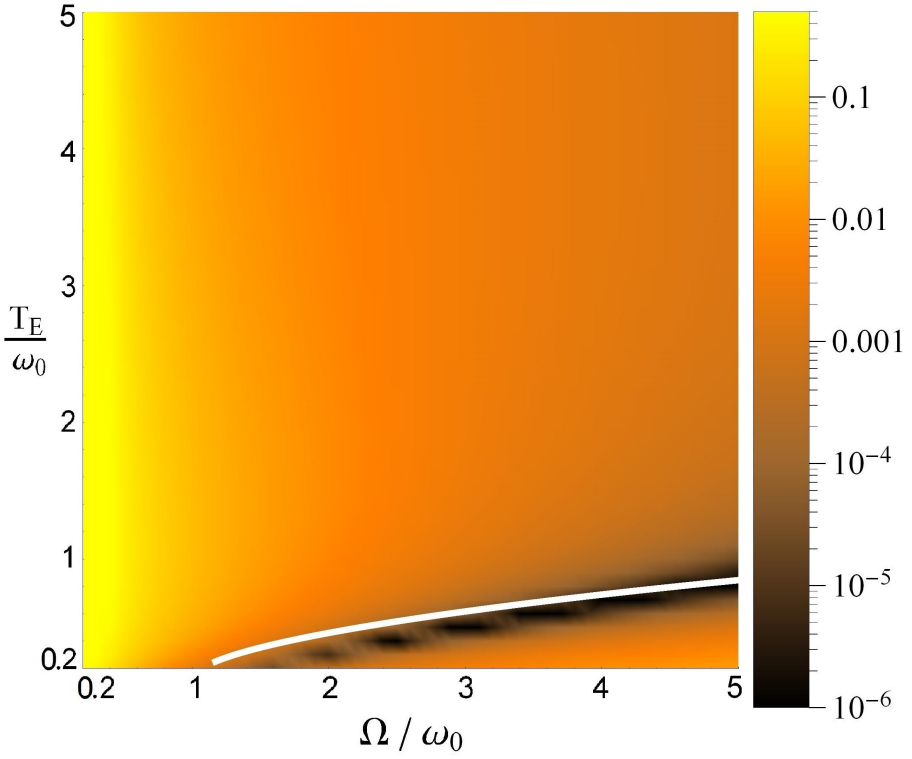

FIGURE 5.5: (Color online) Plot of the non-Markovianity measure $\mathcal{N}(\Omega, T_E)$ up to integration time $t = 100\omega_0^{-1}$, for $\lambda = 0.1$ and for values of the parameters $(\Omega/\omega_0, T_E/\omega_0)$ in the range $(0.2, 5) \times (0.2, 5)$. The white line corresponds to the resonance curve (5.116), which provides an approximate estimate of the region of Markovianity of the dynamics

.

First of all, a comparison with Fig. 3 of [134] shows that, even in this case, the high-frequency part of the spectrum does not affect significantly the non-Markovianity measure. This can be understood by reasoning that, for large values of the cutoff frequency Ω ($\simeq 10\omega_0$), the spectral density can be approximated with $J(\omega) \simeq \lambda\omega$, this leading to a Markovian dynamics [21]. On the other hand, for decreasing values of the cutoff frequency Ω the amount of non-Markovianity, in general, increases, the only exception being represented by the region of parameters in which the resonance condition (5.111) holds. Such condition expresses the requirement of local flatness of the effective spectral density around the system's transition frequency, and describes a curve in the $(\Omega\,,\, T_E)$ plane called resonance curve along which a predominantly Markovian regime

is expected and found [134]. In the case here considered of exponential cutoff, the resonance curve, plotted in Fig. 5.5 as a white line, reads

$$\Omega_{res}(T_E) = \frac{T_E}{\frac{T_E}{\omega_0} - \text{Cosech}\left(\frac{\omega_0}{T_E}\right)}, \tag{5.116}$$

and it is evident how it continues to retrace well the observed Markovian region at low temperatures of the bath.

A comparison between Figs. 5.2 and 5.5 clearly shows that the amount of non-Markovianity of the dynamical map as measured by (5.115) and the amount of heat backflow as quantified by (5.69) are connected to each other. First of all, in fact, for every value of the cutoff frequency Ω, both quantities increase with increasing values of the temperature, this being related to the fact that in this model, when T_E grows, the lower frequency part of the effective spectrum $J_{eff}(\omega, \Omega, T_E)$ is enhanced. Moreover, both the non-Markovianity and the heat backflow measures generally increase for decreasing values of the cutoff frequency. This is due to the fact that the correlation time of the noise kernel reduces for growing values of Ω, so that the correlation function of the bath is almost δ correlated in time, which leads to a semigroup (and therefore Markovian) dynamics. Finally, as already highlighted before, both quantities are strongly related to the resonance condition (5.111). In particular, while the non-Markovianity measure (5.115) vanishes only when (5.111) holds strictly, the heat backflow is suppressed even when (5.111) is approximately satisfied. This result, together with the one discussed above in the Born-Markov regime, makes it possible to conclude that in a Markovian regime heat backflow is suppressed. The opposite is, however, in general, not true; namely, the absence of heat backflow does not imply absence of information backflow, thus preventing a one-to-one relation between these two concepts, as expected from both a mathematical and a conceptual point of view.

The occurrence of heat backflow, in conclusion, appears in this model as a stricter condition than non-Markovianity. On the other hand, however, for values of the parameters Ω and T_E for which the amount of non-Markovianity is significant, it becomes possible to measure a backflow of energy, as witnessed by the colored region in Fig. 5.2. We also stress that the relationship between the amount of heat backflow and non-Markovianity has to be intended at the level of the respective measures (5.69) and (5.115), which are properties of the dynamical map uniquely determined by the choice of the parameters λ, Ω, and T_E. The connection we have found between non-Markovianity and heat backflow measures can finally represent a powerful hint in relation to the practical usefulness of non-Markovianity: It is, in fact, clear from this result that a convenient engineering of the reservoir such to achieve non-Markovianity [139] allows to have heat backflow and therefore to treat the environment as a potential quantum energy buffer.

5.3.3 The quantum brownian motion

We now apply the outlined formalism to a quantum harmonic oscillator linearly coupled to an infinite number of bosonic modes, i.e. the so-called Quantum Brownian Motion

(QBM). The Hamiltonian of the composite system has the form $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{\rm int}$, with:

$$\mathcal{H}_S = \frac{\omega_0}{2}\left(a^\dagger a + 1/2\right),\ \mathcal{H}_E = \sum_k \omega_k b_k^\dagger b_k,\ \mathcal{H}_{SE} = X \otimes B_E, \tag{5.117}$$

where $\hbar$ is set to 1, $a, a^\dagger$ denote the system's annihilation and creation operators, B_E is the same as in Eq. (5.70), $X = 2^{-1/2}(a + a^\dagger)$ ($P = 2^{-1/2}i(a^\dagger - a)$), ω_k stands for the energy of the kth bosonic mode and g_k is the coupling strength between the mode and the system. In the weak coupling limit the master equation for the modified statistical operator $\rho_S(\eta, t)$ reduces to

$$\begin{aligned}\frac{d}{dt}\rho_S(\eta,t) &= -i\left[\mathcal{H}_S, \rho_S(\eta,t)\right] \\ &- \int_0^t ds\ \left[XX(-s)\rho_S(\eta,t)\Phi(s) + \rho_S(\eta,t)X(-s)X\Phi(-s)\right. \\ &\qquad \left. -X\rho_S(\eta,t)X(-s)\Phi(-s-\eta) - X(-s)\rho_S(\eta,t)X\Phi(s-\eta)\right],\end{aligned} \tag{5.118}$$

where

$$\Phi(s) = \mathrm{Tr}_E\left[B_E B_E(-s)\rho_E\right], \qquad \Phi(s-\eta) = \mathrm{Tr}_E\left[B_E^{(-\eta)} B_E^{(\eta)}(-s)\rho_E\right], \tag{5.119}$$

with $B_E^{(-\eta)} = e^{(i/2)\eta\mathcal{H}_E} B_E e^{-(i/2)\eta\mathcal{H}_E}$. Using the fact that $X(t) = X\cos(\omega_0 t) + P\sin(\omega_0 t)$ in the interaction picture with respect to $\mathcal{H}_S$, after some calculations Eq.(5.118) can be re-expressed as

$$\frac{d}{dt}\rho_S(\eta,t) = \Xi(t)\left[\rho_S(\eta,t)\right] + \mathcal{L}_\eta(t)\left[\rho_S(\eta,t)\right], \tag{5.120}$$

where

$$\Xi(t)\left[\cdot\right] = -i\left[\mathcal{H}_S, \cdot\right] - \Delta(t)\left[X,[X,\cdot]\right] + \Pi(t)\left[X,[P,\cdot]\right] + \frac{i}{2}r(t)\left[X^2,\cdot\right] - i\gamma(t)\left[X,\{P,\cdot\}\right] \tag{5.121}$$

is the usual dynamical generator [131, 133] with

$$\begin{aligned}\Delta(t) &= \frac{1}{2}\int_0^t ds D_1(s)\cos(\omega_0 s), \qquad \Pi(t) = \frac{1}{2}\int_0^t ds D_1(s)\sin(\omega_0 s), \\ \gamma(t) &= \frac{1}{2}\int_0^t ds D_2(s)\sin(\omega_0 s), \qquad r(t) = \int_0^t ds D_2(s)\cos(\omega_0 s), \\ D_1(t) &= \Phi(t) + \Phi(-t), \qquad D_2(t) = i\left(\Phi(t) - \Phi(-t)\right),\end{aligned} \tag{5.122}$$

while the non-trace preserving superoperator $\mathcal{L}_\eta(t)\left[\cdot\right]$ is given by

$$\mathcal{L}_\eta(t)\left[\cdot\right] \equiv f_+(t)\, a\cdot a + f_-(t)\, a^\dagger\cdot a^\dagger + g_+(t)\, a\ \cdot a^\dagger + g_-(t)\, a^\dagger\cdot a, \tag{5.123}$$

with

$$f_{\pm}(\eta,t)=\frac{1}{2}\int_0^t ds\Delta D_1^{(\eta)}(s)e^{\pm i\omega_0 s}, \tag{5.124}$$

$$g_{\pm}(\eta,t)=\frac{1}{2}\int_0^t ds\left(\Delta D_1^{(\eta)}(s)\cos(\omega_0 s)\pm\Delta D_2^{(\eta)}(s)\sin(\omega_0 s)\right), \tag{5.125}$$

$$\Delta D_{1,2}^{(\eta)}(t)\equiv D_{1,2}^{(\eta)}(t)-D_{1,2}(t),$$

$$D_1^{(\eta)}(t)=\Phi(t-\eta)+\Phi(-t-\eta),\quad D_2^{(\eta)}(t)=i\left(\Phi(t-\eta)-\Phi(-t-\eta)\right). \tag{5.126}$$

After performing the secular approximation [140], one is left with

$$\begin{aligned}\frac{d}{dt}\rho_S(\eta,t)=&-i\omega_0\left[a^\dagger a,\rho_S(\eta,t)\right]\\&-\left(\frac{\Delta(t)+\gamma(t)}{2}\right)\left\{a^\dagger a,\,\rho_S(\eta,t)\right\}-\left(\frac{\Delta(t)-\gamma(t)}{2}\right)\left\{aa^\dagger,\,\rho_S(\eta,t)\right\}\\&+\left(\Delta(t)+\gamma(t)+g_+(\eta,t)\right)a\,\rho_S(\eta,t)a^\dagger+\left(\Delta(t)-\gamma(t)+g_-(\eta,t)\right)a^\dagger\,\rho_S(\eta,t)a,\end{aligned} \tag{5.127}$$

where the term proportional to $r(t)$ has been considered negligible, which is justified in the weak-coupling limit as long as the environmental cut-off frequency remains finite [131]. As shown in the previous Section, in order to obtain $\rho_S(\eta,t)$, we move to the correspondent Fokker-Planck differential equation for its characteristic function $\chi^{(\eta)}(q,p,t)$ [92]. This is done with for following set of formal substitutions

$$a\rho\longleftrightarrow-\frac{1}{\sqrt{2}}\left[\partial_q+i\partial_p+\frac{1}{2}(q+ip)\right]\chi^{(\eta)}(q,p,t), \tag{5.128}$$

$$a^\dagger\rho\longleftrightarrow\frac{1}{\sqrt{2}}\left[\partial_q-i\partial_p-\frac{1}{2}(q-ip)\right]\chi^{(\eta)}(q,p,t), \tag{5.129}$$

$$\rho a\longleftrightarrow-\frac{1}{\sqrt{2}}\left[\partial_q+i\partial_p-\frac{1}{2}(q+ip)\right]\chi^{(\eta)}(q,p,t), \tag{5.130}$$

$$\rho a^\dagger\longleftrightarrow\frac{1}{\sqrt{2}}\left[\partial_q-i\partial_p+\frac{1}{2}(q-ip)\right]\chi^{(\eta)}(q,p,t), \tag{5.131}$$

which lead to express the various operatorial terms in (5.127) as

$$\begin{aligned}&a^\dagger a\rho\longleftrightarrow-\frac{1}{2}\left[\partial_q-i\partial_p-\frac{1}{2}(q-ip)\right]\left(\partial_q+i\partial_p+\frac{q}{2}+\frac{ip}{2}\right)\chi^{(\eta)}(q,p,t),\\&\rho a^\dagger a\longleftrightarrow-\frac{1}{2}\left[\partial_q+i\partial_p-\frac{1}{2}(q+ip)\right]\left(\partial_q-i\partial_p+\frac{q}{2}-\frac{ip}{2}\right)\chi^{(\eta)}(q,p,t),\\&\Rightarrow\left[a^\dagger a,\rho\right]\longleftrightarrow i\left(q\partial_p-p\partial_q\right)\chi^{(\eta)}(q,p,t),\end{aligned} \tag{5.132}$$

$$\left\{a^\dagger a,\rho\right\}\longleftrightarrow-\left(\partial_{qq}^2+\partial_{pp}^2+1-\frac{q^2+p^2}{4}\right)\chi^{(\eta)}(q,p,t), \tag{5.133}$$

$$
\begin{aligned}
aa^\dagger\rho &\longleftrightarrow -\frac{1}{2}\left[\partial_q + i\partial_p + \frac{1}{2}(q+ip)\right]\left(\partial_q - i\partial_p - \frac{q}{2} + \frac{ip}{2}\right)\chi^{(\eta)}(q,p,t),\\
\rho aa^\dagger &\longleftrightarrow -\frac{1}{2}\left[\partial_q - i\partial_p + \frac{1}{2}(q-ip)\right]\left(\partial_q + i\partial_p - \frac{q}{2} - \frac{ip}{2}\right)\chi^{(\eta)}(q,p,t),\\
\Rightarrow \left[aa^\dagger,\rho\right] &\longleftrightarrow -\left(\partial_{qq}^2 + \partial_{pp}^2 - 1 - \frac{q^2+p^2}{4}\right)\chi^{(\eta)}(q,p,t),
\end{aligned}
\tag{5.134}
$$

and finally

$$
a\rho a^\dagger \longleftrightarrow -\frac{1}{2}\left(\partial_{qq}^2 + \partial_{pp}^2 + \frac{q^2+p^2}{4} + 1 + q\partial_q + p\partial_p\right)\chi^{(\eta)}(q,p,t), \tag{5.135}
$$

$$
a^\dagger\rho a \longleftrightarrow -\frac{1}{2}\left(\partial_{qq}^2 + \partial_{pp}^2 + \frac{q^2+p^2}{4} - 1 - q\partial_q - p\partial_p\right)\chi^{(\eta)}(q,p,t). \tag{5.136}
$$

Putting all these results together, we obtain the differential equation

$$
\begin{aligned}
\frac{d}{dt}\chi^{(\eta)}(q,p,t) = \Big\{&\omega_0\left(q\partial_p - p\partial_q\right) - V_1(\eta,t)\left(\partial_{qq}^2 + \partial_{pp}^2\right) - \left(2\Delta(t) + V_1(\eta,t)\right)\frac{q^2+p^2}{4}\\
&+ \left(V_2(\eta,t) - \gamma(t)\right)\left(q\partial_q + p\partial_p\right) + V_2(\eta,t)\Big\}\chi^{(\eta)}(q,p,t),
\end{aligned}
\tag{5.137}
$$

where we have introduced the quantities

$$
V_{1,2}(\eta,t) = \frac{1}{2}\left(g_-(\eta,t) \pm g_+(\eta,t)\right). \tag{5.138}
$$

Due to the quadratic nature of the Hamiltonian (5.117), the Gaussian shape of the characteristic function is granted [43, 46, 141] and thus an educated ansatz is

$$
\chi^{(\eta)}(q,p,t) = \Psi(\eta,t)\exp\left[i\,(q,p)^T\begin{pmatrix}X_m(\eta,t)\\ P_m(\eta,t)\end{pmatrix} - \frac{1}{2}(q,p)^T\begin{pmatrix}\sigma_{XX}(\eta,t) & \sigma_{XP}(\eta,t)\\ \sigma_{PX}(\eta,t) & \sigma_{PP}(\eta,t)\end{pmatrix}\begin{pmatrix}q\\ p\end{pmatrix}\right], \tag{5.139}
$$

where $(X_m(\eta,t), P_m(\eta,t))^T \equiv (\mathrm{Tr}_S\left[\rho_S(\eta,t)X\right], \mathrm{Tr}_S\left[\rho_S(\eta,t)P\right])^T$ and, $\boldsymbol{\sigma}(\eta,t)$ is the covariance matrix (which is symmetric). Finally, $\Psi(\eta,t)$ represents a time-dependent amplitude which is not conserved during the evolution due to the action of the non trace-preserving superoperator $\mathcal{L}_\eta(t)\left[\cdot\right]$. Having assumed this ansatz for the characteristic function $\chi^{(\eta)}(q,p,t)$, Eq.(5.66) can be expressed as

$$
\theta(t) = \frac{\partial\dot{\Psi}(\eta,t)}{\partial(i\eta)}|_{\eta=0}. \tag{5.140}
$$

Plugging (5.139) into (5.137) and separating the different moments of q and p, it is straightforward to show that the evolution equation for the mean values $X_m(t), P_m(t)$ as well as for the off-diagonal elements of the covariance matrix $\sigma_{XP}(t) = \sigma_{PX}(t)$ has the following structure:

$$
\partial_t O_i(t) = \sum_{j=1}^{3} G_{ij}O_j(t), \qquad O_j \equiv \{X_m, P_m, \sigma_{XP}\}. \tag{5.141}
$$

