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Regularizations and exact methods for non-Markovian open quantum systems

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Candidate

Antonio D'Abbruzzo

Supervisor

Prof. Vittorio Giovannetti

Co-supervisor

Dr. Vasco Cavina

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Abstract

Any realistic physical object ought to be regarded as open to influences from an external uncontrollable environment. Consequently, one of the main topics in the theory of open quantum systems is to derive expressive dynamical laws—master equations—from a microscopic description of the system-environment compound. While plenty has been said in the Markovian regime, where there is a unilateral flow of information from the system to the environment, much less is known beyond it. In this thesis we discuss new techniques to address situations framed in the non-Markovian phenomenology. First, we propose two state-of-art methods to regularize master equations affected by the issue of positivity breaking: such phenomenon is known to occur after weak-coupling expansions, with the celebrated Redfield equation being the primary example of defective occurrence. Then, in order to make progress in the opposite strong-coupling scenario, we discuss methods that are applicable under certain Gaussianity assumptions. Adopting a fruitful marriage between the language of master equations and the Schwinger-Keldysh contour idea from many-body physics, we are able to construct exact stochastic and deterministic master equations with an unprecedented degree of generality and relative simplicity and intuitiveness.

Contents

List of Publications

Publications discussed in the thesis

- A. D'Abbruzzo, V. Cavina, and V. Giovannetti, *A time-dependent regularization of the Redfield equation*, SciPost Phys. **15**, 117 (2023).
- A. D'Abbruzzo, D. Farina, and V. Giovannetti, *Recovering complete positivity of non-Markovian quantum dynamics with Choi-proximity regularization*, Phys. Rev. X **14**, 031010 (2024).
- V. Cavina, A. D'Abbruzzo, and V. Giovannetti, *Unifying quantum stochastic methods using Wick's theorem on the Keldysh contour*, Phys. Rev. Research **7**, 043262 (2025).
- A. D'Abbruzzo, V. Giovannetti, and V. Cavina, *Exact non-Markovian master equations: A generalized derivation for Gaussian systems*, Phys. Rev. Lett. **135**, 240401 (2025).

Publications excluded from the thesis

- A. D'Abbruzzo, V. Alba, and D. Rossini, *Logarithmic entanglement scaling in dissipative free-fermion systems*, Phys. Rev. B **106**, 235149 (2022).
- A. D'Abbruzzo, D. Rossini, V. Giovannetti, and V. Alba, *Steady-state entanglement scaling in open quantum systems: A comparison between several master equations*, arXiv:2409.06326 [quant-ph] (2024).

Publications produced before the Ph.D. course

- A. D'Abbruzzo and D. Rossini, *Self-consistent microscopic derivation of Markovian master equations for open quadratic quantum systems*, Phys. Rev. A **103**, 052209 (2021).
- A. D'Abbruzzo and D. Rossini, *Topological signatures in a weakly dissipative Kitaev chain of finite length*, Phys. Rev. B **104**, 115139 (2021).

Chapter 1

Introduction

Quantum mechanics is the most fundamental physical theory we currently possess to describe the behavior of matter and energy at the atomic and subatomic scales. Many astonishing effects we are capable of observing in nature, such as interference, tunneling, and entanglement, simply cannot be accounted for by the framework of classical mechanics [1].

The standard presentation of non-relativistic quantum mechanics treats physical objects as perfectly isolated systems and puts its law of motion—the Schrödinger equation—in the same role as Newton's laws of classical physics. However, like in classical physics itself, this is an idealization: any realistic system is subjected to the non-trivial influence of an external uncontrollable *environment*. The study of this influence is fundamental for describing effects like dissipation, decoherence, and relaxation—topics which are extremely important throughout many fields of physics, such as quantum computing [2], quantum thermodynamics [3], many-body physics [4], or quantum biology [5].

In the vast majority of cases, studying the entire system-environment setup is not only unfeasible in practice but also beyond our needs, since we are typically not interested in the overwhelming amount of information provided by the environment's internal dynamics. It is the theory of *open quantum systems* [6–8] which provides the tools to apply quantum mechanics in those settings where the presence of the environment cannot be ignored, while still providing reasonably effective dynamical laws for the system alone. Such laws, typically known as *master equations*, necessarily constitute the bulk of the theory and writing them down with a sufficient degree of accuracy is one of the most important tasks one has to address when modeling an open quantum system. Unfortunately, this is far from simple and many unresolved questions still remain.

From the mathematical point of view, much has been said in the *Markovian* regime, where excitations injected by the system into the environment are not allowed to be absorbed back by the system, thus creating a unilateral flow of information from the system to the environment [9, 10]. This hypothesis usually effectively describes large, memory-less environments that are weakly coupled to the system. In such framework, the celebrated *Lindblad-Gorini-Kossakowski-Sudarshan (LGKS) theorem* provides the most general shape the master equation must have in order to represent a physically realizable dynamics [11, 12]. Alas, much less is known beyond this regime and the study of *non-Markovian* master equations is a very active contemporary research field [13–16].

From the practical point of view, there are basically two fundamental ways to approach the modeling problem. A first possibility stems from knowing the elementary processes expected to characterize the dynamics, which leads to a *phenomenological* master equation.

This top-down approach is suitable in those situations where the environment's effect is experimentally well characterized and the objective is to find predictions. Popular examples include LGKS equations constructed with *ad hoc* local Lindblad operators [17, 18]. A second possibility, instead, is the *microscopic derivation*: starting from a detailed microscopic description of the constituents of the system-environment compound, one can explicitly eliminate the environment's degrees of freedom to arrive at an effective description solely for the system's variables. This bottom-up approach seeks to make dissipation and similar effects emerge from the microscopic structure and is better suited for the exploration of potentially new phenomena.

Unfortunately, approaching a microscopic derivation in complete generality without further assumptions is a hopelessly complex task. A possible way forward lies on the path of the Markovian hypothesis. Specifically—as is common in physics—one can attack the problem perturbatively using a *weak-coupling expansion*. At the lowest non-trivial order this leads to the so-called *Redfield equation*, a well-established tool that brought over the decades several remarkable results, especially in thermodynamics and chemistry [19, 20]. Nonetheless, the weak-coupling expansion exposes a mathematical flaw that sometimes hinders the application of the resulting master equations: the *breaking of positivity*. This means that the dynamical law no longer ensures positive measurement probabilities, a requirement that must be taken seriously if we expect to make valid physical predictions [21].

In particular, the issue of positivity breaking displayed by the Redfield equation has been the subject of an intense debate in the literature. While some argue that the effects of such violations lie beyond the approximations used to derive the equation itself [22, 23], others take this fact as a signal that the weak-coupling expansion should be approached with more sophisticated techniques to provide well-founded approximation theories [24–26]. On this line of thinking, several ideas to *regularize* the Redfield equation appeared, each with its pros and cons [27–39]. As we will discuss later on, the first part of this thesis presents new state-of-art techniques that can be applied to regularize any "defective" master equation.

But what if the coupling is inherently strong and the Redfield equation is no longer suitable, along with the whole weak-coupling expansion idea? If we cannot perform approximations, we can surely add simplifying *assumptions* instead. For example, one can start from the hypothesis that parts of the setup can be modeled using analytically tractable *Gaussian systems*. It is probably superfluous to highlight here the importance of Gaussian systems throughout all of physics and the great array of experimental platforms that are well-modeled as such. In quantum physics, bosonic Gaussian states are fundamentally important for quantum optics and continuous-variable quantum information [40], while fermionic Gaussian states are crucial in condensed matter theory and quantum transport to describe, e.g., spin chains, superconductivity, and topological phases [41]. When assuming Gaussian system and/or Gaussian environment, several scattered results can be found in the literature regarding strong-coupling non-Markovian dynamics, as we will explore in the following pages.

At this point it is worth pointing out that the standard theory of open quantum systems, which focuses on finding master equations, is not the only existent approach to the study of non-equilibrium quantum systems. Condensed matter theory and many-body physics are filled with instances of non-equilibrium setups that are usually attacked with the language of *Green's functions*. Powerful tools emerged over the decades on this parallel line of research, and a prominent role is occupied by the so-called *Schwinger-Keldysh contour* [42, 43], a technique whose main power can be summarized as "simplification through rewriting", as we will better discuss later on. In many-body theory it led to the development of *Keldysh field theory*, a structured framework to perturbatively analyze complex non-equilibrium interacting systems and transport setups [44–46].

It is natural to ask how the Green's functions language interfaces with the theory of open quantum systems. While several works attempted the construction of a solid link between master equations and Keldysh field theory [47–52], we believe there are much more unexplored possibilities to incorporate the powerful tools of many-body physics into the problem of microscopically deriving master equations. The second part of this thesis is dedicated to the formulation of a *contour formalism* which allows us to make important statements about the dynamics of open Gaussian systems, surpassing in generality existing results and unifying statements coming from papers commonly read by distinct communities.

Having established the context, motivations, and basic research questions underlying this work, we will now sketch the structure of the thesis by providing a brief description of the content of the following chapters.

- Chapter 2: **Open Quantum Systems**
  In this preliminary chapter we present the fundamental concepts of the theory of open quantum systems, which constitute the backbone of the entire discussion. We focus especially on the structure of time-local master equations, the difference between Markovian and non-Markovian dynamics, the weak-coupling approach to a microscopic derivation, and the Redfield equation.

- Chapter 3: **Regularization Techniques**

  Based on the following publications:

  [38] A. D'Abbruzzo, V. Cavina, and V. Giovannetti, *A time-dependent regularization of the Redfield equation*, SciPost Phys. **15**, 117 (2023).

  [39] A. D'Abbruzzo, D. Farina, and V. Giovannetti, *Recovering complete positivity of non-Markovian quantum dynamics with Choi-proximity regularization*, Phys. Rev. X **14**, 031010 (2024).

  Following the presentation of the Redfield equation, here we discuss various techniques to regularize master equations that violate positivity. After discussing a few famous approaches to regularize the (time-independent) Redfield equation, we illustrate two novel techniques that can be employed to successfully regularize any master equation: the *dynamical regularization* and the *Choi-proximity regularization*. The former enforces Markovianity but keeps the time dependence of the master equation coefficients into account, thus boosting the performance with respect to other methods. The latter, instead, goes beyond the Markovian regime at the cost of increasing the complexity to a tomography-like scheme.

- Chapter 4: **Contour Formulation**
  Here we introduce a contour formulation of quantum dynamics which takes inspiration from Keldysh theory but is simplified and adapted to the evolution of density operators, as this is what one is usually interested in for open quantum systems. We also introduce the Gaussian assumption and we explain how the celebrated Wick's theorem can be applied on contour variables. The result is a compact expression for the propagator that can easily be generalized to incorporate several non-trivial extensions, like initial system-environment correlations and counting statistics.

- Chapter 5: **Non-Markovian Stochastic Dynamics**

  Based on the following publication:

  [53] V. Cavina, A. D'Abbruzzo, and V. Giovannetti, *Unifying quantum stochastic methods using Wick's theorem on the Keldysh contour*, Phys. Rev. Research **7**, 043262 (2025).

  In this chapter we apply the contour formalism developed in Chap. 4 to elaborate a non-Markovian stochastic description of open quantum dynamics in the presence of a Gaussian environment. This approach unifies several results found in the literature under the banner of a single contour noise. We are also able to use this insight to dress the master equation with an interesting semiclassical measurement interpretation.

- Chapter 6: **The Gaussian Master Equation**

  Based on the following publication:

  [54] A. D'Abbruzzo, V. Giovannetti, and V. Cavina, *Exact non-Markovian master equations: A generalized derivation for Gaussian systems*, Phys. Rev. Lett. **135**, 240401 (2025).

  This chapter present a central achievement of the thesis. Specifically, we obtain the *exact* master equation for a generic Gaussian system linearly coupled to a Gaussian environment, which we dub the *Gaussian master equation (GME)*. In doing so, we generalize existing scattered results and provide an intuitive and approachable equation with a clear link to the weak-coupling expansion and the Redfield equation. The chapter contains a detailed derivation of the GME, its reformulation in physical-time variables, and a small example to showcase its relative simplicity.

- Chapter 7: **Conclusions**
  Finally, here we draw our conclusions and outline the prospects of possible future research efforts this work could spark.

Chapter 2

Open Quantum Systems

This preliminary chapter introduces selected topics in the theory of open quantum systems, with the aim of describing the context from which the rest of the thesis is developed.

In Sec. 2.1 we recall the basic concepts of density operator and CPT map. Then, in Sec. 2.2 we explore how time evolution is mathematically accounted for in both closed and open quantum systems. We also discuss the canonical form of time-local master equations and the difference between Markovian and non-Markovian dynamics. Finally, in Sec. 2.3 we present the standard microscopic derivation based on the weak-coupling expansion, culminating in the famous Redfield equation.

2.1 Quantum states

2.1.1 Density operators

Let us consider a quantum system which, for simplicity, is represented by a finite-dimensional Hilbert space $\mathcal{H}$. Let us also indicate with $\mathrm{L}(\mathcal{H})$ the space of linear operators $X : \mathcal{H} \to \mathcal{H}$. According to the axioms of quantum theory [55–57], a *state* of the system is represented by a *density operator*, i.e., a Hermitian operator $\rho \in \mathrm{L}(\mathcal{H})$ that is positive semidefinite[1], $\rho \geq 0$, and normalized to have $\mathrm{Tr}\,\rho = 1$. Such properties are directly related to the fact that measurement probabilities should be non-negative and should sum up to one. The set of quantum states,

$$\mathfrak{S}(\mathcal{H}) := \left\{\rho \in \mathrm{L}(\mathcal{H}) : \rho \geq 0,\ \mathrm{Tr}\,\rho = 1\right\} \tag{2.1}$$

is a closed convex subset of $\mathrm{L}(\mathcal{H})$. In case $\rho = |\psi\rangle\langle\psi|$ for a certain $|\psi\rangle \in \mathcal{H}$, we say that the state is *pure*; otherwise, it is *mixed*. Any density operator can be written as a convex combination of pure states: $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$, with $p_k \geq 0$ and $\sum_k p_k = 1$. Moreover, given a state ρ and an observable $X \in \mathrm{L}(\mathcal{H})$, the expectation value associated with the distribution of measurement outcomes of X is given by the *Born rule* $\langle X\rangle_\rho := \mathrm{Tr}\big[X\rho\big]$. We assume the reader is already familiar with the concept of density operator and we refer to standard treatments for additional clarifications [55–57].

Since the universe is not exhausted by a single quantum system, we should consider what happens when we combine multiple systems. By the axioms of quantum theory, the Hilbert

[1] Recall that $P \in \mathrm{L}(\mathcal{H})$ is a *positive semidefinite* operator, and we write $P \geq 0$, when its eigenvalues are all non-negative, so that $\langle v|P|v\rangle \geq 0$ for any $|v\rangle \in \mathcal{H}$.

space of two distinguishable[2] systems A and B with Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ is given by the tensor product $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. A general state of the whole AB compound must then have the form

$$\rho_{AB} = \sum_{i,j} \alpha_{ij} \rho_{A,i} \otimes \rho_{B,j}, \tag{2.2}$$

where $\rho_{A,i} \in \mathfrak{S}(\mathcal{H}_A)$, $\rho_{B,j} \in \mathfrak{S}(\mathcal{H}_B)$, and $\{\alpha_{ij}\} \subset \mathbb{C}$ (with appropriate constraints to ensure that ρ_{AB} is a valid density operator). In case the sum has a single term, $\rho_{AB} = \rho_A \otimes \rho_B$, we say that the state is *factorized*—the two systems live in complete respective isolation; otherwise we say that the state is *correlated*. If α is diagonal, then ρ_{AB} describes an ensemble of factorized states: we say that it is *classically correlated*, or *separable*. Finally, if α is not diagonal we say that ρ_{AB} is *quantumly correlated*, or *entangled*.

Given a certain ρ_{AB}, suppose now we want to perform a measurement on system A only. We are naturally brought to the following question: can we find $\rho_A \in \mathfrak{S}(\mathcal{H}_A)$ such that

$$\mathrm{Tr}\big[(X \otimes \mathbb{1})\rho_{AB}\big] = \mathrm{Tr}\big[X\rho_A\big] \tag{2.3}$$

for every $X \in \mathrm{L}(\mathcal{H}_A)$? The answer is yes, and the only possible choice is

$$\rho_A = \mathrm{Tr}_B[\rho_{AB}], \tag{2.4}$$

where $\mathrm{Tr}_B : \mathrm{L}(\mathcal{H}_{AB}) \to \mathrm{L}(\mathcal{H}_A)$ is called *partial trace over B*, defined as $\mathrm{Tr}_B[X \otimes Y] = (\mathrm{Tr}\, Y)X$ on factorized inputs and then linearly extended to the whole $\mathrm{L}(\mathcal{H}_{AB})$. The proof can be found in standard treatments, such as Ref. [55].

Note that once we have composite systems, the formulation of quantum theory with (mixed) density operators becomes necessary. In fact, even if we always start from a pure state $|\Psi\rangle \in \mathcal{H}_{AB}$ of the compound, we need to take a partial trace $\mathrm{Tr}_B |\Psi\rangle\langle\Psi|$ to describe the state of system A. This is not a pure state, unless $|\Psi\rangle$ is factorized[3]. Therefore, the density matrix formulation is necessary to account for systems that may be correlated with something else: this is precisely the setting we are interested in when talking about open quantum systems.

2.1.2 CPT maps

Physical objects are not static. Something eventually happens to them, and they react by changing their state. In our context, since states are represented using operators, it is natural to describe such transformations using maps of the form $\Phi : \mathrm{L}(\mathcal{H}) \to \mathrm{L}(\mathcal{H})$, often referred to as *superoperators* (since they act on operators).

Of course, not every such Φ is suitable as a transformation of states: a necessary condition for having a physically reasonable Φ is that the space of states $\mathfrak{S}(\mathcal{H})$ should be left invariant by Φ: this imposes few constraints.

[2] In case the systems are composed of indistinguishable particles, more care is needed. Specifically, the presence of fermionic particles requires a re-examination of the concepts of tensor product and partial trace [58]. Nevertheless, it is possible to re-obtain standard tensor products with an appropriate modification of the involved operators. In the context of the thesis, we will not encounter explicit problems in this regard, but we encourage the reader to keep in mind such issue.

[3] If $|\Psi\rangle = |\psi\rangle \otimes |\phi\rangle$, clearly $\mathrm{Tr}_B\, |\Psi\rangle\langle\Psi| = |\psi\rangle\langle\psi|$, which is pure. Assume instead $|\Psi\rangle = \sum_{i,j} \alpha_{ij} |\psi_i\rangle \otimes |\phi_j\rangle$ with $\{|\psi_i\rangle\}$ and $\{|\phi_j\rangle\}$ orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, and $\mathrm{rank}(\alpha) > 1$. Then, $\mathrm{Tr}_B\, |\Psi\rangle\langle\Psi| = \sum_{i,j} (\alpha\alpha^\dagger)_{ij} |\psi_i\rangle\langle\psi_j|$. This is mixed because $\alpha\alpha^\dagger$ has more than one nonzero eigenvalue, since $\mathrm{rank}(\alpha\alpha^\dagger) = \mathrm{rank}(\alpha)$.

First, we ask to preserve the convexity of $\mathfrak{S}(\mathcal{H})$. A natural way to fulfill this requirement is by making a linearity assumption:[4]

$$\Phi\left(\sum_i \alpha_i X_i\right) = \sum_i \alpha_i \Phi(X_i), \quad \forall\{\alpha_i\} \subset \mathbb{C}, \quad \forall\{X_i\} \subset \mathrm{L}(\mathcal{H}). \tag{2.5}$$

Second, we should require preservation of positive semidefiniteness:

$$X \geq 0 \quad \Rightarrow \quad \Phi(X) \geq 0. \tag{2.6}$$

If this is the case, we say that Φ is *positive*. Note that if Φ is positive, then it is also *Hermitian-preserving*, meaning that if $X = X^\dagger$ then $\Phi(X) = [\Phi(X)]^\dagger$. In fact, for any Hermitian X we can write $X = X_+ - X_-$ with $X_\pm \geq 0$ (just take the "positive" and "negative" parts of the spectral decomposition), so that $\Phi(X)^\dagger = [\Phi(X_+) - \Phi(X_-)]^\dagger = \Phi(X_+) - \Phi(X_-) = \Phi(X)$. Finally, if $\mathrm{Tr}\, X = 1$ we should have $\mathrm{Tr}\, \Phi(X) = 1$. It is convenient to require then

$$\mathrm{Tr}\, \Phi(X) = \mathrm{Tr}\, X, \quad \forall X \in \mathrm{L}(\mathcal{H}). \tag{2.7}$$

If this is the case, we say that Φ is *trace-preserving*.

A linear positive trace-preserving superoperator leaves the set of states invariant. However, this is not the whole story: we should check what happens when our system A is considered in combination with another one B. More specifically, if Φ leaves $\mathfrak{S}(\mathcal{H}_A)$ invariant, can we be sure that $\Phi \otimes \mathbb{1}_B$, with $\mathbb{1}_B$ being the identity on B, leaves $\mathfrak{S}(\mathcal{H}_{AB})$ invariant? If Φ is a reasonable physical transformation, we expect the answer to be yes. If the whole setup is prepared in a separable state,

$$(\Phi \otimes \mathbb{1}_B)\left(\sum_i \alpha_i \rho_{A,i} \otimes \rho_{B,i}\right) = \sum_i \alpha_i \Phi(\rho_{A,i}) \otimes \rho_{B,i}, \tag{2.8}$$

which is still a valid separable state of the compound when Φ is positive and trace-preserving. However, we cannot say the same if the input to $\Phi \otimes \mathbb{1}_B$ is an entangled state [55–57].

As an example, consider the case in which A and B are two-dimensional systems, with Hilbert spaces spanned by orthonormal bases indicated with $\{|0\rangle, |1\rangle\}$. Take then as Φ the transpose map $\Phi(X) = X^T$. Of course, this is a linear positive trace-preserving operation, since transposition does not alter the eigenvalues. However, consider what happens if we prepare the whole setup in the entangled state $|\Psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. Then,

$$(\Phi \otimes \mathbb{1}_B)\,|\Psi\rangle\langle\Psi| = \frac{1}{2}\big(\,|00\rangle\langle 00| + |10\rangle\langle 01| + |10\rangle\langle 01| + |11\rangle\langle 11|\,\big). \tag{2.9}$$

A simple computation reveals that the operator on the right-hand side possesses a negative eigenvalue: thus, it cannot be a valid state of the compound.

In order to keep into consideration that our system can be entangled with another one, positivity is not enough: we must require *complete positivity*, which is to say that $\Phi \otimes \mathbb{1}_B$ must be positive for every choice of "ancillary" system B. Of course, a completely positive map is also a positive map, but the converse is not true, as we just showed.

[4] An immediate consequence of linearity is that equivalent ensembles stay equivalent after the application of Φ. Interestingly, rejecting this statement—and therefore, rejecting linearity—leads to the possibility of instantaneous signaling, which is certainly undesirable [59].

We can now finally make the following statement: *a physically reasonable transformation of quantum states must be represented by a linear, completely positive, and trace-preserving superoperator* Φ. These requirements are often abbreviated by saying that Φ is a *CPT map*, a *quantum channel*, or a *quantum operation*.

A natural question follows: can we characterize the form of CPT maps out of all possible maps? In order to answer, we first establish a seemingly unrelated notational device. Fix an orthonormal basis $\{|n\rangle\} \subset \mathcal{H}$ of the system and consider the maximally entangled state

$$|\mathcal{E}\rangle := \frac{1}{\sqrt{d}} \sum_n |n\rangle \otimes |n\rangle \in \mathcal{H} \otimes \mathcal{H}, \tag{2.10}$$

where $d := \dim \mathcal{H}$. Then, for a given map Φ, we define its *Choi operator* as

$$J(\Phi) := (\Phi \otimes \mathbb{1}) |\mathcal{E}\rangle\langle\mathcal{E}| = \frac{1}{d} \sum_{n,m} \Phi(|n\rangle\langle m|) \otimes |n\rangle\langle m| \in \mathrm{L}(\mathcal{H} \otimes \mathcal{H}). \tag{2.11}$$

By inspection, it is easy to see that, for any $X = \sum_{i,j} x_{ij} |i\rangle\langle j| \in \mathrm{L}(\mathcal{H})$,

$$\begin{aligned} \Phi(X) &= \sum_{i,j} x_{ij} \Phi(|i\rangle\langle j|) = d \sum_{i,j} x_{ij} (\mathbb{1} \otimes \langle i|) J(\Phi) (\mathbb{1} \otimes |j\rangle) \\ &= d \sum_{i,j} x_{ij} \operatorname{Tr}_2[J(\Phi)(\mathbb{1}_A \otimes |j\rangle\langle i|)] = d \operatorname{Tr}_2[J(\Phi)(\mathbb{1} \otimes X^T)], \end{aligned} \tag{2.12}$$

where Tr_2 stands for the partial trace over the second copy of the system. This means that there is a one-to-one correspondence between linear superoperators Φ and Choi operators $J(\Phi)$: such a correspondence is often referred to as *Choi-Jamiołkowski isomorphism*.

The importance of the Choi operator is established by the following fundamental result, whose proof can be found in any quantum information textbook [55–57].