Note that the heat flow per unit of time $\theta(t)$ is uniquely determined by the time-dependent amplitude $\Psi(\eta,t)$ Eq. (5.140), which only depends on the diagonal matrix elements of the covariance matrix, see Eq. (5.142). The evolution equation for the latter, in turn, can be seen to be decoupled from one for the off-diagonal elements of the covariance matrix (coherences). This indicates that, for the case at hand, it is sufficient to consider initial thermal states relative to an effective temperature T_S which must be chosen to be greater or equal to the initial environmental temperature T_E to ensure the energy backflow is not in the direction of the temperature gradient [2]. In this case we have that $\sigma_{XP}(0) = X_m(0) = P_m(0) = 0$, and thus $\sigma_{XP}(t) = X_m(t) = P_m(t) = 0\ \forall t$. Moreover we have that $\sigma_{XX}(\eta,t) = \sigma_{PP}(\eta,t) \equiv \sigma(\eta,t)$ [43, 46, 141]. The number of evolution equations for the Gaussian parameters therefore reduce to two, namely

$$\partial_t \Psi(\eta,t) = \Psi(\eta,t)\left(2V_1(\eta,t)\sigma(\eta,t) + V_2(\eta,t)\right), \tag{5.142}$$

$$\partial_t \sigma(\eta,t) = \frac{1}{2}\left[2\Delta(t) + V_1(\eta,t)\right] + 2\left[V_2(\eta,t) - \gamma(t)\right]\sigma(\eta,t) + 2V_1(\eta,t)\sigma^2(\eta,t) \tag{5.143}$$

We stress that, since $\lim_{\eta\to 0} V_j(\eta,t) = 0 (j = 1,2)$, we have

$$\partial_t \Psi(0,t) = 0 \tag{5.144}$$

$$\partial_t \sigma(0,t) = \Delta(t) - 2\gamma(t)\sigma(0,t). \tag{5.145}$$

which leads to the well-known solution for the characteristic function [131–133, 142]

$$\chi(q,p,t) = \exp\left[-\frac{q^2+p^2}{2}\sigma(0,t)\right], \tag{5.146}$$

with

$$\sigma(0,t) = e^{-2\int_0^t ds\gamma(s)}\left(\sigma(0,0) + \int_0^t ds\Delta(s)e^{2\int_0^s d\tau\gamma(\tau)}\right). \tag{5.147}$$

Some further calculations lead to the final expression for the heat flow per unit of time Eq.(5.140) that can be expressed as

$$\theta(t) = 2\sigma(0,t)\left(\frac{1}{2}D_2(t)\cos(\omega_0 t) + \omega_0\gamma(t)\right) + \frac{1}{2}D_1(t)\sin(\omega_0 t) - \omega_0\Delta(t), \tag{5.148}$$

where we have used that $\Psi(0,t) = 1$ and where the diagonal element $\sigma(0,t)$ of the covariance matrix is the solution of Eq. (5.144) with the initial condition $\sigma(0,0) = 1/2(1 + 2N(T_S))$, with $N(T_S) = [\exp(1/T_S) - 1]^{-1}$ (T_S being the effective system's initial temperature). As in [2], in order to properly speak of heat backflow , T_S is chosen to be greater or equal to the initial environmental temperature T_E, condition that would lead to a steady non-negative mean energy transfer from the reduced system to the environment in the Born-Markov semigroup limiting case.

5.3.3.1 Numerical evaluation of the heat backflow measure

In conformity with the choice made for the spin - boson model, we assume the spectral density characterizing the environmental correlation function to be of Ohmic form with

exponential cut-off (5.108).

Note that the initial effective temperature T_S of the system must be chosen to be greater or equal to the initial environmental temperature T_E to ensure the heat backflow is not in the direction of the temperature gradient [2].

In Fig. 5.6(a) we show the heat flow per unit of time $\theta(t)$ as given by Eq. (5.148), in the weak coupling limit $\lambda = 0.01$ and in units of ω_0, for $\Omega = 0.25\omega_0$, $T_E = \omega_0$ and for three different values of the effective system's temperature $T_S/\omega_0 = 1,\ 2,\ 3$.

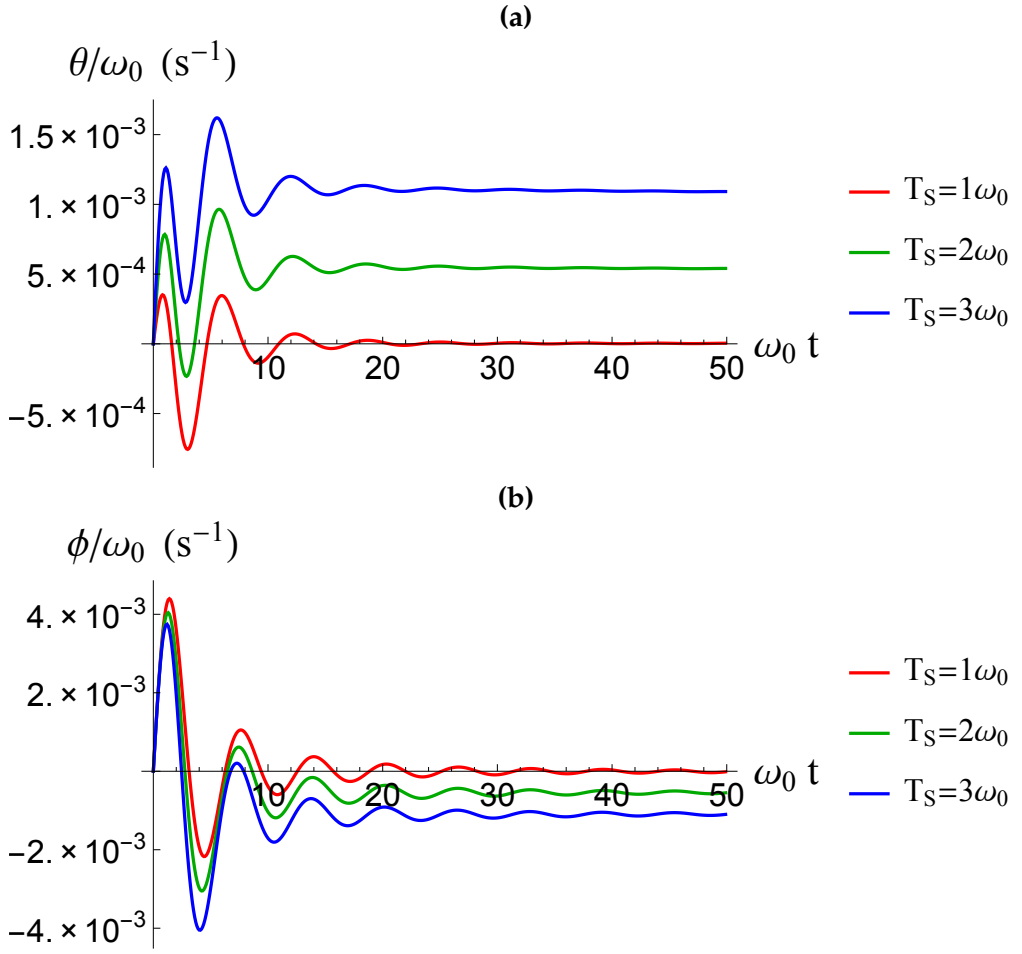

FIGURE 5.6: (Color online) Time evolution of: (a) $\theta(t)$ and (b) $\phi(t)$, in units of ω_0, for $\Omega = 0.25\omega_0$, $\lambda = 0.01$ and $T_E = \omega_0$ and for different values of the initial system's temperature $T_S/\omega_0 = 1,\ 2,\ 3$.

An interesting feature of the heat flow is represented by the first positive peak of $\theta(t)$, which can be observed even when the initial temperatures of the reduced system and of the environment are equal to each other. Such peak, which was observed also in the case of a spin-boson model [2], is a general feature due to the choice of dealing with an initial factorized state, which is essential in order to have a well-defined dynamical map [21]. In fact, even if system and environment are in Gibbs form relative to the same temperature T, i.e. $\rho_{SE}(0) = \frac{e^{-\mathcal{H}_S/T}}{Z_S} \otimes \frac{e^{-\mathcal{H}_E/T}}{Z_E}$, with Z_S and Z_E being the partition functions of the reduced system and environment respectively, the state does not represent an equilibrium

preparation [2, 137, 138]. In particular, the contribution of the interaction Hamiltonian is absent before $t = 0$, i.e. when the first measurement of the environmental energy in the two-time measurement protocol outlined above is performed. The switching on of the interaction term results in a net heat flow both into the environment and into the system that takes place at the early stage of the coupled evolution. In fact, if we compute the change in the system's energy

$$\langle \Delta \mathcal{H}_S \rangle_t \equiv \mathrm{Tr}_S \left[\mathcal{H}_S \left(\rho_S(t) - \rho_S(0) \right) \right] = \sigma(0,t) - \sigma(0,0), \tag{5.149}$$

we still observe a first positive peak in its time-derivative $\phi(t) \equiv \frac{d}{dt}\langle \Delta \mathcal{H}_S \rangle$, as shown in Fig. 5.6(b) [138]. The last equality in Eq. (5.149) has been obtained by noting that $\langle \mathcal{H}_S \rangle_t = \frac{1}{2}\langle X^2 + P^2 \rangle_t \equiv \sigma(0,t)$.

It is also interesting to consider the time behavior of the change in the mean values of the energies of the environment $\langle \Delta q \rangle_t$ Eq. (5.65) and of the system $\langle \Delta \mathcal{H}_S \rangle_t$ Eq. (5.149). While the latter is always a positive quantity, it turns out that the energy of the environment, for different values of cut-off frequency and initial temperatures, shows in the weak coupling regime a decrease over time with respect to its initial value, given $T_E = T_S$. This lower energy value persists in the long time limit. Being in the weak coupling regime, we can assume the final state of the composite system to be effectively factorized, with an environmental reduced density matrix that can therefore be cast into a Gibbs form relatively to an inverse temperature which is lower than the initial one. In this sense one could speak of a non-externally induced *cooling effect*.

Finally, from the analysis of Fig. 5.6(a), it emerges how the heat backflow measure, i.e. the area of the negative region of $\theta(t)$, is maximized for $T_E = T_S$; strong numerical evidences suggest that this trend is maintained for all values of the relevant parameters λ, Ω, T_E. This fact, in agreement also with what happens in the case of a spin-boson model [2], can be understood considering that there is no initial temperature gradient when the two temperatures initially match, this favouring a more symmetric situation of energy exchange. Exploiting this result, we can then evaluate the amount of heat backflow , as estimated by Eq. (5.69).

In Fig. 5.8 we show the behaviour of the heat backflow measure $\langle \Delta q \rangle_{back}$ with respect to its dependence on the various parameters λ, Ω, $T_E (= T_S)$ in the range $\lambda \in [0.01, 0.1]$. In such weak coupling regime the measure turns out to be monotonically increasing with the coupling strength and possesses a non trivial behavior with respect to the cut-off frequency Ω: for intermediate values of the initial temperatures $T_E = T_S$, $\langle \Delta q \rangle_{back}$ decreases for large Ω, while for very low temperature ($T_E = T_S = 0.25\omega_0$) there seems to be an almost linear increment of the latter with Ω.

5.3.3.2 Heat backflow in the strong coupling regime

Here we present a numerical approach to calculate the quantities $\langle \Delta q \rangle_{back}$ and $\theta(t)$, defined in Eqs.(5.69) and (5.66) respectively, in the QBM without relying on the FCS. The results obtained this way will encompass both the dynamical regimes of weak coupling,

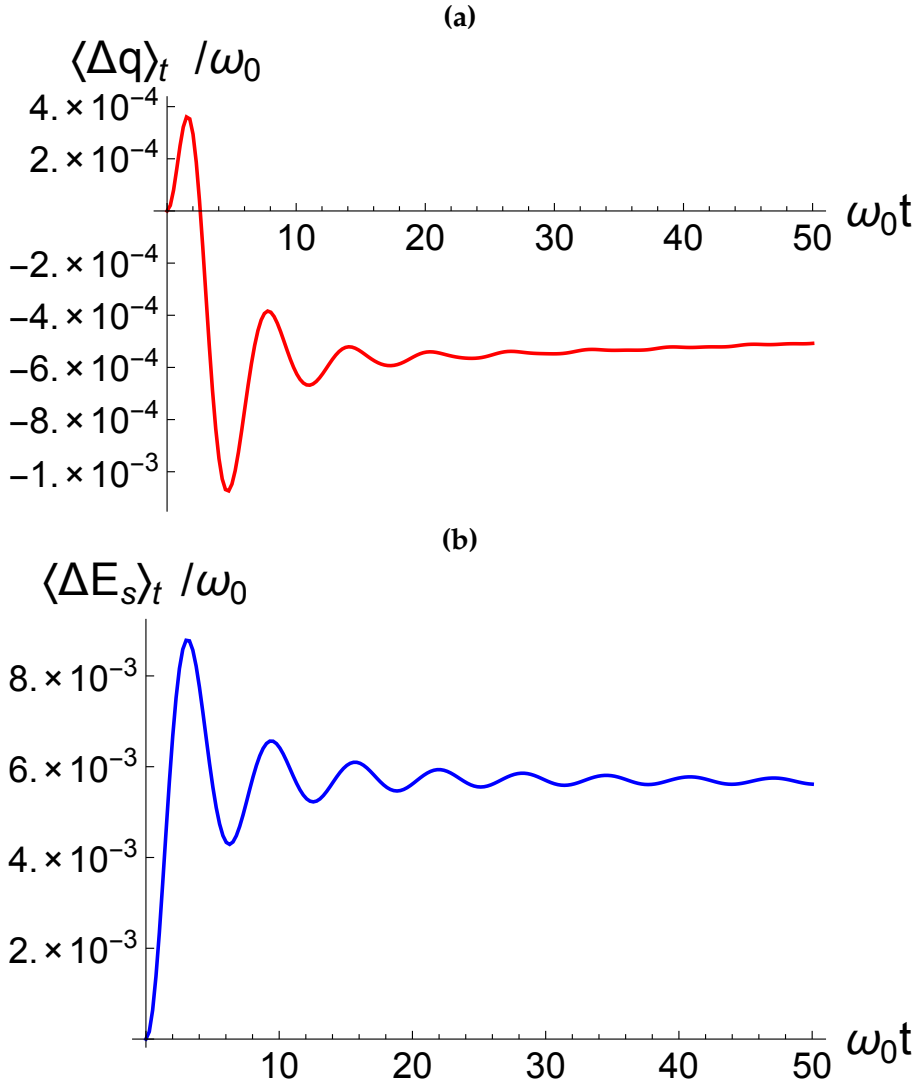

FIGURE 5.7: (Color online) Time evolution of: (a) $\langle \Delta q \rangle_t$ and (b) $\langle \Delta E_S \rangle_t$, in units of ω_0, for $\Omega = 0.25\omega_0$, $\lambda = 0.01$ and $T_E = T_S = \omega_0$. Note that the final value of the internal energy of the environment is lower than its initial value, meaning that the environment has cooled down.

where we will show the agreement with those obtained in the previous Section 5.3.3, and of strong coupling. The essential starting point of this method [143] is to consider the environment as composed by an arbitrary but *finite* number N of bosonic modes, so that the total Hamiltonian (5.117) is now represented by a $(N+1) \times (N+1)$ matrix of the form

$$\mathcal{H} = \frac{\mathbf{P}^T \mathbf{P}}{2} + \mathbf{X}^T \mathbf{M} \mathbf{X}, \tag{5.150}$$

with $\mathbf{X} = (X_1, X_2, \cdot, X_N, X_{N+1})^T$ and $\mathbf{P} = (P_1, P_2, \cdot, P_N, P_{N+1})^T$, where X_{N+1}, P_{N+1} denote the position and momentum operators of the reduced system while the remaining N operators refer to the environmental modes. Finally, the matrix $\mathbf{M}$ has elements $\mathbf{M}_{i,i} = \frac{\omega_i^2}{2}$ for $i = 1, \cdot N$, $\mathbf{M}_{N+1,N+1} = \frac{\omega_0}{2}$ and $\mathbf{M}_{i,N+1} = \mathbf{M}_{N+1,i} = -\frac{g_i}{2}$. We point out that the QBM studied in the previous Section is retrieved when we take the limit $N \to +\infty$, in

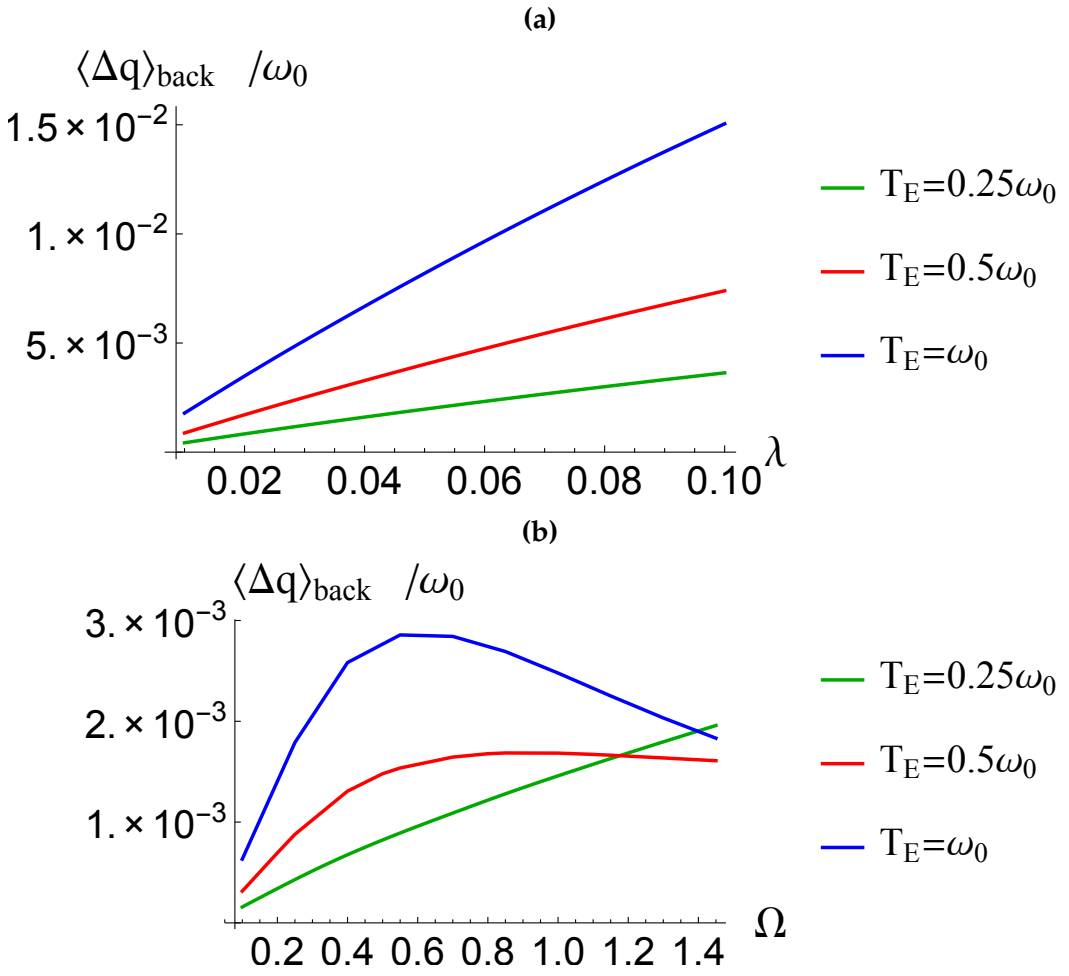

FIGURE 5.8: (Color online) heat backflow measure as a function of the coupling strength λ for different values of the parameters Ω and T_E which characterize the dynamical map.

which case however the numerical approach is not treatable. Since Eq.(5.150) is quadratic in position and momentum it can always be diagonalized by means of an orthogonal transformation $\mathbf{O}$ [143], i.e. $\mathbf{M} = \mathbf{ODO}^T$ with $\mathbf{D}$ a diagonal matrix made of the eigenvalues $\{\sqrt{2d_i}\}_{i=1,\cdot,N+1}$ (often referred to as *eigenfrequencies*) of $\mathbf{M}$. By moving to the new coordinates $\tilde{\mathbf{X}} = \mathbf{O}^T\mathbf{X}$ and $\tilde{\mathbf{P}} = \mathbf{O}^T\mathbf{P}$, referred to as normal modes, we can express Eq.(5.150) as

$$\mathcal{H} = \sum_{i=1}^{N+1} \frac{1}{2}\left(\tilde{P}_i^2 + d_i^2\tilde{X}_i^2\right), \tag{5.151}$$

which leads to a free evolution

$$\tilde{X}_i(t) = \tilde{X}(0)\cos(d_i t) + \frac{\tilde{P}_i(0)}{d_i}\sin(d_i t), \tag{5.152}$$

$$\tilde{P}_i(t) = -d_i\tilde{X}(0)\sin(d_i t) + \tilde{P}_i(0)\cos(d_i t). \tag{5.153}$$

Finally, coming back to the original picture and defining the diagonal matrices $\mathbf{Cos}, \mathbf{Sin}$ and $\tilde{\mathbf{D}}$ with elements $\mathbf{Cos}_{i,i} = \cos(d_i t)$, $\mathbf{Sin}_{i,i} = \sin(d_i t)$ and $\tilde{\mathbf{D}}_{i,i} = d_i$ respectively, we

get the exact evolution of the position and momentum operators

$$X_i(t) = \sum_{j=1}^{N+1} \left[\mathbf{M}_{ij}^{XX}(t)X_j(0) + \mathbf{M}_{ij}^{XP}(t)P_j(0)\right],$$
$$P_i(t) = \sum_{j=1}^{N+1} \left[\mathbf{M}_{ij}^{PX}(t)X_j(0) + \mathbf{M}_{ij}^{PP}(t)P_j(0)\right], \tag{5.154}$$

where $\mathbf{M}^{XX}(t) = \mathbf{M}^{PP}(t) \equiv \mathbf{O}\,\mathbf{Cos}\,\mathbf{O}^T$, $\mathbf{M}^{XP}(t) \equiv \mathbf{O}\,\mathbf{Sin}\,\tilde{\mathbf{D}}^{-1}\,\mathbf{O}^T$ and finally $\mathbf{M}^{PX}(t) \equiv \mathbf{O}\,\mathbf{Sin}\,\tilde{\mathbf{D}}\,\mathbf{O}^T$. Building on (5.154), we can straightforwardly obtain the time-evolution of the mean values of the energy of the environment $\langle\mathcal{H}_E\rangle_t = \frac{1}{2}\sum_{i=1}^{N}\left(\langle X_i^2\rangle_t + \langle P_i^2\rangle_t\right)$ and of the system $\langle\mathcal{H}_S\rangle_t = \frac{1}{2}\left(\langle X_{N+1}^2\rangle_t + \langle P_{N+1}^2\rangle_t\right)$, as well as their time derivatives $\theta(t)$ and $\phi(t)$.

We stress that Eq. (5.154) requires no assumption but the finite number of harmonic oscillators. This gives rise to a different evolution at very long times (longer the higher is N), when the dynamics in the case of the finite environment leads to Poincaré revivals. However, since no weak coupling or secular approximations are involved in this exact numerical approach, it is possible to extend our study of heat backflow for this model also to the strong coupling regime $\lambda > 0.1$, while confronting the numerical evidences with the analytical predictions in the weak coupling regime. Building on Eq. (5.154), we can straightforwardly obtain the heat flow per unit of time $\theta(t)$, which we plot in Fig. 5.9(a) having chosen $N = 150$ modes in the environment for the simulation. We have chosen this value for N because we have observed that all the results do not change with higher numbers of bath modes. Also, the Poincaré recurrence time is well beyond the considered propagation time.

Fig. 5.9(a) clearly shows that in the weak coupling regime the numerical solution (solid line) retraces perfectly the predictions of the analytical approach based on the full-counting statistics (dashed line), while for strong coupling the difference between the two becomes marked, see Fig. 5.9(b). Having $\theta(t)$ as a result of the numerical simulation and by means of Eq. (5.69), it is then immediate to obtain the heat backflow measure, which we show as a function of λ and of Ω in Figs. 5.9(c) and (d) respectively. Note that the range of the coupling strength in Fig. 5.9(c), being $\lambda \in [0.01,\, 1.8]$, encompasses also the strong coupling regime; looking at the lower bottom-left corner, i.e. for $\lambda \in [0.01,\, 0.1]$, we can see that we recover the results obtained using the analytic approach shown in Fig. 5.8.

It is evident from Fig. 5.9(c) the existence of a threshold value of the coupling strength $\lambda^*\left(\Omega, T_E\right)$ above which the heat backflow measure vanishes. It can be shown that this behavior is maintained for any value of the cut-off frequency and temperature, proving therefore a general feature of the dynamics of this model. In order to understand this result, we make use of Eq. (5.154) to calculate all the separate contributions to the total mean energy, i.e the time-evolution of the change in the mean values of the energy of the

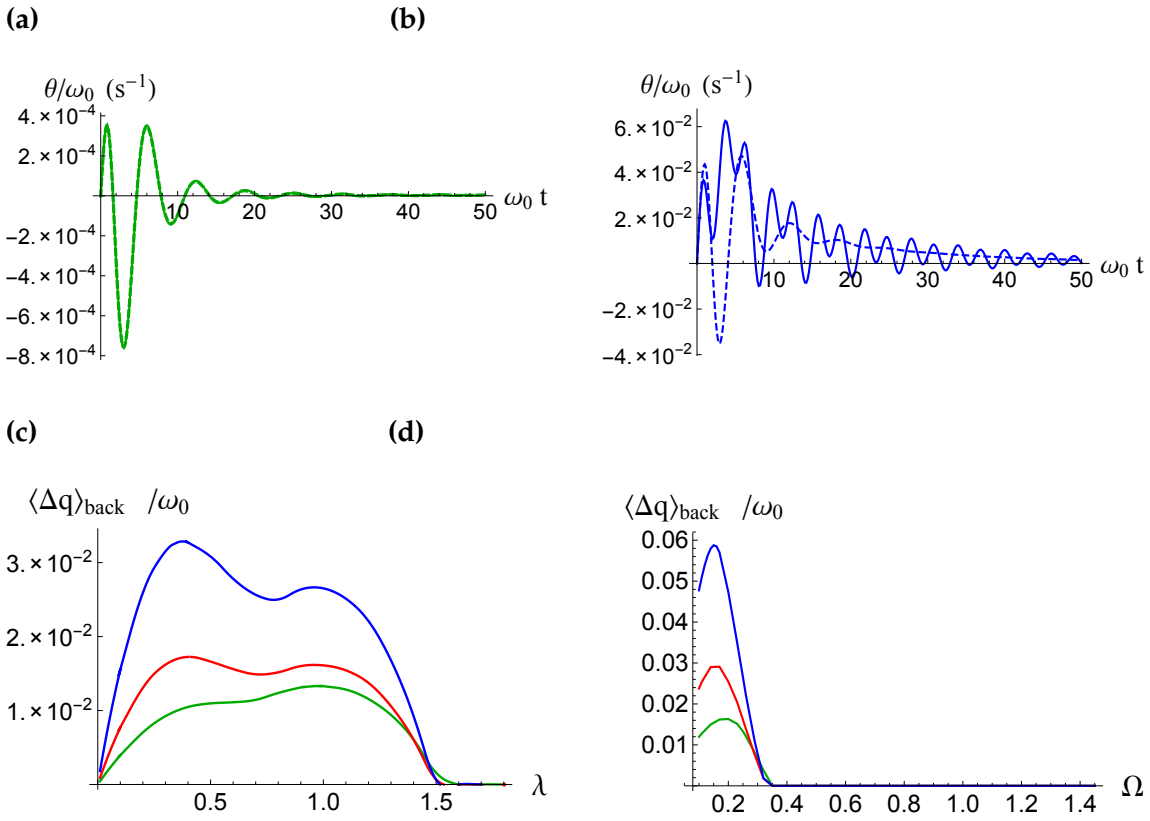

FIGURE 5.9: (Color online) Time behavior of the heat flow per unit of time $\theta(t)$ in units of ω_0 for $\Omega = 0.25\omega_0$, $T_E = T_S = \omega_0$ and coupling strength $\lambda = 0.01$ **(a)** and $\lambda = 1$ **(b)**. The solid lines refer to the solution obtained with the numerical method, while the dashed lines are the curves predicted by the analytical approach relying on the FCS methods. Plot of the heat backflow measure in units of ω_0 as a function of the coupling strength λ for $\Omega = 0.25\omega_0$ **(c)** and as a function of the coupling strength Ω for $\lambda = 1$ **(d)**, for three different values of the initial temperatures: $T_E = T_S = 0.25\omega_0$ (green line), $T_E = T_S = 0.5\omega_0$ (red line) and $T_E = T_S = \omega_0$ (blue line). These curves were produced by means of the numerical simulation with $N = 150$ environmental bosonic modes.

environment

$$\langle \Delta q \rangle_t = \frac{1}{2} \sum_{i=1}^{N} \left[\left(\langle X_i^2 \rangle_t + \langle P_i^2 \rangle_t \right) - \left(\langle X_i^2 \rangle_0 + \langle P_i^2 \rangle_0 \right) \right],$$

of the system

$$\langle \Delta E_S \rangle_t = \frac{1}{2} \left[\left(\langle X_{N+1}^2 \rangle_t + \langle P_{N+1}^2 \rangle_t \right) - \left(\langle X_{N+1}^2 \rangle_0 + \langle P_{N+1}^2 \rangle_0 \right) \right], \tag{5.155}$$

and finally of the interaction Hamiltonian $\langle \Delta \mathcal{H}_I \rangle_t$.

Fig. 5.10 shows these three different contributions for $\Omega = 0.25\omega_0$ and $T_E = T_S = \omega_0$ in the cases of weak coupling $\lambda = 0.01$ (top three plots) and of strong coupling $\lambda = 0.8$ (middle three plots) and $\lambda = 1.8$ (bottom three plots), the latter corresponding to a situation for which the heat backflow measure vanishes. The heat backflow contributions correspond to the time regions where the mean internal energy of the environment [red

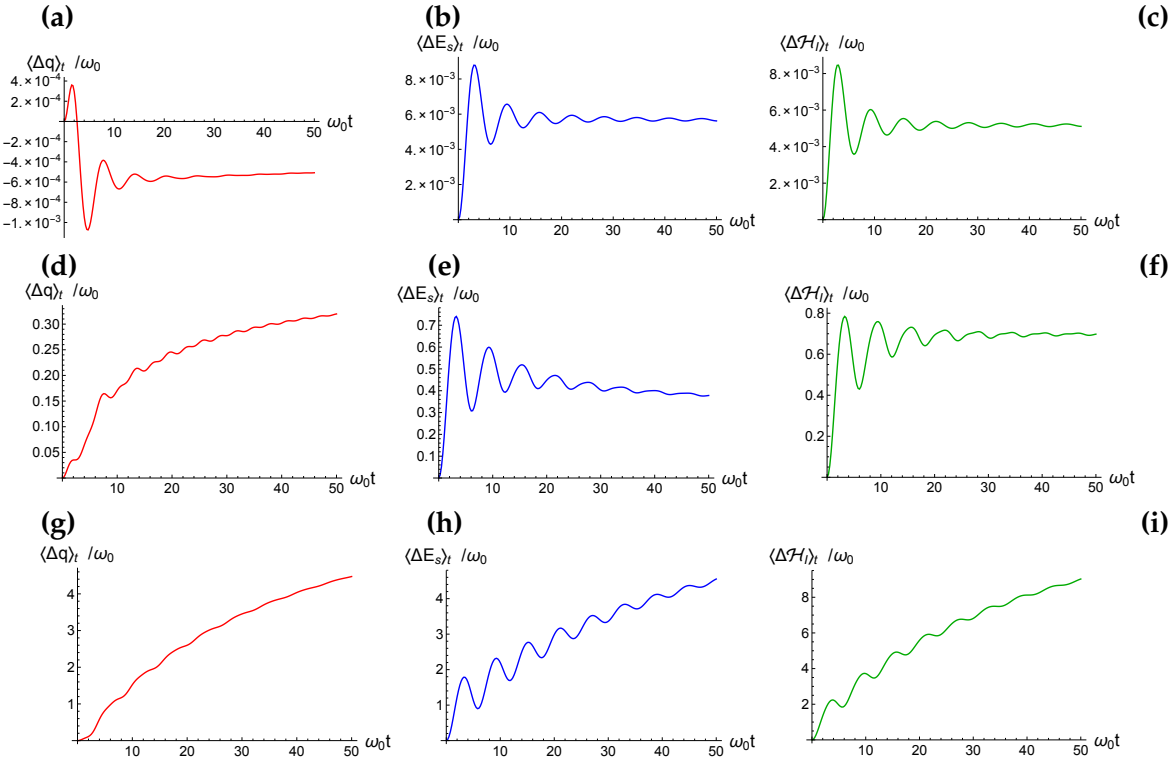

FIGURE 5.10: Separate contributions to the time behavior of the mean total energy in units of ω_0, for $\Omega = 0.25\omega_0$, $T_E = T_S = \omega_0$. The top three panels (a-c) refer to the weak coupling case $\lambda = 0.01$, the middle three (d-f) to $\lambda = 0.8$ and finally the bottom three (g-i) to strong coupling $\lambda = 1.8 > \lambda^*$. (a), (d) and (g) Mean values of the change in the environmental Hamiltonian Eq. (5.65); (b), (e) and (h) Mean values of the change in the system Hamiltonian Eq. (5.149); (c), (f) and (i) Mean values of the change in the interaction Hamiltonian.

curves in panels (a), (d) and (g)] temporarily decreases. The measure introduced in Eq. (5.69) is just the sum of all these contributions.

Fig. 5.10 shows the different time behavior of the average energy of the environment [panels (a), (d) and (g)]. In particular, in the weak coupling regime the latter decreases, see Fig. 5.10(a), this leading to the cooling effect previously put into evidence using FCS methods. An opposite behavior is observed in the strong coupling, where the change in the average energy of the environment increases with time, see Fig. 5.10(d) and (g). For strong coupling the three contributions become of the same order of magnitude, at variance with what happens in the weak coupling case, where the change in the system's internal energy and in the mean value of the interaction Hamiltonian were roughly an order of magnitude bigger than the change in the environmental energy. An analysis of these two cases shows then that in the weak coupling the time-variation of $\langle \Delta E_S \rangle_t$, which is always positive in our setup, is due both to the switching on of the interaction Hamiltonian at $t = 0^+$ (after the energy measurement on the environment in the two-time measurement protocol) but also to the backflow of energy from the environment, which, despite at the same initial temperature, loses to it a part of its energy. In the strong coupling regime this no longer happens, and the increment in the mean system's energy is only due to $\langle \Delta \mathcal{H}_I \rangle_t$, which becomes dominant and ceases energy also to the

environment, thus opposing the occurrence of heat backflow which is in fact very much reduced and eventually, when the threshold coupling strength $\lambda^*(\Omega, T_E)$ is reached and overcome (bottom three panels), stops.

5.3.3.3 Relationship with the non-Markovianity of the reduced dynamics

Here we study the parameter dependence of the non-Markovianity in this QBM setting and compare it with the behaviour of the heat backflow. To this purpose, we consider a recently introduced measure of non-Markovianity [76], based on the time behaviour of the Quantum Interferometric Power (QIP) in the case of Gaussian states evolving through Gaussian channels, see Chapter 3 Subection 3.2.3.5, also referred to as Gaussian Interferometric Power. Employing the quantum Fisher information, the GIP measures the ability to estimate, according to black-box interferometry, a local phase shift in a worst case scenario with a two-mode Gaussian probe [74, 75] characterizing the state of the reduced system plus an ancilla.

While the non-Markovianity measure $\mathcal{N}_{\mathcal{Q}}(\Lambda)$ [76] includes a maximization over all possible initial two-mode Gaussian states:

$$\begin{aligned} \mathcal{N}_{\mathcal{Q}}(\Lambda) &= \max_{\boldsymbol{\sigma}_{SA}} \mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}(\Lambda), \\ \mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}(\Lambda) &\equiv \frac{1}{2}\int_0^{+\infty} dt\ \left(|\mathscr{D}(t)| + \mathscr{D}(t)\right), \end{aligned} \tag{5.156}$$

$\mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}(\Lambda)$ represents a (more easily computable) lower bound for the latter. Analytic expressions for $\mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}(\Lambda)$ for the QBM in the weak coupling and secular approximation are given in [74] for two important classes of initial two-mode Gaussian states: the mixed thermal states (MTS) and the squeezed thermal states (STS), respectively characterized by covariance matrices of the form

$$\boldsymbol{\sigma}_{SA}^{MTS} = k e^{2r_1} \begin{pmatrix} \mathbf{x}_1 & \mathbf{y}_1 \\ \mathbf{y}_1 & \mathbf{x}_1 \end{pmatrix}, \quad \boldsymbol{\sigma}_{SA}^{STS} = k \begin{pmatrix} \mathbf{x}_2 & \mathbf{y}_2 \\ \mathbf{y}_2 & \mathbf{x}_2 \end{pmatrix}, \tag{5.157}$$

where $\mathbf{x}_{1,2} = \mathrm{diag}(x_{1,2}, x_{1,2})$ with $x_{1,2} = \cosh(2r_{1,2})$ and where $\mathbf{y}_1 = \mathrm{diag}(y_1, y_1)$, $\mathbf{y}_2 = \mathrm{diag}(y_2, -y_2)$ with $y_{1,2} = \sinh(2r_{1,2})$. In these expressions $k = \nu + 1/2$, with r_1 being the strength of the Gaussian operations, r_2 the squeezing parameter and ν the average number of thermal photons.