Theorem 2.1. *Let Φ be a linear superoperator on $\mathrm{L}(\mathcal{H})$. Then:*

- *(i) Φ is completely positive if and only if $J(\Phi) \geq 0$. Equivalently, $\Phi(X) = \sum_\alpha K_\alpha X K_\alpha^\dagger$ for some $\{K_\alpha\} \subset \mathrm{L}(\mathcal{H})$.*
- *(ii) Φ is trace-preserving if and only if $\mathrm{Tr}_1 J(\Phi) = \mathbb{1}/d$, where Tr_1 is the partial trace over the original system. Equivalently, $\Phi(X) = \sum_\alpha K_\alpha X Q_\alpha$ for some $\{K_\alpha\}, \{Q_\alpha\} \subset \mathrm{L}(\mathcal{H})$ satisfying $\sum_\alpha Q_\alpha K_\alpha = \mathbb{1}$.*
- *(iii) Φ is CPT if and only if $J(\Phi) \geq 0$ and $\mathrm{Tr}_1 J(\Phi) = \mathbb{1}/d$. Equivalently, $\Phi(X) = \sum_\alpha K_\alpha X K_\alpha^\dagger$ for some $\{K_\alpha\} \subset \mathrm{L}(\mathcal{H})$ satisfying $\sum_\alpha K_\alpha^\dagger K_\alpha = \mathbb{1}$.*

The expression in (i) is usually called *Kraus representation* of Φ, and the operators K_α are consequently called *Kraus operators*. From this representation, it is immediate to see that products of CPT maps are CPT maps too.

There are two remarkable facts about this theorem. First, even though the definition of complete positivity involves an arbitrary ancillary system, we actually only need to consider one with the same Hilbert space as the original system. Second, we do not need to check that $(\Phi \otimes \mathbb{1})P$ is positive for every possible choice of $P \geq 0$ when investigating complete positivity: it is sufficient to just take $P = |\mathcal{E}\rangle\langle\mathcal{E}|$. This is why the Choi operator is so important in the characterization of completely positive maps.

Theorem 2.1 thus establishes a one-to-one correspondence between the set of CPT maps and the closed convex set of *physical Choi operators*

$$\mathfrak{J}(\mathcal{H}) := \{P \in \mathrm{L}(\mathcal{H} \otimes \mathcal{H}) : P \geq 0, \mathrm{Tr}_1 P = \mathbb{1}/\dim \mathcal{H}\}. \tag{2.13}$$

Note that $\mathfrak{J}(\mathcal{H}) \subset \mathfrak{S}(\mathcal{H}\otimes\mathcal{H})$, which means that physical Choi operators are actual admissible states of the combined system-ancilla setup.

We conclude this section by discussing a concept which will be useful later. Given two states $\rho_1, \rho_2 \in \mathfrak{S}(\mathcal{H})$, it is a known fact of quantum information theory that the maximal probability of correctly distinguish ρ_1 from ρ_2 with a one-shot measurement is directly linked to the trace distance [55–57]

$$D(\rho_1, \rho_2) := \frac{1}{2}\left\|\rho_1 - \rho_2\right\|_1, \tag{2.14}$$

where $\|X\|_1 := \mathrm{Tr}\,|X| = \mathrm{Tr}\,\sqrt{X^\dagger X}$ is the trace norm. The question we want to ask is the following: how does the action of a CPT map affects the distinguishability of two states, as measured by their trace distance? The answer is the following known result [56, 60].

Theorem 2.2. *Let Φ be a positive and trace-preserving linear map on $\mathrm{L}(\mathcal{H})$. Then,*

$$D(\Phi(\rho_1), \Phi(\rho_2)) \leq D(\rho_1, \rho_2), \quad \forall \rho_1, \rho_2 \in \mathfrak{S}(\mathcal{H}). \tag{2.15}$$

In other words, a physical transformation of states must necessarily bring states closer to each other, making them less distinguishable. This is a structural fact that will play an important role when discussing non-Markovianity in Sec. 2.2.4. Note that complete positivity is not required for this argument and that plain positivity is enough.

2.2 Time evolution

In the previous section we saw that the state of a quantum system can be described using density operators, and that a physically reasonable transformation of such states must be represented by a CPT map. A particularly important instance of state transformation is naturally given by *time evolution*. However, since time is a continuous parameter in standard quantum theory, it is more appropriate to study parameterized families $\{\Phi_t\}$ of CPT maps, with t being time.

2.2.1 Time evolution in closed systems

For exposition purposes, we start the discussion by reviewing how time evolution works in the easier setting of *closed* systems, i.e., systems which are assumed to evolve independently of any other system that may be present in the universe. This is of course an idealized scenario, but it forms the fundamental basis for all the subsequent discussion.

According to the axioms of quantum theory, the state of a closed system $|\psi_t\rangle \in \mathcal{H}$ at time t obeys the *Schrödinger equation* [1]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi_t\rangle = -iH(t)\,|\psi_t\rangle\,, \tag{2.16}$$

for a suitable system-dependent Hermitian *Hamiltonian* operator $H(t) \in \mathrm{L}(\mathcal{H})$. Note that if $|\psi_t\rangle$ satisfies (2.16) then $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t|\psi_t\rangle = 0$, hence normalization is correctly preserved. Since (2.16) is a first-order linear differential equation, its solution satisfies

$$|\psi_t\rangle = U_{t,s}\,|\psi_s\rangle\,, \quad \forall t \geq s, \tag{2.17}$$

where $U_{t,s} \in \mathrm{L}(\mathcal{H})$ is called *evolution operator* or *propagator*. Clearly, $U_{s,s} = \mathbb{1}$ and, since $\langle\psi_t|\psi_t\rangle = \langle\psi_s|U_{t,s}^\dagger U_{t,s}|\psi_s\rangle$, the propagator must be unitary, $U_{t,s}^\dagger U_{t,s} = U_{t,s}U_{t,s}^\dagger = \mathbb{1}$. Moreover,

$$|\psi_s\rangle = U_{t,s}^\dagger |\psi_t\rangle\,, \quad \forall t \geq s, \tag{2.18}$$

hence $U_{t,s}^\dagger$ can be seen as an "inverse" propagator. Occasionally, we may write $U_{t,s}^\dagger \equiv U_{s,t}$. We can also infer the composition law

$$U_{t,s} = U_{t,t'}U_{t',s}, \quad \forall\, s \leq t' \leq t. \tag{2.19}$$

Of course, the Schrödinger equation can equivalently be written as a differential equation for the propagator as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}U_{t,s} = -iH(t)U_{t,s}, \quad U_{s,s} = \mathbb{1}. \tag{2.20}$$

An important result is that the unique solution to Eq. (2.20) is

$$U_{t,s} = \mathbb{1} + \sum_{n=1}^{\infty}(-i)^n \int_s^t \mathrm{d}\tau_1 \int_s^{\tau_1} \mathrm{d}\tau_2 \ldots \int_s^{\tau_{n-1}} \mathrm{d}\tau_n\, H(\tau_1)H(\tau_2)\ldots H(\tau_n), \tag{2.21}$$

which can be proved by directly taking the time derivative.

Note that the string of operators $H(\tau_1)H(\tau_2)\ldots H(\tau_n)$ is laid out such that $\tau_1 > \tau_2 > \ldots > \tau_n$. As a consequence, it is typical to rewrite the above equation using the following convenient notational device. Given n parameterized operators $X_1(t_1), \ldots, X_n(t_n)$, there exists a permutation $\varphi : \{1, \ldots, n\} \to \{1, \ldots, n\}$ such that $t_{\varphi(1)} > t_{\varphi(2)} > \ldots > t_{\varphi(n)}$. We define the *time-ordering operation* $\mathbb{T}$ by

$$\mathbb{T}\{X_1(t_1)\ldots X_n(t_n)\} := X_{\varphi(1)}(t_{\varphi(1)})\ldots X_{\varphi(n)}(t_{\varphi(n)}). \tag{2.22}$$

In other words, $\mathbb{T}$ takes as input a product of operators and has the effect of reordering them such that the time parameter increases from right to left. Sometimes it will be convenient to consider also an *anti-time-ordering operation* $\widetilde{\mathbb{T}}$ which orders time in the opposite direction:

$$\widetilde{\mathbb{T}}\{X_1(t_1)\ldots X_n(t_n)\} := X_{\varphi(n)}(t_{\varphi(n)})\ldots X_{\varphi(1)}(t_{\varphi(1)}). \tag{2.23}$$

Note that all operators can be thought of as commuting with each other when put inside $\mathbb{T}$, since $\mathbb{T}$ will eventually order them in the same way. More explicitly,

$$\mathbb{T}\big\{X_{\sigma(1)}(t_{\sigma(1)})\ldots X_{\sigma(n)}(t_{\sigma(n)})\big\} = \mathbb{T}\{X_1(t_1)\ldots X_n(t_n)\} \tag{2.24}$$

for any permutation σ of $\{1, \ldots, n\}$.

Now, let $\mathfrak{S}_n$ be the set of permutations of $\{1, \ldots, n\}$. We can write

$$\begin{aligned}
\int_s^t \mathrm{d}\tau_1 \int_s^{\tau_1} \mathrm{d}\tau_2 \ldots \int_s^{\tau_{n-1}} \mathrm{d}\tau_n\, H(\tau_1)H(\tau_2)\ldots H(\tau_n)& \\
= \int_s^t \mathrm{d}\tau_1 \int_s^{\tau_1} \mathrm{d}\tau_2 \ldots \int_s^{\tau_{n-1}} \mathrm{d}\tau_n\, \mathbb{T}\{H(\tau_1)H(\tau_2)\ldots H(\tau_n)\}& \\
= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n} \int_s^t \mathrm{d}\tau_1 \int_s^{\tau_1} \mathrm{d}\tau_2 \ldots \int_s^{\tau_{n-1}} \mathrm{d}\tau_n\, \mathbb{T}\big\{H(\tau_{\sigma(1)})H(\tau_{\sigma(2)})\ldots H(\tau_{\sigma(n)})\big\}& \\
= \frac{1}{n!}\int_s^t \mathrm{d}\tau_1 \int_s^t \mathrm{d}\tau_2 \ldots \int_s^t \mathrm{d}\tau_n\, \mathbb{T}\{H(\tau_1)H(\tau_2)\ldots H(\tau_n)\},&
\end{aligned} \tag{2.25}$$

where in the first equality we used the fact that $H(\tau_1)\dots H(\tau_n)$ is already ordered, in the second equality we applied the symmetry property (2.24), and in the third equality we used the known expression for the integral over the n-dimensional hypercube $[s,t]^n$. As a consequence,

$$U_{t,s} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_s^t \mathrm{d}^n\boldsymbol{\tau}\, \mathbb{T}\{H(\tau_1)\dots H(\tau_n)\}, \tag{2.26}$$

where $\mathrm{d}^n\boldsymbol{\tau} \equiv \mathrm{d}\tau_1\dots\mathrm{d}\tau_n$, and it is understood that the term with $n=0$ is equal to the identity. This expression is known as *Dyson series*. It can also be written as a more compact *ordered exponential* [1]

$$U_{t,s} = \mathbb{T}\exp\left[-i\int_s^t H(\tau)\,\mathrm{d}\tau\right], \tag{2.27}$$

where it is understood that the time ordering $\mathbb{T}$ is applied to the integrands after the exponential is expanded. Of course, in case the Hamiltonian does not change with time, $H(t)\equiv H$, then time ordering is unnecessary and $U_{t,s} = e^{-iH(t-s)}$.

In the following it will be useful to note that the ordered exponential can be written as the product of an infinite number of infinitesimal exponentials[5]:

$$U_{t,s} = \lim_{n\to\infty}\left[e^{-iH(t_n)\Delta t}e^{-iH(t_{n-1})\Delta t}\dots e^{-iH(t_0)\Delta t}\right], \tag{2.28}$$

where $\Delta t = (t-s)/n$ and $t_j = s + j\Delta t$ for $j\in\{0,\dots,n\}$. The proof is simple:

$$\begin{aligned}\lim_{n\to\infty}\left[e^{-iH(t_n)\Delta t}\dots e^{-iH(t_0)\Delta t}\right] &= \lim_{n\to\infty}\mathbb{T}\left\{e^{-iH(t_n)\Delta t}\dots e^{-iH(t_0)\Delta t}\right\}\\ &= \lim_{n\to\infty}\mathbb{T}\exp\left[-i\sum_{j=0}^{n}H(t_j)\Delta t\right] = \mathbb{T}\exp\left[-i\int_s^t H(\tau)\,\mathrm{d}\tau\right],\end{aligned} \tag{2.29}$$

where in the first equality we used the fact that the exponentials are already ordered, in the second equality we thought of the exponentials as commuting operators inside $\mathbb{T}$—and thus we compacted them into a single exponential—and in the third equality we recognized a Riemann sum which turns into an integral upon taking the limit.

Summarizing, we showed that the Schrödinger equation (2.16) for the evolution of pure states is solved by Eq. (2.17) with the propagator (2.27). But what about mixed states? Since density operators can be written as convex combinations of pure states, it is immediate to realize that

$$\rho(t) = U_{t,s}\rho(s)U_{t,s}^\dagger \equiv \mathcal{U}_{t,s}[\rho(s)]. \tag{2.30}$$

Since $U_{t,s}$ is unitary, this is a valid Kraus decomposition, so that $\mathcal{U}_{t,s}$ is a CPT map for every $t\geq s$. By taking the derivative with respect to t, we see that this is the unique solution to the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i[H(t),\rho(t)], \tag{2.31}$$

where $[X,Y] \coloneqq XY - YX$ is the commutator between the operators X and Y. Eq. (2.31) is known as the *von Neumann equation* and it is the generalization of the Schrödinger equation to density operators [61].

[5] In mathematical terms, this is known as a *left product integral*.

2.2.2 Time evolution in open systems

The moment we let our system of interest interact with other systems, we can no longer expect its evolution to be dictated by a von Neumann equation. We will now discuss how to formally describe the time evolution in this more complex scenario, involving *open* quantum systems [6–8].

Let S be our system of interest, and let E be its surrounding *environment*, i.e., all the other systems in the universe of discourse which are not S. By definition, the compound SE is a closed system, and its density operator $\rho_{SE}(t) \in \mathfrak{S}(\mathcal{H}_{SE})$ evolves unitarily, as in Eq. (2.31). Let us fix an initial time point t_0 at which we agree that the state of the universe is $\rho_{SE}(t_0)$. Then, the state of S at time $t \geq t_0$, $\rho(t) = \mathrm{Tr}_E[\rho_{SE}(t)]$, is given by

$$\rho(t) = \mathrm{Tr}_E[\boldsymbol{\mathcal{U}}_{t,t_0}\rho_{SE}(t_0)]. \tag{2.32}$$

Since S is what we care about, we would like a *dynamical map* Φ_t such that $\rho(t) = \Phi_t[\rho(t_0)]$, with $\rho(t_0) = \mathrm{Tr}_E[\rho_{SE}(t_0)]$. Unfortunately, it is impossible to do so if we make no assumption about $\rho_{SE}(t_0)$ [62, 63]. Consider in fact the following example. Suppose both system and environment are two-dimensional systems spanned by orthonormal bases indicated with $\{|0\rangle, |1\rangle\}$, and suppose the whole dynamics is described by the one-shot CNOT gate

$$U_{t,t_0} = \mathbb{1}_S \otimes |0\rangle\langle 0| + \sigma_x \otimes |1\rangle\langle 1|, \tag{2.33}$$

where σ_x is the Pauli operator with actions $\sigma_x |0\rangle = |1\rangle$ and $\sigma_x |1\rangle = |0\rangle$. Consider now the following two different initial states:

$$\rho_{SE}^{(1)}(t_0) = \frac{1}{2}\big[\,|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|\,\big], \tag{2.34a}$$

$$\rho_{SE}^{(2)}(t_0) = \frac{1}{2}\big[\,|1\rangle\langle 1| \otimes |0\rangle\langle 0| + |0\rangle\langle 0| \otimes |1\rangle\langle 1|\,\big]. \tag{2.34b}$$

The reduced state of the system is the same in the two cases, $\rho(t_0) = \mathrm{Tr}_E\, \rho_{SE}^{(1,2)}(t_0) = \mathbb{1}_S/2$. However, if we first apply the dynamics,

$$\boldsymbol{\mathcal{U}}_{t,t_0}\rho_{SE}^{(1)}(t_0) = |0\rangle\langle 0| \otimes \frac{\mathbb{1}_E}{2}, \qquad \boldsymbol{\mathcal{U}}_{t,t_0}\rho_{SE}^{(2)}(t_0) = |1\rangle\langle 1| \otimes \frac{\mathbb{1}_E}{2}, \tag{2.35}$$

and then we take the partial trace over the environment, the system ends up in two different states. We conclude that $\rho(t)$ is not uniquely defined as a function of $\rho(t_0)$ alone.

The easiest way out of this problem is to assume that system and environment are initially not correlated:

$$\rho_{SE}(t_0) = \rho(t_0) \otimes \Omega_0, \tag{2.36}$$

where $\Omega_0 \in \mathfrak{S}(\mathcal{H}_E)$ is a fixed state of the environment. In this case, we indeed have

$$\rho(t) = \Phi_t[\rho(t_0)], \qquad \Phi_t(X) := \mathrm{Tr}_E[\boldsymbol{\mathcal{U}}_{t,t_0}(X \otimes \Omega_0)]. \tag{2.37}$$

It is easy to show that this is a CPT map for every $t \geq t_0$, and therefore it describes an admissible physical evolution for S[6].

[6] Actually, the expression in (2.37) is another way to characterize CPT maps, and it is known as the *Stinespring representation* of Φ_t, or as a *Stinespring dilation* [55–57].

The assumption of initial factorized state can be slightly relaxed if we adopt a more operational viewpoint [63]. Since a dynamical map Φ_t should be able to describe the evolution of an arbitrary initial state of the system S, we can imagine to employ the following procedure[7]: starting from a naturally occurring universe state $\rho_{SE}(t_0)$, discard the system S and prepare it anew in a desired state $\rho(t_0)$. The "input" to the unitary evolution is still a factorized state $\rho(t_0) \otimes \Omega_0$, but this time Ω_0 is not an arbitrary state of the environment: it is obtained by tracing out the system from the initial universe state, $\Omega_0 = \mathrm{Tr}_S[\rho_{SE}(t_0)]$.

Writing Φ_t in Eq. (2.37) is not the end of the story. The environment E is typically an incredibly large object, and the map $\mathcal{U}_{t,t_0}$ cannot be practically handled in the vast majority of scenarios. These difficulties can be softened if we manage to write a differential equation for $\rho(t)$ using only the information about the environment that is relevant for the evolution of $\rho(t)$. Since S is usually much more manageable and under our control, solving such equation of motion is much easier than calculating the whole $\mathcal{U}_{t,t_0}$. Note also that if we are only interested in the evolution of S, the object $\mathcal{U}_{t,t_0}$ contains a huge amount of unwanted information concerning the evolution of E.

There are many ways to approach the problem of writing an equation of motion of which Φ_t is the solution. Here we describe a path that makes use of an additional assumption about Φ_t. We say that the dynamical map Φ_t is *regular* if, for any $t \geq t_0$, there exists a map Φ_t^{-1} such that $\Phi_t \Phi_t^{-1} = \Phi_t^{-1} \Phi_t = \mathbb{1}_S$. When viewed as a linear operator, Φ_t^{-1} is just the inverse of Φ_t; however, Φ_t^{-1} will not be a CPT map in general[8], and it does not represent any physical transformation. What we are practically requiring is that different initial states never cross each other during the evolution, i.e., $\rho_1 \neq \rho_2 \Rightarrow \Phi_t(\rho_1) \neq \Phi_t(\rho_2)$. Regularity thus indeed restricts the set of evolutions we can cover, but it is usually accepted as a mild condition [64].

Suppose we are allowed to take the time derivative $\mathrm{d}\Phi_t/\mathrm{d}t$ of a regular dynamical map Φ_t—otherwise there is little hope of writing an equation of motion. Then, we define the *generator* of Φ_t as

$$\mathcal{L}_t := \frac{\mathrm{d}\Phi_t}{\mathrm{d}t} \Phi_t^{-1}. \tag{2.38}$$

From the generator, we obviously have the following first-order linear differential equation:

$$\frac{\mathrm{d}\Phi_t}{\mathrm{d}t} = \mathcal{L}_t \Phi_t, \qquad \Phi_{t_0} = \mathbb{1}_S. \tag{2.39}$$

Equivalently, if we write $\rho(t) = \Phi_t(\rho_0)$ with $\rho_0 \in \mathfrak{S}(\mathcal{H}_S)$ being an arbitrary initial state,

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = \mathcal{L}_t[\rho(t)], \qquad \rho(t_0) = \rho_0. \tag{2.40}$$

This is called a *master equation* for $\rho(t)$, or a *time-local master equation* to emphasize that the generator $\mathcal{L}_t$ depends on time t only. We can formally write the solution using an ordered exponential:

$$\rho(t) = \mathbb{T} \exp\left[\int_{t_0}^{t} \mathrm{d}\tau \, \mathcal{L}_\tau\right] \rho_0. \tag{2.41}$$

[7] This is the prescription proposed in Ref. [63], where it is shown that this is the natural choice if one wants to interpret the dynamical map as a "law of motion".

[8] One can show that Φ_t^{-1} is a CPT map if and only if $\Phi_t(X) = UXU^\dagger$ for some U unitary [7]. Therefore, for a truly open system, Φ_t^{-1} is never CPT: this is why irreversibility is such an important concept in open system dynamics.

The fact that Φ_t is a CPT map imposes some constraints on $\mathcal{L}_t$: we cannot expect an arbitrary superoperator to be a valid generator for a master equation. Unfortunately, at the time of writing, there is no known general characterization of generators giving rise to CPT dynamical maps (or even just positive trace-preserving ones) [16, 65]. This is arguably the most important unsolved problem in the mathematical theory of open quantum systems. However, an important characterization can be given if we just use preservation of Hermiticity and trace, as shown in the following theorem [64].

Theorem 2.3. *Let Φ_t be a dynamical map on $\mathrm{L}(\mathcal{H}_S)$ satisfying the master equation* (2.40)*. Then Φ_t is Hermitian- and trace-preserving if and only if, for every $t \geq t_0$, there exists a Hermitian operator $h(t) \in \mathrm{L}(\mathcal{H}_S)$, a Hermitian coefficient matrix $\chi(t)$, and a set $\{L_i\} \subset \mathrm{L}(\mathcal{H}_S)$ of operators such that the generator of Φ_t is*

$$\mathcal{L}_t(X) = -i[h(t), X] + \sum_{i,j} \chi_{ij}(t) \left[L_i X L_j^\dagger - \frac{1}{2} \left\{ L_j^\dagger L_i, X \right\} \right], \tag{2.42}$$

where $[X, Y] := XY - YX$ is the commutator and $\{X, Y\} := XY + YX$ is the anticommutator.

Proof. First, suppose Φ_t is Hermitian- and trace-preserving. Its generator, being a linear map on $\mathrm{L}(\mathcal{H}_S)$, can be written as $\mathcal{L}_t(X) = \sum_\alpha K_\alpha(t) X Q_\alpha^\dagger(t)$ for some operators $\{K_\alpha(t)\}$ and $\{Q_\alpha(t)\}$ in $\mathrm{L}(\mathcal{H}_S)$. Let $\{G_i\}$ be an orthonormal basis of $\mathrm{L}(\mathcal{H}_S)$ and expand $K_\alpha(t) = \sum_i k_{\alpha,i}(t) G_i$ and $Q_\alpha(t) = \sum_i q_{\alpha,i}(t) G_i$, so that

$$\mathcal{L}_t(X) = \sum_{i,j} \ell_{ij}(t) G_i X G_j^\dagger, \tag{2.43}$$

where $\ell_{ij}(t) := \sum_\alpha k_{\alpha,i}(t) q_{\alpha,j}^*(t)$. Since Φ_t is Hermitian-preserving, we have $\Phi_t(X)^\dagger = \Phi_t(X)$ whenever $X = X^\dagger$. Therefore, from the master equation,

$$\mathcal{L}_t[\Phi_t(X)]^\dagger = \frac{\mathrm{d}}{\mathrm{d}t} \Phi_t(X)^\dagger = \frac{\mathrm{d}}{\mathrm{d}t} \Phi_t(X) = \mathcal{L}_t[\Phi_t(X)]. \tag{2.44}$$

This implies that the coefficient matrix $\ell(t)$ is Hermitian, $\ell_{ji}^*(t) = \ell_{ij}(t)$. Moreover, we can always choose the orthonormal set $\{G_i\}$ in such a way that one element is proportional to the identity and the other elements are traceless: specifically, we call $G_0 = \mathbb{1}_S/\sqrt{d}$ (where d is the dimension of $\mathcal{H}_S$), so that

$$\begin{aligned} \mathcal{L}_t(X) &= \frac{\ell_{00}(t)}{d} X + \frac{1}{\sqrt{d}} \sum_{i \neq 0} \ell_{i0}(t) G_i X + \frac{1}{\sqrt{d}} \sum_{j \neq 0} \ell_{0j}(t) X G_j^\dagger + \sum_{i,j \neq 0} \ell_{ij}(t) G_i X G_j^\dagger \\ &= F(t) X + X F(t)^\dagger + \sum_{i,j \neq 0} \ell_{ij}(t) G_i X G_j^\dagger, \end{aligned} \tag{2.45}$$

where $F(t) := \ell_{00}(t)/2d + \sum_{i \neq 0} \ell_{i0}(t) G_i/\sqrt{d}$. Moreover, since Φ_t is trace-preserving,

$$\mathrm{Tr}\, \mathcal{L}_t[\Phi_t(X)] = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Tr}\, \Phi_t(X) = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Tr}\, X = 0. \tag{2.46}$$

Therefore, we must have

$$F(t) + F(t)^\dagger = -\sum_{i,j \neq 0} \ell_{ij}(t) G_j^\dagger G_i. \tag{2.47}$$

Using the relation $F(t)X + XF(t)^\dagger = \frac{1}{2}[F(t) - F(t)^\dagger, X] + \frac{1}{2}\{F(t) + F(t)^\dagger, X\}$, we finally conclude

$$\mathcal{L}_t(X) = \frac{1}{2}\left[F(t) - F(t)^\dagger, X\right] + \sum_{i,j\neq 0} \ell_{ij}(t)\left[G_i X G_j^\dagger - \frac{1}{2}\left\{G_j^\dagger G_i, X\right\}\right], \tag{2.48}$$

which has the form in Eq. (2.42) once we define $h(t) := -\frac{i}{2}[F(t) - F(t)^\dagger]$, $\chi_{ij}(t) := \ell_{ij}(t)$ for $i, j \neq 0$, and $L_i := G_i$ for $i \neq 0$. Note that $h(t)$ is a Hermitian operator by construction, and that the Hermiticity of $\chi(t)$ follows from the Hermiticity of $\ell(t)$.

For the converse direction of the theorem, suppose the generator $\mathcal{L}_t$ of Φ_t is given by Eq. (2.42). By inspection, we see that

$$\mathcal{L}_t(X)^\dagger = \mathcal{L}_t(X^\dagger), \qquad \operatorname{Tr}\mathcal{L}_t(X) = 0, \tag{2.49}$$

for any $X \in \mathrm{L}(\mathcal{H}_S)$. But we also have

$$\Phi_t(X) = \mathbb{T}\exp\left[\int_{t_0}^{t} \mathrm{d}\tau\, \mathcal{L}_\tau\right]X = X + \sum_{n=1}^{\infty}\int_{t_0}^{t}\mathrm{d}\tau_1 \int_{t_0}^{\tau_1}\mathrm{d}\tau_2 \ldots \int_{t_0}^{\tau_{n-1}}\mathrm{d}\tau_n\, \mathcal{L}_{\tau_1}\mathcal{L}_{\tau_2}\ldots\mathcal{L}_{\tau_n}X. \tag{2.50}$$

In case $X = X^\dagger$, we can easily prove by induction on n that $[\mathcal{L}_{\tau_1}\ldots\mathcal{L}_{\tau_n}X]$ is Hermitian, allowing us to conclude that $\Phi_t(X)$ is Hermitian too. Finally, the property $\operatorname{Tr}\Phi_t(X) = \operatorname{Tr}X$ immediately follows from $\operatorname{Tr}\mathcal{L}_t(X) = 0$. □

Eq. (2.42) is called *canonical form* of the generator. Since $h(t)$ is Hermitian, the first term resembles the right-hand side of the von Neumann equation, and is thus called *unitary term*. The remaining part is instead called *dissipative term*. The coefficient matrix $\chi(t)$ is sometimes known as *Kossakowski matrix*, while the operators $\{L_i\}$ are called *Lindblad operators*. Note that since the Kossakowski matrix is Hermitian, it can be unitarily diagonalized:

$$\chi_{ij}(t) = \sum_k u_{ik}(t)\Delta_k(t)u_{jk}^*(t), \tag{2.51}$$

where $\Delta_k(t) \in \mathbb{R}$ and $u(t)$ is unitary. Then, if we define $V_k(t) := \sum_i u_{ik}(t)L_i$,

$$\mathcal{L}_t(X) = -i[h(t), X] + \sum_k \Delta_k(t)\left[V_k(t)XV_k^\dagger(t) - \frac{1}{2}\left\{V_k^\dagger(t)V_k(t), X\right\}\right], \tag{2.52}$$

which is a *diagonal* canonical form for the generator. The operators $V_k(t)$ are also sometimes called Lindblad operators, even though in this case they are in general time-dependent.

2.2.3 Markovian dynamics

It is crucial to understand the following fact: we are allowed to talk about a master equation because of the existence of an initial time point t_0 at which system and environment are taken to be uncorrelated. This is what yields a dynamical map Φ_t in the first place. However, taken time points $t_0 < s < t$, we cannot define in the same way a CPT dynamical map $\Phi_{t,s}$ such that $\rho(t) = \Phi_{t,s}[\rho(s)]$, because system and environment are typically not factorized at time s. We cannot write a composition law of the form $\Phi_t = \Phi_{t,s}\Phi_s$, in stark contrast with the closed-system scenario.

In case of regular dynamics, we can formally define a "propagator"

$$\Lambda_{t,s} := \Phi_t \Phi_s^{-1}, \quad t_0 \leq s \leq t, \tag{2.53}$$

in such a way that the dynamical map is *divisible* as [66]

$$\Phi_t = \Lambda_{t,s} \Phi_s. \tag{2.54}$$

A composition law holds for $\Lambda_{t,s}$, meaning that $\Lambda_{t,s} = \Lambda_{t,t'}\Lambda_{t',s}$ for any $t' \in [s,t]$, and if Φ_t obeys the master equation (2.40) then $\Lambda_{t,s}$ obeys the same master equation in t for any fixed $s \leq t$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Lambda_{t,s} = \mathcal{L}_t \Lambda_{t,s}, \quad \Lambda_{s,s} = \mathbb{1}, \tag{2.55}$$

so that

$$\Lambda_{t,s} = \mathbb{T}\exp\left[\int_s^t \mathrm{d}\tau\, \mathcal{L}_\tau\right], \tag{2.56}$$

which is the analogue of the unitary propagator in the closed-system case. The problem is that a map defined through Eq. (2.53) is not CPT in general. In case it happens that $\Lambda_{t,s}$ is actually CPT for any $t \geq s$, then it can be interpreted as a propagator and it can be used to describe the evolution: we say that the dynamics is *CP-divisible*[9]. Of course, a CP-divisible dynamical map is necessarily CPT, since we can always write $\Phi_t = \Lambda_{t,t_0}$.

Studying CP-divisible evolutions is considerably simpler than studying general evolutions: in the divisibility relation (2.54), s can be arbitrarily close to t, and if $\Lambda_{t,s}$ is an actual propagator this means that the state of the system at time t directly depends only on the state at a time s infinitesimally earlier than t. In classical physics, this is what one would call *Markovian dynamics*, with the composition law being the analogue of the Chapman-Kolmogorov relation for probability distributions [67]. For this reason, it is common to identify Markovianity with CP-divisibility in the quantum setting[10].

Remarkably, the simplification introduced by the CP-divisibility assumption is sufficient to complement Theorem 2.3 with a complete characterization of when Φ_t is guaranteed to be CPT, as explained in the following theorem.

Theorem 2.4 (LGKS). *Let Φ_t be a dynamical map on* $\mathrm{L}(\mathcal{H}_S)$ *satisfying the master equation* (2.40). *Then Φ_t is CP-divisible if and only if its generator has the canonical form* (2.42) *with $\chi(t) \geq 0$ for all $t \geq t_0$.*

Proof. Assume first that Φ_t is CP-divisible and let $\Lambda_{t,s}$ be the associated propagator. From the master equation, it follows that

$$\mathcal{L}_t[\Phi_t(X)] = \frac{\mathrm{d}}{\mathrm{d}t}\Phi_t(X) = \lim_{\epsilon\to 0}\frac{\Phi_{t+\epsilon}(X) - \Phi_t(X)}{\epsilon} = \lim_{\epsilon\to 0}\frac{\Lambda_{t+\epsilon,t} - \mathbb{1}_S}{\epsilon}\Phi_t(X). \tag{2.57}$$

Therefore, for the purpose of writing the master equation, we can think of $\mathcal{L}_t$ as

$$\mathcal{L}_t = \lim_{\epsilon\to 0}\frac{\Lambda_{t+\epsilon,t} - \mathbb{1}_S}{\epsilon}. \tag{2.58}$$

[9] The prefix CP stands for "completely positive" and it is used to distinguish this concept of divisibility from situations in which $\Lambda_{t,s}$ has less properties. For example, the study of *P-divisible* maps, where $\Lambda_{t,s}$ is just positive, is rich in results [16].

[10] It is worth pointing out that the description using dynamical maps ignores the possibility of performing multi-time measurement processes. The *process tensor formalism* [68] includes such processes into the picture, and in that scenario different notions of Markovianity emerge that are not equivalent to CP-divisibility [69, 70].

Since $\Lambda_{t,s}$ is assumed to be CPT, we can write it in Kraus representation:

$$\Lambda_{t,s}(X) = \sum_\alpha K_\alpha(t,s) X K_\alpha^\dagger(t,s). \tag{2.59}$$

Let $\{G_i\}$ be an orthonormal basis of $\mathrm{L}(\mathcal{H}_S)$ with $G_0 = \mathbb{1}_S/\sqrt{d}$ and $d = \dim \mathcal{H}_S$. Then we can expand $K_\alpha(t,s) = \sum_i k_{\alpha,i}(t,s) G_i$ and

$$\Lambda_{t,s}(X) = \sum_{i,j} \lambda_{ij}(t,s) G_i X G_j^\dagger, \quad \lambda_{ij}(t,s) := \sum_\alpha k_{\alpha,i}(t,s) k^*_{\alpha,j}(t,s). \tag{2.60}$$

Note that $\lambda(t,s)$ is a positive semidefinite matrix by construction. Moreover,

$$\mathcal{L}_t(X) = \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\sum_{i,j} \lambda_{ij}(t+\epsilon,t) G_i X G_j^\dagger - X\right] \equiv \sum_{i,j} \ell_{ij}(t) G_i X G_j^\dagger, \tag{2.61}$$

where

$$\ell_{00}(t) := \lim_{\epsilon\to 0} \frac{\lambda_{00}(t+\epsilon,t) - d}{\epsilon}, \qquad \ell_{ij}(t) := \lim_{\epsilon\to 0} \frac{\lambda_{ij}(t+\epsilon,t)}{\epsilon}. \tag{2.62}$$

Thanks to the positive semidefiniteness of $\lambda(t,s)$, we see that $\ell(t)$ is also a positive semidefinite matrix. But, according to the proof of Theorem 2.3, $\ell(t)$ is exactly the Kossakowski matrix $\chi(t)$ once we restrict its indices to $i,j \neq 0$.

For the converse part of the theorem, suppose $\mathcal{L}_t$ has the canonical form with $\chi(t) \geq 0$, and consider the map $\Lambda_{t,s}$ defined through Eq. (2.56). Using an argument similar to the one employed in the proof of Theorem 2.3, we immediately conclude that $\Lambda_{t,s}$ is trace-preserving, since $\operatorname{Tr} \mathcal{L}_t(X) = 0$: we only need to prove that $\Lambda_{t,s}$ is completely positive. According to Eq. (2.28), we can write

$$\Lambda_{t,s} = \lim_{n\to\infty} \left[e^{\mathcal{L}_{t_n}\Delta t} e^{\mathcal{L}_{t_{n-1}}\Delta t} \dots e^{\mathcal{L}_{t_0}\Delta t}\right], \tag{2.63}$$

where $\Delta t = (t-s)/n$ and $t_j = s + j\Delta t$ for $j \in \{0,\dots,n\}$. Since products of CPT maps are CPT maps, it is sufficient to prove that $\exp[\tau \mathcal{L}_t]$ is completely positive for any τ and t. Let us write $\mathcal{L}_t$ in diagonal canonical form (2.52). Since we assumed $\chi(t) \geq 0$, we know that $\Delta_k(t) \geq 0$. Hence,

$$\mathcal{L}_t(X) = F(t)X + XF^\dagger(t) + \sum_k \widetilde{V}_k(t) X \widetilde{V}_k^\dagger(t), \tag{2.64}$$

where $F(t) := -ih(t) - \sum_k \Delta_k(t) V_k^\dagger(t) V_k(t)/2$ and $\widetilde{V}_k(t) := \sqrt{\Delta_k(t)}\, V_k(t)$. In other words,

$$\mathcal{L}_t = \mathcal{L}_t^{(0)} + \sum_k \mathcal{L}_t^{(k)}, \qquad \mathcal{L}_t^{(0)}(X) := F(t)X + XF^\dagger(t), \quad \mathcal{L}_t^{(k)}(X) := \widetilde{V}_k(t) X \widetilde{V}_k^\dagger(t). \tag{2.65}$$

One easily checks by differentiation that

$$e^{\tau \mathcal{L}_t^{(0)}}(X) = e^{\tau F(t)} X e^{\tau F^\dagger(t)}, \tag{2.66}$$

which proves that $\exp[\tau \mathcal{L}_t^{(0)}]$ is completely positive. Moreover,

$$e^{\tau \mathcal{L}_t^{(k)}}(X) = \sum_{n=0}^\infty \frac{\tau^n}{n!} [\widetilde{V}_k(t)]^n X [\widetilde{V}_k^\dagger(t)]^n, \tag{2.67}$$

which is also completely positive. But, using a Trotter expansion,

$$e^{\tau\mathcal{L}_t} = \lim_{n\to\infty}\left[e^{\tau\mathcal{L}_t^{(0)}/n}\prod_k e^{\tau\mathcal{L}_t^{(k)}/n}\right]^n, \tag{2.68}$$

which is completely positive because it is a limit of products of completely positive maps. □

Theorem 2.4 is the generalization of a famous result developed by Gorini, Kossakowski, and Sudarshan in Ref. [12], independently extended to the bounded infinite-dimensional case by Lindblad in [11]. Therefore, we will refer to it as the *LGKS theorem*. The original theorem focused on the special case in which the generator does not depend on time, $\mathcal{L}_t \equiv \mathcal{L}$, so that the expression (2.56) for the propagator simplifies as

$$\Lambda_{t,s} = e^{(t-s)\mathcal{L}}. \tag{2.69}$$

In this case $\Lambda_{t,s} \equiv \Lambda_{t-s}$ is *homogeneous in time*, meaning that it only depends on the time difference $\tau = t-s$ instead of t and s separately. $\{\Lambda_\tau\}$ is known as a *dynamical semigroup* [10], in order to remind ourselves of the composition law, which in the Markovian case translates into compositions of actual physical transformations.

According to the LGKS theorem, the eigenvalues $\Delta_k(t)$ of the Kossakowski matrix for CP-divisible evolution are all non-negative. An interesting physical interpretation for this is that they can be seen as *transition rates*. More specifically, let us assume for simplicity that $h(t)$ and $V_k(t)$ are time-independent, and let us also assume that we can write $h = \sum_\alpha E_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ and $V_k \equiv V_{\alpha\beta} = |\psi_\alpha\rangle\langle\psi_\beta|$ (for $\alpha \neq \beta$), with $\{|\psi_\alpha\rangle\}$ being a spectral basis for h. If we write the system state as $\rho(t) = \sum_\alpha p_\alpha(t)|\psi_\alpha\rangle\langle\psi_\alpha|$, one can check by direct computation that the master equation turns into the following differential equation for $p_\alpha(t)$:

$$\frac{\mathrm{d}p_\alpha(t)}{\mathrm{d}t} = \sum_{\beta\neq\alpha}\left[\Delta_{\alpha\beta}(t)p_\beta(t) - \Delta_{\beta\alpha}(t)p_\alpha(t)\right]. \tag{2.70}$$

This is nothing more than a standard *rate equation* for a classical Markovian process [67]. The coefficients $\Delta_{\alpha\beta}(t)$ represent probability rates of jumping from state $|\psi_\beta\rangle$ to state $|\psi_\alpha\rangle$.

Of course, if $\Delta_k(t) < 0$ for some t, this interpretation falls apart and, in fact, we must have non-Markovian dynamics. It is important to stress out that we do not have a characterization theorem for CPT dynamical maps in case $\Delta_k(t) < 0$. An arbitrary generator in canonical form with $\Delta_k(t) < 0$ at some time t may or may not represent a valid evolution. We only know for sure that if it represents a valid evolution, then the corresponding dynamical map must be non-Markovian. The problem of detecting when a generator gives rise to CPT non-Markovian dynamics is very relevant [13–16].

2.2.4 Measures of non-Markovianity

In certain situations one could be interested in measuring how much a non-Markovian dynamics under consideration deviates from a Markovian one. There are several non-equivalent ways to approach this question, each with its pros and cons. Here we will consider two of them, since they will turn out to be useful in the following chapter.

In case a time-local master equation is given in canonical form, a natural choice to measure the degree of non-Markovianity is to determine how much the eigenvalues $\Delta_k(t)$ of the Kossakowski matrix are far from being all non-negative. More specifically, we can use

$$m(t) := \sum_k \max\{-\Delta_k(t), 0\}, \tag{2.71}$$

or its integrated version over a time interval if we are interested in a more global measure. This is called *Rivas-Huelga-Plenio (RHP) measure* [71]. Assuming the master equation under consideration is guaranteed to generate CPT evolution, we can be sure that $m(t) = 0$ if and only if the dynamics is Markovian and the more $m(t)$ increases the farther we are from Markovianity. Interestingly, one can show that $m(t)$ can also be written in terms of the Choi operator of the propagator [71]:

$$m(t) \propto \lim_{\epsilon \to 0} \frac{\|J(\Lambda_{t+\epsilon,t})\|_1 - 1}{\epsilon}, \tag{2.72}$$

which clearly shows that $m(t)$ measures how far the propagator is from being a CPT map—which is precisely the definition of Markovianity as CP-divisibility.

Unfortunately, in many situations one does not have access to a master equation in canonical form, and calculating $m(t)$ may be cumbersome. Suppose instead that only Φ_t is available, perhaps as the result of a numerical simulation: can we define some quantity that is able to detect whether the evolution is non-Markovian or not? Consider two initial states ρ_1, ρ_2 of the system at initial time t_0 and denote $\rho_1(t) = \Phi_t(\rho_1)$ and $\rho_2(t) = \Phi_t(\rho_2)$ for any $t \geq t_0$. Given two time points $t \geq s$, the distinguishability between ρ_1 and ρ_2, as defined by Eq. (2.14), obeys

$$\begin{aligned} D[\rho_1(t), \rho_2(t)] &= \frac{1}{2}\left\|\rho_1(t) - \rho_2(t)\right\|_1 = \frac{1}{2}\left\|\Phi_t(\rho_1) - \Phi_t(\rho_2)\right\|_1 = \frac{1}{2}\left\|\Phi_t(\rho_1 - \rho_2)\right\|_1 \\ &= \frac{1}{2}\left\|\Lambda_{t,s}\Phi_s(\rho_1 - \rho_2)\right\|_1 = \frac{1}{2}\left\|\Lambda_{t,s}[\rho_1(s) - \rho_2(s)]\right\|_1 \\ &= D[\Lambda_{t,s}\rho_1(s), \Lambda_{t,s}\rho_2(s)]. \end{aligned} \tag{2.73}$$

In case of Markovian dynamics, the propagator $\Lambda_{t,s}$ is a CPT map, and Theorem 2.2 implies

$$D[\Lambda_{t,s}\rho_1(s), \Lambda_{t,s}\rho_2(s)] \leq D[\rho_1(s), \rho_2(s)]. \tag{2.74}$$

In other words, the distinguishability $D[\rho_1(t), \rho_2(t)]$ is a monotonically non-increasing function of time:

$$\sigma(\rho_1, \rho_2; t) := \frac{\mathrm{d}}{\mathrm{d}t} D[\rho_1(t), \rho_2(t)] \leq 0. \tag{2.75}$$

If, for a certain choice of ρ_1, ρ_2, we observe $\sigma > 0$ at a certain time, we can be sure that the evolution under consideration is non-Markovian: this is called the *Breuer-Laine-Piilo (BLP) condition* [72]. The interpretation is that when $\sigma \leq 0$ at all times, the states of the system are destined to become more and more indistinguishable, since information is completely lost to the environment. Instead, when $\sigma > 0$ in a certain time interval, there is an *information backflow* from the environment to the system: this regain is what allows states to acquire previously lost distinguishability, and constitutes a purely non-Markovian mechanism. However, note that the BLP condition says nothing in case we observe $\sigma \leq 0$ all the way through: we could still have a non-Markovian evolution that happens to not show information backflow for the considered choice of ρ_1, ρ_2 (or for any other reason). The BLP condition is then just a *non-Markovianity witness*, and not a measure. If an evolution is witnessed to be non-Markovian by the BLP condition then it must have non-zero RHP measure, $m(t) \neq 0$, but the converse is not necessarily true [73].

2.3 Standard microscopic approach

The discussion about time evolution in open quantum systems was purely structural and formal. An important question remains to be answered: how do we write the generator of a master equation in practical situations? Is there a way to construct the quantities $h(t)$, $\chi(t)$, $\{L_i\}$ appearing in the canonical form starting from a given microscopic description of the system and its environment [74, 75]? In the closed-system case, the "microscopic description" is exhaustively provided by the Hamiltonian operator, but in the open case it is not yet clear what we need. In this section, we will discuss the standard way to derive master equations under a number of suitable assumptions and approximations, especially towards a Markovian setting. In the rest of the thesis we will explore various methods to generalize this construction by progressively relaxing such approximations.

2.3.1 Nakajima-Zwanzig equation

Since the system-environment compound is closed by definition, let us start by specifying its Hamiltonian, assumed for simplicity time-independent:

$$H = H_0 + \lambda V, \quad H_0 = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E. \tag{2.76}$$

Here, H_0 is a "free" term, containing the Hamiltonians of system and environment H_S and H_E as if they were independent of each other. Instead, V is the term that accounts for the interaction. We introduced a parameter λ, having the dimension of energy, in order to keep track of the order with which V appears in the following expressions. We can imagine λ to be a constant representing the "strength" of the interaction. Furthermore, we can always write V in the form

$$V = \sum_\alpha A_\alpha \otimes B_\alpha, \tag{2.77}$$

where $\{A_\alpha\} \subset \mathrm{L}(\mathcal{H}_S)$ and $\{B_\alpha\} \subset \mathrm{L}(\mathcal{H}_E)$. Even though one could always take A_α and B_α as Hermitian operators with appropriate rearrangements [6, 7], here we will not make this assumption. Of course, V must be a Hermitian operator: as a consequence, the sets $\{A_\alpha\}$ and $\{B_\alpha\}$ need to satisfy a consistency requirement. Specifically, for each *interaction index* α, there must exist a unique index $\overline{\alpha}$ such that

$$A_\alpha^\dagger = A_{\overline{\alpha}}, \qquad B_\alpha^\dagger = B_{\overline{\alpha}}. \tag{2.78}$$

This ensures that if A_α and B_α appear in the sum (2.77), then $A_\alpha^\dagger$ and $B_\alpha^\dagger$ appear too and V is guaranteed to be Hermitian.

The density operator $\rho_{SE}(t)$ of the universe evolves according to the von Neumann equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{SE}(t) = -i[H, \rho_{SE}(t)]. \tag{2.79}$$

Since the interaction V is what makes the problem non-trivial, it is convenient as a first step to "hide" the free evolution by changing the reference frame. If we define

$$\varrho_{SE}(t) \coloneqq e^{iH_0 t}\rho_{SE}(t)e^{-iH_0 t}, \tag{2.80}$$

one can easily check that

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho_{SE}(t) = -i\lambda[V(t), \varrho_{SE}(t)], \qquad V(t) \coloneqq e^{iH_0 t}Ve^{-iH_0 t}. \tag{2.81}$$

This is a common procedure in quantum mechanics, called moving to the *interaction picture* [1, 61]. Remembering Eq. (2.77), we can also write

$$V(t) = \sum_\alpha A_\alpha(t) \otimes B_\alpha(t), \qquad A_\alpha(t) \coloneqq e^{iH_S t}A_\alpha e^{-iH_S t}, \quad B_\alpha(t) \coloneqq e^{iH_E t}B_\alpha e^{-iH_E t}. \tag{2.82}$$

If we define the superoperator $\mathcal{V}(t)$ through $\mathcal{V}(t)X \coloneqq -i[V(t), X]$, we equivalently have

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho_{SE}(t) = \lambda\mathcal{V}(t)\varrho_{SE}(t). \tag{2.83}$$

For what concerns the initial condition, we will assume there is an initial time t_0 at which system and environment can be taken to be uncorrelated:

$$\varrho_{SE}(t_0) = \varrho(t_0) \otimes \Omega_0, \tag{2.84}$$

where $\varrho(t_0)$ is an arbitrary initial state of the system and Ω_0 is a fixed environment state.