Fig. 5.11 shows $\mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}$ as a function of the coupling strength λ and as a function of the cut-off frequency Ω for fixed values of the remaining parameters T_E, k and $r_{1,2}$.

A comparison between Fig. 5.11 and Figs. 5.8 and 5.10 clearly highlights common features between the amount of non-Markovianity of the dynamical map as measured by (5.156) and the amount of energy backflow as quantified by (5.69) once they are seen as functions of the parameters which determine the dynamical map describing the dynamics (i.e. λ, Ω and T_E), i.e. after the maximization procedure which makes them independent from the choice of initial state of the system. It turns out in fact that $\mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}$

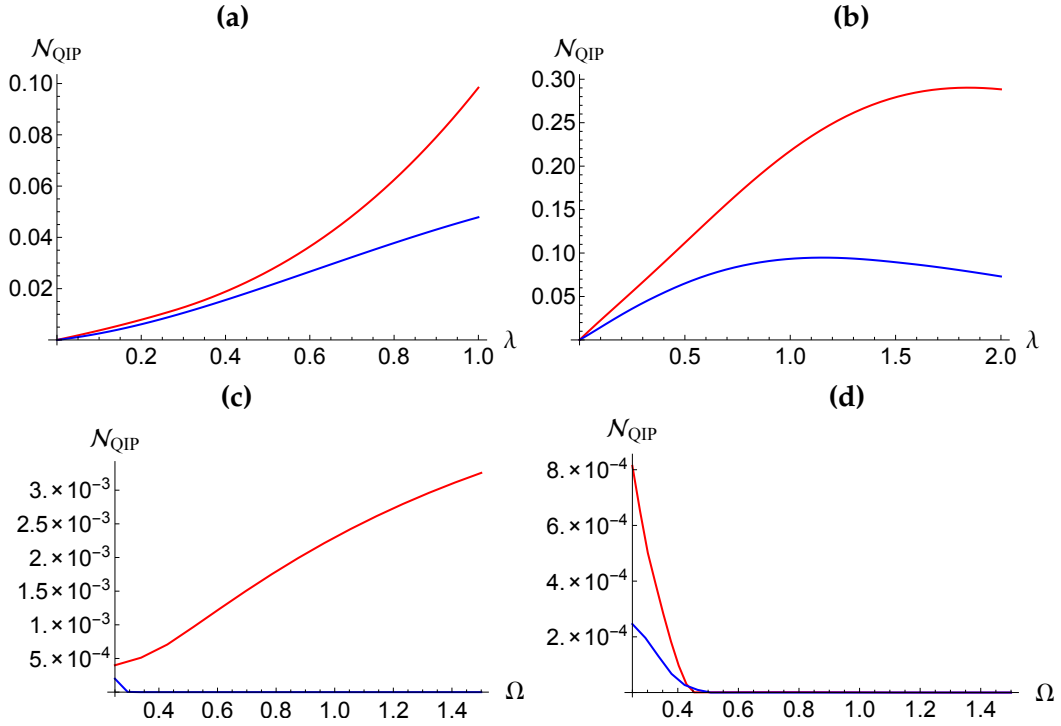

FIGURE 5.11: (Color online) Plots of the non-Markovianity measure $\mathcal{N}_{\mathcal{Q}}^{\boldsymbol{\sigma}}$ for the class of STS (blue lines) and of MTS (red lines), with $k_{1,2} = 1$, $r_1 = r_2 = 0.658$ (otherwise stated), as function of λ [panels (a) and (b)] and of the cut-off frequency [panels (c) and (d)] for fixes values of the remaining parameters. In particular: (a) $\Omega = 0.25\omega_0$ and $T_E = 0.25\omega_0$; (b) $\Omega = 0.25\omega_0$ and $T_E = \omega_0$; (c) $\lambda = 0.01$ and $T_E = 0.25\omega_0$ and $r_1 = 10^{-2}$; (d) $\lambda = 0.01$, $T_E = \omega_0$ and $r_1 = r_2 = 0.22$.

and $\langle \Delta q \rangle_{back}$ present a very similar dependence on the cut-off frequency: in the low-temperature $T_E = 0.25\omega_0$ and weak-coupling $\lambda = 0.01$ regime they both show a monotonic increase with Ω, see Figs. 5.11(c) and green curve of Fig. 5.8(b), while for increasing values of the environmental temperature, both vanish above a certain value of the cut-off around $\Omega \simeq 0.4\omega_0$ [see Figs. 5.11(d) and 5.10(d)]. This behavior can be explained by remembering that, for increasing values of the cut-off Ω, the environmental correlation function (5.74) becomes progressively more sharply correlated in time, this leading to a limiting reduced dynamics which is that of a semigroup, thus Markovian. For very small values of the environmental temperature, memory effects however persist for larger values of the cut-off frequency, as witnessed by (5.156) and shown in Fig. 5.11(c).

Our results moreover show that the property of a reduced dynamical map to be non-Markovian does not in general guarantee the occurrence of energy backflow. This can be seen by looking at the behavior of the energy backflow quantifier and of the non-Markovianity measure in their dependence on the coupling strength: the former in fact vanishes once a certain threshold $\lambda^*(\Omega, T_E)$ is reached, see Fig. 5.10(a), above which the dynamics is still non-Markovian, see Fig. 5.11(a) and (b). Also in their dependence on the cut-off frequency, see Figs. 5.10(b) and 5.11(d), the value of Ω below which the dynamics is still non-Markovian is slightly larger than the same threshold for the occurrence of energy backflow.

These considerations allow to conclude that the occurrence of energy backflow appears as a stricter condition than non-Markovianity, in agreement with [2]. $\langle \Delta q \rangle_{back}$ has turned out, in fact, to be different from zero for values of the parameters λ, Ω, T_E for which the dynamics is non-Markovian, vice versa vanishing whenever the reduced dynamics becomes Markovian.

In conclusion, using the FCS formalism obtained in terms of a two-time measurement protocol, we have studied in this Chapter the mean value of the energy exchange between a system of interest, both of finite and infinite dimensions, and its environment in the framework of the second-order time-convolutionless GME, introducing a suitable condition and quantifier for the occurrence of heat backflow from the environment back to the system. We have then applied this construction firstly to the spin-boson model and secondly to the quantum brownian motion. In both cases, we have chosen an Ohmic spectral density with exponential cutoff to describe the distribution of bosonic bath modes and their interaction with the open quantum system. Direct evaluation of the mean value of heat and of the heat backflow measure have shown that for certain values of the parameters determining the dynamics (i.e. the environmental temperature T_E, the cut-off frequency Ω and the coupling strength λ), the heat can actually flow back from the environment to the system. We have finally considered suitable estimators of non-Markovianity which were suitable for the models considered and discussed their relationship with the heat backflow measure. These comparative analyses have shown that non-Markovianity allows for the observation of heat backflow while Markovianity prevents it: occurrence of heat backflow poses therefore itself as a stricter condition to be fulfilled than non-Markovianity.

6

Landauer's principle in non-Markovian open quantum systems

In the previous Chapter we focused our attention on the study of the dynamics of heat in relation with the first law of thermodynamics. The discussion in this Chapter will still have the heat as one of the main quantities under investigation, though instead from an angle revolving around the second law of thermodynamics in the context of open quantum systems. In particular, we will discuss in detail the proper statement of the so-called Landauer's principle in this context, which states that, in order to irreversibly erase some information from a system (quantified through its entropy) an expenditure of heat (thus dissipated) is required. This deep result, which therefore involves and binds together the fields of quantum thermodynamics and quantum information theory, will be recalled in Section 6.2 in its original statement by Landauer and improved by a purely quantum correction due to the finite size of the environment which performs the erasure [4]. Finally, we will discuss the introduction of a new family of lower bounds to the mean dissipated heat in Landauer's fashion, showing how a direct application to an interesting and not studied physical finite-dimensional quantum systems proves that they can be tighter than both Landauer's result and its finite-size-corrected improvement. Remarkably, the techniques employed to derive these bounds will be based on the same FCS analysis presented in Section 5.2, making therefore possible to apply them, at variance with the usual Landauer's bound, also to the scenario of non-equilibrium quantum systems.

6.1 The second law of quantum thermodynamics in open quantum systems

In the previous Chapter we studied the first law of thermodynamics in the quantum realm, where we focused on the concepts of energy, heat and work. In particular, we introduced the so-called *full counting statistics* formalism, by means of which we reconstructed the mean value of the change in the environmental energy in a non-Markovian regime according to a two-time measurement protocol.

In this Chapter we will deal with the second law of thermodynamics in the framework of open quantum systems. In particular our attention will be drawn by the *Landauer's principle*, a theoretical result of paramount importance only recently adapted to the quantum scenario, which not only can be seen as a more fundamental formulation of the second law, but also bridges the world of thermodynamics with the one of information theory. In this regard, we will show how the application of the very same full-counting statistics and two-time measurement protocol techniques can lead to a new family of lower bounds to the mean dissipated heat in an environmental-assisted erasure of information in Landauer's fashion, which can prove to be tighter than the latter (at least for finite dimensional systems) when applied to a specific model.

Let us consider an open quantum system scenario, where a system S interacts with an environment E so that the total Hamiltonian describing the evolution of the composite system is given by $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{SE}$. The total state at the initial time is assumed to be factorized

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_\beta, \tag{6.1}$$

with $\rho_\beta = e^{-\beta\mathcal{H}_E}/Z_E$ and $Z_E = \mathrm{Tr}_E\left[e^{-\beta\mathcal{H}_E}\right]$. First of all, the second law of thermodynamics is very well-known to be intimately related with the concept of *irreversibility*, which inevitably brings along the notions of fluctuation theorems and micro-reversibility. Since Boltzmann's work, several attempts have been made to find a microscopic derivation of the second law, the main difficulty in this task being that the most natural candidate, the von Neumann entropy $S(\rho_{SE}) = -\mathrm{Tr}_{SE}\left[\rho_{SE}\ln\rho_{SE}\right]$ represents a constant of motion (in absence of an external driving field). However, it is precisely this time invariance which naturally induces a splitting of the change in the system's entropy $S(\rho_S)(t) = -\mathrm{Tr}_S\left[\rho_S(t)\ln\rho_S(t)\right]$, which instead is a function of time, in two contributions: an entropy flow and an entropy production. Consider in fact that

$$-\mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\rho_{SE}(t)\right] = -\mathrm{Tr}_{SE}\left[\rho_{SE}(0)\ln\rho_{SE}(0)\right] = -\mathrm{Tr}_S\left[\rho_S(0)\ln\rho_S(0)\right] - \mathrm{Tr}_E\left[\rho_\beta\ln\rho_\beta\right], \tag{6.2}$$

where we used the additivity of the von Neumann entropy for product states. In light of this relation, since we are interested in the manifestation of irreversibility in the reduced system, we have that [122]

$$\begin{aligned}\Delta S(t) &\equiv S(\rho_S)(0) - S(\rho_S(t)) = \mathrm{Tr}_S\left[\rho_S(t)\ln\rho_S(t)\right] - \mathrm{Tr}_S\left[\rho_S(0)\ln\rho_S(0)\right] \\ &= \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\rho_S(t)\right] - \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\rho_{SE}(t)\right] + \mathrm{Tr}_E\left[\rho_\beta\ln\rho_\beta\right] \\ &= \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\left(\rho_S(t)\otimes\rho_\beta\right)\right] - \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\rho_{SE}(t)\right] - \mathrm{Tr}_E\left[\left(\rho_E(t)-\rho_\beta\right)\ln\rho_\beta\right].\end{aligned} \tag{6.3}$$

By inserting the explicit expression of the initial environmental state (which is in Gibbs form), it is easy to see that the last term is equal to

$$\mathrm{Tr}_E\left[\left(\rho_E(t)-\rho_\beta\right)\ln\rho_\beta\right] = -\beta Q_E(t) \equiv -\Delta S_r(t) \tag{6.4}$$

with $Q_E(t)$, defined in Equation (5.7), being the change in the environmental energy, i.e. the heat. The latter quantity is thus associated to the *reversible* change in the system's entropy. The first two terms in Equation (6.3) are nothing but a quantum relative entropy

between the total state at time t and the product state which was prepared at initial time $t = 0$

$$S(\rho_{SE}(t)||\,(\rho_S(t)\otimes\rho_\beta)) = \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\rho_{SE}(t)\right] - \mathrm{Tr}_{SE}\left[\rho_{SE}(t)\ln\left(\rho_S(t)\otimes\rho_\beta\right)\right] \equiv -\Delta S_i(t). \tag{6.5}$$

Due to Klein's inequality [21, 144], this contribution, commonly referred to as *entropy production*, is always non-negative, i.e. $\Delta S_i(t) \geq 0$, with the equality being saturated if and only if no correlations between system and environment build up during the evolution. To summarize, one has therefore the relation

$$\Delta S(t) = \Delta S_i(t) + \Delta S_r(t), \tag{6.6}$$

which highlights the splitting of the entropy change in a reversible and an irreversible contribution [122]. Equation (6.6) can also be cast in an equivalent form [4], which has the merit to be more clearly connected to the so-called Landauer's principle, which we will discuss in a short while. In order to do that, given the marginals ρ_S, ρ_E of a generic state ρ_{SE}, we recall the definition of *mutual information*

$$I(\rho_S : \rho_E) \equiv S(\rho_S) + S(\rho_E) - S(\rho_{SE}), \tag{6.7}$$

which is a broadly employed concept in quantum information theory to characterize, for example, the amount of correlations between a system and an environment (or an ancilla) or, when maximized over all possible separable states, to calculate Holevo's channel capacity [145]. This quantity naturally comes into stage when we consider the change in the environmental entropy $\Delta S_E(t) \equiv S(\rho_E(t)) - S(\rho_\beta)$ alongside with the system's one. In fact

$$\begin{aligned} -\Delta S(t) + \Delta S_E(t) &= S(\rho_S(t)) - S(\rho_S(0)) + S(\rho_E(t)) - S(\rho_\beta) \\ &= S(\rho_S(t)) + S(\rho_E(t)) - S(\rho_S(0)\otimes\rho_\beta) \\ &= S(\rho_S(t)) + S(\rho_E(t)) - S(\rho_{SE}(t)) = I(\rho_S(t) : \rho_E(t)), \end{aligned} \tag{6.8}$$

where we have used the additivity property in the case of product states and the invariance of the total entropy. The property of the mutual information to be a non-negative quantity, i.e. $I(\rho_S(t) : \rho_E(t)) \geq 0$, can be seen as another statement of the second law of quantum thermodynamics. We will go back to this expression of the second law in the following Subsection, showing how it relates with the Landauer's principle.

Before moving to that however, it is worth to finally discuss the relationship between the entropy contributions in Equation (6.6) and the first law of quantum thermodynamics (5.4). To this aim, recall the discussion made in Section 5.1 about the first law in the framework of open quantum systems and consider in particular the quantities defined in Eqs. (5.7), (5.10) and (5.13). In light of Equation (6.6), if we introduce the non-equilibrium free energy of the 'system + interaction'

$$\Delta F_S(t) \equiv \Delta U_S(t) - \beta^{-1}\Delta S(t), \tag{6.9}$$

we have that the entropy production (6.5) corresponds to

$$\Delta S_i(t) = \beta \left(W(t) - \Delta F(t) \right), \tag{6.10}$$

which is known in the literature also as the *dissipated work* associated with an entropy increase in the system during an irreversible process [146].

6.2 The Landauer principle and the environmental-assisted erasure protocol

Thermodynamics has been unavoidably related to information theory since Maxwell seemed to show that the bare knowledge about a system allows to extract work from the system, thus apparently violating the second law. This paradox, known as Maxwell's demon, is the result of a thought experiment where a box full of a gas and partitioned in the middle is monitored by a demon who can get information about the microscopic details of all the particles. The demon controls a small gate in the partition and selectively opens the gate to let fast particles pass to the left box and slow particles to the right box. Since the velocity of the particles is related to their temperature, this process creates a temperature gradient between the two chambers of the box, at no expenditure of work, in violation of the second law. Moreover, this temperature gradient can in turn be exploited to extract work.

The resolution to this apparent paradox came from Landauer [23] and Bennett [147–149], who realized that the amount of work needed to prepare the demon's memory to store the information about the particles at the beginning of the procedure or, equivalently, to erase the demon's memory about the information he acquired about the particles at the end of the procedure precisely matches and compensate the extracted work, thus restoring the second law of thermodynamics. In other words, Landauer recognized that any information erasure from the information-bearing memory causes entropy to flow (and thus heat) to the non information-bearing system. If the latter acts at inverse temperature β, then a dissipated heat

$$\beta Q_E \geq \Delta S \tag{6.11}$$

is dissipated in the process, with ΔS denoting the entropy decrease in the memory. The inequality (6.11) is known as *Landauer's bound* and represents a lower bound to the mean dissipated heat in an erasure protocol scenario. It is only very recently that a solid mathematical background was given for this protocol to be valid in the quantum scenario, where a quantum counterpart of the Landauer's bound can be studied. In [4] the authors provided the minimal setup in which they proved and improved Landauer's lower bound to the mean dissipated heat, which are

- both the information - bearing degree of freedom, i.e. the memory or system S and the non - information - bearing one, i.e. the environment or reservoir E, are described in terms of Hilbert spaces $\mathscr{H}_S$ and $\mathscr{H}_E$;

- the environment is initially described in terms of a thermal state $\rho_\beta = e^{-\beta\mathcal{H}_E}/Z_E$, with $\mathcal{H}_E$ being a self-adjoint Hamiltonian operator on $\mathscr{H}_E$, $\beta \in [-\infty, +\infty]$ its inverse temperature and $Z_E = \mathrm{Tr}_E\left[e^{-\beta\mathcal{H}_E}\right]$;
- the total initial state is uncorrelated $\rho_{SE}(0) = \rho_S(0) \otimes \rho_\beta$;
- the evolution of the overall system $S + E$ is given in terms of an unitary operator, i.e. $\rho_{SE}(t) = U(t,0)\rho_{SE}(0)\, U^\dagger(t,0)$.