From here, we are interested in tracing out the environment to obtain a differential equation involving solely the system's state. Note that the partial trace operation is preserved by the passage to the interaction picture, since if $\rho(t) = \mathrm{Tr}_E\, \rho_{SE}(t)$ then

$$\begin{aligned} \mathrm{Tr}_E\, \varrho_{SE}(t) &= \mathrm{Tr}_E[e^{iH_0 t}\rho_{SE}(t)e^{-iH_0 t}] = e^{iH_S t}\,\mathrm{Tr}_E[e^{iH_E t}\rho_{SE}(t)e^{-iH_E t}]e^{-iH_S t} \\ &= e^{iH_S t}\,\mathrm{Tr}_E[\rho_{SE}(t)]e^{-iH_S t} = e^{iH_S t}\rho(t)e^{-iH_S t} \eqqcolon \varrho(t). \end{aligned} \tag{2.85}$$

In order to extract $\varrho(t)$, let us define a *projection superoperator* $\mathcal{P}$ on $\mathrm{L}(\mathcal{H}_{SE})$, and its complementary $\mathcal{Q}$, through

$$\mathcal{P}[X] \coloneqq \mathrm{Tr}_E[X] \otimes \Omega_0, \qquad \mathcal{Q} \coloneqq \mathbb{1}_{SE} - \mathcal{P}. \tag{2.86}$$

We call $\mathcal{P}$ projector because $\mathcal{P}^2 = \mathcal{P}$, thanks to the fact that $\mathrm{Tr}\,\Omega_0 = 1$. If we apply $\mathcal{P}$ and $\mathcal{Q}$ to Eq. (2.83), we obtain the following pair of equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda\mathcal{P}\mathcal{V}(t)\varrho_{SE}(t) = \lambda\mathcal{P}\mathcal{V}(t)[\mathcal{P}\varrho_{SE}(t)] + \lambda\mathcal{P}\mathcal{V}(t)[\mathcal{Q}\varrho_{SE}(t)], \tag{2.87a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{Q}\varrho_{SE}(t)] = \lambda\mathcal{Q}\mathcal{V}(t)\varrho_{SE}(t) = \lambda\mathcal{Q}\mathcal{V}(t)[\mathcal{P}\varrho_{SE}(t)] + \lambda\mathcal{Q}\mathcal{V}(t)[\mathcal{Q}\varrho_{SE}(t)], \tag{2.87b}$$

with initial conditions $\mathcal{P}\varrho_{SE}(t_0) = \varrho_{SE}(t_0)$ and $\mathcal{Q}\varrho_{SE}(t_0) = 0$.

Before moving on, we make a simplifying assumption. For any $X \in \mathrm{L}(\mathcal{H}_{SE})$,

$$\begin{aligned} \mathcal{P}\mathcal{V}(t)\mathcal{P}X &= \mathcal{P}\mathcal{V}(t)(\mathrm{Tr}_E\, X \otimes \Omega_0) = -i\mathcal{P}[V(t), \mathrm{Tr}_E\, X \otimes \Omega_0] = -i\,\mathrm{Tr}_E[V(t), \mathrm{Tr}_E\, X \otimes \Omega_0] \otimes \Omega_0 \\ &= -i\sum_\alpha \mathrm{Tr}[B_\alpha(t)\Omega_0][A_\alpha(t), \mathrm{Tr}_E\, X] \otimes \Omega_0. \end{aligned} \tag{2.88}$$

We will assume the so-called *stability condition*:

$$\mathrm{Tr}[B_\alpha(t)\Omega_0] = 0, \quad \forall\alpha, \tag{2.89}$$

so that $\mathcal{PV}(t)\mathcal{P} = 0$. Such condition can always be ensured when Ω_0 is a stationary state of the environment, i.e., when $[\Omega_0, H_E] = 0$. In fact, in case $\mathrm{Tr}[B_\alpha\Omega_0] = 0$ for all α, one simply has $\mathrm{Tr}[B_\alpha(t)\Omega_0] = \mathrm{Tr}\left[e^{iH_Et}B_\alpha e^{-iH_Et}\Omega_0\right] = \mathrm{Tr}[B_\alpha\Omega_0] = 0$. Instead, if $\mu_\alpha := \mathrm{Tr}[B_\alpha\Omega_0] \neq 0$ for some α, define

$$\widetilde{B}_\alpha := B_\alpha - \mu_\alpha \mathbb{1}_E \tag{2.90}$$

and

$$\widetilde{V} := V - \sum_\alpha \mu_\alpha A_\alpha \otimes \mathbb{1}_E = \sum_\alpha A_\alpha \otimes \widetilde{B}_\alpha, \qquad \widetilde{H}_0 := H_0 + \sum_\alpha \mu_\alpha A_\alpha \otimes \mathbb{1}_E. \tag{2.91}$$

If we make the substitutions $H_0 \mapsto \widetilde{H}_0$ and $V \mapsto \widetilde{V}$, the total Hamiltonian H stays the same, $\widetilde{H}_0$ still does not contain interactions, and $\widetilde{V}$ is defined in terms of environment operators satisfying $\mathrm{Tr}\,[\widetilde{B}_\alpha\Omega_0] = 0$ for all α.

Since $\mathcal{PV}(t)\mathcal{P} = 0$, we can write Eq. (2.87a) as

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda\mathcal{PV}(t)[\mathcal{Q}\varrho_{SE}(t)]. \tag{2.92}$$

We can close this equation if we formally solve Eq. (2.87b) for $\mathcal{Q}\varrho_{SE}(t)$. But this can be easily done using the operator version of the variation of parameters formula, well known from the theory of ordinary differential equations:

$$\mathcal{Q}\varrho_{SE}(t) = \lambda \int_{t_0}^{t} \mathrm{d}s\, \mathcal{G}(t,s)\mathcal{QV}(s)\mathcal{P}\varrho_{SE}(s), \tag{2.93}$$

where we used that $\mathcal{Q}\varrho_{SE}(t_0) = 0$ and where $\mathcal{G}(t,s)$ is the propagator associated with the homogeneous version of Eq. (2.87b),

$$\mathcal{G}(t,s) = \mathbb{T}\exp\left[\lambda \int_s^t \mathrm{d}\tau\, \mathcal{QV}(\tau)\right]. \tag{2.94}$$

Substituting in Eq. (2.92),

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda^2 \int_{t_0}^{t} \mathrm{d}s\, \mathcal{PV}(t)\mathcal{G}(t,s)\mathcal{QV}(s)[\mathcal{P}\varrho_{SE}(s)]. \tag{2.95}$$

This is known as *Nakajima-Zwanzig equation*, and provides an exact master equation for the system state, albeit with a highly nontrivial dependence on microscopic parameters [6, 7]. This complexity makes the equation almost useless for practical purposes, at least if we do not make further assumptions about the setup.

Note that the Nakajima-Zwanzig equation is not a time-local equation as the ones we discussed in Sec. 2.2.2, because the right-hand side of Eq. (2.95) depends on $\mathcal{P}\varrho_{SE}(s)$ for all values of $s \in [t_0, t]$. Nevertheless, for regular dynamics, it is always possible to express it as a time-local equation, as discussed in Ref. [6].

2.3.2 Weak coupling and Redfield equation

Suppose system and environment are just *weakly coupled* to each other, so that we are entitled to imagine λ as a small expansion parameter. In case we stop at the lowest order, the Nakajima-Zwanzig equation considerably simplifies, as we will now show.

Since the universe evolves unitarily, we can write $\varrho_{SE}(s)$ in terms of $\varrho_{SE}(t)$ using the inverse total propagator:

$$\varrho_{SE}(s) = \mathcal{U}^{\dagger}_{t,s}\varrho_{SE}(t), \tag{2.96}$$

where

$$\mathcal{U}_{t,s} := \mathbb{T}\exp\left[\lambda \int_s^t \mathrm{d}\tau\, \mathcal{V}(\tau)\right]. \tag{2.97}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda^2 \int_{t_0}^t \mathrm{d}s\, \mathcal{P}\mathcal{V}(t)\mathcal{G}(t,s)\mathcal{Q}\mathcal{V}(s)\mathcal{P}\mathcal{U}^{\dagger}_{t,s}\varrho_{SE}(t). \tag{2.98}$$

Suppose now we expand the exponentials that define $\mathcal{G}(t,s)$ and $\mathcal{U}^{\dagger}_{t,s}$. Assuming V to be a bounded operator, a simple norm estimate shows that the nth term of such expansion is of order $O(\lambda^n t^n)$. As a consequence, at lowest order,

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda^2 \int_{t_0}^t \mathrm{d}s\, \mathcal{P}\mathcal{V}(t)\mathcal{Q}\mathcal{V}(s)[\mathcal{P}\varrho_{SE}(t)] + O\big(\lambda^3 t^2\big). \tag{2.99}$$

We should keep in mind that λt is the relevant expansion parameter here: for a finite value of the coupling λ, we cannot expect the truncated master equation to be accurate at arbitrarily large time t.

Assume now $\lambda \ll t^{-1}$ and let us ignore the $O\big(\lambda^3 t^2\big)$ term: we are left with a time-local master equation that is free of ordered exponentials. Let us write it more explicitly. First, since $\mathcal{Q} = \mathbb{1}_{SE} - \mathcal{P}$ and $\mathcal{P}\mathcal{V}(s)\mathcal{P} = 0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{P}\varrho_{SE}(t)] = \lambda^2 \int_{t_0}^t \mathrm{d}s\, \mathcal{P}\mathcal{V}(t)\mathcal{V}(s)[\mathcal{P}\varrho_{SE}(t)]. \tag{2.100}$$

Moreover, for any $X \in \mathrm{L}(\mathcal{H}_{SE})$,

$$\begin{aligned}
\mathcal{P}\mathcal{V}(t)\mathcal{V}(s)\mathcal{P}X &= \mathcal{P}\mathcal{V}(t)\mathcal{V}(s)(\mathrm{Tr}_E X \otimes \Omega_0) = -i\mathcal{P}\mathcal{V}(t)[V(s), \mathrm{Tr}_E X \otimes \Omega_0] \\
&= -\mathcal{P}[V(t), [V(s), \mathrm{Tr}_E X \otimes \Omega_0]] \\
&= -\mathrm{Tr}_E[V(t), [V(s), \mathrm{Tr}_E X \otimes \Omega_0]] \otimes \Omega_0 \\
&= -\mathrm{Tr}_E[V(t), V(s)(\mathrm{Tr}_E X \otimes \Omega_0)] \otimes \Omega_0 + \mathrm{H.c.},
\end{aligned} \tag{2.101}$$

therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \int_{t_0}^t \mathrm{d}s\, \mathrm{Tr}_E[V(t), V(s)(\varrho(t) \otimes \Omega_0)] + \mathrm{H.c.} \tag{2.102}$$

At this point it is convenient to define the so-called *environment correlation function*[11]

$$c_{\alpha\beta}(t,s) := \mathrm{Tr}\big[B_\alpha(t)B_\beta(s)\Omega_0\big]. \tag{2.103}$$

[11]Some authors define this function using $B^{\dagger}_{\alpha}(t)$ instead of $B_\alpha(t)$, but for our purposes it will be more useful to keep this notation. The two definitions can of course be linked to each other.

Thanks to Eq. (2.78), it has the symmetry

$$c^*_{\alpha\beta}(t,s) = c_{\overline{\beta}\overline{\alpha}}(s,t). \tag{2.104}$$

Moreover, in case Ω_0 is stationary, this function is homogeneous in time, meaning that

$$\begin{aligned} c_{\alpha\beta}(t,s) &= \mathrm{Tr}\left[e^{iH_E t}B_\alpha e^{-iH_E t}e^{iH_E s}B_\beta e^{-iH_E s}\Omega_0\right] = \mathrm{Tr}\left[e^{iH_E t}B_\alpha e^{-iH_E(t-s)}B_\beta \Omega_0 e^{-iH_E s}\right] \\ &= \mathrm{Tr}\left[e^{iH_E(t-s)}B_\alpha e^{-iH_E(t-s)}B_\beta\Omega_0\right] = \mathrm{Tr}\left[B_\alpha(t-s)B_\beta\Omega_0\right] =: c_{\alpha\beta}(t-s). \end{aligned} \tag{2.105}$$

Carrying out the partial trace in Eq. (2.102) and using the definition of environment correlation function, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}s\, c_{\alpha\beta}(t-s)[A_\alpha(t), A_\beta(s)\varrho(t)] + \mathrm{H.c.} \tag{2.106}$$

This is known as the *Redfield equation* [19, 20], and it will be a central object of study in the thesis. It is also typically rewritten using the change of variables $\tau := t - s$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta}\int_{0}^{t-t_0} \mathrm{d}\tau\, c_{\alpha\beta}(\tau)[A_\alpha(t), A_\beta(t-\tau)\varrho(t)] + \mathrm{H.c.} \tag{2.107}$$

Before moving on, it is convenient to put this master equation in canonical form. Even though there are infinite ways to achieve this, a natural starting point is provided by the spectral decomposition of the free system Hamiltonian:

$$H_S = \sum_k \omega_k \left|\psi_k\right\rangle\!\left\langle\psi_k\right|. \tag{2.108}$$

Each interaction operator A_α can be expanded in such energy eigenbasis,

$$A_\alpha = \sum_{k,q} A_{\alpha,kq}E_{kq}, \qquad A_{\alpha,kq} := \langle\psi_k|A_\alpha|\psi_q\rangle, \quad E_{kq} := \left|\psi_k\right\rangle\!\left\langle\psi_q\right|. \tag{2.109}$$

Since $e^{iH_S t}E_{kq}e^{-iH_S t} = e^{-i\omega_{kq}t}E_{kq}$, with $\omega_{kq} := \omega_q - \omega_k$, we can also write

$$A_\alpha(t) = \sum_{k,q} e^{-i\omega_{kq}t}A_{\alpha,kq}E_{kq} = \sum_{k,q} e^{i\omega_{kq}t}A^*_{\overline{\alpha},kq}E^\dagger_{kq}, \tag{2.110}$$

where in the second equality we exchanged $k \leftrightarrow q$. Therefore,

$$[A_\alpha(t), A_\beta(t-\tau)\varrho(t)] = \sum_{k,q,n,m} e^{i\omega_{kq}t}e^{-i\omega_{nm}(t-\tau)}A^*_{\overline{\alpha},kq}A_{\beta,nm}[E^\dagger_{kq}, E_{nm}\varrho(t)], \tag{2.111}$$

which leads to

$$\begin{aligned} \frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} &= -\lambda^2 \sum_{\alpha,\beta}\sum_{k,q,n,m} \Gamma_{\alpha\beta}(\omega_{nm};t)e^{i(\omega_{kq}-\omega_{nm})t}A^*_{\alpha,kq}A_{\beta,nm}[E^\dagger_{kq}, E_{nm}\varrho(t)] + \mathrm{H.c.} \\ &= -\lambda^2 \sum_{k,q,n,m} K_{kq,nm}(t)e^{i(\omega_{kq}-\omega_{nm})t}[E^\dagger_{kq}, E_{nm}\varrho(t)] + \mathrm{H.c.}, \end{aligned} \tag{2.112}$$

where we defined the quantities

$$\Gamma_{\alpha\beta}(\omega;t) := \int_0^{t-t_0} \mathrm{d}\tau\, c_{\overline{\alpha}\beta}(\tau)e^{i\omega\tau}, \qquad K_{kq,nm}(t) := \sum_{\alpha,\beta} \Gamma_{\alpha\beta}(\omega_{nm};t)A^*_{\alpha,kq}A_{\beta,nm}. \tag{2.113}$$

Now we want to expand the commutator and the H.c. term, with the aim of grouping the various terms according to the structure of the canonical form. For future convenience, we wrap this calculation in a general lemma.

Lemma 2.5. *Consider a collection of operators* $\{X_a\}$*, a Hermitian operator* ρ*, and a set of complex coefficients* $\{f_{ab}\}$*. Then,*

$$-\sum_{a,b} f_{ab}[X_a^\dagger, X_b\rho] + H.c. = -i\sum_{a,b}\frac{f_{ab}-f_{ba}^*}{2i}[X_a^\dagger X_b, \rho] + \sum_{a,b}(f_{ab}+f_{ba}^*)\left[X_b\rho X_a^\dagger - \frac{1}{2}\{X_a^\dagger X_b, \rho\}\right]. \tag{2.114}$$

Proof. We can write

$$\begin{aligned}
-\sum_{a,b} f_{ab}[X_a^\dagger, X_b\rho] + \mathrm{H.c.} &= -\sum_{a,b} f_{ab}\left(X_a^\dagger X_b\rho - X_b\rho X_a^\dagger\right) - \sum_{a,b} f_{ab}^*\left(\rho X_b^\dagger X_a - X_a\rho X_b^\dagger\right) \\
&= \sum_{a,b}(f_{ab}+f_{ba}^*)X_b\rho X_a^\dagger - \sum_{a,b}\left(f_{ab}X_a^\dagger X_b\rho + f_{ba}^*\rho X_a^\dagger X_b\right),
\end{aligned} \tag{2.115}$$

where we made the substitution $a \leftrightarrow b$ in the second sum. The conclusion follows once we realize that

$$f_{ab}X_a^\dagger X_b\rho + f_{ba}^*\rho X_a^\dagger X_b = \frac{1}{2}(f_{ab}+f_{ba}^*)\{X_a^\dagger X_b, \rho\} + \frac{1}{2}(f_{ab}-f_{ba}^*)[X_a^\dagger X_b, \rho]. \tag{2.116}$$

□

According to Lemma 2.5, if we define the coefficients

$$\chi_{kq,nm}(t) := K_{kq,nm}(t) + K^*_{nm,kq}(t), \tag{2.117a}$$

$$\eta_{kq,nm}(t) := \frac{1}{2i}[K_{kq,nm}(t) - K^*_{nm,kq}(t)], \tag{2.117b}$$

we end up with the canonical master equation

$$\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} = -i\lambda^2[\widetilde{H}_{LS}(t), \varrho(t)] + \lambda^2 \sum_{k,q,n,m} \chi_{kq,nm}(t)e^{i(\omega_{kq}-\omega_{nm})t}\left[E_{nm}\varrho(t)E_{kq}^\dagger - \frac{1}{2}\{E_{kq}^\dagger E_{nm}, \varrho(t)\}\right], \tag{2.118}$$

where

$$\widetilde{H}_{LS}(t) := \sum_{k,q,n,m} \eta_{kq,nm}(t)e^{i(\omega_{kq}-\omega_{nm})t}E_{kq}^\dagger E_{nm}. \tag{2.119}$$

It is sometimes convenient to group the sums over energy indices according to the value of ω_{kq}. Specifically, consider the set of *Bohr frequencies* of the system,

$$\mathcal{B} := \left\{\omega_{kq}\right\}_{k,q=1}^{d}, \tag{2.120}$$

and for each operator A_α and $\omega \in \mathcal{B}$, define

$$A_\alpha(\omega) := \sum_{k,q} \delta_{\omega,\omega_{kq}} A_{\alpha,kq} E_{kq}, \tag{2.121}$$

which is basically a jump operator between eigenstates of the system separated by an energy gap ω, with each possible jump weighted by the corresponding matrix element of A_α. Then, it is easy to see that

$$\begin{aligned}\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} = -i\lambda^2[\widetilde{H}_{LS}(t), \varrho(t)] + \lambda^2 \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} \chi_{\alpha\beta}(\omega,\omega';t) e^{i(\omega-\omega')t} \\ \times \left[A_\beta(\omega')\varrho(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega'), \varrho(t)\} \right],\end{aligned} \tag{2.122}$$

where

$$\widetilde{H}_{LS}(t) = \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} \eta_{\alpha\beta}(\omega,\omega';t) e^{i(\omega-\omega')t} A_\alpha^\dagger(\omega) A_\beta(\omega'), \tag{2.123}$$

and

$$\chi_{\alpha\beta}(\omega,\omega';t) := \Gamma_{\alpha\beta}(\omega';t) + \Gamma_{\beta\alpha}^*(\omega;t), \tag{2.124a}$$

$$\eta_{\alpha\beta}(\omega,\omega';t) := \frac{1}{2i}\left[\Gamma_{\alpha\beta}(\omega';t) - \Gamma_{\beta\alpha}^*(\omega;t) \right]. \tag{2.124b}$$

All these equations can also be easily transformed back into master equations for the original density operator $\rho(t)$ by reverting the interaction-picture transformation. Since $\rho(t) = e^{-iH_S t}\varrho(t)e^{iH_S t}$,

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H_S, \rho(t)] + e^{-iH_S t}\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t}e^{iH_S t}. \tag{2.125}$$

But we also know that $e^{-iH_S t}E_{kq}e^{iH_S t} = e^{i\omega_{kq}t}E_{kq}$, which is enough to conclude that

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H_S + \lambda^2 H_{LS}(t), \rho(t)] + \lambda^2 \sum_{k,q,n,m} \chi_{kq,nm}(t) \left[E_{nm}\rho(t)E_{kq}^\dagger - \frac{1}{2}\{E_{kq}^\dagger E_{nm}, \rho(t)\} \right] \tag{2.126}$$

or

$$\begin{aligned}\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H_S + \lambda^2 H_{LS}(t), \rho(t)] + \lambda^2 \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} \chi_{\alpha\beta}(\omega,\omega';t) \\ \times \left[A_\beta(\omega')\rho(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega'), \rho(t)\} \right],\end{aligned} \tag{2.127}$$

with

$$H_{LS}(t) := \sum_{k,q,n,m} \eta_{kq,nm}(t) E_{kq}^\dagger E_{nm} = \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} \eta_{\alpha\beta}(\omega,\omega';t) A_\alpha^\dagger(\omega) A_\beta(\omega'). \tag{2.128}$$

2.3.3 Markov approximation

The Redfield equation is a master equation with time-dependent generator, hence, in principle, it is able to describe non-Markovian effects. In this subsection, we will show that if the environment is sufficiently big and if we neglect some short-time dynamics arising at the beginning of the evolution, we can approximate the master equation using a time-independent generator: for this reason, the procedure is dubbed *Markov approximation* [6, 7].

Suppose for the moment that the environment is a finite-dimensional quantum system, so that we can write the spectral decomposition of its free Hamiltonian as $H_E = \sum_k \varepsilon_k |\phi_k\rangle\langle\phi_k|$. Similarly to what we did on the system's side, we can write $B_\alpha = \sum_{k,q} B_{\alpha,kq} |\phi_k\rangle\langle\phi_q|$, with $B_{\alpha,kq} := \langle\phi_k|B_\alpha|\phi_q\rangle$. By direct computation, we find

$$c_{\overline{\alpha}\beta}(\tau) = \sum_{k,q,n} e^{i(\varepsilon_q-\varepsilon_k)\tau} B^*_{\alpha,kq} B_{\beta,kn} \langle\phi_n|\Omega_0|\phi_q\rangle . \tag{2.129}$$

Since $c_{\overline{\alpha}\beta}(\tau)$ is a correlation function defined in terms of the interaction operators B_α, we expect it to contain information about how the environment handles excitations arising because of the interaction with the system. Note that the right-hand side of Eq. (2.129) is a quasi-periodic function of τ: by the *Poincaré recurrence theorem*, it will eventually bounce back to its initial value [7]. For a finite environment, this is an expected non-Markovian effect in which information recoils back into the system. However, if the environment is instead constituted by a large number of particles or modes, the recurrence time becomes extremely large or, in practice, infinite. In this scenario, we expect $c_{\overline{\alpha}\beta}(\tau)$ to decay to zero after a typical decay time τ_E, roughly describing how much time the environment needs in order to recover after having received an "interaction pulse" from the system.

Now, suppose we are interested in times t such that $t - t_0$ is sufficiently larger than τ_E, meaning that we do not intend to resolve the environment's relaxation dynamics. Since we assumed $\lambda t \ll 1$ when we performed the weak-coupling expansion, we are now additionally requiring that the interaction strength should be weak with respect to the environment's relaxation timescale:

$$\lambda\tau_E \ll 1. \tag{2.130}$$

In standard literature, this is usually also referred to as *weak coupling*; however, one should keep in mind that this condition alone is not sufficient to derive the Redfield equation using the procedure we adopted above.

Assuming $t - t_0 \gg \tau_E$ brings the following advantage: since $c_{\overline{\alpha}\beta}(\tau)$ is practically zero for $\tau > \tau_E$, we can extend the integration region in Eq. (2.113) from $[0, t - t_0]$ to $[0, +\infty)$ without making much of a difference:

$$\Gamma_{\alpha\beta}(\omega; t) \mapsto \lim_{t\to\infty} \Gamma_{\alpha\beta}(\omega; t) = \int_0^\infty \mathrm{d}\tau\, c_{\overline{\alpha}\beta}(\tau) e^{i\omega\tau} =: \Gamma_{\alpha\beta}(\omega). \tag{2.131}$$

For this to be admissible, we must of course require the environment correlation function to have a sufficiently strong decay at infinity: rigorous sufficient conditions can be found in the literature [7, 9]. The effect is that the quantities $\chi_{kq,nm}(t)$, $\eta_{kq,nm}(t)$, $\chi_{\alpha\beta}(\omega, \omega'; t)$, and $\eta_{\alpha\beta}(\omega, \omega'; t)$ all become time-independent.

Note that the same result can be derived by performing the extension of the integration domain directly in Eq. (2.107),

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta} \int_0^\infty \mathrm{d}\tau\, c_{\alpha\beta}(\tau)[A_\alpha(t), A_\beta(t-\tau)\varrho(t)] + \mathrm{H.c.} \tag{2.132}$$

In the rest of the thesis, we will distinguish Eq. (2.132) and Eq. (2.107) by calling the former *time-independent Redfield equation* and by calling the latter *time-dependent Redfield equation*—and similarly for the corresponding canonical forms.

2.3.4 Non-positivity of the Redfield equation

While the Redfield equation seems to be a convenient time-local master equation, it was obtained under a number of approximations: it is then natural to ask whether the associated dynamical map is CPT or not. In general, this is a non-trivial question. Since the trace of a commutator is always zero, it is immediate to verify that $\mathrm{Tr}\left[\mathrm{d}\rho(t)/\mathrm{d}t\right] = 0$ for Eq. (2.107), hence the trace of $\rho(t)$ is correctly preserved. Unfortunately, the same cannot be said for positivity, as the following example shows [21].

Consider a two-dimensional system, with Hilbert space spanned by $\{|0\rangle, |1\rangle\}$ and free Hamiltonian $H_S = \varepsilon |1\rangle\langle 1|$. As the environment, we take a set of bosonic harmonic oscillators, so that $H_E = \sum_p \varepsilon_p c_p^\dagger c_p$, with $c_p, c_p^\dagger$ being creation and annihilation operators obeying the canonical commutation relations $[c_p, c_{p'}^\dagger] = \delta_{pp'}$ and $[c_p, c_{p'}] = 0$. The system-environment interaction is taken to be

$$V = (|0\rangle\langle 1| + |1\rangle\langle 0|) \otimes \sum_p g_p (c_p + c_p^\dagger), \tag{2.133}$$

where g_p is a real coupling constant.

The Kossakowski matrix in energy basis for the time-independent Redfield equation is

$$\chi_{kq,nm} = \left[\Gamma(\omega_{nm}) + \Gamma^*(\omega_{kq})\right] \left(\delta_{k0}\delta_{q1} + \delta_{k1}\delta_{q0}\right)\left(\delta_{n0}\delta_{m1} + \delta_{n1}\delta_{m0}\right), \tag{2.134}$$

which means that it has non-zero entries only in the diagonal block Ξ corresponding to the indices $(k, q) \in \{(0, 1), (1, 0)\}$, with

$$\Xi = \begin{bmatrix} 2\,\mathrm{Re}\,\Gamma(\varepsilon) & \Gamma(-\varepsilon) + \Gamma^*(\varepsilon) \\ \Gamma(\varepsilon) + \Gamma^*(-\varepsilon) & 2\,\mathrm{Re}\,\Gamma(-\varepsilon) \end{bmatrix}. \tag{2.135}$$

Clearly, $\chi \geq 0$ if and only if $\Xi \geq 0$. A straightforward computation shows that the eigenvalues of Ξ are

$$\ell_\pm = \mathrm{Re}[\Gamma(\varepsilon) + \Gamma(-\varepsilon)] \pm \sqrt{\mathrm{Re}^2[\Gamma(\varepsilon) - \Gamma(-\varepsilon)] + |\Gamma(\varepsilon) + \Gamma^*(-\varepsilon)|^2}, \tag{2.136}$$

and that $\ell_+ \geq \ell_-$. One finds that the lowest eigenvalue ℓ_- obeys the implication

$$\ell_- \geq 0 \quad \Leftrightarrow \quad \Gamma(\varepsilon) = \Gamma(-\varepsilon). \tag{2.137}$$

But the condition on the right is false, in general, which implies that χ is not positive semidefinite and that the associated master equation does not generate CPT evolution.

It is interesting to observe how the diagonal entries of Ξ are non-negative. In fact, with a direct calculation one finds

$$2\,\mathrm{Re}\,\Gamma(\varepsilon) = 2\pi \sum_p g_p^2 \left[\frac{\delta(\varepsilon - \varepsilon_p)}{1 - e^{-\beta\varepsilon_p}} + \frac{\delta(\varepsilon + \varepsilon_p)}{e^{\beta\varepsilon_p} - 1}\right] \geq 0. \tag{2.138}$$

Unfortunately, this is not enough to infer positive semidefiniteness of Ξ because of the presence of non-diagonal terms. Positivity of diagonal terms will play a role when discussing the secular approximation in the next subsection.

Note that it is not possible to straightforwardly extend the above argument to the case of the time-dependent Redfield equation because it could still be possible for the evolution to be CPT (and non-Markovian) when the Kossakowski matrix is not positive semidefinite. Nevertheless, there are examples in which such equation displays non-positive behavior, even though it typically does so in a less dramatic way with respect to its time-independent variant [22, 23].

To date, there is still a lot of debate going on among experts for what concerns the problem of positivity breaking that affects the Redfield equation. Some argue that such violations only appear when pushing the equation beyond its limits by considering not-so-weak coupling values [23]. One should also appreciate how well it works when violations are not detected: for example, it is probably the only known weak-coupling master equation that correctly reproduces the relaxation phenomenon to the mean-force Gibbs state [76, 77]. However, others argue that this mathematical flaw has the potential of ruining other physical requirements even without explicit positivity violations [24–26]. For example, it has been shown that the Redfield equation violates the generalized quantum detailed balance condition [78], and that in certain cases can yield long-lived local generation of entanglement [79].

2.3.5 Secular approximation

We will now illustrate the traditional way of curing the non-positivity problem of the Redfield equation, at the price of introducing an additional assumption about the system. This procedure exclusively applies to the time-independent Redfield equation.

In the example discussed in the previous subsection, we saw how the breaking of positivity was caused by the presence of non-diagonal terms with $\omega \neq \omega'$ in the frequency representation of the Kossakowski matrix $\chi_{\alpha\beta}(\omega, \omega')$. If we could neglect such non-diagonal terms, positivity would be guaranteed: it turns out that this idea can be applied in general. Consider the time independent-version of Eq. (2.122): in case the typical value of $|\omega - \omega'|^{-1}$ is much shorter than the typical evolution timescale, the exponential $e^{i(\omega-\omega')t}$ is rapidly oscillating and thus roughly averages to zero, provided $\omega \neq \omega'$. More specifically, if we assume the Bohr frequencies of the system to be well-separated with respect to the environment correlation time,

$$\lambda \ll \tau_E^{-1} \ll \min_{\omega \neq \omega' \in \mathcal{B}} |\omega - \omega'|, \tag{2.139}$$

then we can effectively substitute $e^{i(\omega-\omega')t} \mapsto \delta_{\omega,\omega'}$ in Eq. (2.122). This is called *secular approximation*, and it yields the so-called *secular master equation*:

$$\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} = -i[\lambda^2 H_{LS}, \varrho(t)] + \lambda^2 \sum_{\alpha,\beta} \sum_{\omega \in \mathcal{B}} \chi_{\alpha\beta}(\omega) \left[A_\beta(\omega)\varrho(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega), \varrho(t)\} \right], \tag{2.140}$$

where

$$H_{LS} = \lambda^2 \sum_{\alpha,\beta} \sum_{\omega \in \mathcal{B}} \eta_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \tag{2.141}$$

and we abbreviated for simplicity $\chi_{\alpha\beta}(\omega, \omega) \equiv \chi_{\alpha\beta}(\omega)$ and $\eta_{\alpha\beta}(\omega, \omega) \equiv \eta_{\alpha\beta}(\omega)$.

Before proceeding, let us discuss some properties of the coefficients $\chi_{\alpha\beta}(\omega)$ and $\eta_{\alpha\beta}(\omega)$.

Thanks to the symmetry property (2.104) of the environment correlation function,

$$\Gamma^*_{\beta\alpha}(\omega) = \int_0^\infty \mathrm{d}\tau\, c^*_{\overline{\beta}\alpha}(\tau)e^{-i\omega\tau} = \int_{-\infty}^0 \mathrm{d}\tau\, c_{\overline{\alpha}\beta}(\tau)e^{i\omega\tau}, \tag{2.142}$$

from which we see that $\chi_{\alpha\beta}(\omega)$ is just a full Fourier transform:

$$\chi_{\alpha\beta}(\omega) = \int_{-\infty}^\infty \mathrm{d}\tau\, c_{\overline{\alpha}\beta}(\tau)e^{i\omega\tau}. \tag{2.143}$$

Instead, $\eta_{\alpha\beta}(\omega)$ can be computed from the Kossakowski matrix using a *Kramers-Krönig relation*. In fact,

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2\pi}\int_0^\infty \mathrm{d}\tau \int_{-\infty}^\infty \mathrm{d}\omega'\, \chi_{\alpha\beta}(\omega')e^{-i\omega'\tau}e^{i\omega\tau}. \tag{2.144}$$

The integration over τ can be performed using the following well-known formula,

$$\int_0^\infty \mathrm{d}\tau\, e^{i(\omega-\omega')\tau} = \pi\delta(\omega-\omega') + i\mathbb{P}\frac{1}{\omega-\omega'}, \tag{2.145}$$

where $\mathbb{P}$ stands for the Cauchy's principal value sign. We obtain

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\chi_{\alpha\beta}(\omega) + i\eta_{\alpha\beta}(\omega) \tag{2.146}$$

with

$$\eta_{\alpha\beta}(\omega) = \frac{1}{2\pi}\mathbb{P}\int_{-\infty}^\infty \mathrm{d}\omega'\, \frac{\chi_{\alpha\beta}(\omega')}{\omega-\omega'}. \tag{2.147}$$

One clearly sees that the $\eta_{\alpha\beta}(\omega)$ appearing here is the same $\eta_{\alpha\beta}(\omega)$ appearing in the secular master equation. Additionally, one can easily show that H_{LS} commutes with H_S, meaning that its only effect is to shift the "bare" system's energy levels. For this reason, one usually refers to H_{LS} as the *Lamb shift Hamiltonian*, in analogy to a similar phenomenon appearing in atomic physics[12]. Note that this does not happen in general for the Redfield equation.

We are now ready to prove that the secular master equation, contrary to the Redfield equation, generates a proper CPT Markovian evolution. Thanks to the LGKS theorem 2.4, it is sufficient to show that the Kossakowski matrix is positive semidefinite. Define the collective index $i = (\alpha, \omega)$. The entry $(i, j) = ((\alpha, \omega), (\beta, \omega'))$ of the Kossakowski matrix is then given by $\chi_{ij} \equiv \chi_{\alpha\beta}(\omega, \omega')$. In the secular case, $\chi_{ij} = 0$ for $\omega \neq \omega'$, hence χ can be arranged in block-diagonal form, where each block χ^ω can be associated with a specific frequency ω and has entries $\chi^\omega_{ij} \equiv \chi^\omega_{\alpha\beta} \equiv \chi_{\alpha\beta}(\omega)$. It is then sufficient to prove that $\chi^\omega \geq 0$ for any $\omega \in \mathcal{B}$. Given an arbitrary vector $\mathbf{v} = (v_\alpha)$, we need to show that the following quantity is non-negative:

$$\langle \mathbf{v}, \chi^\omega \mathbf{v}\rangle = \sum_{\alpha,\beta} v^*_\alpha \chi^\omega_{\alpha\beta} v_\beta = \int_{-\infty}^\infty \mathrm{d}\tau\, f(\tau)e^{i\omega\tau}, \qquad f(\tau) := \sum_{\alpha,\beta} v^*_\alpha c_{\overline{\alpha}\beta}(\tau) v_\beta. \tag{2.148}$$

To do that, we invoke a standard result in the theory of Fourier transforms, which is *Bochner's theorem*: it says that the Fourier transform of $f(\tau)$ is nonnegative when the matrix $\{f(\tau_n - \tau_m)\}$,

[12] It is worth pointing out that the usual Lamb shift in atomic physics is caused by vacuum fluctuations exclusively. In our case, any environment effect can be responsible for the shift, including thermal fluctuations.

obtained by varying the time points τ_n and τ_m, is positive semidefinite. In our case, first we write

$$f(\tau_n - \tau_m) = \sum_{\alpha,\beta} v_\alpha^* \operatorname{Tr}\big[B_\alpha^\dagger(\tau_n) B_\beta(\tau_m)\Omega_0\big] v_\beta = \operatorname{Tr}\big[N^\dagger(\tau_n) N(\tau_m)\Omega_0\big], \tag{2.149}$$

with $N(\tau) := \sum_\alpha v_\alpha B_\alpha(\tau)$. Then, for an arbitrary vector (w_n),

$$\begin{aligned}\sum_{n,m} w_n^* f(\tau_n - \tau_m) w_m &= \sum_{n,m} w_n^* \operatorname{Tr}\big[N^\dagger(\tau_n) N(\tau_m)\Omega_0\big] w_m \\ &= \sum_{n,m} \operatorname{Tr}\Big[w_n^* \sqrt{\Omega_0} N^\dagger(\tau_n) N(\tau_m) \sqrt{\Omega_0} w_m\Big] = \operatorname{Tr}\big[M^\dagger M\big] \geq 0,\end{aligned} \tag{2.150}$$

with $M := \sum_n w_n N(\tau_n)\sqrt{\Omega_0}$.

We conclude with an interesting remark. Since we derived the secular master equation from the Redfield equation, it seems reasonable to expect that the condition $\lambda t \ll 1$ which allowed us to perform the weak-coupling expansion should be kept here too. Surprisingly, under suitable assumptions on $c_{\overline{\alpha}\beta}(\tau)$, it is possible to show that the secular master equation can accurately be applied all the way to $t \to \infty$ even for a finite value of λ, provided of course that $\lambda \ll \tau_E^{-1} \ll \min_{\omega \neq \omega' \in \mathcal{B}} |\omega - \omega'|$ [80].

Chapter 3

Regularization Techniques

This chapter describes the results originally published in the following papers:

[38] A. D'Abbruzzo, V. Cavina, and V. Giovannetti, *A time-dependent regularization of the Redfield equation*, SciPost Phys. **15**, 117 (2023).

[39] A. D'Abbruzzo, D. Farina, and V. Giovannetti, *Recovering complete positivity of non-Markovian quantum dynamics with Choi-proximity regularization*, Phys. Rev. X **14**, 031010 (2024).

In the previous chapter we discussed how one of the fundamental problems in the theory of open quantum systems is to derive accurate master equations starting from a microscopic description of the system-environment compound. Using a weak-coupling expansion, we obtained the Redfield equation (2.106), which was showed to exhibit positivity breaking. However, we were able to recover CPT evolution after an additional secular approximation, which required us to assume a system with well-separated transition energies. As a consequence, the resulting master equation (2.140) displays independent evolution of the system's modes associated with specific Bohr frequencies.

The secular approximation was originally devised in the context of quantum optics, where it can be applied with the same spirit as the well-known *rotating-wave approximation*[1] [84]. However, the hypothesis of well-separated energy levels is not necessarily an appropriate assumption when considering many-body systems or modern solid-state devices, where energy levels tend to be dense. This is the main reason why recent research efforts have been devoted to the study of *beyond-secular* master equations [22, 27–37].

Since weak coupling is a more reasonable assumption that does not put limits to the energy structure of the system, a natural reference point is given by the Redfield equation[2]. However, as we argued in Sec. 2.3.4, the lack of a CPT guarantee can potentially "taint" results towards non-physical predictions. It is still under scrutiny among researchers whether such possibility should be regarded as a serious practical problem or not. Here we take a pragmatic approach: when using the Redfield equation, the CPT condition should be strictly monitored and when violations are observed one should try to correct them. Of course, we assume that no other master equation is available for a more accurate description of the dynamics.

[1] The difference is that the rotating-wave approximation is applied at the level of the interaction Hamiltonian V before tracing out the environment, while the secular approximation is applied at the level of the system's master equation. Therefore, even though they share a similar spirit, they are different approximations: see Refs. [81–83] for a more in-depth comparison.

[2] Few approaches to beyond-secular physics have been proposed in the literature without taking the Redfield equation as a starting point: see, e.g., the so-called *refined weak-coupling limit* described in Ref. [24].

We call *regularization* the act of modifying a master equation to make it satisfy the CPT requirement, possibly without spoiling accuracy and other nice properties the original master equation could have. Since this is a vague task, it comes without surprises that a great number of approaches exist to achieve this purpose, each with its set of pros and cons. The mathematical origin of this vagueness lies in the lack of a general characterization theorem for the generator of a CPT dynamical map. However, we do have a tool in case we are willing to turn the equation into a Markovian one—which may be appropriate or not according to the situation: the LGKS theorem. If we manage to write the master equation at hand in canonical form and if we turn the Kossakowski matrix into a positive semidefinite matrix, then regularization has been achieved. The secular approximation is just one way of doing this, by making the following substitution in Eq. (2.122):

$$\chi_{\alpha\beta}(\omega,\omega';t) \mapsto \delta_{\omega,\omega'}\chi_{\alpha\beta}(\omega). \tag{3.1}$$

The purpose of this chapter is to present a set of regularization techniques beyond the secular one. Specifically, in Sec. 3.1 we begin by reviewing few famous beyond-secular master equations from this point of view. Then, in Secs. 3.2 and 3.3 we present two new proposals to perform the regularization of general master equations, highlighting their pros and cons with respect to preexisting techniques.

3.1 Beyond-secular master equations

As we discussed above, we are interested in providing regularizations beyond the reach of the secular approximation. As a preliminary step, in this section we will briefly discuss a restricted selection of beyond-secular master equations—taken from Refs. [29, 32, 33, 37]—from the point of view of the regularization language.

3.1.1 Partial secular master equation

Let us consider the interaction-picture version of the time-independent Redfield equation, expressed in terms of the system's Bohr frequencies. We rewrite it here for convenience:

$$\begin{aligned}\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} &= -i\sum_{\alpha,\beta}\sum_{\omega,\omega'\in\mathcal{B}}\eta_{\alpha\beta}(\omega,\omega')e^{i(\omega-\omega')t}[A^\dagger_\alpha(\omega)A_\beta(\omega'),\varrho(t)]\\ &\quad+\sum_{\alpha,\beta}\sum_{\omega,\omega'\in\mathcal{B}}\chi_{\alpha\beta}(\omega,\omega')e^{i(\omega-\omega')t}\left[A_\beta(\omega')\varrho(t)A^\dagger_\alpha(\omega)-\frac{1}{2}\{A^\dagger_\alpha(\omega)A_\beta(\omega'),\varrho(t)\}\right].\end{aligned} \tag{3.2}$$

A quite physically-grounded approach consists in making a *coarse-graining transformation* [27, 29]: suppose we do not have access to $\varrho(t)$ at an arbitrary resolution in time, so that we are bound to measure time with a finite error Δ. More specifically, we alter the master equation by averaging both sides over the time span $[t-\Delta/2, t+\Delta/2]$, which means to apply the operation

$$\mathscr{C}_\Delta[X(t)] := \frac{1}{\Delta}\int_{t-\Delta/2}^{t+\Delta/2}\mathrm{d}s\, X(s). \tag{3.3}$$

Suppose Δ is much smaller than the typical evolution timescale of $\varrho(t)$, so that we can still hope to resolve the relevant part of the dynamics. Then, approximately speaking, on the left-hand side nothing changes:

$$\mathscr{C}_\Delta\left[\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t}\right] = \frac{\varrho(t+\Delta/2) - \varrho(t-\Delta/2)}{\Delta} \simeq \frac{\mathrm{d}\varrho(t)}{\mathrm{d}t}. \tag{3.4}$$

For the same reason, on the right-hand side the density operator can be brought out of the integral (since it changes very little over the integration region):

$$\mathscr{C}_\Delta[e^{i(\omega-\omega')t}\varrho(t)] \simeq \frac{\varrho(t)}{\Delta}\int_{t-\Delta/2}^{t+\Delta/2} \mathrm{d}s\, e^{i(\omega-\omega')s} = e^{i(\omega-\omega')t}\mathrm{sinc}\left[\frac{(\omega-\omega')\Delta}{2}\right]\varrho(t), \tag{3.5}$$

where $\mathrm{sinc}(x) := \sin(x)/x$ stands for the cardinal sine. The effect of the coarse graining is thus the substitution

$$\begin{aligned} \chi_{\alpha\beta}(\omega,\omega') &\mapsto \chi^{(\Delta)}_{\alpha\beta}(\omega,\omega') := \chi_{\alpha\beta}(\omega,\omega')S^{(\Delta)}_{\omega-\omega'}, \\ \eta_{\alpha\beta}(\omega,\omega') &\mapsto \eta^{(\Delta)}_{\alpha\beta}(\omega,\omega') := \eta_{\alpha\beta}(\omega,\omega')S^{(\Delta)}_{\omega-\omega'}, \end{aligned} \tag{3.6}$$

where

$$S^{(\Delta)}_\omega := \mathrm{sinc}\left(\frac{\omega\Delta}{2}\right) \tag{3.7}$$

is a *sampling factor*. Note that in the limit $\Delta \to \infty$, we have $S^{(\Delta)}_\omega \to \delta_{\omega,0}$ and we recover the effect of the secular approximation reported in Eq. (3.1)[3]. For this reason, the transformation (3.6) with finite Δ is called *partial secular approximation*. The importance of this procedure lies in the following result, whose proof can be found in Ref. [29].

Theorem 3.1. *There exists $\Delta_0 > 0$ such that $\chi^{(\Delta)}_{\alpha\beta}(\omega,\omega')$ is positive semidefinite for any $\Delta \geq \Delta_0$. Specifically,*

$$\Delta_0 = \frac{4(|\mathcal{B}|-1)\gamma_{\max}}{\lambda_{\min}\nu_{\min}}, \tag{3.8}$$

where $|\mathcal{B}|$ is the number of Bohr frequencies, $\gamma_{\max} := \max_\omega \|\Gamma(\omega)\|_\infty$ with $\|\cdot\|_\infty$ being the uniform norm [56], $\lambda_{\min} := \min_\omega \lambda(\omega)$ with $\lambda(\omega)$ being the minimum eigenvalue of $\chi(\omega)$, and finally $\nu_{\min} := \min_{\omega\neq\omega'} |\omega-\omega'|$. All maximizations and minimizations are here intended for $\omega \in \mathcal{B}$.

If the coarse graining parameter Δ is carefully chosen, the partial secular master equation generates CPT evolution and is thus a valid regularization of the Redfield equation. It is interesting to observe how Δ_0 in Eq. (3.8) is structured. First, Δ_0 increases when the minimum eigenvalue of $\chi(\omega)$ approaches zero: in particular, this means that the full secular choice $\Delta \to \infty$ is the only possibility for a singular χ—at least according to the bound in Eq. (3.8), which is however not tight [29]. Interestingly, Δ_0 increases also when the spacing between Bohr frequencies decreases, signaling that the denser the levels the greater the timescales we need to ignore by coarse graining.

[3] Sending $\Delta \to \infty$ is a formal violation of the hypothesis of having Δ smaller than the evolution timescale of $\varrho(t)$, hence this is not a proper derivation of the secular master equation.

3.1.2 Geometric-arithmetic master equation

While the partial secular approach improves upon the full secular one, it does not solve the problem in case of extremely dense system levels, since $\Delta_0 \to \infty$ when $\nu_{\min} \to 0$ in Eq. (3.8). Our desire is to perform a regularization that is independent of the system properties as much as possible. A different approach can be devised if we remember that

$$\chi(\omega, \omega') = \Gamma(\omega') + \Gamma^\dagger(\omega) \tag{3.9}$$

is defined as a sum of two contributions: it would be easier to ensure $\chi \geq 0$ if it were expressed as a product instead.

Suppose first that a single interaction channel is involved, so that $\chi(\omega, \omega')$ is a scalar-valued function. Using the fact that $\Gamma(\omega) = \frac{1}{2}\chi(\omega) + i\eta(\omega)$, where $\chi(\omega) = \chi(\omega, \omega)$ and $\eta(\omega) = \eta(\omega, \omega)$,

$$\begin{aligned} \chi(\omega, \omega') &= \frac{1}{2}[\chi(\omega) + \chi(\omega')] + i\left[\eta(\omega') - \eta(\omega)\right] \\ &= \sqrt{\chi(\omega)\chi(\omega')} + \frac{1}{2}\left[\sqrt{\chi(\omega)} - \sqrt{\chi(\omega')}\right]^2 + i\left[\eta(\omega') - \eta(\omega)\right] \\ &\equiv \sqrt{\chi(\omega)\chi(\omega')} + D(\omega, \omega'), \end{aligned} \tag{3.10}$$

where D is a "detuning" function, since $D(\omega, \omega) = 0$. In Refs. [33, 37], Davidović empirically showed that the contribution of the detuning to the dynamics can be practically ignored, provided that the coupling is smaller than the system's frequency spread. Note that this is a much weaker requirement with respect to the secular approximation, since no mention is made of the gaps between Bohr frequencies. The above argument has been heuristically extended to the case of multiple interaction channels with the use of a matrix square root:

$$\chi(\omega, \omega') \mapsto \sqrt{\chi(\omega)}\sqrt{\chi(\omega')}. \tag{3.11}$$

Recall that $\chi(\omega) \geq 0$, so that the above substitution is effectively a valid regularization of the Redfield equation. The resulting equation has been dubbed *geometric-arithmetic master equation (GAME)* [37], as it is obtained by approximating the arithmetic mean in Eq. (3.9) with the geometric mean in Eq. (3.11).

An interesting direct derivation of this Kossakowski matrix was independently obtained in Ref. [32], where the resulting master equation was called *universal Lindblad equation (ULE)*. We will now briefly show how such derivation can be compactly carried out.