This set of assumptions is minimal in the sense that, whenever anyone of them is dropped, Landauer's bound can be violated, as reported in the literature [4]. More specifically, the first and last assumptions imply that all the parts involved in the erasure process are described quantum mechanically and that no other third part plays any role. The violation of the assumption of no initial correlations between system and environment is proven to lead in some cases to violations of the Landauer's bound. Moreover, this assumption is in line with the point of view of many thermodynamical protocols, such as error correction or quantum computing, where the memory register is taken to be independent of the reservoir. Finally, the assumption of dealing with an initial reservoir in Gibbs form is essential for two reasons: the first and more practical one is to have a well-defined inverse temperature β entering the Landauer's principle; the second one is that thermal states are in fact the only completely passive states (i.e. states from which one cannot extract work by means of unitary operations [150]) and its drop can lead to violations of Landauer's bound [4].

Within this framework, we can now prove the following Theorem by Reeb and Wolf by using the quantities introduced in Eqs. (6.6) and (6.7)

$$\begin{aligned} I(\rho_S(t) : \rho_E(t)) + \Delta S(t) &= \Delta S_E(t) \\ &= -\mathrm{Tr}_E\left[\rho_E(t)\ln\rho_E(t)\right] + \mathrm{Tr}_E\left[\rho_\beta \ln \rho_\beta\right] \\ &= -\mathrm{Tr}_E\left[\rho_E(t)\ln\rho_E(t)\right] + \mathrm{Tr}_E\left[\rho_\beta \ln \rho_\beta\right] - \beta\mathrm{Tr}_E\left[\mathcal{H}_E\rho_E(t)\right] \\ &= -D(\rho_E(t)||\rho_\beta) + \beta Q_E(t), \end{aligned} \tag{6.12}$$

with $Q_E(t)$ defined as in Equation (5.7). This result is the equality form of Landauer's principle, from which the lower bound to the mean dissipate heat $Q_E(t)$ is derived by simply using the argument that both the relative entropy $D(\rho_E(t)||\rho_\beta)$ and the mutual information $I(\rho_S(t) : \rho_E(t))$ are non-negative quantities of their argument

$$\beta Q_E(t) = \Delta S(t) + I(\rho_S(t) : \rho_E(t)) + D(\rho_E(t)||\rho_\beta) \geq \Delta S(t). \tag{6.13}$$

We stress that the equality in Equation (6.13) can be proven to be equivalent to Equation (6.6) [4], thus explicitly showing the deep link between the second law of thermodynamics and Landauer's principle.

The above relation allows to evaluate how much the Landauer's bound deviates from the value $\beta Q_E(t) = \Delta S(t)$. From Equation (6.13) it follows immediately that the heat flow equals the change in system's entropy if and only if $I(\rho_S(t) : \rho_E(t)) = D(\rho_E(t)||\rho_\beta) = 0$, being both these quantities non - negative. These requirements are however equivalent

to impose that $\rho_{SE}(t) = \rho_S(t) \otimes \rho_E(0)$, i.e. $Q_E(t) = \Delta S(t) = 0$ at any time. In light of such considerations, only trivial evolutions lead to the saturations of the Landauer's bound in the case of a finite dimensional system, thus suggesting that tighter versions of $\beta Q_E(t) \geq \Delta S(t)$ can be found. The interested reader is referred to [4] for details and proofs of this tighter lower bound to the mean dissipated heat. It is worth of stress that, while for $\Delta S(t) \geq 0$ the above bound is tight, for processes which increase the system's entropy the bound is not tight. In the next Subsection, following a rather radically different approach with respect to Landauer's and Reeb-Wolf's, we will derive a new family of lower bounds to the mean dissipated heat which will be valid also in the context of non-equilibrium systems and moreover which will be tight irrespectively of the sign of $\Delta S(t)$.

6.3 Full - counting statistics approach to a lower bound to the mean dissipated heat

We will present here the derivation of a new one-parameter family of lower bounds to the mean dissipated heat which, within the framework of the erasure protocol illustrated above, are also valid in a non-equilibrium scenario and improve both Landauer's and Reeb - Wolf's results.

To achieve this goal, the first observation is that the dissipated heat $Q_E(t)$ entering the Landauer's bound (6.13) can be studied relying on the two-time measurement protocol of the environmental energy discussed in Chapter 5 Section 5.2, i.e. $Q_E(t) = \mathrm{Tr}_E\left[\mathcal{H}_E\left(\rho_E(t) - \rho_\beta\right)\right]$, where we have already assumed $\rho_\beta = e^{-\beta\mathcal{H}_E}/Z_E$ as the initial environmental state according to Reeb-Wolf setup.

The starting point is the cumulant generating function (5.23) for the heat $Q_E(t)$, which is given by

$$\tilde{\Theta}(\eta, \beta, t) \equiv \ln\langle e^{-\eta Q_E}\rangle_t = \ln \int dQ_E\, p_t(Q_E) e^{-\eta Q_E}, \tag{6.14}$$

where, for future convenience, we have decided to made explicit reference to the inverse temperature β of the bath, which enters through the initial environmental state ρ_β. The key observation is to notice that the $\tilde{\Theta}(\eta, \beta, t)$ is a convex function with respect to the counting parameter η [126]. This can be proven exploiting Hölder's inequality which, given a measure space (Ω, Σ, μ), states that, for all measurable function f, g on Ω,

$$\| fg \|_1 \leq \| f \|_p \| g \|_q, \qquad 0 \leq q, p, \leq 1, \ \frac{1}{p} + \frac{1}{q} = 1, \tag{6.15}$$

where

$$\| f \|_r \equiv \left(\int_\Omega d\mu\, |f|^r \right)^{\frac{1}{r}} \forall r \in [1, +\infty). \tag{6.16}$$

If the measure μ is, as in our case, a probability measure, then (6.15) is equivalent to

$$\langle |fg| \rangle \leq \left(\langle |f|^p \rangle\right)^{\frac{1}{p}} \left(\langle |g|^q \rangle\right)^{\frac{1}{q}}. \tag{6.17}$$

By exploiting the property of the logarithm to be convexity preserving, we immediately have that

$$\begin{aligned}\tilde{\Theta}([\alpha\eta_1 + (1-\alpha)\eta_2], \beta, t) &= \ln\langle e^{-[\alpha\eta_1+(1-\alpha)\eta_2]Q}\rangle_t \\ &\leq \alpha \ln\langle e^{-\eta_1 Q}\rangle_t + (1-\alpha)\ln\langle e^{-\eta_2 Q}\rangle_t = \alpha\tilde{\Theta}(\eta_1,\beta,t) + (1-\alpha)\tilde{\Theta}(\eta_2,\beta,t), \quad (6.18)\end{aligned}$$

where we used Equation (6.17) with the substitution $\alpha \leftrightarrow 1/p$, $(1-\alpha) \leftrightarrow 1/q$. Equation (6.18) expresses the convexity of the cumulant generating function. If we combine this property, equivalently expressed as [151]

$$\tilde{\Theta}(\eta,\beta,t) \geq \eta \frac{\partial}{\partial\eta}\tilde{\Theta}(\eta,\beta,t)|_{\eta=0}, \quad (6.19)$$

with the fact that, in light of Equation (5.24),

$$Q_E(t) = -\frac{\partial}{\partial\eta}\tilde{\Theta}(\eta,\beta,t)|_{\eta=0}, \quad (6.20)$$

we immediately obtain a one-parameter family of lower bounds for the mean dissipated heat $Q_E(t)$ which, for positive values of η, reads

$$\beta Q_E(t) \geq -\frac{\beta}{\eta}\tilde{\Theta}(\eta,\beta,t) \equiv \mathcal{B}^{\eta}_{\mathcal{Q}}(t), \quad \eta > 0, \quad (6.21)$$

We stress that the derivation of this result relies only on the assumptions taken into account in the erasure protocol setup.

This family of lower bounds can be understood as follows. The left hand side of Equation (6.21) is, apart from the factor β, the derivative of the cumulant generating function, evaluated for $\eta = 0$ and changed of sign. The right hand side instead, for small enough η, can be seen as the incremental quotient, taken for positive increments, of the cumulant generating function around the origin $\eta = 0$.

On the one hand, for $\eta \to 0$ one therefore recovers the actual derivative and the bound is saturated. This fact implies that this bound is always *asymptotically tight* to the mean dissipated heat $Q_E(t)$ irrespectively of its sign, in the sense that for any possible dissipated heat there exist a process and a suitable value of the parameter η such that the difference $\beta Q_E(t) - \mathcal{B}^{\eta}_{\mathcal{Q}}(t) < \delta$ ($\delta > 0$) at any time.

On the other hand, for $\eta = \beta$ one remarkably obtains the Landauer's bound derived in [152]. If we substitute in fact the counting parameter η with β in the generating function Equation (6.14), we obtain that

$$e^{\tilde{\Theta}(\beta,\beta,t)} = \langle e^{-\beta Q_E(t)}\rangle_t = \mathrm{Tr}_E\left[U(t,0)\left(\rho_S(0)\otimes \mathbb{1}_E\right)U^{\dagger}(t,0)\right], \quad (6.22)$$

which corresponds to the result Equation (6) of [152]. Note however that $\tilde{\Theta}(\beta,\beta,t)$ no longer represents a proper cumulant generating function of the moments of the heat distribution, i.e. the average dissipated heat $\langle Q\rangle_t$, for example, could not have been

obtained as

$$Q_E(t) \neq -\frac{\partial}{\partial\beta}\langle e^{\beta Q}\rangle|_{\beta=0}, \tag{6.23}$$

because of the additional dependence on β of the initial state of the environment. Nevertheless, the application of Jensen's inequality as in [152] allows to access $Q_E(t)$, this leading to the lower bound found in that reference

$$\mathcal{B}^{\beta}_{\mathcal{Q}} \equiv -\tilde{\Theta}(\beta,\beta,t) = \ln \mathrm{Tr}_E\left[U(t,0)\left(\rho_S(0)\otimes \mathbb{1}_E\right)U^{\dagger}(t,0)\right]. \tag{6.24}$$

6.3.1 Relationship with non-unitality of the environmental channel

It is interesting to consider the relationship that the new family of lower bound $\mathcal{B}^{\eta}_{\mathcal{Q}}(t)$ for $\eta=\beta$ has with the degree of non-unitality of the channel, which governs the evolution of the environmental state. The latter condition is in fact expressed by the request that

$$\sum_k A_k(t)A_k^{\dagger}(t) = \mathbb{1}_E, \tag{6.25}$$

where the various $A_k(t) \equiv A_{ij}(t) = \sqrt{\lambda_j}\,\langle i|\,U(t,0)\,|j\rangle$ denote the Kraus operators for the environment obtained from the usual evolution operator $U(t,0)$, $\{|j\rangle\,,\lambda_j\}$ being the eigenstates and eigenvalues of the initial density matrix of the system, i.e. $\rho_S(0) = \sum_j \lambda_j\,|j\rangle\,\langle j|$. To show this connection, we have to consider the expression of the cumulant generating function

$$\tilde{\Theta}(\eta,\beta,t) = \ln \mathrm{Tr}_{SE}\left[e^{-(\eta/2)\mathcal{H}_E}U(t,0)e^{(\eta/2)\mathcal{H}_E}\rho_{SE}(0)e^{(\eta/2)\mathcal{H}_E}U^{\dagger}(t,0)e^{-(\eta/2)\mathcal{H}_E}\right]. \tag{6.26}$$

Exploiting the ciclicity of the trace and the condition $\left[e^{(\eta/2)\mathcal{H}_E},\rho_\beta\right]=0$, we have that

$$\begin{aligned}
\tilde{\Theta}(\eta,\beta,t) &= \ln \mathrm{Tr}_{SE}\left[e^{-\eta\mathcal{H}_E}U(t,0)\left(\rho_S(0)\otimes\frac{e^{-(\beta-\eta)\mathcal{H}_E}}{Z}\right)U^{\dagger}(t,0)\right]\\
&= \ln \mathrm{Tr}_{SE}\left[\frac{e^{-\beta\mathcal{H}_E}}{Z}e^{(\beta-\eta)\mathcal{H}_E}U(t,0)\left(\rho_S(0)\otimes e^{-(\beta-\eta)\mathcal{H}_E}\right)U^{\dagger}(t,0)\right]\\
&= \ln \mathrm{Tr}_{SE}\left[\left(\mathbb{1}_S\otimes\rho_\beta\right)\,e^{\frac{(\beta-\eta)}{2}\mathcal{H}_E}U(t,0)e^{\frac{-(\beta-\eta)}{2}\mathcal{H}_E}\,\left(\rho_S(0)\otimes\mathbb{1}_E\right)\,e^{\frac{-(\beta-\eta)}{2}\mathcal{H}_E}U^{\dagger}(t,0)e^{\frac{(\beta-\eta)}{2}\mathcal{H}_E}\right]\\
&= \ln \mathrm{Tr}_{SE}\left[\left(\mathbb{1}_S\otimes\rho_\beta\right)\,U_{\beta-\eta}(t,0)\,\left(\rho_S(0)\otimes\mathbb{1}_E\right)\,\left(U_{\beta-\eta}(t,0)\right)^{\dagger}\right],
\end{aligned} \tag{6.27}$$

where

$$U_{\beta-\eta}(t,0) \equiv e^{\frac{(\beta-\eta)}{2}\mathcal{H}_E}U(t,0)e^{\frac{-(\beta-\eta)}{2}\mathcal{H}_E}. \tag{6.28}$$

As a result of (6.27), we get

$$\tilde{\Theta}(\eta,\beta,t) = \ln \mathrm{Tr}_E\left[\rho_\beta \mathbf{A}^{\eta}(t)\right], \tag{6.29}$$

with

$$\mathbf{A}^{\eta}(t) \equiv \mathrm{Tr}_S\left[U_{\beta-\eta}(t,0)\,\left(\rho_S(0)\otimes\mathbb{1}_E\right)\,\left(U_{\beta-\eta}(t,0)\right)^{\dagger}\right], \tag{6.30}$$

where $U_{\beta-\eta}(t,0) = e^{-(\eta-\beta)\mathcal{H}_E/2}U(t,0)e^{(\eta-\beta)\mathcal{H}_E/2}$ represents the evolution conditional to the two-time measurement of the environmental energy. Equation (6.29) puts into evidence the peculiar role of the $\eta = \beta$ choice: for this value of the counting field parameter in fact we find that the operator defined in Equation (6.30) reduces to

$$\mathbf{A}^{\beta}(t) = \mathrm{Tr}_E \left[U(t,0) \left(\rho_S(0) \otimes \mathbb{1}_E \right) U^{\dagger}(t,0) \right] \tag{6.31}$$

$$\equiv \sum_k A_k(t) A_k^{\dagger}(t). \tag{6.32}$$

In light of Eqs. (6.21) and (6.25), it is immediate to see that if the environmental map is unital the new family of lower bounds vanishes. In the erasure protocol framework here considered however, the dynamical map $\Lambda_E : \rho_\beta \mapsto \rho_E(t)$ is by construction non-unital, since the dissipative dynamics inevitably perturbs the initial Gibbs state of the environment in order to erase information stored in S [152].

To relate these concepts more quantitatively, we introduce the following figure of merit which gives an estimate of the degree of non-unitality of the map Λ_E

$$\mathcal{N}_E(t) = \| \mathbf{A}^{\beta}(t) - \mathbb{1}_E \|, \tag{6.33}$$

where $\| \cdot \|$ denotes the Frobenius norm.

6.3.2 Relationship between the new family of lower bounds and the $\alpha-$Rényi divergence

Coming back to the generic η case, it is also worth noticing that, in the case the open system starts in the maximally mixed state $\rho_S(0) = \mathbb{1}_S$, the newly found family of lower bounds $\mathcal{B}_{\mathcal{Q}}^{\eta}(t)$ can be written in terms of a quantum Rényi divergence. The latter quantity is defined as follows

$$S_\alpha(\rho||\sigma) \equiv \frac{1}{\alpha - 1} \ln \mathrm{Tr} \left[\rho^\alpha \sigma^{1-\alpha} \right], \qquad \alpha \in (0,1) \cup (1, +\infty). \tag{6.34}$$

The assumption $\rho_S(0) = \mathbb{1}_S/N_S$ is actually considered from the very beginning in many discussions of the Landauer's principle [153, 154] as well as in the original derivation by Landauer himself [23], with the target state of the process being instead a pure state. According to the above notation, in such process $\Delta S(t) \equiv S(\rho_S(0)) - S(\rho_S(t))$ is therefore positive and so is the mean dissipated heat. It is important in fact to keep in mind that,contrary to intuition, the information here refers to the entropy of a system and thus to its uncertainty. It is for this reason that Landauer therefore referred to the erasure process as a process which leads to an *increase of certainty* in the system's state [23, 120]. To see the above mentioned relation, we first re-write the cumulant generating function

$\tilde{\Theta}(\eta,\beta,t)$ as follows

$$\begin{aligned}\tilde{\Theta}(\eta,\beta,t) &= \ln \mathrm{Tr}_{SE}\left[e^{-(\eta/2)\mathcal{H}_E}U(t,0)e^{(\eta/2)\mathcal{H}_E}\left(\rho_S(0)\otimes\rho_\beta\right)e^{(\eta/2)\mathcal{H}_E}U^\dagger(t,0)e^{-(\eta/2)\mathcal{H}_E}\right]\\ &= \ln \mathrm{Tr}_{SE}\left[e^{-\eta\mathcal{H}_E}U(t,0)\left(\rho_S(0)\otimes\frac{e^{-(\beta-\eta)\mathcal{H}_E}}{Z}\right)U^\dagger(t,0)\right]\\ &= \ln \mathrm{Tr}_{SE}\left[\left(\mathbb{1}_S\otimes(\frac{e^{-\beta\mathcal{H}_E}}{Z})^{\frac{\eta}{\beta}}\right)U(t,0)\left(\rho_S(0)\otimes(\frac{e^{-\beta\mathcal{H}_E}}{Z})^{1-\frac{\eta}{\beta}}\right)U^\dagger(t,0)\right].\end{aligned} \tag{6.35}$$