Let us start with the following expression for the time-independent Redfield equation:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) &= -\lambda^2 \sum_{\alpha,\beta} \int_0^\infty \mathrm{d}\tau\, c_{\alpha\beta}(\tau)[A_\alpha(t), A_\beta(t-\tau)\varrho(t)] + \text{H.c.} \\ &= -\lambda^2 \sum_{\alpha,\beta} \int_{-\infty}^\infty \mathrm{d}s'\, \theta(t-s')c_{\overline{\alpha}\beta}(t-s')[A_\alpha^\dagger(t), A_\beta(s')\varrho(t)] + \text{H.c.} \end{aligned} \tag{3.12}$$

Remember that $c_{\overline{\alpha}\beta}(\tau)$ is the inverse Fourier transform of $\chi_{\alpha\beta}(\omega)$. We introduce the so-called *jump correlator* [32] as the inverse Fourier transform of $\sqrt{\chi(\omega)}$:

$$g(\tau) := \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}\omega\, \sqrt{\chi(\omega)}e^{-i\omega\tau}. \tag{3.13}$$

By the convolution theorem for Fourier transforms, we get the relation

$$\sum_{\mu} \int_{-\infty}^{\infty} \mathrm{d}s \, g_{\alpha\mu}(t-s) g_{\mu\beta}(s-s') = c_{\overline{\alpha}\beta}(t-s'), \tag{3.14}$$

which leads us to

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta,\mu} \int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}s' \, \theta(t-s') g_{\alpha\mu}(t-s) g_{\mu\beta}(s-s') [A_\alpha^\dagger(t), A_\beta(s')\varrho(t)] + \mathrm{H.c.} \tag{3.15}$$

Under the weak-coupling assumption, $c_{\overline{\alpha}\beta}(\tau)$ quickly decays to zero and by the same reasoning the jump correlator $g_{\alpha\beta}(\tau)$ should also quickly decay to zero. We can then substitute $t \leftrightarrow s$ inside the integral without making much of an impact:

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta,\mu} \int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}s' \, \theta(s-s') g_{\alpha\mu}(s-t) g_{\mu\beta}(t-s') [A_\alpha^\dagger(s), A_\beta(s')\varrho(t)] + \mathrm{H.c.} \tag{3.16}$$

Rigorous error bounds for this substitution can be found in Ref. [32]. Introducing again the Bohr representation for the interaction operators,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = -\lambda^2 \sum_{\alpha,\beta,\mu} \sum_{\omega,\omega' \in \mathcal{B}} \int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}s' \, \theta(s-s') \\ \times g_{\alpha\mu}(s-t) e^{i\omega s} g_{\mu\beta}(t-s') e^{-i\omega' s'} [A_\alpha^\dagger(\omega), A_\beta(\omega')\varrho(t)] + \mathrm{H.c.} \end{aligned} \tag{3.17}$$

At this point we make the decomposition

$$\theta(s-s') = \frac{1}{2}\left[1 + \mathrm{sgn}(s-s')\right], \tag{3.18}$$

which yields two contributions. In the first one, we recognize the known Fourier transforms of the jump correlators:

$$\begin{aligned} &-\frac{\lambda^2}{2} \sum_{\alpha,\beta,\mu} \sum_{\omega,\omega' \in \mathcal{B}} e^{i(\omega-\omega')t} \sqrt{\chi(\omega)}_{\alpha\mu} \sqrt{\chi(\omega')}_{\mu\beta} [A_\alpha^\dagger(\omega), A_\beta(\omega')\varrho] + \mathrm{H.c.} \\ &= \lambda^2 \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} e^{i(\omega-\omega')t} \left[\sqrt{\chi(\omega)}\sqrt{\chi(\omega')}\right]_{\alpha\beta} \left[A_\beta(\omega')\varrho(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\left\{A_\alpha^\dagger(\omega)A_\beta(\omega'), \varrho\right\}\right], \end{aligned} \tag{3.19}$$

where we used Lemma 2.5 to arrange the result in canonical form. This is precisely the interaction-picture dissipator of the geometric-arithmetic master equation.

The second term originating from the decomposition (3.18) is what differentiates the ULE from the GAME. Specifically, such term is

$$-i\lambda^2 \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} e^{i(\omega-\omega')t} \eta_{\alpha\beta}(\omega,\omega') [A_\alpha^\dagger(\omega), A_\beta(\omega')\varrho(t)] + \mathrm{H.c.} \tag{3.20}$$

with

$$\eta_{\alpha\beta}(\omega,\omega') = -\frac{i}{2} \sum_{\mu} \int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}s' \, \mathrm{sgn}(s-s') g_{\alpha\mu}(s-t) e^{i\omega(s-t)} g_{\mu\beta}(t-s') e^{i\omega'(t-s')}. \tag{3.21}$$

It is immediate to check that $\eta^*_{\beta\alpha}(\omega', \omega) = -\eta_{\alpha\beta}(\omega, \omega')$, hence this effectively turns out to be a Lamb shift contribution by Lemma 2.5:

$$-i\lambda^2 \sum_{\alpha,\beta} \sum_{\omega,\omega' \in \mathcal{B}} e^{i(\omega-\omega')t} \eta_{\alpha\beta}(\omega, \omega') [A^\dagger_\alpha(\omega) A_\beta(\omega), \varrho(t)]. \tag{3.22}$$

Following Ref. [32], we can also show that $\eta(\omega, \omega')$ can be written in a more compact form in terms of $\sqrt{\chi}$. First, we use the definition of jump correlator to write

$$\begin{aligned} \eta_{\alpha\beta}(\omega, \omega') = &-\frac{i}{2(2\pi)^2} \sum_\mu \int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}s' \,\mathrm{sgn}(s - s') \int_{-\infty}^{\infty} \mathrm{d}E \int_{-\infty}^{\infty} \mathrm{d}E' \\ &\times \sqrt{\chi(E)}_{\alpha\mu} e^{-iE(s-t)} e^{i\omega(s-t)} \sqrt{\chi(E')}_{\mu\beta} e^{-iE'(t-s')} e^{i\omega'(t-s')}. \end{aligned} \tag{3.23}$$

This can be arranged as

$$\eta_{\alpha\beta}(\omega, \omega') = -\frac{i}{2(2\pi)^2} \int_{-\infty}^{\infty} \mathrm{d}E \int_{-\infty}^{\infty} \mathrm{d}E' \left[\sqrt{\chi(E)} \sqrt{\chi(E')} \right]_{\alpha\beta} \mathcal{R}(\omega - E, E' - \omega'), \tag{3.24}$$

where

$$\mathcal{R}(\omega, \omega') := \int_{-\infty}^{\infty} \mathrm{d}\tau \int_{-\infty}^{\infty} \mathrm{d}\tau' \,\mathrm{sgn}(\tau - \tau') e^{i\omega\tau + i\omega'\tau'}. \tag{3.25}$$

This quantity can be explicitly computed as follows:

$$\begin{aligned} \mathcal{R}(\omega, \omega') &= \int_{-\infty}^{\infty} \mathrm{d}\tau \int_{-\infty}^{\tau} \mathrm{d}\tau' \left[e^{i\omega\tau + i\omega'\tau'} - e^{i\omega\tau' + i\omega'\tau} \right] \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \int_{0}^{\infty} \mathrm{d}\overline{\tau} \left[e^{i\omega\tau + i\omega'(\tau - \overline{\tau})} - e^{i\omega(\tau - \overline{\tau}) + i\omega'\tau} \right] \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \, e^{i(\omega+\omega')\tau} \int_{0}^{\infty} \mathrm{d}\overline{\tau} \left[e^{-i\omega'\overline{\tau}} - e^{-i\omega\overline{\tau}} \right] \\ &= 2\pi\delta(\omega + \omega') \left[\pi\delta(\omega') - i\mathbb{P}\frac{1}{\omega'} - \pi\delta(\omega) + i\mathbb{P}\frac{1}{\omega} \right] = 4\pi i \delta(\omega + \omega') \mathbb{P}\frac{1}{\omega}, \end{aligned} \tag{3.26}$$

Substituting above, we finally obtain

$$\eta(\omega, \omega') = \frac{1}{2\pi} \mathbb{P} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{E} \sqrt{\chi(\omega - E)} \sqrt{\chi(\omega' - E)}. \tag{3.27}$$

Note how this expression reduces to the secular case, where η is given by the Kramers-Krönig relation (2.147), if we restrict to $\omega = \omega'$.

3.2 Dynamical regularization

In the previous section we discussed how some common procedures employed to regularize the time-independent Redfield equation essentially amount to substituting the original Kossakowski matrix with a certain positive semidefinite matrix, thus making the dynamics CPT—and Markovian—by the LGKS theorem. Such approaches were tailored to the particular structure of the Kossakowski matrix and can hardly be generalized to other scenarios, such as for the *time-dependent* Redfield equation.

In this section we will describe a simple proposal we put forward in Ref. [38] to regularize *any* time-local master equation, such as the time-dependent Redfield equation, once it is written in canonical form. The idea is the following: what if, at every time instant t, we "project" the Kossakowski matrix $\chi(t)$ onto the set of positive semidefinite matrices? In this way, we are making an optimal minimal-disturbance choice for a positive χ, while being capable of keeping into account its time dependence. Using an exactly solvable example, we will show how this idea yields a master equation that is more accurate with respect to the previous approaches, especially at small times.

Of course, Markovian dynamics is enforced by this procedure: in Sec. 3.3 we will see how a similar projection technique can be employed to regularize any time-local master equation while keeping its eventual non-Markovian features.

3.2.1 Dynamical projection idea

In the system's energy basis, any time-local master equation in canonical form (2.42) can be written in the form

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i[H_S + \lambda^2 H_{LS}(t), \rho(t)] + \lambda^2 \sum_{i,j} \chi_{ij}(t)\left[E_j \rho(t) E_i^\dagger - \frac{1}{2}\left\{E_i^\dagger E_j, \rho(t)\right\}\right], \tag{3.28}$$

where $H_{LS}(t) = \sum_{i,j} \eta_{ij}(t) E_i^\dagger E_j$ and we defined for convenience d^2 collective indices $i = (k, q)$ and $j = (n, m)$ [cf. Eq. (2.126) for the case of the Redfield equation]. With this notation it is obvious that the Kossakowski matrix $\chi(t)$ can be seen as a Hermitian $d^2 \times d^2$ complex matrix.

Suppose we fix a norm $\|\cdot\|$ on the space of $d^2 \times d^2$ complex matrices, such as the Frobenius norm $\|X\| := \sqrt{\operatorname{Tr} X^\dagger X}$. Then, we consider the problem

$$\chi^+(t) := \arg \min_{P = P^\dagger \geq 0} \|\chi(t) - P\|. \tag{3.29}$$

Standard convex analysis ensures that this is a well-defined expression [85, 86]. Specifically, this is a projection onto the closed convex cone of positive semidefinite matrices. In other words, $\chi^+(t)$ is the (unique) positive semidefinite matrix which is "closest" to $\chi(t)$ according to the norm $\|\cdot\|$. If we focus on the Frobenius norm, an explicit formula for $\chi^+(t)$ can be written. While this is a well-known result in statistics and optimization theory, we reproduce a proof here, given its importance for the present discussion [87].

Theorem 3.2. *Let $\|\cdot\|$ be the Frobenius norm and let χ be a Hermitian matrix, with unitary spectral decomposition $\chi = U \operatorname{diag}(\ell_i) U^\dagger$. Then,*

$$\chi^+ = U \operatorname{diag}(\max\{\ell_i, 0\}) U^\dagger = \frac{\chi + |\chi|}{2}, \tag{3.30}$$

where $|\chi| = \sqrt{\chi^2}$ is the matrix absolute value. In other words, χ^+ is obtained by putting to zero the negative eigenvalues of χ while keeping the eigenvectors unchanged.

Proof. Let P be an arbitrary Hermitian positive semidefinite matrix of the same dimension as χ. Since the Frobenius norm is unitarily invariant, we can write

$$\|\chi - P\|^2 = \left\|U \operatorname{diag}(\ell_i) U^\dagger - P\right\|^2 = \left\|\operatorname{diag}(\ell_i) - U^\dagger P U\right\|^2. \tag{3.31}$$

The matrix $Y := U^\dagger P U$ is still positive semidefinite. Therefore, since $\|X\|^2 = \sum_{i,j} |X_{ij}|^2$,

$$\|\chi - P\|^2 = \sum_{i\neq j} |Y_{ij}|^2 + \sum_i |\ell_i - Y_{ii}|^2 \geq \sum_i |\ell_i - Y_{ii}|^2 \geq \sum_{i:\ell_i<0} |\ell_i - Y_{ii}|^2 \geq \sum_{i:\ell_i<0} \ell_i^2, \tag{3.32}$$

where in the last inequality we used the fact that $Y_{ii} \geq 0$. This bound is tight and is uniquely saturated by the choice $Y = \mathrm{diag}(\max\{\ell_i, 0\})$, for which $P = UYU^\dagger = U\mathrm{diag}(\max\{\ell_i, 0\})U^\dagger$. □

Our *dynamical regularization* proposal amounts then to the substitution [38]

$$\chi(t) \mapsto \chi^+(t), \qquad \forall t \geq t_0. \tag{3.33}$$

By the LGKS theorem, this is enough to guarantee CPT Markovian evolution, therefore it is a proper regularization that is capable of keeping into account the time dependence of $\chi(t)$, unlike the techniques described in Sec. 3.1. Moreover, this procedure is well-defined not only for the Redfield equation but for any time-local master equation that is written in canonical form.

It is worth mentioning that a somewhat similar (but less general) optimization has been proposed in Ref. [35]: there, the authors parametrically splitted the Redfield equation into a "positive" and a "negative" contribution, minimizing the latter with an appropriate choice of parameters. Such approach was tailored to the case of single interaction channel, and can be extended to multiple uncorrelated channels by optimizing each channel separately. As we will show in a moment, this is basically equivalent to our proposal in the case of single interaction channel. However, with the dynamical regularization we are not limited to such scenario and we are able to handle arbitrary interaction structures using a more "global" optimization.

3.2.2 Explicit formula for single interaction channel

In the most general case, the dynamical regularization (3.33) can be efficiently carried out by numerical diagonalization. The projection can, however, be performed analytically in the case of a single interaction channel: this calculation will allow us to gain some insight into when we expect the regularized dynamics to be sufficiently close to the original one.

For single interaction channel the Kossakowski matrix has the form

$$\chi_{ij}(t) = \left[\Gamma_j(t) + \Gamma_i^*(t)\right] A_i^* A_j = A_i^* G_j(t) + G_i^*(t) A_j, \tag{3.34}$$

where $\Gamma_i(t) \equiv \Gamma(\omega_i; t)$ and we defined $G_i(t) := \Gamma_i(t) A_i$. From now on, we will drop the time index t for ease of notation. Excluding trivial scenarios, we must now distinguish between two situations.

If $\Gamma_i \equiv \Gamma$ is constant, then $\chi_{ij} = (2\,\mathrm{Re}\,\Gamma) A_i^* A_j$ becomes a rank-one matrix with unique non-zero eigenvalue $\ell = (2\,\mathrm{Re}\,\Gamma)\|\mathbf{A}\|^2$ and associated eigenvector $\mathbf{A}^*/\|\mathbf{A}\|$, where $\mathbf{A}$ is the vector with components A_i and we denoted $\|\mathbf{A}\| = \sum_i |A_i|^2$. If $\ell \geq 0$, then χ is already positive semidefinite and no regularization is needed. Otherwise, if $\ell < 0$, the projection would lead to the zero matrix $\chi^+ = 0$. Therefore, this case is of little interest.

Provided the Γ_i are not all equal, then $\mathbf{A}$ and $\mathbf{G}$ are linearly independent vectors and χ is a rank-two matrix. Only two non-zero eigenvalues are allowed, and the corresponding eigenvectors must be of the form $\mathbf{V} = a\mathbf{A}^* + b\mathbf{G}^*$. Imposing $\chi\mathbf{V} = \ell\mathbf{V}$ and equating the coefficients, we find

$$\ell a = a\langle \mathbf{A}, \mathbf{G}\rangle + b\|\mathbf{G}\|^2, \qquad \ell b = a\|\mathbf{A}\|^2 + b\langle \mathbf{G}, \mathbf{A}\rangle, \tag{3.35}$$

where $\langle \mathbf{A}, \mathbf{G}\rangle = \sum_i A_i^* G_i$. From the first equation we get

$$\frac{b}{a} = \frac{\ell - \langle \mathbf{A}, \mathbf{G}\rangle}{\|\mathbf{G}\|^2}, \tag{3.36}$$

which substituted into the second yields a second-order equation for ℓ, with solutions

$$\ell_\pm = \mathrm{Re}\langle \mathbf{A}, \mathbf{G}\rangle \pm \sqrt{\|\mathbf{A}\|^2\|\mathbf{G}\|^2 - [\mathrm{Im}\langle \mathbf{A}, \mathbf{G}\rangle]^2}. \tag{3.37}$$

By the Cauchy-Schwarz inequality, we immediately see that $\ell_+ \geq 0$ and $\ell_- \leq 0$, which confirms that χ is not positive semidefinite, in general.

It is instructive to rewrite $\ell_\pm$ explicitly in terms of physical quantities. To do that, let us introduce the following notation:

$$\langle \mathbf{x}^\alpha\rangle := \frac{\sum_i x_i^\alpha |A_i|^2}{\sum_i |A_i|^2}, \tag{3.38}$$

meaning that we treat $|A_i|^2/\|\mathbf{A}\|^2$ as a probability distribution. Then, if we split Γ_i in its real and imaginary parts as $\Gamma_i = J_i + iS_i$,

$$\langle \mathbf{A}, \mathbf{G}\rangle = \sum_i A_i^* G_i = \sum_i \Gamma_i |A_i|^2 = \|\mathbf{A}\|^2[\langle \mathbf{J}\rangle + i\langle \mathbf{S}\rangle], \tag{3.39a}$$

$$\|\mathbf{G}\|^2 = \sum_i |G_i|^2 = \sum_i |\Gamma_i|^2 |A_i|^2 = \sum_i (J_i^2 + S_i^2)|A_i|^2 = \|\mathbf{A}\|^2\left[\langle \mathbf{J}^2\rangle + \langle \mathbf{S}^2\rangle\right]. \tag{3.39b}$$

We conclude that

$$\ell_\pm = \|\mathbf{A}\|^2[\langle \mathbf{J}\rangle \pm \mathcal{V}], \qquad \mathcal{V} := \sqrt{\langle \mathbf{J}\rangle^2 + \mathrm{Var}(\mathbf{J}) + \mathrm{Var}(\mathbf{S})}, \tag{3.40}$$

where $\mathrm{Var}(\mathbf{x}) := \langle \mathbf{x}^2\rangle - \langle \mathbf{x}\rangle^2$. Similar results were also reported in Refs. [22, 35, 37]. The bigger the variances associated with Γ_i, the bigger the magnitude of the negative eigenvalue ℓ_-, hence the regularization is expected to cause minimum disturbance when the environment correlation function is quite flat over the set of Bohr frequencies of the system. This is consistent with a Markovian dynamics requirement. In fact, remember that the magnitude of the negative eigenvalues of the Kossakowski matrix can be used to measure non-Markovianity according to the RHP measure (see Sec. 2.2.4).

The regularized Kossakowski matrix can now be written as $\chi_{ij}^+ = \ell_+ V_i V_j^*$, where $\mathbf{V}$ is the normalized eigenvector associated with ℓ_+. We can write

$$\mathbf{V} = \frac{\mathbf{W}}{\|\mathbf{W}\|}, \qquad \mathbf{W} = \|\mathbf{G}\|^2\mathbf{A}^* + (\ell_+ - \langle \mathbf{A}, \mathbf{G}\rangle)\mathbf{G}^*, \tag{3.41}$$

from which

$$\chi_{ij}^+ = \frac{\ell_+ A_i^* A_j}{\|\mathbf{W}\|^2}\left[\|\mathbf{G}\|^4 + \|\mathbf{G}\|^2(\ell_+ - \langle \mathbf{A}, \mathbf{G}\rangle^*)\Gamma_j + \|\mathbf{G}\|^2(\ell_+ - \langle \mathbf{A}, \mathbf{G}\rangle)\Gamma_i^* + |\ell_+ - \langle \mathbf{A}, \mathbf{G}\rangle|^2\Gamma_i^*\Gamma_j\right]. \tag{3.42}$$

After some manipulation, this acquires the form

$$\chi^+_{ij} = \frac{\ell_+ A_i^* A_j}{\|\mathbf{W}\|^2} \|\mathbf{A}\|^2 \|\mathbf{G}\|^2 \left[\langle \mathbf{J}^2 \rangle + \langle \mathbf{S}^2 \rangle + (\mathcal{V} - i\langle \mathbf{S} \rangle)\Gamma_j + (\mathcal{V} + i\langle \mathbf{S} \rangle)\Gamma_i^* + \Gamma_i^* \Gamma_j\right]. \tag{3.43}$$

Moreover, a straightforward calculation shows that

$$\|\mathbf{W}\|^2 = 2\ell_+ \|\mathbf{A}\|^2 \|\mathbf{G}\|^2 \mathcal{V}, \tag{3.44}$$

from which we obtain the following final result for the regularized Kossakowski matrix:

$$\chi^+_{ij} = \frac{A_i^* A_j}{2\mathcal{V}} \left[\langle \mathbf{J}^2 \rangle + \langle \mathbf{S}^2 \rangle + (\mathcal{V} - i\langle \mathbf{S} \rangle)\Gamma_j + (\mathcal{V} + i\langle \mathbf{S} \rangle)\Gamma_i^* + \Gamma_i^* \Gamma_j\right]. \tag{3.45}$$

3.2.3 Example

It is worth comparing the dynamical regularization (3.33) with the approaches discussed in Sec. 3.1, in order to assess if there is indeed an advantage in terms of better approximating the exact underlying dynamics. For this reason we now look for a simple example where the system's evolution can be obtained exactly, and the various regularizations will be put to the test against such evolution.

Probably the simplest exactly-solvable open quantum system is a qubit coupled to the field vacuum through an excitation-preserving interaction [6]. Specifically, the system is spanned by two states $|0\rangle, |1\rangle$ and has Hamiltonian $H_S = \varepsilon\,|1\rangle\langle 1|$, the environment is a collection of harmonic oscillators $H_E = \sum_p \varepsilon_p c_p^\dagger c_p$, and the interaction is

$$V = \sum_p \left[g_p\,|1\rangle\langle 0| \otimes c_p + g_p^*\,|0\rangle\langle 1| \otimes c_p^\dagger\right]. \tag{3.46}$$

Unfortunately, the Kossakowski matrix of the Redfield equation associated with this model turns out to be rank-one: as we argued above, this is not suitable for the application of the dynamical regularization. This fact can be seen as follows. First, we identify the interaction operators,

$$A_1 = |1\rangle\langle 0|, \quad A_2 = |0\rangle\langle 1|, \quad B_1 = \sum_p g_p c_p, \quad B_2 = \sum_p g_p^* c_p^\dagger. \tag{3.47}$$

Since the environment is assumed to be in its vacuum state at the beginning of the evolution, the only non-zero component of the correlation function is $c_{\overline{2}2}(\tau)$, hence

$$\chi_{kq,nm}(t) = \left[\Gamma_{22}(\omega_{nm};t) + \Gamma_{22}^*(\omega_{kq};t)\right] A_{2,kq}^* A_{2,nm} = 2\,\mathrm{Re}[\Gamma_{22}(\varepsilon;t)]\delta_{k0}\delta_{q1}\delta_{n0}\delta_{m1}, \tag{3.48}$$

which has only one non-zero entry, namely $\chi_{01,01}(t)$.

We can avoid this problem by moving to higher-dimensional systems. In Ref. [88] one can find the exact solution of a three-dimensional open system, spanned by the states $|0\rangle, |1\rangle, |2\rangle$: this is better suited for the purpose of our discussion and we choose it for illustrating the performance of the dynamical regularization [38]. The environment is still described by a collection of harmonic oscillators in the vacuum state, but system Hamiltonian and interaction are now given by

$$H_S = \omega_1\,|1\rangle\langle 1| + \omega_2\,|2\rangle\langle 2|, \qquad V = \sum_p \left[g_{1,p}\,|0\rangle\langle 1| + g_{2,p}\,|0\rangle\langle 2|\right] \otimes c_p^\dagger + \mathrm{H.c.} \tag{3.49}$$

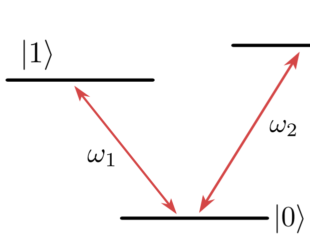

Figure 3.1: Energy levels of an open three-level V-system. The arrows indicate transitions induced by an external bosonic environment in its vacuum state.

Such interaction causes transitions solely between the levels $|0\rangle$ and $|1\rangle$, and between the levels $|0\rangle$ and $|2\rangle$: it is customary to say that the system is put in a *V configuration* (see Fig. 3.1).

Similarly to the qubit case, not all interaction operators appear in the Redfield equation if the environment starts out in its vacuum state. Specifically, only the operators

$$A_\alpha = |0\rangle\langle\alpha| \,, \qquad B_\alpha = \sum_p g_{\alpha,p} c_p^\dagger, \qquad \alpha \in \{1,2\} \tag{3.50}$$

matter, and correspondingly we only have to consider the components $c_{\overline{\alpha}\beta}(\tau)$, $\alpha, \beta \in \{1,2\}$ of the correlation function. Here we follow Ref. [88] and we assume

$$c_{\overline{\alpha}\beta}(\tau) = \frac{\gamma_{\alpha\beta}\mu}{2} e^{-\mu|\tau|} e^{-i\omega_0\tau}, \tag{3.51}$$

where $\mu, \omega_0 > 0$ and $\gamma_{\alpha\beta} = \sqrt{\gamma_\alpha \gamma_\beta}$ with $\gamma_{1,2} > 0$. In the simplifying case $\gamma_1 = \gamma_2 = \gamma$, we can consider γ as a measure of the system-environment coupling, and hence of the inverse typical evolution time of the system (in interaction picture). Instead, μ can be thought of as the inverse decay time of environment's correlations. In this context, the Markov approximation translates in the requirement $\gamma \ll \mu$.

We proceed by showing a comparison between the exact solution and what we obtain by numerically solving the Redfield equation and various regularizations of it. Such master equations can straightforwardly be approached numerically with a vectorization of the generator followed by the application of a standard Runge-Kutta integrator [89, 90] (see Refs. [38, 39] for additional details). In Fig. 3.2 we report the results for the density matrix elements when the system starts out from the pure initial state $(|1\rangle + |2\rangle)/\sqrt{2}$, choosing as parameters $\omega_1 = 1$, $\omega_2 = 2$, $\omega_0 = 1.5$, $\gamma_1 = \gamma_2 = 0.3$, and $\mu = 2$ (as usual, we work in units such that $\hbar = k_B = 1$). At this level all equations behave more or less similarly. Except for the fact that the secular-approximated one globally provides the worst results, it is hard to tell which of the others performs better. The situation is similar for other choices of parameters.

If we want to assess more carefully the quality of a regularization we should compare the predictions with the exact dynamics in a way that is independent from the initial state. Here we adopt a simple technique to compare two evolution in a pointwise fashion[4] using the Choi-Jamiołkowski isomorphism (see Sec. 2.1.2). Specifically, let $\Phi_t^{(1)}$ and $\Phi_t^{(2)}$ be two linear superoperators that map the initial state to the state at time t according to two different procedures (such as the exact dynamics or a certain master equation). Then, it is meaningful

[4] More global comparisons should be possible and are left to future work.

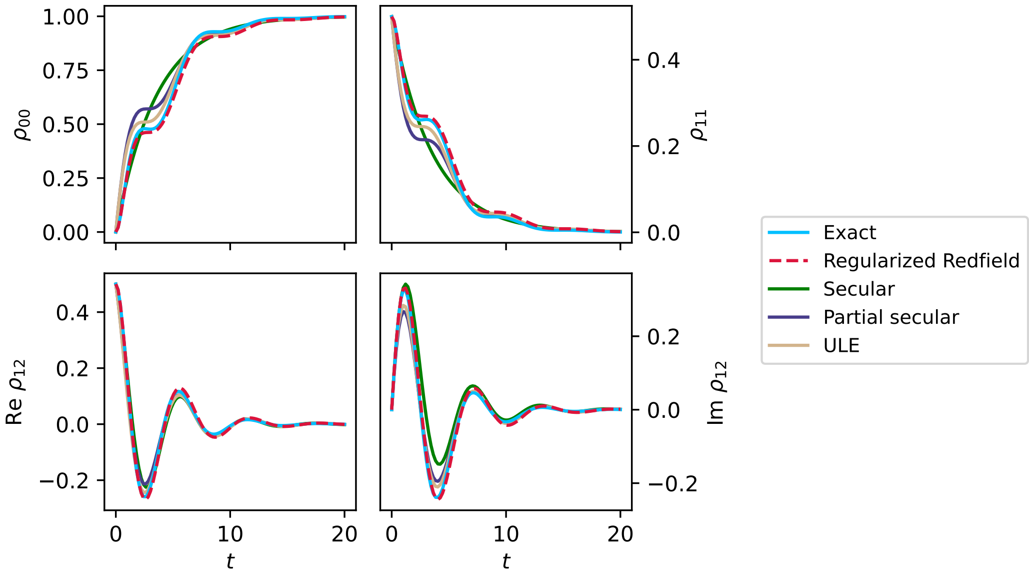

Figure 3.2: Time evolution of the three-level density matrix elements starting from the pure state $(|1\rangle + |2\rangle)/\sqrt{2}$. The label "Regularized Redfield" refers to the dynamical regularization. The partial secular case is obtained by finding the smallest coarse-graining time Δ_0 that guarantees positivity of the Kossakowski matrix. The label "ULE" refers to the universal Lindblad equation. The parameters of the model are $\omega_1 = 1$, $\omega_2 = 2$, $\omega_0 = 1.5$, $\gamma_1 = \gamma_2 = 0.3$, and $\mu = 2$.

to consider the distance between the corresponding Choi operators as measured by some arbitrarily defined norm:

$$\delta(t) := \| J(\Phi_t^{(1)}) - J(\Phi_t^{(2)}) \| \,. \tag{3.52}$$

This provides a measure of the difference between two dynamics that does not depend on the initial state[5].

In Fig. 3.3 we report examples for $\delta(t)$ between the exact solution and the various master equations, calculated with the Frobenius norm. Parameters are here fixed at $\omega_1 = 1$, $\omega_2 = 2$, $\omega_0 = 1.5$, $\gamma_1 = \gamma_2 = 0.05$, and we present results for several values of μ. We find that the performance of the dynamical regularization depends on the ratio between μ and the frequency spread of the system $\omega_R := \max\{\omega_1, \omega_2\}$.

For values of μ that are sufficiently larger that ω_R, the procedure has little effect on the already good accuracy of the Redfield equation, as expected from the fact that the Kossakowski matrix is essentially positive semidefinite in a deep Markovian regime. For smaller values of μ—while still being greater than ω_R—we can instead observe how the dynamical regularization well approximates the exact dynamics in a more consistent way with respect to the other master equations, especially at short times. This was not clear with a direct comparison at the level of the density matrix, and it is a consequence of the ability to retain time dependence in the Kossakowski matrix.

However, a change in the trend can be observed when lowering the value of μ below

[5]Of course, other choices are possible. From a quantum information perspective, it would make sense to consider, e.g., the *diamond norm* [56]. The choice we make here is primarily dictated by simplicity and convenience.

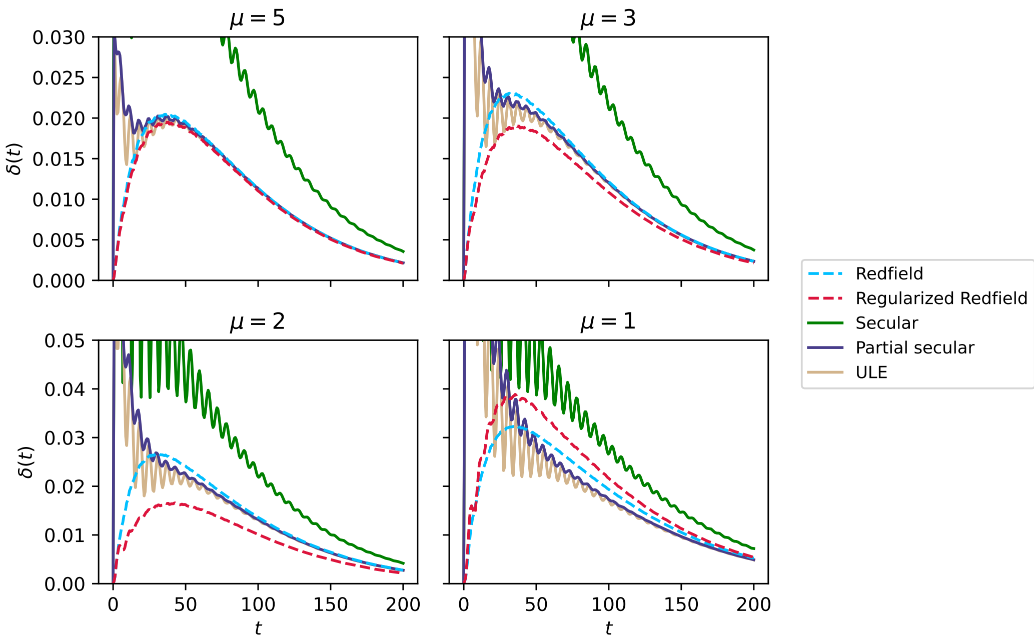

Figure 3.3: Distance from the exact dynamics for the three-level system as represented by the quantity $\delta(t)$, defined in Eq. (3.52) using the Frobenius norm, for several values of μ while fixing $\omega_1 = 1$, $\omega_2 = 2$, $\omega_0 = 1.5$, $\gamma_1 = \gamma_2 = 0.05$. The various master equations are chosen as in Fig. 3.2.

ω_R, where the regularization provides results worse than Redfield itself. In this essentially non-Markovian regime, the truncation of the negative part of the Kossakowski matrix has a drastic effect on the dynamics. This situation is of course out of reach for the approaches presented up to now, since they all enforce CP-divisible dynamics.

3.3 Choi-proximity regularization

The regularization procedures approached so far are meant to provide well-defined *Markovian* evolutions, in the spirit of improving upon the secular approximation. The dynamical regularization of Sec. 3.2 is applicable beyond the realm of the Redfield equation, even though CP-divisibility is inevitably imposed by the projection of the Kossakowski matrix. In principle, time-local master equation can display non-Markovian features, which are all missed by such manipulation.

In this section we discuss the technique we proposed in Ref. [39] to treat CPT violations in a general dynamical map without imposing CP-divisibility. The idea is to apply the projection technique at the level of the Choi operator instead of the Kossakowski matrix: this is inspired by recent work in quantum process tomography, where such projections are employed to recover proper quantum channels from a set of imprecise or partial measurements [91–94]. In the course of the section, we will show that this *Choi-proximity regularization* produces well-defined evolutions, retains non-Markovianity, and necessarily improves accuracy with respect to the unknown exact dynamics, a feature not shared with the dynamical regularization.

3.3.1 Projection onto the physical Choi space

Let Φ be a Hermitian-preserving linear superoperator. Its Choi operator $J(\Phi)$, defined back in Eq. (2.11), is obviously a Hermitian operator. We also know by Theorem 2.1 that Φ is CPT if and only if $J(\Phi)$ belongs to the set

$$\mathfrak{J} := \{P \geq 0 : \mathrm{Tr}_1 P = \mathbb{1}/d\}. \tag{3.53}$$

We will refer to $\mathfrak{J}$ as the space of *physical Choi operators*. Since $\mathfrak{J}$ is the intersection of a closed convex cone with an affine subspace, it is itself a closed convex set. It is then meaningful to consider the projection of $J(\Phi)$ onto $\mathfrak{J}$:

$$\widetilde{J} := \arg\min_{P \in \mathfrak{J}} \|J(\Phi) - P\|. \tag{3.54}$$

For mathematical convenience, we assume $\|\cdot\|$ to be the Frobenius norm, as we did in Sec. 3.2[6]. Thanks to the Choi-Jamiołkowski isomorphism, we can always find a map $\widetilde{\Phi}$ such that $J(\widetilde{\Phi}) = \widetilde{J}$. It is in fact sufficient to take [cf. Eq. (2.12)]

$$\widetilde{\Phi}(X) := d\,\mathrm{Tr}_2[\widetilde{J}(\mathbb{1} \otimes X^T)]. \tag{3.55}$$

We argue that $\widetilde{\Phi}$ can work as a minimally-invasive CPT substitute for Φ [39].

In general, it is difficult to solve the optimization problem (3.54) in closed form, and one has to attack it from a numerical standpoint. Because of the requirement on the partial trace, this is quite a different problem with respect to the one we encountered in the dynamical regularization (3.29). As often happens in quantum information, Eq. (3.54) can be formulated as a semidefinite program [56, 86]. However, more tailored approaches can be devised if one exploits the specific structure of $\mathfrak{J}$. In the mathematical literature, this is referred to as a *semidefinite least-squares problem*, a well-studied subclass of non-linear convex programming with applications in numerical linear algebra and statistics [85]. As an example of state-of-the-art approach for solving (3.54) we cite the following duality theorem [95, 96].

Theorem 3.3. *The solution to Eq.* (3.54) *can be written as*

$$\widetilde{J} = \Pi\Big[J(\Phi) + \mathbb{1} \otimes \widetilde{Y}\Big], \tag{3.56}$$

where Π is the projection onto the cone of positive semidefinite matrices, which by Theorem 3.2 can be expressed as $\Pi[X] = (X + |X|)/2$, and $\widetilde{Y}$ is the solution of the following unconstrained optimization problem:

$$\widetilde{Y} := \arg\min_{Y = Y^\dagger} \theta(Y), \tag{3.57}$$

where

$$\theta(Y) = \frac{1}{2}\|\Pi[J(\Phi) + \mathbb{1} \otimes Y]\|^2 - \mathrm{Tr}\, Y \tag{3.58}$$

is a convex differentiable objective function with Lipschitz-continuous gradient

$$\nabla\theta(Y) = \mathrm{Tr}_1(\Pi[J(\Phi) + \mathbb{1} \otimes Y]) - \frac{\mathbb{1}}{d}. \tag{3.59}$$

[6]It is interesting to point out that physical significance can be given to the choice of the Frobenius norm in terms of maximizing the likelihood function in measurement experiments [91].

The interesting fact about this theorem is that the problem of finding $\widetilde{Y}$ is much easier than (3.54), since it is unconstrained and can be approached using standard non-linear convex optimizers, such as (accelerated) gradient descent or quasi-Newton techniques [97, 98]. Moreover, we only need d^2 real parameters to describe a Hermitian matrix Y, instead of d^4 to describe P in Eq. (3.54).

Suppose now that Φ is the result of some approximation of an underlying unknown channel Φ^{ex}. Since $J(\Phi^{\mathrm{ex}}) \in \mathfrak{J}$, one can prove that $\widetilde{\Phi}$ is necessarily closer to Φ^{ex} than Φ. This is a consequence of the convexity of the problem and can be deduced by standard arguments in convex analysis [85]. Given its relevance for our discussion, we reproduce a proof here.

Theorem 3.4. $\|J(\Phi) - J(\Phi^{\mathrm{ex}})\| \geq \|J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\|$.

Proof. By convexity, we know that $\alpha J(\Phi^{\mathrm{ex}}) + (1-\alpha) J(\widetilde{\Phi}) \in \mathfrak{J}$ for any $\alpha \in [0,1]$. By definition of projection, such operator must be more distant to $J(\Phi)$ than $J(\widetilde{\Phi})$, hence

$$\begin{aligned}
\frac{1}{2}\left\|J(\Phi) - J(\widetilde{\Phi})\right\|^2 &\leq \frac{1}{2}\left\|J(\Phi) - \alpha J(\Phi^{\mathrm{ex}}) - (1-\alpha) J(\widetilde{\Phi})\right\|^2 = \frac{1}{2}\left\|J(\Phi) - J(\widetilde{\Phi}) + \alpha J(\widetilde{\Phi}) - \alpha J(\Phi^{\mathrm{ex}})\right\|^2 \\
&= \frac{1}{2}\left\|J(\Phi) - J(\widetilde{\Phi})\right\|^2 + \frac{\alpha^2}{2}\left\|J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\right\|^2 + \alpha\langle J(\Phi) - J(\widetilde{\Phi}), J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\rangle,
\end{aligned} \tag{3.60}$$

where $\langle X, Y\rangle := \mathrm{Tr}\left[X^\dagger Y\right]$. This inequality can be rearranged as

$$\langle J(\Phi) - J(\widetilde{\Phi}), J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\rangle + \frac{\alpha}{2}\left\|J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\right\|^2 \geq 0, \tag{3.61}$$

which leads to $\langle J(\Phi) - J(\widetilde{\Phi}), J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\rangle \geq 0$ after taking the limit $\alpha \to 0$. With this, we can write

$$\begin{aligned}
\left\|J(\Phi) - J(\Phi^{\mathrm{ex}})\right\|^2 &= \left\|J(\Phi) - J(\widetilde{\Phi}) + J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\right\|^2 \\
&= \left\|J(\Phi) - J(\widetilde{\Phi})\right\|^2 + \left\|J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\right\|^2 + 2\langle J(\Phi) - J(\widetilde{\Phi}), J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\rangle \\
&\geq \left\|J(\widetilde{\Phi}) - J(\Phi^{\mathrm{ex}})\right\|^2,
\end{aligned} \tag{3.62}$$

which is what we wanted to prove. □

3.3.2 Application to dynamical maps

Suppose now we have a set $\{\Phi_t\}_{t \geq t_0}$ of Hermitian-preserving maps, which are meant to approximate some exact evolution $\{\Phi_t^{\mathrm{ex}}\}_{t\geq t_0}$. Applying the projection described above to every Φ_t, we can construct a set $\{\widetilde{\Phi}_t\}_{t\geq t_0}$ of CPT maps defining the regularized dynamics (see Fig. 3.4). Such projection needs to be performed only once for every $t \geq t_0$: the evolution of any initial state can then be obtained from Eq. (3.55). Moreover, thanks to Theorem 3.4, the regularized dynamics $\widetilde{\Phi}_t$ is necessarily more accurate than Φ_t with respect to the unknown exact evolution Φ_t^{ex}.

To better see how Φ_t and $\widetilde{\Phi}_t$ differ, let us consider the difference between the corresponding Choi operators:

$$\Delta(t) := J(\widetilde{\Phi}_t) - J(\Phi_t). \tag{3.63}$$

The norm $\|\Delta(t)\|$ can be seen as a measure of CPT violation of Φ_t and quantifies the impact of the Choi-proximity regularization on the original dynamics. Clearly, for any ρ,

$$\widetilde{\Phi}_t(\rho) = \Phi_t(\rho) + d\,\mathrm{Tr}_2\left[\Delta(t)(\mathbb{1} \otimes \rho^T)\right]. \tag{3.64}$$

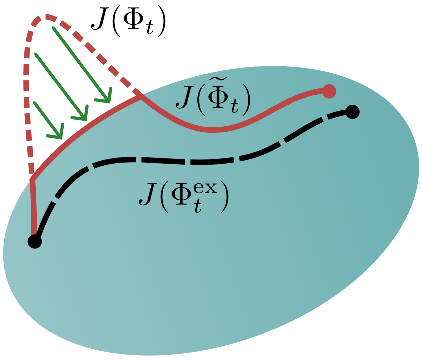

Figure 3.4: Choi-proximity regularization of a dynamical map Φ_t obtained from approximating an exact evolution Φ_t^{ex}. In those time regions where the Choi operator $J(\Phi_t)$ exits the space of physical Choi operators (depicted as a colored oval), we project it back, resulting in a CPT map $\widetilde{\Phi}_t$. Thanks to the convexity of the physical Choi space, the result is closer to the exact dynamics Φ_t^{ex}, as stated in Theorem 3.4.

Suppose now that Φ_t obeys some time-local master equation $\partial_t \Phi_t = \mathcal{L}_t \Phi_t$. Assuming $\Delta(t)$ to be differentiable[7], we can put forward a time-local master equation for $\widetilde{\Phi}_t$:

$$\partial_t \widetilde{\Phi}_t = \mathcal{L}_t \widetilde{\Phi}_t - d\mathcal{L}_t \operatorname{Tr}_2 \left[\Delta(t)(\mathbb{1} \otimes \rho^T)\right] + d \operatorname{Tr}_2 \left[\partial_t \Delta(t)(\mathbb{1} \otimes \rho^T)\right]. \tag{3.65}$$

The same can be done in case Φ_t obeys an integral equation of the Nakajima-Zwanzig type $\partial_t \Phi_t = \int_0^t \mathrm{d}s\, \mathcal{K}_{t-s} \Phi_s$,

$$\partial_t \widetilde{\Phi}_t = \int_0^t \mathrm{d}s\, \mathcal{K}_{t-s} \widetilde{\Phi}_s - d \int_0^t \mathrm{d}s\, \mathcal{K}_{t-s} \operatorname{Tr}_2 \left[\Delta(s)(\mathbb{1} \otimes \rho^T)\right] + d \operatorname{Tr}_2 \left[\partial_t \Delta(t)(\mathbb{1} \otimes \rho^T)\right]. \tag{3.66}$$

The most important fact we can get from these equations is that they contain a dependence on the initial state ρ, which was absent in the original evolution. This hints at the fact that non-Markovianity can be displayed by the regularized dynamics. Of course, no guarantee is given for the "amount" of non-Markovianity with respect to the original evolution. Nevertheless, as we will show in the next subsection, the possibility of non-Markovianity is concrete and offers a net advantage with respect to other regularizations.

3.3.3 Examples

Let us consider again the problem of a two-level system coupled to a vacuum environment with excitation-preserving interaction, whose Hamiltonian was defined back in Sec. 3.2.3. This setup constitutes one of the few exactly solvable models in the theory of open quantum systems, and has been thoroughly studied. Such exact solution, which can be found, e.g., in Ref. [6], can be written as

$$\rho_{00}(t) = \rho_{00}(t_0)\mathcal{A}(t) + 1 - \mathcal{A}(t), \qquad \rho_{11}(t) = \rho_{11}(t_0)\mathcal{A}(t), \qquad \rho_{01}(t) = \rho_{01}(t_0)\mathcal{B}(t)e^{i\varepsilon t}, \tag{3.67}$$

[7] The differentiability of $\Delta(t)$ could be assessed using the implicit function theorem on the Karush-Kuhn-Tucker conditions [85, 86] associated with the optimization problem, as done in Ref. [99]. In any case, the Choi-proximity regularization can be performed without explicit mention to a master equation.

where

$$\mathcal{A}(t) = |G(\alpha, t)|^2, \qquad \mathcal{B}(t) = G(\alpha, t) \tag{3.68}$$

with $\alpha = \sqrt{\mu^2 - 2\gamma\mu}$ and

$$G(\alpha, t) = e^{-\mu t/2}\left[\cosh\left(\frac{\alpha t}{2}\right) + \frac{\mu}{\alpha}\sinh\left(\frac{\alpha t}{2}\right)\right]. \tag{3.69}$$

In Ref. [6] it is also discussed how the time-dependent Redfield equation for this model can be explicitly solved to give again Eq. (3.67) but with

$$\mathcal{A}(t) = e^{-R(t)}, \qquad \mathcal{B}(t) = e^{-R(t)/2}, \qquad R(t) = \gamma\left(t + \frac{e^{-\mu t} - 1}{\mu}\right). \tag{3.70}$$

For the subsequent discussion, it is also instructive to consider the so-called *Born equation*: this is obtained from the Nakajima-Zwanzig expression (2.95) by expanding at second order in the coupling without inverting the evolution from $\varrho(s)$ to $\varrho(t)$. The result is the same as the Redfield equation, but with $\varrho(s)$ instead of $\varrho(t)$. It is expected for such an equation to be more accurate than the Redfield one, even though it is not a time-local master equation. In this specific case, the Born equation can however be explicitly solved to give, again, Eq. (3.67) but with

$$\mathcal{A}(t) = G(\alpha', t), \qquad \mathcal{B}(t) = G(\alpha, t), \tag{3.71}$$

where $\alpha' = \sqrt{\mu^2 - 4\gamma\mu}$, as discussed in Ref. [6].

Let us first ask about the Markovianity displayed by these solutions. Given two arbitrary states ρ, σ it is easy to see that, under the evolution dictated by Eq. (3.67), the distinguishability, as defined by Eq. (2.14), writes

$$D_t(\rho, \sigma) = \sqrt{|\rho_{11} - \sigma_{11}|^2\mathcal{A}^2(t) + |\rho_{01} - \sigma_{01}|^2\mathcal{B}(t)}. \tag{3.72}$$

In case $\mathcal{B}^2(t) = \mathcal{A}(t)$ for all $t \geq t_0$, which happens for the exact solution and the Redfield equation, Eq. (3.67) describes a qubit amplitude damping channel: it is known that in this case the BLP condition (cf. Sec. 2.2.4) provides a necessary and sufficient condition for CP-divisibility [16]. In this case,

$$D_t(\rho, \sigma) = |\rho_{11} - \sigma_{11}|\mathcal{A}(t) \tag{3.73}$$

and CP-divisibility is equivalent to have non-increasing $\mathcal{A}(t)$ for all $t \geq t_0$. Note that

$$\frac{\mathrm{d}}{\mathrm{d}t}e^{-R(t)} = -\gamma e^{-R(t)}(1 - e^{-\mu t}) \geq 0, \tag{3.74}$$

hence the Redfield solution is always Markovian in this case. Instead, for the exact solution we compute

$$\frac{\mathrm{d}}{\mathrm{d}t}|G(\alpha, t)|^2 = \left(1 - \frac{\mu^2}{\alpha^2}\right)\alpha e^{-\mu t/2}\sinh\left(\frac{\alpha t}{2}\right)G(\alpha, t). \tag{3.75}$$

When $\mu \geq 2\gamma$, it turns out that α is a non-negative real number satisfying $\mu^2/\alpha^2 \geq 1$ and $G(\alpha, t) \geq 0$. This implies that $|G(\alpha, t)|^2$ is non-increasing as a function of t and the dynamics is Markovian. On the other hand, if $\mu < 2\gamma$ then α is an imaginary number: the above derivative oscillates and can take positive values. This means that for sufficiently small μ the qubit's evolution can display non-Markovianity.

In case $\mathcal{B}^2(t) \neq \mathcal{A}(t)$, which happens for the Born equation, the BLP condition is only necessary for CP-divisibility. Nevertheless, for initial states ρ, σ with equal coherences the distinguishability still acquires the form in Eq. (3.73) and we can again focus our attention solely on $\mathcal{A}(t)$. Now,

$$\frac{\mathrm{d}}{\mathrm{d}t}G(\alpha', t) = \frac{1}{2}\left(1 - \frac{\mu^2}{\alpha'^2}\right)e^{-\mu t/2}\sinh\left(\frac{\alpha' t}{2}\right). \tag{3.76}$$

If $\mu < 4\gamma$ this derivative oscillates and can acquire positive values: this indicates that for sufficiently small μ the Born equation can display non-Markovianity.