If we then assume that $\rho_S(0)=\mathbb{1}_S/N_S$, we have that

$$\begin{aligned}&U(t,0)\left(\rho_S(0)\otimes(\rho_\beta)^{1-\frac{\eta}{\beta}}\right)U^\dagger(t,0) = N_S^{-\frac{\eta}{\beta}}U(t,0)\left(\rho_S(0)\otimes\rho_\beta\right)^{1-\frac{\eta}{\beta}}U^\dagger(t,0)\\ &N_S^{-\frac{\eta}{\beta}}\left(U(t,0)\,\rho_S(0)\otimes\rho_\beta U^\dagger(t,0)\right)^{1-\frac{\eta}{\beta}} = N_S^{-\frac{\eta}{\beta}}\left(\rho_{SE}(t)\right)^{1-\frac{\eta}{\beta}},\end{aligned} \tag{6.36}$$

where we have exploited the unitarity of $U(t,0)$ to insert $(1-\frac{\eta}{\beta})$ resolutions of the identity $\mathbb{1}_{SE}=U^\dagger(t,0)U(t,0)$. It is therefore immediate to see that

$$\tilde{\Theta}(\eta,\beta,t)=\ln \mathrm{Tr}_{SE}\left[(\rho_{SE}(0))^{\frac{\eta}{\beta}}\left(\rho_{SE}(t)\right)^{(1-\frac{\eta}{\beta})}\right]=\left(\frac{\eta}{\beta}-1\right)S_{\frac{\eta}{\beta}}\left(\rho_{SE}(0)||\rho_{SE}(t)\right). \tag{6.37}$$

where we have moved the factor $N_S^{-\frac{\eta}{\beta}}$ to the first term appearing in with in the trace in Equation (6.35), i.e. $\left(\mathbb{1}_S\otimes(\frac{e^{-\beta\mathcal{H}_E}}{Z})^{\frac{\eta}{\beta}}\right)$, to give $\left(\rho_S(0)\otimes(\frac{e^{-\beta\mathcal{H}_E}}{Z})^{\frac{\eta}{\beta}}\right)$. The mean dissipated heat is then lower bounded by

$$\beta Q_E(t)\geq\mathcal{B}^\eta_{\mathcal{Q}}(t)_{|\rho_S(0)=\mathbb{1}_S}=\left(\frac{\beta}{\eta}-1\right)S_{\frac{\eta}{\beta}}\left(\rho_{SE}(0)||\rho_{SE}(t)\right). \tag{6.38}$$

We note in passing that a *fluctuation relation* for the heat distribution can be immediately obtained from (6.37) simply by substituting the value $\eta=\beta$ in the expressions and employing the definition of the cumulant generating function

$$\langle e^{\tilde{\Theta}(\beta,\beta,t)}\rangle_t\equiv\langle e^{-\beta Q_E(t)}\rangle_t=1. \tag{6.39}$$

Equation (6.38) can be re-written by making use of the skew-symmetry of $S_\alpha(\rho||\sigma)$:

$$S_\alpha(\rho||\sigma)=\frac{\alpha}{1-\alpha}S_{1-\alpha}(\sigma||\rho),\qquad\forall\alpha\neq0,1\,, \tag{6.40}$$

as

$$\beta Q_E(t)\geq\mathcal{B}^\eta_{\mathcal{Q}}(t)_{|\rho_S(0)=\mathbb{1}_S}=S_{1-\frac{\eta}{\beta}}\left(\rho_{SE}(t)||\rho_{SE}(0)\right),\qquad\forall\eta\in(0,\beta)\cup(\beta,+\infty]. \tag{6.41}$$

This last expression, in combination with the properties [155–157]

$$S_\alpha(\rho||\sigma)\geq0,\qquad\forall\rho,\sigma>0,\ \forall\alpha\in(0,+\infty], \tag{6.42}$$

$$S_\alpha(\rho||\sigma)>S_\beta(\rho||\sigma),\qquad\forall\alpha>\beta, \tag{6.43}$$

allows us to conclude that

$$\beta Q_E(t)_{|\rho_S(0)=\mathbb{1}_S} \geq 0, \qquad \text{for any } \forall \eta > 0, \tag{6.44}$$

thus in accordance with the original observation by Landauer mentioned above that the mean dissipated heat in this particular case is always non - negative (with the equality being reached only for trivial dynamics).

Finally, the following interesting relation can be found for this particular choice of initial system's state

$$\beta Q_E(t) = \lim_{\eta \to 0^+} S_{1-\frac{\eta}{\beta}} \left(\rho_{SE}(t) || \rho_{SE}(0)\right) = D\left(\rho_{SE}(t) || \rho_{SE}(0)\right), \tag{6.45}$$

where $D\left(\sigma||\rho\right) \equiv -\mathrm{Tr}\left[\sigma \ln \sigma\right] + \mathrm{Tr}\left[\sigma \ln \rho\right]$ is the *relative quantum entropy* between the total state of the composite system at time t and the total state at initial time $t = 0$. Since the latter is factorized, we have that [21]

$$D\left(\rho_{SE}(t) || \rho_{SE}(0)\right) = S(\rho_S(0)) + S(\rho_\beta) - S(\rho_{SE}(t)), \tag{6.46}$$

is thus the mean dissipated heat is in this case a measure of the change of the von-Neumann entropy resulting from the traces over the subsystems S and E, thus providing a measure for the corresponding information loss.

6.4 The XX-coupled pumped V-system

6.4.1 The model

Here we show the application of our results to an original model consisting of a three level V-system $|0\rangle$, $|1\rangle$, $|2\rangle$, where the $|0\rangle - |1\rangle$ transition is externally pumped by a laser with frequency Ω_1 while the transition between $|0\rangle - |2\rangle$ is dictated by the interaction with the environment, a two-level system, through an XX-type interaction. Moreover both the environmental qubit and the $|0\rangle - |2\rangle$ transition feel an external magnetic field along the z direction. See Fig. 6.1.

A straightforward generalization of this model, which we have called *XX-coupled pumped V-system*, is obtained by considering the environment made of a chain of two-level systems coupled through XX-interactions, which however can be tackled only through numerical simulations as the size increases. Despite quantitative changes, the qualitative behavior of the thermodynamical quantities of interest is however already captured by the analytically-solvable case of a single-spin environment and for this reason we will study it in detail.

This model is moreover interesting since it has not (to the best of our knowledge) been studied in the literature and represents a non-trivial variant of the well-known spin-chain model investigated, for example, in [152, 158, 159]. The latter, in fact, consists of a qubit instead of a three-level system and the coupling is again through an XX-type

interaction (which has the property to preserve the number of excitations). Its wide applications range from quantum simulations to quantum information.

Moreover, it is intuitively clear that the presently considered model reduces to the one consisting of two spins just mentioned in the particular situation where the pump Ω_1 is switched off and the system starts in the excited state $|2\rangle\langle 2|$, thus leaving with an effective two-level system interacting through an XX coupling with another spin. This result will be rigorously confirmed below, this way providing an useful check between the results obtained in this model and those derived in [152].

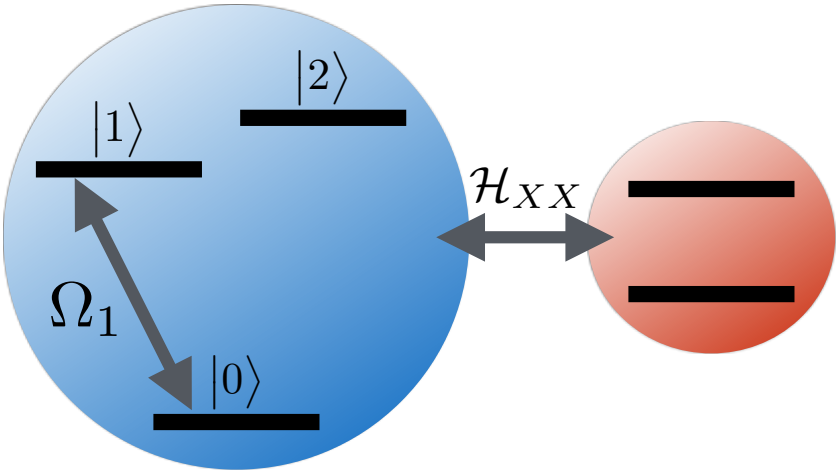

FIGURE 6.1: The XX-coupled pumped V-system. The $|0\rangle - |1\rangle$ transition of the open system is externally pumped by a laser with frequency Ω_1 while the transition between $|0\rangle - |2\rangle$ is dictated by the interaction with the environment, a two-level system, through an XX-type interaction. Moreover both the environmental qubit and the $|0\rangle - |2\rangle$ transition feel an external magnetic field along the z direction.

The total Hamiltonian is given by $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{XX} + \mathcal{H}_{SF}$ (with F denoting the laser field), with

$$\mathcal{H}_S = BS_z^{20}, \quad \mathcal{H}_E = B\sigma_z, \quad \mathcal{H}_{XX} = J\left(S_x^{20}\otimes\sigma_x + S_y^{20}\otimes\sigma_y\right), \quad \mathcal{H}_{SF} = \underline{D}^{20}\cdot\underline{E}, \tag{6.47}$$

where $\sigma_x, \sigma_y, \sigma_z$ denote the Pauli matrices for the environmental qubit,

$$S_x^{10} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \; S_y^{10} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \; S_z^{10} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$S_x^{20} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \; S_y^{20} = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \; S_z^{20} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

and finally $\underline{D}^{20} = \underline{d}S_-^{20} + \underline{d}^* S_+^{20}$, with $S_\pm^{20} = \frac{1}{2}\left(S_x^{20} \pm iS_y^{20}\right)$, is the dipole operator and $\underline{E} = \varepsilon + \varepsilon^*$, with $\varepsilon = i\sum_{\mathbf{k}}\sum_{\lambda=1,2}(\sqrt{2\pi\omega_{\mathbf{k}}/V})\,\mathbf{e}_\lambda(\mathbf{k})b_\lambda(\mathbf{k})$, is the electric field of the laser in the Shrödinger picture [21]. We remind that we have chosen for simplicity $\hbar = k_B = 1$ and continue to do so henceforth.

6.4.2 The master equation

In the present Section we derive an exact master equation in the interaction picture for the evolution of the reduced system's statistical operator by applying the concepts presented in Chapter 2 Sections 2.2.3 and 2.2.4.1.

First of all we move to the interaction picture with respect to the free Hamiltonian $\mathcal{H}_S + \mathcal{H}_E$. In this case the interaction terms become

$$\mathcal{H}_{XX}(t) + \mathcal{H}_{SF}(t) = J\left(S_x^{20} \otimes \sigma_x + S_y^{20} \otimes \sigma_y\right) + \underline{D}^{20}(t) \cdot \underline{E}(t), \tag{6.48}$$

where we have used the fact that

$$S_x^{20}(t) \otimes \sigma_x(t) + S_y^{20}(t) \otimes \sigma_y(t) = S_x^{20} \otimes \sigma_x + S_y^{20} \otimes \sigma_y, \tag{6.49}$$

and where explicitly

$$\begin{aligned}\underline{D}^{20}(t) \cdot \underline{E}(t) = \underline{d} \cdot \underline{\varepsilon} e^{-i(\omega_0+B)t} S_-^{20} + \underline{d}^* \cdot \underline{\varepsilon}^* e^{i(\omega_0+B)t} S_+^{20} \\ + \underline{d} \cdot \underline{\varepsilon}^* e^{-i(\omega_0-B)t} S_-^{20} + \underline{d}^* \cdot \underline{\varepsilon} e^{i(\omega_0-B)t} S_-^{20}.\end{aligned} \tag{6.50}$$

By assuming the so-called rotating-wave approximation (RWA), which amounts to drop the fast oscillating terms in the previous expression, and choosing the frequency of the external field to match with the magnetic field, i.e. $\omega_0 = B$, we are left with

$$\underline{D}^{20}(t) \cdot \underline{E}(t) = \Omega_1 S_+^{20} + \Omega_1^* S_-^{20}, \tag{6.51}$$

where $\Omega_1 = |\Omega_1| e^{i\phi} \equiv \underline{d}^* \cdot \underline{\varepsilon}$ is the Rabi frequency. In what follows, we will also choose the phase of the external field in order for Ω_1 to be real, so that

$$\mathcal{H}_{XX}(t) + \mathcal{H}_{SF}(t) = J\left(S_x^{20} \otimes \sigma_x + S_y^{20} \otimes \sigma_y\right) + \Omega_1 S_x^{20} \otimes \mathbb{1}_2. \tag{6.52}$$

By direct exponentiation of the Hamiltonian (6.52), the overall unitary evolution operator $U(t,0)$ governing the evolution of the composite system can be analytically found and reads

$$U(t,0) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{4\cos(t\omega_1)J^2+\Omega_1^2}{\omega_1^2} & \frac{2J(\cos(t\omega_1)-1)\Omega_1}{\omega_1^2} & 0 & -\frac{2iJ\sin(t\omega_1)}{\omega_1} & 0 \\ 0 & \frac{2J(\cos(t\omega_1)-1)\Omega_1}{\omega_1^2} & \frac{4J^2+\cos(t\omega_1)\Omega_1^2}{\omega_1^2} & 0 & -\frac{i\sin(t\omega_1)\Omega_1}{\omega_1} & 0 \\ 0 & 0 & 0 & \cos(t\Omega_1) & 0 & -i\sin(t\Omega_1) \\ 0 & -\frac{2iJ\sin(t\omega_1)}{\omega_1} & -\frac{i\sin(t\omega_1)\Omega_1}{\omega_1} & 0 & \cos(t\omega_1) & 0 \\ 0 & 0 & 0 & -i\sin(t\Omega_1) & 0 & \cos(t\Omega_1) \end{pmatrix}, \tag{6.53}$$

where $\omega_1 = \sqrt{\Omega_1^2 + 4J^2}$ represents a Rabi frequency modified by the coupling J. Note that the above expression is given by assuming the following lexicographic order to expand the vectors $|\Psi\rangle \in \mathscr{H}_S \otimes \mathscr{H}_E = (|21\rangle, |20\rangle, |11\rangle, |10\rangle, |01\rangle, |00\rangle)^T$, where the first digit refers to the the V-system while the second to the environmental qubit.

In order to find the time-local master equation

$$\frac{d}{dt}\rho_S(t) = \mathcal{K}_{TCL}(t)\rho_S(t), \tag{6.54}$$

i.e. determining the time-local generator governing the evolution of the V-system, we need, first of all, to find the quantum dynamical map $\Lambda(t,0)$. Consider to this purpose that the initial state of the composite system is of factorized form $\rho_{SE}(0) = \rho_S(0) \otimes \rho_\beta$,

$$\rho_S(0) = |\Psi_0\rangle\langle\Psi_0|, \quad |\Psi_0\rangle = \cos(\phi)|0\rangle + \sin(\phi)\sin(\alpha)|1\rangle + \sin(\phi)\cos(\alpha)|2\rangle, \tag{6.55}$$

and

$$\rho_\beta = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|, \qquad p = \frac{1}{2}(1 + \tanh(\beta B)). \tag{6.56}$$

This choice is also in accordance with the assumptions made in the erasure protocol mentioned at the beginning of Section 6.2. We have then that

$$\begin{aligned}
\rho_S(t) &= \mathrm{Tr}_E\left[U(t,0)\left(\rho_S(0)\otimes\rho_\beta\right)U^\dagger(t,0)\right] \\
&= \sum_{j=0}^{1}\Big[\langle j|\sqrt{1-p}U(t,0)|1\rangle\rho_S(0)\langle 1|\sqrt{1-p}U(t,0)|j\rangle \\
&\qquad\qquad + \langle j|\sqrt{p}U(t,0)|0\rangle\rho_S(0)\langle 0|\sqrt{p}U(t,0)|j\rangle\Big] \\
&= \sum_{i,j=0}^{1} K_{ij}(t)\rho_S(0)K_{ij}^\dagger(t),
\end{aligned} \tag{6.57}$$

with $K_{ij}(t) = \sqrt{1-3p+j(2p-1)}\,\langle i|\,U(t,0)\,|j\rangle$ being the Kraus operators. Inserting the explicit expression of the unitary operator (6.53), these operators read

$$
\begin{aligned}
K_{00}(t) &= \begin{pmatrix} \frac{\sqrt{p}\left(\omega_1^2 - 8J^2\mathrm{Sin}^2\left(\frac{t\omega_1}{2}\right)\right)}{\omega_1^2} & 0 & 0 \\ 0 & \sqrt{p}\cos\left(t\Omega_1\right) & -i\sqrt{p}\sin\left(t\Omega_1\right) \\ 0 & -i\sqrt{p}\sin\left(t\Omega_1\right) & \sqrt{p}\cos\left(t\Omega_1\right) \end{pmatrix}, \\
K_{01}(t) &= \begin{pmatrix} 0 & 0 & 0 \\ \frac{2J\sqrt{p}(\cos(t\omega_1)-1)\Omega_1}{\omega_1^2} & 0 & 0 \\ -\frac{2iJ\sqrt{p}\sin(t\omega_1)}{\omega_1} & 0 & 0 \end{pmatrix}, \\
K_{10}(t) &= \begin{pmatrix} 0 & \frac{2J\sqrt{1-p}(\cos(t\omega_1)-1)\Omega_1}{\omega_1^2} & -\frac{2iJ\sqrt{1-p}\sin(t\omega_1)}{\omega_1} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
K_{11}(t) &= \begin{pmatrix} \sqrt{1-p} & 0 & 0 \\ 0 & \sqrt{1-p}\cos\left(t\omega_1\right) & -\frac{i\sqrt{1-p}\sin(t\omega_1)\Omega_1}{\omega_1} \\ 0 & -\frac{i\sqrt{1-p}\sin(t\omega_1)\Omega_1}{\omega_1} & \sqrt{1-p}\cos\left(t\omega_1\right) \end{pmatrix}.
\end{aligned} \tag{6.58}
$$

We now consider an basis of $\mathcal{L}\left(\mathbb{C}^3\right)$ which is orthonormal with respect to the Hilbert-Schmidt product and satisfies the constraints (2.86). The latter is represented by the eight Gell-Mann matrices $\{\lambda_i\}_{i=1,\dots,8}$, which form a basis for the $su(3)$ algebra [16], plus the identity

$$
\begin{aligned}
\lambda_0 &= \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \lambda_1 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \lambda_2 = \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\lambda_3 &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \ \lambda_4 = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}, \ \lambda_5 = \begin{pmatrix} 0 & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 0 & 0 \\ \frac{i}{\sqrt{2}} & 0 & 0 \end{pmatrix}, \\
\lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \ \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \ \lambda_8 = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{6}} & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}} \end{pmatrix}.
\end{aligned} \tag{6.59}
$$

By means of Equations (6.58) and (6.59), we can immediately find the expression of the 9×9matrix $\mathbf{\Lambda}$ associated to the representation of the quantum dynamical map $\Lambda(t,0)$ on basis $\{E_{\alpha\beta}\}$ (2.36)

$$
\Lambda_{\alpha\beta} = \mathrm{Tr}_S\left[\lambda_\alpha^\dagger\left(\sum_{i,j=0}^{1} K_{ij}(t)\lambda_\beta K_{ij}^\dagger(t)\right)\right]. \tag{6.60}
$$

By exploiting$\mathbf{\Lambda}$, whose explicit expression we prefer to leave out due to its length, the matrix form of the time-local generator $\mathbf{K}_{TCL}$ on the same Hilbert-Schmidt basis is readily obtained by means of Equation (2.82).

Since the dynamical map was obtained from the overall unitary evolution operator, it is by construction trace and hermiticity preserving and completely positive. We can

therefore exploit these properties to better specify the structure of the time-local master equation (6.54) as shown in Subsection 2.2.4.1. Firstly, we need to express the time-local generator on the basis $\{F_{\alpha\beta}\}$ (2.38), a task straightforwardly carried out by applying the change of basis (2.40). This leads to the 9×9 matrix $\mathbf{K}'_{TCL}$ with entries $[\mathcal{K}'_{TCL}]_{\alpha\beta}$, by means of which a master equation in the form of (2.95) can be expressed. We give the result in the case of an initially cold environment (case $\beta \to +\infty$), which reads

$$\frac{d}{dt}\rho(t) = -i\left[\tilde{\mathcal{H}}(t), \rho(t)\right] + d_1(t)\left(G_-(t)\rho(t)G_-^\dagger(t) - \frac{1}{2}\{G_-^\dagger(t)G_-(t), \rho(t)\}\right) + d_2(t)\left(H_-(t)\rho(t)H_-^\dagger(t) - \frac{1}{2}\{H_-^\dagger(t)H_-(t), \rho(t)\}\right), \quad (6.61)$$

where

$$\tilde{\mathcal{H}}(t) = \Omega_1 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (6.62)$$

is the effective Hamiltonian obtained through Equation (2.93), where

$$d_{1,2}(t) = b(t) \mp \sqrt{b^2(t) + 4a^2(t)}, \qquad a(t) = \frac{2J^2\left[1 - \cos(\omega_1 t)\right]}{\omega_1^2 - 4J^2\left[1 - \cos(\omega_1 t)\right]},$$
$$b(t) = \frac{4J^2\omega_1 \sin(\omega_1 t)}{\omega_1^2 - 4J^2\left[1 - \cos(\omega_1 t)\right]} \quad (6.63)$$

are the only two non-zero eigenvalues of the submatrix $\tilde{\mathbf{K}}'_{TCL}$ obtained from $\mathbf{K}'_{TCL}$ by removing the first row and column and where, finally, the Lindblad operators $G_-(t)$ and $H_-(t)$ are the corresponding eigen-operators

$$G_-(t) = -v_-(t)\left|1\right\rangle\left\langle 2\right| + i\sqrt{1 - v_-^2(t)}\left|0\right\rangle\left\langle 2\right| \equiv -v_-(t)\sigma_-^{21} + i\sqrt{1 - v_-^2(t)}\sigma_-^{20}, \quad (6.64)$$

$$H_-(t) = v_+(t)\left|1\right\rangle\left\langle 2\right| + i\sqrt{1 - v_+^2(t)}\left|0\right\rangle\left\langle 2\right| \equiv v_+(t)\sigma_-^{21} + i\sqrt{1 - v_+^2(t)}\sigma_-^{20}, \quad (6.65)$$

$$v_\pm(t) = \pm\frac{\sqrt{2}a(t)}{\sqrt{b(t)\left(b(t) \pm \sqrt{4a^2(t) + b^2(t)}\right) + 4a^2(t)}}, \quad (6.66)$$

have been obtained through Equation (2.96).

We stress that the operators $G_-(t)$ and $H_-(t)$ are normalized to 1 and mutually orthogonal with respect to the Hilbert-Schmidt product, i.e. $\mathrm{Tr}_S\left[G_-^\dagger H_-(t)\right] = 0$.

If the pump Ω_1 is switched off, the function $a(t)$ vanishes while $b(t) \to 2J\tan(2Jt)$, thus leaving with the following master equation

$$\frac{d}{dt}\rho(t) = 2J\tan(2Jt)\left(\sigma_-^{20}\rho(t)\sigma_+^{20} - \frac{1}{2}\{\sigma_+^{20}\sigma_-^{20}, \rho(t)\}\right), \quad (6.67)$$

which describes an amplitude damping involving the $|0\rangle - |2\rangle$ transition [37, 152, 158].

Finally note that the dynamical map $\Lambda(t,0)$, despite being CPTP by construction, is not CP-divisible since the time-dependent damping rates $d_{1,2}(t)$ can assume both positive and negative values.

6.4.3 The dissipated heat statistics and new lower bound

In this Subsection we will evaluate the quantities introduced in Subsection 6.3 for the model at hand. First of all, we note that the passage to the interaction picture leaves the expression of consider the cumulant generating function $\tilde{\Theta}(\eta,\beta,t)$ defined in Equation (6.14) unchanged. This is readily seen by exploiting (6.26), the ciclicity property of the trace and the relation $[\mathcal{H}_0,\mathcal{H}_E]=0$:

$$\begin{aligned}\tilde{\Theta}(\eta,\beta,t)&=\ln\mathrm{Tr}_{SE}\left[e^{-(\eta/2)\mathcal{H}_E}U_0(t,0)U_I(t,0)e^{(\eta/2)\mathcal{H}_E}\rho_{SE}(0)e^{(\eta/2)\mathcal{H}_E}U_I^\dagger(t,0)U_0^\dagger(t,0)e^{-(\eta/2)\mathcal{H}_E}\right]\\&=\ln\mathrm{Tr}_{SE}\left[e^{-(\eta/2)\mathcal{H}_E}U_I(t,0)e^{(\eta/2)\mathcal{H}_E}\rho_{SE}(0)e^{(\eta/2)\mathcal{H}_E}U_I^\dagger(t,0)e^{-(\eta/2)\mathcal{H}_E}\right].\end{aligned}\tag{6.68}$$

Every quantity derived from the latter, consequently, do not depend on the picture chosen either.

We then employ the unitary operator in interaction picture (6.53) in expression (6.68) in order to obtain the cumulant generating function and the Landauer bound $\mathcal{B}_{\mathcal{Q}}^{\eta}(t)$. The cumulant generating function $\tilde{\Theta}(\eta,\beta,t)$ and the mean dissipated heat $Q_E(t)$ can be found analytically for a generic initial state of the system (6.55). Since their expressions are however quite lengthy, we give them in Appendix A, reporting here only their form for the choice $\rho_S(0)=|2\rangle\langle 2|$, which corresponds to the choice $\theta=0,\phi=\pi/2$:

$$\begin{aligned}\tilde{\Theta}(\eta,\beta,t)=\log\Bigg(&[1+\tanh(\beta B)]\,\frac{16J^2\Omega_1^2e^{-2B\eta}\sin^4\left(\frac{\omega_1}{2}t\right)+4J^2e^{-2B\eta}\sin^2\left(\omega_1 t\right)}{2\omega_1^4}\\&+[1+\tanh(\beta B)]\,\frac{\left(4J^2\cos\left(\omega_1 t\right)+\Omega_1^2\right)^2}{2\omega_1^4}\,\frac{1-\tanh(\beta B)}{2}\Bigg),\end{aligned}\tag{6.69}$$

$$Q_E(t)=[1+\tanh(\beta B)]\,\frac{16BJ^2\sin^2\left(\frac{\omega_1}{2}t\right)\left[-4J^2\sin^2\left(\frac{\omega_1}{2}t\right)+\omega_1^2\right]}{\omega_1^4}.\tag{6.70}$$

Both these quantities are always positive for every value of the parameters J,Ω_1,B and at every time t.

Fig. 6.2 clearly shows that, for decreasing values of the ratio η/β, the bound increasingly approaches the blue curve representing $\beta\langle Q\rangle_t$, which can be calculated analytically for this model using Equation (6.20). We stress that the red line in Fig.(6.2), correspondent to the choice $\eta=\beta$, reproduces the Landauer lower bound obtained in [152]. By taking instead larger values of η/β, the bound increasingly approaches to zero.

By means of the analytic expression of the unitary evolution operator $U(t,0)$ (6.53), the Kraus operators for the environmental channel A_k can be found simply by taking the partial trace over the system. The quantifier of the non-unitality degree of the environmental channel, given by the Frobenius norm of the difference between $\mathbf{A}^\beta(t)=\sum_k A_k(t)A_k^\dagger(t)$

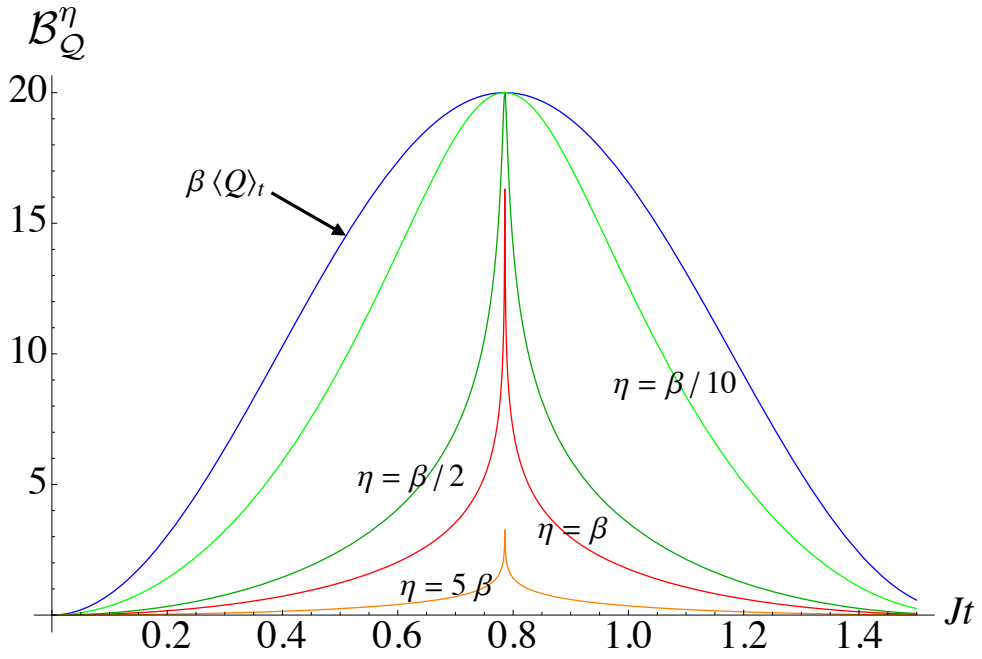

FIGURE 6.2: The blue line represents $\beta\langle Q\rangle_t$, while the other lines are the bound $\mathcal{B}_{\mathcal{Q}}^{\eta}$ for several different values of the counting parameter. In particular, the red line corresponds to the choice $\eta = \beta$ which reproduces the Landauer's bound $\mathcal{B}_{\mathcal{Q}}$ also considered in [152]. The other parameters have been fixed to $J = 1$, $B = 1$, $\beta = 10$ and $\Omega_1 = 0.1$.

and the identity $\mathbb{1}_E$ can be expressed in a closed form. In the case $\rho_S(0) = |2\rangle\langle 2|$ it reduces to

$$\mathcal{N}_E(t) = \frac{16\sqrt{2}J^2\sin^2\left(\frac{\omega_1}{2}t\right)\left[-4J^2\sin^2\left(\frac{\omega_1}{2}t\right)+\omega_1^2\right]}{\omega_1^4}. \tag{6.71}$$

By direct confrontation of Eqs. (A.4) and (6.71), it follows that

$$\mathcal{N}_E(t) = \frac{\sqrt{2}}{1+\tanh(\beta B)}Q_E(t), \tag{6.72}$$

which however holds true only for the choice $\rho_S(0) = |2\rangle\langle 2|$. In general however, this quantity is always positive and vanishes whenever the coupling J goes to zero, or whenever the argument of the $\sin^2$ goes to zero (which happens when the two degrees of non-unitality as well as the family of lower bounds and dissipated heat go to zero).

In Fig. 6.3 we plot the behavior of the rescaled non-unitality $\beta\mathcal{N}_E$ (black line) against the dissipated heat and the lower bound for $\eta = \beta$ in the cases of cold, $\beta = 10$, and relatively hot, $\beta = 1$, environment. It is evident that the zeros and the maxima of the three curves are attained at the same times.

A remarkable feature that occurs in Fig. 6.3 **(a)** is the cusp appearing in $\mathcal{B}_{\mathcal{Q}}^{\eta}$ when the dissipated heat is maximized. Here, the environment qubit is effectively in the ground state when $\beta = 10$. At the cusp, the bound is as close as possible to the actual dissipated heat. Contrarily, when $\beta = 1$, we see these features are smoothed out and the dissipated heat

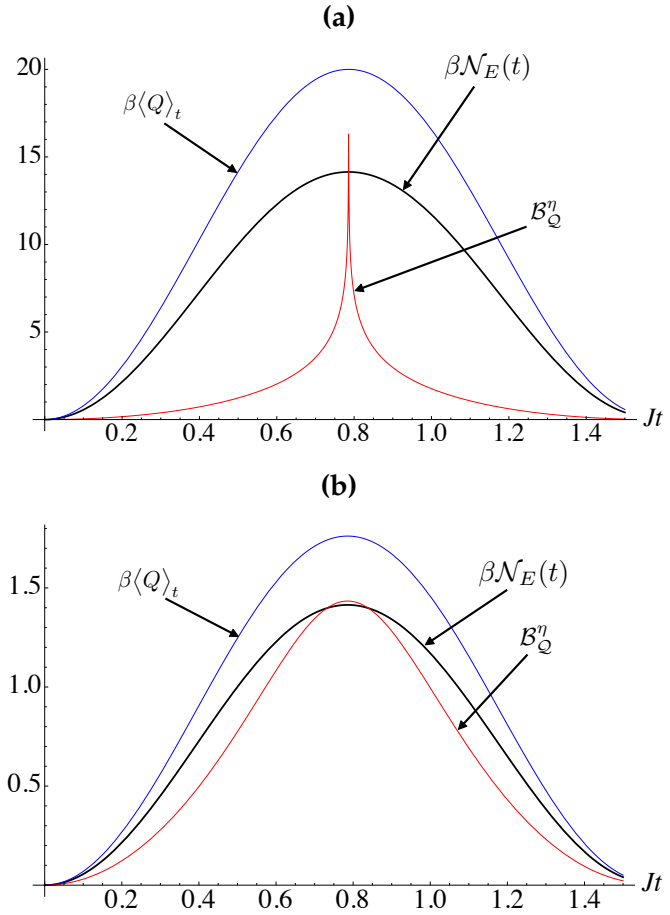

FIGURE 6.3: Mean dissipated heat $\beta\langle Q\rangle_t$ (top-most blue curve), rescaled non-unitality $\beta\mathcal{N}_E(t)$ (middle, black curve) and the lower bound $\mathcal{B}_Q^\eta$ for $\eta = \beta$ (bottom-most red curve). In both panels we fix $B = J = 1$, $\Omega_1 = 0.1$ and **(a)** $\beta = 10$ **(b)** $\beta = 1$.

is significantly reduced. Furthermore, the bound is now a smoothly varying function, closely tracking the same functional form $\beta Q_E(t)$.

This behavior can be explained by studying the populations, ρ_S^{00}, ρ_S^{11}, ρ_S^{22}, of the V-system, shown in Fig. 6.4 for the same parameters used in Fig. 6.3. Focusing on panel **(a)**, and recalling that we always assume our system is initialized in $\rho_S(0) = |2\rangle\langle 2|$, we see that, as the the system evolves, the population of the $|2\rangle$ state is completely transferred to the $|0\rangle$ state. The point at which both $\beta Q_E(t)$ and $\mathcal{B}_Q^\eta$ are maximized corresponds exactly to when $\rho_S^{22} = 0$. At this point all of the energy initially contained in the system is 'emptied' into the environment qubit, which due to being initially in its ground state is able to accept and store all of this energy. When $\beta = 1$, panel **(b)**, the situation is markedly different due to the fact that the environment is comparatively warm, with a sizeable population initially in the excited state. In this case, the environment is unable to store *all* the energy initially in the system. Therefore the population ρ_S^{22} cannot reach 0 and the dissipated heat is accordingly reduced.

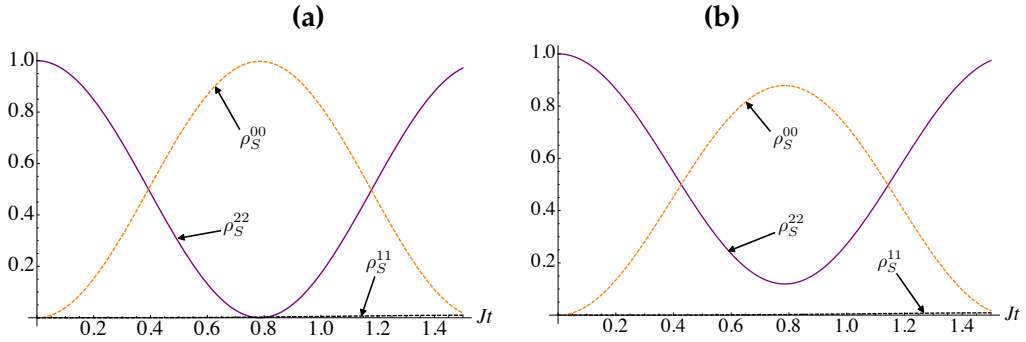

FIGURE 6.4: Dynamics of the populations, ρ_S^{00} (dashed, orange), ρ_S^{11} (dashed, black), and ρ_S^{22} (solid, purple). of the three-level system. **(a)** For $B=1$, $J=1$, $\beta=10$ and $\Omega_1=0.1$. **(b)** As for the previous panel except $\beta=1$.

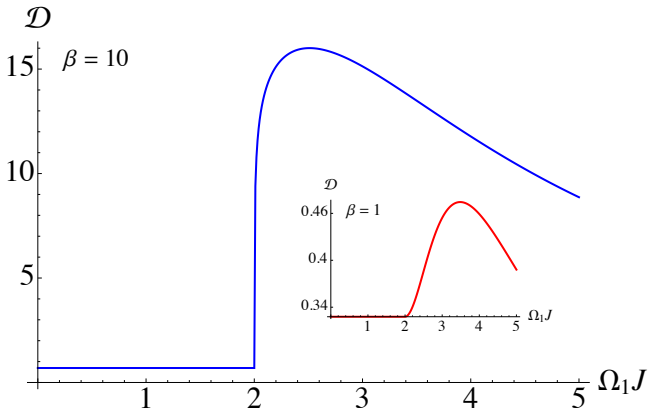

FIGURE 6.5: Difference, $\mathcal{D}$, between the maximum of the mean dissipated heat and maximum of the lower bound $\mathcal{B}_{\mathcal{Q}}^{\eta}$ for $\eta = \beta$ as a function of the pump frequency Ω_1. Here we take $J = 1$, $B = 1$, and $\beta = 10$. *Inset:* As for main panel except setting $\beta = 1$.

Closer examination of the cusp in Fig. 6.3 **(a)** reveals a peculiar feature. Defining

$$\mathcal{D} \equiv \mathrm{Max}_t \left[\beta Q_E(t) - \mathcal{B}_{\mathcal{Q}}^{\beta}(t)\right], \tag{6.73}$$

as the difference between the maximum dissipated heat and maximum of the bound, we find that for the same parameters in Fig. 6.3 **(a)**, $\mathcal{D} = \ln 2$. In Fig. 6.5 we examine the quantity in (6.73) more closely and we see there exists a 'critical' pump strength. If the environment is initially cold, $\beta = 10$, then for $\Omega_1 \leq 2J$ we find $\mathcal{D}$ is constant and always $\ln 2$. This occurs because in this regime, the population of ρ_S^{22} is always able to reach exactly 0. If $\Omega > 2J$ then the pump begins to dominate the dynamics. Now, due to the strong pumping of the $|0\rangle - |1\rangle$ transition, some of the population is trapped in the system and the ρ_S^{22} population is never completely empty. We see a sudden increase in $\mathcal{D}$, due to the fact that for $\Omega_1 > 2J$ the bound is significantly reduced compared to the dissipated heat. Interestingly the same qualitative behavior persists even when the environment is initially warm, $\beta = 1$. In the inset we see that for $\Omega_1 \leq 2J$, $\mathcal{D}$ is again

constant and only changes when $\Omega_1 > 2J$.

In conclusion, in this Chapter we have derived a new family of lower bounds to the mean dissipated heat in an environmental-assisted erasure protocol scenario, i.e. a framework where the fundamental Landauer's principle holds. This has been achieved using full-counting statistics methods introduced in Chapter 5 Section 5.2 and so the results are valid also in a non-equilibrium setting. The obtained family of lower bounds can be shown to be asymptotically tight by construction to the mean dissipated heat, at variance with Landauer's and Reeb-Wolf's bounds which in general are not always tight. The latter however are more related to the quantum information point of view while our result sticks more to the side of thermodynamics. We have moreover shown an application of this construction on an interesting open quantum system, for which we also have provided an analytical solution. This model consisted of a three-level V-system in which one energetic transition was externally pumped by a laser field, while the other transition is coupled to a two-level system through an XX-interaction. As stressed at the beginning of Section 6.4, the choice of an environment made of a single spin was motivated also by the fact that it provides benchmark results for the case of an environment consisting of a spin-chain, where the inter-spin couplings is dictated by an XX-interaction. The latter is planned to be tackled by means of a numerical simulation in the near future.

7 Conclusions

In this work, several different properties of open quantum systems have been investigated within a non-Markovian dynamical regime. In particular, we started exploring the validity of the quantum regression theorem, which allows to reconstruct multi-time correlation functions, and then moved to the field of quantum thermodynamics, where we studied the concept of heat in non-driven open quantum systems, firstly by characterizing its flow and then by bounding from below its dissipation in an erasure-protocol setup.

The first two Chapters of the Thesis were dedicated to introduce all the open quantum systems' notions later employed. In particular, in Chapter 2 we thoroughly discussed the characterization of the dynamics of a reduced system in terms of quantum dynamical maps and of master equations, with a particular emphasis on their time-local expressions. Moreover we showed how to derive the latter given the knowledge of the former (and vice versa), and discussed how the properties of quantum dynamical maps (such as, for example, trace and hermiticity preservation, complete positivity, CP-divisibility...) are reflected into constraints on the structure of the respective master equations. Explicit applications of this have been carried out in Chapters 4 and 6, where expressions for the exact time-local master equations have been derived for a pure-dephasing spin-boson model and for an externally pumped V-system coupled to a single-site spin chain through an XX interaction.

In Chapter 3 we concentrated on one of the leitmotifs of this work, namely the notion of non-Markovianity, in particular showing how the main criteria in the quantum realm, which have been introduced in the last decade, have their natural classical counterparts in sufficient conditions of non-Markovianity within the framework of stochastic processes. Several estimators for the degree of non-Markovianity have been presented and discussed, the reason being that, even though they all share the same goal to quantify the amount of memory effects in a reduced dynamics, each one of them has different properties which make them more or less suitable for the model at hand. Actually, even considering a single open quantum system, the evaluation of several of these estimators could be useful since they capture distinctive aspects related to non-Markovian dynamics. This fact has been explicitly shown for the pure-dephasing spin-boson system discussed in

Chapter 4, where the measure by Rivas, Huelga and Plenio and the one by Breuer, Laine and Piilo have been calculated. The former identifies the violation of the CP-divisibility of the family of dynamical maps as the signature of non-Markovian reduced quantum dynamics. The latter relies instead on the variation of the distinguishability between two reduced states, quantified in terms of the trace distance, whose eventual non monotonic behavior is interpreted in terms of an information backflow from the environment to the open system. Despite the criteria for the occurrence of non-Markovianity all coincide for this model, these two estimators quantify the degree of non-Markovianity behavior differently with respect to the parameters characterizing the family of dynamical maps.

In Chapter 4 we explored the relationship between the above mentioned criteria of non-Markovianity and the validity of the quantum regression theorem which is a statement relating the behaviour in time of the mean values and of the two-time correlation functions of system operators. After giving a clear ground for the quantum regression theorem, we explicitly calculated all the quantities for two specific models. The first open system considered was a pure-dephasing spin-boson model and the second one consisted in a photonic-realization of a dephasing interaction. For a class of spectral densities with exponential cut-off and power law behaviour at low frequencies we have studied the onset of non-Markovianity as a function of the coupling strength and of the exponent determining the low frequency behaviour, further giving an exact expression for the corresponding non-Markovianity measures. The deviation from the quantum regression theorem has been estimated evaluating the relative error made in replacing the exact two-time correlation function for the system operators with the expression reconstructed by the evolution of the corresponding mean values.

Results have shown that the validity of the quantum regression theorem represents a stronger requirement than Markovianity. The same conclusions have been shown to hold also in the second open quantum system considered, namely an all-optical realization of a dephasing interaction, which has been recently exploited in order to experimentally investigate the non-Markovianity. Also in this model, for different choices of the frequency distribution, significant violations to the quantum regression theorem were observed even in the presence of a Markovian dynamics.

In Chapters 5 and 6 we focused on the concept of heat in non-driven open quantum systems. Borrowing and employing the full-counting statistics formalism from quantum thermodynamics, we studied the time behavior of its mean value in presence of a non-Markovian dynamical regime and we introduced a new family of lower bounds for its dissipation in an erasure-protocol scenario. In the case of semigroup dynamics, it was known that the heat flow turns out to be a monotonic function of time from the hotter to the colder subsystem and vanishes when the initial temperature gradient is absent. In particular, a positive rate of heat exchange would indicate an energy flow from system to environment while a negative rate would mean the opposite, i.e. a heat flowing from the environment towards the open system. In this work we have investigated how the mean heat flow behaves in a non-Markovian dynamical regime. Results have shown that, interestingly, the heat flow becomes an oscillating function of time, which can even change its sign and, interestingly, is different from zero even if the system and the environment start at the same temperature. Starting from dynamical situations which in

the Born-Markov semigroup limit would lead to a non-negative steady heat flow, we were naturally lead to introduce a notion of heat backflow from the environment to the system as the fraction of heat which corresponds to temporarily negative regions of the heat flow. A measure for the total amount of heat flowing out of the environment was then built upon this definition and characterized both for finite-dimensional and infinite-dimensional Gaussian open quantum systems. In order to make the latter a property of the quantum dynamical map only, a maximization over all possible initial states of the system has been incorporated in its definition. Interestingly, numerical evidences have shown that this maximum is achieved whenever the system and the environment start at the same temperature, a condition which, as stressed above, would imply no energy flow in the Born-Markov semigroup limiting case. A thorough analysis of the heat backflow measure has been carried out in two relevant models, representatives of the two above mentioned classes of open systems: the so-called spin-boson model, which is a two-level system coupled to a bosonic bath through a position-position interaction, and the quantum Brownian motion, which differs from the latter in the fact that it is an harmonic oscillator instead of a qubit. An analytic insight of all the quantities of interest has been achieved for both these models in the weak coupling regime, where the dynamics of the open system was approximated by a second-order time-convolutionless master equation. In the case of the quantum bronwian motion, an extension to the strong coupling regime has been performed by relying on a numerical approach which, with the only assumption to deal with a large but finite number of environmental modes, allowed for exact simulations of the equation of motions and, thus, characterization of the time behavior of heat flow. The obtained results have allowed to characterize the dependence of energy exchanges in these non-driven open quantum systems and, in particular, to pinpoint the regions of relevant parameters where the heat backflow was absent or maximum.

The heat backflow measure is reminiscent of a sort of memory effect by virtue of its construction and physical meaning and furthermore vanishes in the case of a semigroup, thus Markovian, dynamics. For these reasons we were naturally led to investigate the relationship between it and suitable non-Markovianity estimators. Results confirm the intuition that the occurrence of heat backflow, being the latter a specific observable and thus representing only one possible contribution of information backflow, represents a stricter condition than non-Markovianity. Otherwise stated, on the one hand an heat backflow from the environment to the system can be observed for those values of the relevant parameters such that the dynamics is non-Markovian, while, on the other hand, a Markovian evolution prevents any observation of the latter. In the case of the spin-boson moreover, a physical explanation and a more stringent connection between the heat backflow measure and the trace-distance based non-Markovianity measure introduced by Breuer, Laine and Piilo has been found due to their mutual relationship with the so-called resonance condition. The latter in fact corresponds to a region of dynamical parameters where the spectral density at resonance is almost locally flat, thus mimicking a white-noise spectrum which is notoriously Markovian. Around this curve also the heat backflow measure is practically absent.

Finally, Chapter 6 was devoted to show how to derive, by means of full-counting statistics formalism, a novel family of lower bounds to the mean dissipated heat, which are always asymptotically tight, in a generic (and thus also non-Markovian) erasure-protocol scenario. The latter calls for the notorious Landauer's principle, which fundamentally express the second law of thermodynamics by bounding from below the mean dissipated heat with the information erasure in the system, quantified through the variation of its entropy. An explicit application of this construction has been shown for an open quantum system consisting of a three-level V-system, externally pumped by a laser on one of its two transitions and coupled on the other transition to a spin chain through an XX interaction. Analytical exact solutions for the dynamics of this model has also been obtained.

In conclusion, this work of Thesis, whose content is collected in [1–3, 5], has been hinged on the investigation of multi-time correlation functions and thermodynamical quantities, such as heat, in a non-Markovian open quantum systems scenario, with the goal to better understand their behavior in the presence of memory effects in the reduced dynamics.

7.1 Outlook

First of all, it is worth to mention that, concerning the topics studied in Chapter 4, other studies have followed [1], such as [91, 160], where projector-operator techniques were employed to derive the equations of motion for the effective density operator (4.14), in order to characterize the contributions leading to the violations to the quantum regression procedure. It would be interesting to perform further studies along these lines such as employing the projection operator technique to operators evolved in Heisenberg picture as in [161]. This formal apparatus would hopefully lead to a more clear relationship with the non-Markovianity criteria. In this regard, in the same philosophy adopted in Chapter 3, further investigation between regression procedure and classical Markovian processes should be worth considering, in order to better characterize their quantum counterparts.

Entering the realm of quantum thermodynamics, there is a plethora of interesting follow-up of the topics introduced and analysed in Chapters 5 and 6. Here we report some of them, which we plan to deal with in our future research. To begin with, while in [2, 3] we have been interested in characterizing the time-behavior of the first cumulant (mean value) of heat, higher-order cumulants can also be considered using the full-counting statistics formalism [162, 163], making it possible to discuss, for example, bunching properties of bosons in the presence of heat backflow. Another aspect to further carry on and clarify is a more precise statement of the relationship between the occurrence of heat backflow and of non-Markovianity. With this aim, other spectral densities such as (4.55) and, of course, other models than the spin-boson and the quantum brownian motion deserve to be considered, in order to make more general statements. Another challenging but very interesting research would be to apply these studies to more complex quantum systems such as, for example, the biological ones. Among the many difficulties that are

involved when dealing with such systems is the fact that a detailed microscopic knowledge of them is usually not feasible, thus preventing the possibility to reconstruct the heat generating function by means of a two-time measurement protocol.

Finally, several aspects related to the newly introduced family of lower bounds, also obtained by means of full-counting statistics methods, can be developed. As we stressed in Chapter 6 in fact, this family of bounds is always asymptotically tight to the mean dissipated heat and, remarkably, reduces to the lower bound obtained in [152] for a specific value of the counting field parameter. This latter case, although bearing a clear physical meaning in terms of the degree of non-unitality of the map which evolves the state of the environment, is not guaranteed to outperform Reeb and Wolf's bound nor even Landauer's original contribution ΔS. A more systematic study of the relative performances of these three bounds with respect to the possible initial conditions of the open system represent an ongoing project. Preliminary results carried out on finite-dimensional systems similar to the one considered in Chapter 6 but subject to random interaction Hamiltonians seem to suggest that Landauer's as well as Reeb and Wolf's bounds provide a more faithful bound whenever the open quantum system starts in a more mixed state, while the bound in [152] outperforms the other two whenever the purity of the state increases. Finally, an important goal would be to provide concrete strategies which would allow to experimentally access this new lower bound and to test it against Landauer's.

A

Analytic solutions for the heat statistics in the XX-coupled pumped V-system

In this Appendix we provide the explicit expressions of the cumulant generating function $\Theta(\eta, \beta, t)$ (6.14) and of the mean dissipated heat (5.7) for the model considered in Chapter 6 Section 6.4 and for a generic initial system state of the form

$$\rho_S(0) = |\Psi_0\rangle\langle\Psi_0|, \quad |\Psi_0\rangle = \cos(\phi)|0\rangle + \sin(\phi)\sin(\alpha)|1\rangle + \sin(\phi)\cos(\alpha)|2\rangle. \tag{A.1}$$

By exploiting the overall unitary evolution operator in interaction picture (6.53), we have that a direct calculation of Equation (6.26) leads to the following result for the cumulant generating function

$$\begin{aligned}
\Theta(\eta,\beta,t) = \ln\Bigg[& -\frac{1}{2}\cos^2(\alpha)\sin^2(\phi)(\tanh(\beta B)-1) \\
& + \frac{e^{-2B\eta}\left(2\sin^2(\phi)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)J^2\cos^2(\alpha)(\tanh(\beta B)+1)\right)}{4J^2+\Omega_1^2} \\
& - \frac{\frac{1}{2}\sin^2(\phi)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\Omega_1^2\sin^2(\alpha)(\tanh(\beta B)-1)}{4J^2+\Omega_1^2} \\
& + \frac{e^{-2B\eta}\left(-\frac{1}{2}e^{2B\eta}\left(4J^2+\Omega_1^2\right)\cos^2(\phi)(\tanh(\beta B)-1)\cos^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\right)}{4J^2+\Omega_1^2} \\
& + \frac{e^{-2B\eta}\left(8J^2\Omega_1^2\cos^2(\alpha)\sin^2(\phi)(\tanh(\beta B)+1)\sin^4\left(\frac{1}{2}t\sqrt{4J^2+\Omega_1^2}\right)\right)}{\left(4J^2+\Omega_1^2\right)^2} \\
& + \frac{e^{-2B\eta}\left(-\frac{1}{2}e^{2B\eta}(\tanh(\beta B)-1)\left(\sin^2(\alpha)\sin^2(\phi)\left(\Omega_1^2\cos\left(t\sqrt{4J^2+\Omega_1^2}\right)+4J^2\right)^2\right)\right)}{\left(4J^2+\Omega_1^2\right)^2} \\
& + \frac{e^{-2B\eta}\left(\left(\Omega_1^2\left(4J^2+\Omega_1^2\right)\cos^2(\phi)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\right)\right)}{\left(4J^2+\Omega_1^2\right)^2}
\end{aligned} \tag{A.2}$$

$$
\begin{aligned}
&+\frac{\frac{1}{2}\cos^2(\alpha)\sin^2(\phi)(\tanh(\beta B)+1)\left(4J^2\cos\left(t\sqrt{4J^2+\Omega_1^2}\right)+\Omega_1^2\right)^2}{\left(4J^2+\Omega_1^2\right)^2}\\
&-\frac{2J^2e^{2B\eta}(\tanh(\beta B)-1)\left(4\Omega_1^2\sin^2(\alpha)\sin^2(\phi)\sin^4\left(\frac{1}{2}t\sqrt{4J^2+\Omega_1^2}\right)\right)}{\left(4J^2+\Omega_1^2\right)^2}\\
&+\frac{2J^2e^{2B\eta}(\tanh(\beta B)-1)\left(\left(4J^2+\Omega_1^2\right)\cos^2(\phi)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\right)}{\left(4J^2+\Omega_1^2\right)^2}\\
&+\frac{1}{2}(\tanh(\beta B)+1)\left(\sin^2(\alpha)\sin^2(\phi)\cos^2\left(t\Omega_1\right)+\cos^2(\phi)\sin^2\left(t\Omega_1\right)\right)\\
&+\frac{1}{2}(\tanh(\beta B)+1)\left(\sin^2(\alpha)\sin^2(\phi)\sin^2\left(t\Omega_1\right)+\cos^2(\phi)\cos^2\left(\Omega_1 t\right)\right)\Bigg]. \qquad \text{(A.3)}
\end{aligned}
$$

By means of Eq.(6.20) the average dissipated heat is given by

$$
\begin{aligned}
Q_E(t) = &\left(4J^2+\Omega_1^2\right)^{-2}\Bigg[4BJ^2\Bigg(-\tanh(\beta B)\Bigg(4\sin^2(\phi)\sin^2\left(\frac{1}{2}t\sqrt{4J^2+\Omega_1^2}\right)\\
&\left(\Omega_1^2\sin^2(\alpha)\sin^2\left(\frac{1}{2}t\sqrt{4J^2+\Omega_1^2}\right)+\cos^2(\alpha)\left(2J^2\cos\left(t\sqrt{4J^2+\Omega_1^2}\right)+2J^2+\Omega_1^2\right)\right)\\
&+\left(4J^2+\Omega_1^2\right)\cos^2(\phi)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\\
&+\cos(2\alpha)\sin^2(\phi)\sin^2\left(\frac{1}{2}t\sqrt{4J^2+\Omega_1^2}\right)\left(\left(\Omega_1^2-4J^2\right)\cos\left(t\sqrt{4J^2+\Omega_1^2}\right)-4J^2-3\Omega_1^2\right)\\
&+\frac{1}{4}\left(4J^2+\Omega_1^2\right)(3\cos(2\phi)+1)\sin^2\left(t\sqrt{4J^2+\Omega_1^2}\right)\Bigg)\Bigg]. \qquad \text{(A.4)}
\end{aligned}
$$

Note how both the mean dissipated heat and the family of lower bounds depend, alongside with the inverse temperature β characterizing the initial Gibbs state ρ_β, on the choice of the initial state of the system. This is an important indication that this choice plays an important characterizing role in the erasure protocol; this aspect however is the subject of further ongoing study.

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