Let us now ask about the CPT requirement for these evolutions. A straightforward computation shows that the Choi operator associated with the evolution (3.67) is given by

$$J = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & \mathcal{B}(t)e^{i\varepsilon t} \\ 0 & 1-\mathcal{A}(t) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \mathcal{B}(t)e^{-i\varepsilon t} & 0 & 0 & \mathcal{A}(t) \end{bmatrix}. \tag{3.77}$$

This always satisfies $\mathrm{Tr}_1 J = \mathbb{1}/2$, in accordance with the fact that all the involved dynamical maps are trace-preserving. On the other hand, the eigenvalues of J are

$$0, \qquad \frac{1-\mathcal{A}(t)}{2}, \qquad \frac{1+\mathcal{A}(t) \pm \sqrt{[1-\mathcal{A}(t)]^2 + 4\mathcal{B}^2(t)}}{4}. \tag{3.78}$$

Since $\mathcal{A}(t) \leq 1$, these eigenvalues are always non-negative, except at most the rightmost one with the minus sign, which is easily seen to be non-negative if and only if $\mathcal{B}^2(t) \leq \mathcal{A}(t)$. Such condition is always satisfied by the exact solution and the Redfield equation, but not by the Born equation, which can then violate the positivity requirement.

We can summarize the previous discussions as follows. The Redfield equation is CPT but it does not capture the non-Markovian features of the exact solution at moderate couplings. On the other hand, the Born equation exhibits non-Markovian effects but in general it is not CPT. It is then reasonable to apply the Choi-proximity regularization procedure to the Born equation.

In Fig. 3.5 (top row) we compare the accuracy of the Born equation, the Redfield equation, and the regularized version of the Born equation against the exact solution, as measured by the Choi distance $\left\|J(\Phi_t) - J(\Phi_t^{\mathrm{ex}})\right\|$ we already used for the dynamical regularization in Sec. 3.2. Here we fix $\gamma = 1$ and we study what happens for several values of μ. Obviously, greater values of μ lead to better accuracy for all master equations, while things get worse when we approach the non-Markovian regime for smaller values of μ. However, note that in all cases the regularized Born equation outperforms the other two: for the Born equation this is expected by Theorem 3.4, but it was not obvious for the Redfield equation. Note also that, for small enough μ, the Born equation develops regions in which it is CPT: unfortunately, our regularization cannot do anything there.

In Fig. 3.5 (bottom row) we also show the dynamics of the distinguishability measure $D_t(\rho, \sigma)$ when $\rho = |0\rangle\langle 0|$ and $\sigma = |1\rangle\langle 1|$. As before, $\gamma = 1$ and several values of μ are investigated. In the Markovian regime (greater values of μ) we see how the prediction of the regularized Born equation is practically exact, while at this level some deviations can be seen for the other two master equations. When entering the non-Markovian regime for smaller values of μ, several things can be noticed. The prediction of the Redfield equation is always

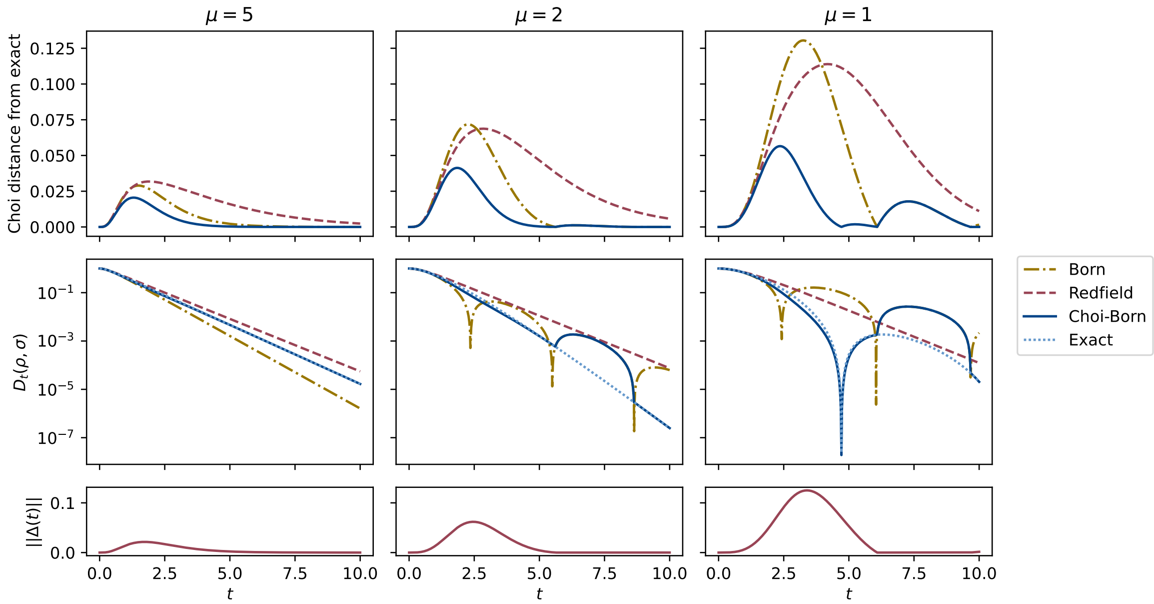

Figure 3.5: Plots obtained for the qubit system with $\gamma = 1$ and $\mu \in \{5, 2, 1\}$. Top row: dynamics of the Choi distance between a certain evolution and the exact one [cf. Eq. (3.52)]. Middle row: dynamics of the distinguishability measure $D_t(\rho, \sigma)$ with $\rho = |0\rangle\langle 0|$ and $\sigma = |1\rangle\langle 1|$. In this case the y-axis is plotted in logarithmic scale for better readability. Bottom row: CPT violation parameter $\|\Delta(t)\|$, with $\Delta(t)$ defined in Eq. (3.63). Note how the Choi-proximity regularization of the Born equation—"Choi-Born" in the legend—outperforms the other two methods and, when activated, reproduces the Markovian and non-Markovian behaviors of the exact dynamics.

monotonic, as expected. The Born equation, instead, is capable of showing non-monotonic behavior but it is quite different from the exact one. The regularized Born equation not only shows non-monotonic behavior as well, but also remarkably follows the exact solution in those time regions where the Born equation is not CPT. Again, the regularization has no power in those regions where the Born equation is already CPT. Finally, notice that there is an intermediate situation in which the Born equation predicts non-Markovianity when the exact solution does not: when activated, our regularization is capable of correcting this behavior.

As a second example we study the more complex spin-boson model, which occupies a prominent role in the theory of open quantum systems and constitutes a paradigmatic playground to study many dissipative and decoherence mechanisms [6, 8]. The system consists of a spin-1/2 particle with Hamiltonian

$$H_S = \frac{\varepsilon}{2}\sigma_z + \frac{\delta}{2}\sigma_x, \tag{3.79}$$

where $\sigma_x, \sigma_y, \sigma_z$ are the usual Pauli matrices, ε is the energy gap between ground state $|0\rangle$ and excited state $|1\rangle$, and δ is a tunneling strength between such states. The spin is coupled to an environment of bosonic oscillators $H_E = \sum_p \varepsilon_p c_p^\dagger c_p$ and the interaction is

$$V = \sigma_z \otimes \sum_p g_p \left(c_p + c_p^\dagger\right). \tag{3.80}$$

In order to keep things simple, we assume again that the environment is characterized by the exponential correlation function (3.51).

There is no explicit exact solution for this model, even though the system is small enough to allow for an easy numerical approach through hierarchical equations of motion (HEOM) [100]. In particular, we rely on the corresponding functions provided by the Python library QuTip [101]: in the following, the result obtained with this procedure will be referred to as "exact solution". The Redfield equation associated with this problem—and its regularizations—can also easily be solved numerically.

It is generally believed that CPT violations of the Redfield equation tend to appear at short times and with at least moderate coupling constant [23]. In this regime the accuracy with respect to the exact solution is not expected to be satisfying. Applying the Choi-proximity regularization can slightly improve performances, but our aim in this example is another one: we want to show how our procedure can give a well-defined dynamics that retains the non-Markovian features of the Redfield equation, contrary to other common regularization schemes.

Let us first focus on the time-dependent Redfield equation. In Fig. 3.6 we show the dynamics of the distinguishability measure $D_t(\rho, \sigma)$ when $\rho = |0\rangle\langle 0|$ and $\sigma = |1\rangle\langle 1|$ in a moderate coupling regime with $\gamma = 1.5$ and $\mu = 0.1$, together with the CPT violation parameter $\|\Delta(t)\|$. In the distinguishability plot we see that the regularization does not make much of a difference with respect to the original time-dependent Redfield evolution, but the dynamics is now guaranteed to be physically well defined. Notice how the time-dependent Redfield equation violates positivity at short times with $\|\Delta(t)\| \sim 10^{-3}$. The moderate impact of the Choi-proximity regularization allows the regularized equation to keep the nice features of the Redfield equation, such as accounting for the non-Markovianity of the model: note how the oscillations in the distinguishability measure are roughly positioned as

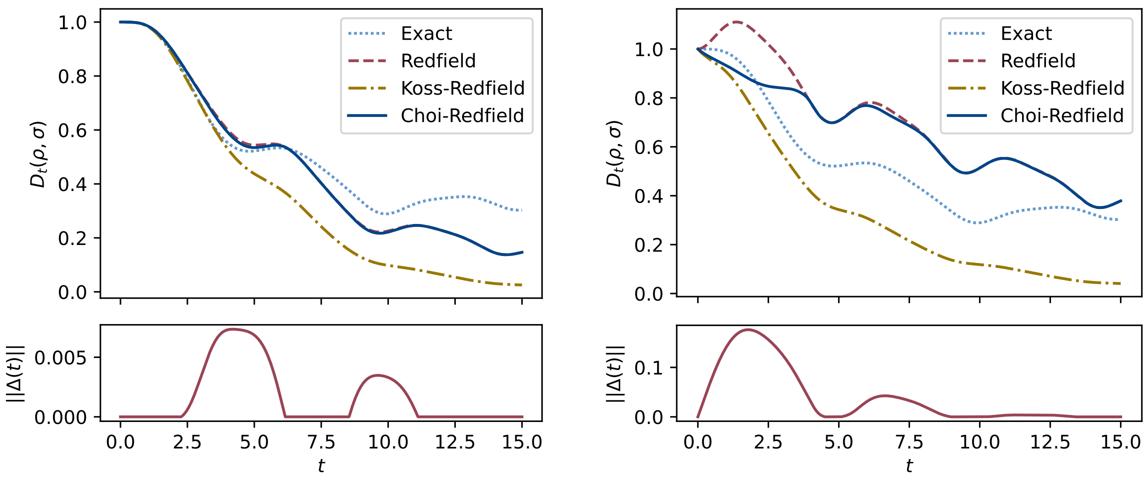

Figure 3.6: (Left) Dynamics of the distinguishability measure $D_t(\rho, \sigma)$ for the spin-boson model with $\rho = |0\rangle\langle 0|$ and $\sigma = |1\rangle\langle 1|$. At the bottom, the CPT violation parameter $\|\Delta(t)\|$. The parameters of the model are $\varepsilon = 1$, $\delta = 0.7$ for the system and $\gamma = 1.5$, $\mu = 0.1$, $\omega_0 = 1$ for the interaction. (Right) Same as on the left but using the time-independent Redfield equation.

in the exact solution. In contrast, we also plot the prediction of the time-dependent Redfield equation regularized by acting on its Kossakowski matrix with the dynamical regularization of Sec. 3.2: in this case a monotonic decrease is observed, in accordance with the fact that we are imposing a CP-divisibility requirement.

In Fig. 3.6 we also show the same plot but starting from the time-independent version of the Redfield equation. This time the positivity violation is clearly visible also in the distinguishability plot, where $D_t(\rho, \sigma)$ unphysically grows beyond the value of one at short times. Correspondingly, we find $\|\Delta(t)\| \sim 10^{-1}$ in this time region. The Choi-proximity regularization corrects this behavior and reproduces non-Markovian oscillations, contrary to the dynamical regularization.

Chapter 4

Contour Formulation

This chapter describes a slightly generalized version of the contour technique that was originally formulated, discussed, and used in:

[53] V. Cavina, A. D'Abbruzzo, and V. Giovannetti, *Unifying quantum stochastic methods using Wick's theorem on the Keldysh contour*, Phys. Rev. Research **7**, 043262 (2025).

In Chap. 3 we discussed the problem of deriving weak-coupling master equations and the related issue of complete-positivity breaking, which led us to various regularization techniques. In the rest of the thesis we will shift our focus towards *exact* descriptions of quantum dynamics, without resorting to assumptions about coupling or other scales at play. In this intrinsically *non-Markovian* setting, the LGKS theorem is not available and the mathematical structure of the dynamics is much less clear [16]. To cope with this, a heterogeneous variety of approaches has been proposed during the years to still find useful predictions in practice, like hierarchical equations of motion [100], reaction-coordinate [102, 103] and pseudomode mappings [104], collision models [105, 106], and tensor-network techniques [107].

At the same time, nonequilibrium quantum field theory has been able to provide important results, e.g., in cosmology, high-energy physics, and condensed matter physics [44–46]. The *Schwinger-Keldysh contour formalism* [42, 43], in particular, has been proved to be a highly efficient analytical tool. Even though some works already approached the construction of a link between these two worlds [47–52, 108, 109], we believe the contour formalism still holds substantial untapped potential for advancing research in the field of open quantum systems. In this chapter we formulate a Keldysh-like contour formalism that is able to exactly describe the time evolution of density operators of open quantum systems. In contrast to usual approaches, we do not make use of field objects, path integrals [110, 111], or involved superoperators [112–114], thus achieving a remarkable degree of clarity in final results.

We begin with a description of the contour in Sec. 4.1.1 in the simpler context of closed quantum systems. Then, in Sec. 4.1.2 we move to the contour formulation for open quantum systems which are initially uncorrelated from their environment, an assumption we usually took for granted in Chaps. 2 and 3. However, in Sec. 4.1.3 we show that initial system-environment correlations, which are fundamental for the description of strongly-coupled systems, can effortlessly be taken into account using a "complexification" of the contour—a technique borrowed from thermal field theory [115]. In Sec. 4.2 we will introduce a Gaussian environment assumption: after generalizing the well-known Wick's theorem [40, 41] to contour operators, we will arrive at a result that is formally equivalent to (a generalization of) the Feynman-Vernon influence functional [110]. This will form the backbone of the discussion for the following chapters. Finally, in Sec. 4.3 we will conclude by summarizing the results obtained so far and by discussing the generalization power of the proposed contour formalism, suggesting a number of possible extensions.

4.1 Quantum dynamics on the contour

4.1.1 Closed system

Let us consider a closed quantum system whose state at time t is described by the density operator $\rho(t)$. If $H(t)$ is the Hamiltonian that characterizes the evolution of such system, we know that the state at time t is obtained from the state at time $t_0 \leq t$ as [cf. Eq. (2.30)]

$$\rho(t) = U(t,t_0)\rho(t_0)U^{\dagger}(t,t_0), \qquad U(t,t_0) = \mathbb{T}\exp\left[-i\int_{t_0}^{t} \mathrm{d}s\, H(s)\right], \tag{4.1}$$

where $\mathbb{T}$ is the time-ordering operation. After expanding the exponentials,

$$\rho(t) = \sum_{k,q=0}^{\infty} \frac{(-i)^{k+q}}{k!q!} \int_{t_0}^{t} \mathrm{d}^k\mathbf{s} \int_{t}^{t_0} \mathrm{d}^q\mathbf{s}'\, \mathbb{T}\{H(s_1)\dots H(s_k)\}\rho(t_0)\widetilde{\mathbb{T}}\{H(s_1')\dots H(s_q')\}, \tag{4.2}$$

where $\widetilde{\mathbb{T}}$ is the anti-time-ordering operation and $\int_{t_0}^{t} \mathrm{d}^k\mathbf{s}$ is intended as a shorthand for the n-dimensional integral $\int_{t_0}^{t} \mathrm{d}s_1 \dots \int_{t_0}^{t} \mathrm{d}s_k$.

The basic idea behind the contour construction originates from the desire of writing Eq. (4.2) in a simpler form. To do that, let us trace the effect of the ordering on the operator string inside the integrals. If we read the time arguments when "moving" from right to left, we quickly realize that time travels from t to t_0 and then back to t. Let us then denote with $\gamma^-(t)$ the domain of the variables $s_1, \dots, s_k$: this is just the interval $[t_0, t]$. Let us also denote with $\gamma^+(t)$ the domain of the variables $s_1', \dots, s_q'$: this is again just the interval $[t_0, t]$ but we distinguish it from $\gamma^-(t)$ for ordering purposes. While $\gamma^-(t)$ is "positively oriented" when going from t_0 to t, the path $\gamma^+(t)$ is "positively oriented" when going from t to t_0. We introduce the notation $z = s^{\pm}$, which stands for the point that lies at value s on $\gamma^{\pm}(t)$. Following the structure of Eq. (4.2), it is meaningful to consider the path

$$\gamma(t) := \gamma^+(t) * \gamma^-(t), \tag{4.3}$$

which is the concatenation of $\gamma^+(t)$ and $\gamma^-(t)$, in that order. For obvious reasons, we call $\gamma^-(t)$ the *forward branch* and $\gamma^+(t)$ the *backward branch*, while $\gamma(t)$ is simply called *contour*: see Fig. 4.1 for a pictorial representation.

After defining the *contour Hamiltonian* $H(z) \equiv H(s^{\pm}) := H(s)$, Eq. (4.2) becomes

$$\rho(t) = \sum_{k,q=0}^{\infty} \frac{(-i)^{k+q}}{k!q!} \int_{\gamma^-(t)} \mathrm{d}^k\mathbf{z} \int_{\gamma^+(t)} \mathrm{d}^q\mathbf{z}'\, \mathbb{T}\{H(z_1)\dots H(z_k)\rho(t_0)H(z_1')\dots H(z_q')\}. \tag{4.4}$$

Here $\mathbb{T}$ is intended as a *contour-ordering operation*, which puts operators with "later" arguments on the left according to the ordering imposed by $\gamma(t)$. It is clear that it acts as the standard time ordering when restricted on the forward branch, while it acts as the anti-time

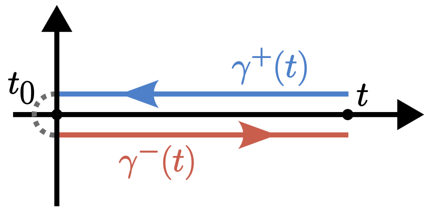

Figure 4.1: Schematic representation of the contour defined in Eq. (4.3). Starting from time t, a backward branch $\gamma^+(t)$ goes straight to the initial time t_0, and then a forward branch $\gamma^-(t)$ returns back to t.

ordering when restricted on the backward branch, but mixed situations are possible. As in the usual scenario, operators commute inside the $\mathbb{T}$ sign, hence

$$\begin{aligned}\rho(t) &= \sum_{k,q=0}^{\infty} \frac{(-i)^{k+q}}{k!q!} \int_{\gamma^-(t)} \mathrm{d}^k\mathbf{z} \int_{\gamma^+(t)} \mathrm{d}^q\mathbf{z}'\, \mathbb{T}\{H(z_1)\dots H(z_k)H(z_1')\dots H(z_q')\rho(t_0)\} \\ &= \sum_{n=0}^{\infty}\sum_{k=0}^{n} \frac{(-i)^n}{k!(n-k)!} \int_{\gamma^-(t)} \mathrm{d}^k\mathbf{z} \int_{\gamma^+(t)} \mathrm{d}^{n-k}\mathbf{z}'\, \mathbb{T}\{H(z_1)\dots H(z_k)H(z_1')\dots H(z_{n-k}')\rho(t_0)\},\end{aligned} \tag{4.5}$$

where in the second equality we rewrote the sums in terms of $n = k + q$. Thanks to the well-known binomial property—which applies because the integrand is completely symmetric upon exchanges of integration variables—this is simply

$$\rho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \mathbb{T}\big\{H(z_1)\dots H(z_n)\rho(t_0)\big\}. \tag{4.6}$$

We can also write this in the suggestive exponential form

$$\rho(t) = \mathbb{T}\left\{\exp\left[-i\int_{\gamma(t)} \mathrm{d}z\, H(z)\right]\rho(t_0)\right\}, \tag{4.7}$$

where, as usual, it is understood that $\mathbb{T}$ is applied to operator strings after the exponential is expanded in its Taylor series.

The expression (4.7) is completely equivalent to (4.2), even though its compactness with respect to (4.2) should be appreciated. In introducing the contour $\gamma(t)$ we simplified the operator structure at the cost of changing the integration domain. Such a rearrangement has already been proved extremely useful in nonequilibrium Green's function theory [45, 46] and, as we will show in the rest of the thesis, it is able to provide interesting results for open quantum systems too.

It is worth noticing the difference between our contour $\gamma(t)$ and the usual *Schwinger-Keldysh contour* that is commonly employed in field theory, many-body physics, and related fields [42, 43]. In those treatments, the focus is on the evolution of field operators in Heisenberg picture rather than density operators in Schrödinger picture. One can verify that the change of picture translates in an "inversion" of the contour, which is obtained by following $\gamma^-(t)$ first and $\gamma^+(t)$ second. Since here we are interested in the evolution of density operators, we will stick with the definition of the contour we gave above.

The contour Hamiltonian $H(z)$ was defined to be equal to the physical Hamiltonian on both branches of the contour. What if we allow it to be different? Suppose, e.g., that $H(s^-) = h(s)$ and $H(s^+) = h'(s)$, with $h \neq h'$. In this case,

$$\rho(t) = \mathbb{T}\exp\left[-i\int_{t_0}^{t} \mathrm{d}s\, h(s)\right] \rho(t_0)\, \widetilde{\mathbb{T}}\exp\left[i\int_{t_0}^{t} \mathrm{d}s\, h'(s)\right]. \tag{4.8}$$

As one can verify by differentiation, this is the unique solution to

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i\left[h(t)\rho(t) - \rho(t)h'(t)\right], \tag{4.9}$$

which reduces to the von Neumann equation when $h = h'$. Equations such as (4.9) emerge, e.g., in *non-Hermitian quantum physics* [116] where $h' = h^\dagger$ and h is a non-Hermitian Hamiltonian. Even though Eq. (4.9) does not conserve probability, it has meaning as an effective description of non-unitary open dynamics that has been post-selected to avoid quantum jumps[1]. The "unbalance" $h \neq h^\dagger$ is neatly captured by the contour formulation, making Eq. (4.9) entirely analogous to the standard von Neumann equation: it is sufficient to focus on Eq. (4.7) with generic contour Hamiltonian $H(z)$.

4.1.2 Open system

Let us now assume our quantum system of interest to be coupled to some external environment. Specifically, as we did back in Sec. 2.3, we assume the Hamiltonian of the system-environment compound to be of the form

$$H = H_0 + V, \qquad H_0 = H_S + H_E, \qquad V = \sum_\alpha A_\alpha \otimes B_\alpha, \tag{4.10}$$

where H_0 is the free term, containing a system Hamiltonian H_S and an environment Hamiltonian H_E, while V is the coupling contribution, written in terms of system operators A_α and environment operators B_α. All these objects can be, in principle, dependent on time t.

It is convenient to move to the interaction picture. Specifically, given the free propagator

$$U_0(t, t_0) = \mathbb{T}\exp\left[-i\int_{t_0}^{t} \mathrm{d}s\, H_0(s)\right], \tag{4.11}$$

we replace the universe state $\rho_{SE}(t)$ with

$$\varrho_{SE}(t) \coloneqq U_0^\dagger(t, t_0)\rho_{SE}(t)U_0(t, t_0). \tag{4.12}$$

Then, we know that the von Neumann equation for $\varrho_{SE}(t)$ writes

$$\frac{\mathrm{d}\varrho_{SE}(t)}{\mathrm{d}t} = -i[\mathcal{V}(t), \varrho_{SE}(t)], \qquad \mathcal{V}(t) \coloneqq U_0^\dagger(t, t_0)V(t)U_0(t, t_0). \tag{4.13}$$

Using the contour $\gamma(t)$, it is immediate to realize that the above equation is solved by

$$\varrho_{SE}(t) = \mathbb{T}\left\{\exp\left[-i\int_{\gamma(t)} \mathrm{d}z\, \mathcal{V}(z)\right]\varrho_{SE}(t_0)\right\}, \tag{4.14}$$

[1] Consider for example the canonical form of a LGKS generator (2.42). If we drop the term $\sum_{i,j}\chi_{ij}L_i\rho L_j^\dagger$, what remains is Eq. (4.9) with $h' = h^\dagger$ and $h = H - \frac{i}{2}\sum_{i,j}\chi_{ij}L_j^\dagger L_i$, which is non-Hermitian.

where $\mathcal{V}(z) \equiv \mathcal{V}(s^{\pm}) := \mathcal{V}(s)$ is defined to be the same on both branches.

We are however interested in writing the reduced density operator $\varrho(t) = \mathrm{Tr}_E\, \varrho_{SE}(t)$, and to do that we need to take the partial trace over the environment. For the moment, let us assume that the initial universe state is factorized:

$$\varrho_{SE}(t_0) = \varrho(t_0) \otimes \varrho_E, \tag{4.15}$$

where $\varrho(t_0)$ is the initial state of the system and ϱ_E is the initial state of the environment. This is the same assumption we made when discussing dynamical maps in Sec. 2.2.2 and the Nakajima-Zwanzig equation in Sec. 2.3.1. By definition,

$$\mathcal{V}(t) = \sum_{\alpha} \mathcal{A}_\alpha(t) \otimes \mathcal{B}_\alpha(t), \tag{4.16a}$$

$$\mathcal{A}_\alpha(t) = U_0^\dagger(t,t_0) A_\alpha(t) U_0(t,t_0), \qquad \mathcal{B}_\alpha(t) = U_0^\dagger(t,t_0) B_\alpha(t) U_0(t,t_0). \tag{4.16b}$$

Therefore, after we expand the exponential in Eq. (4.14), the partial trace over the environment immediately yields

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{\gamma(t)} \mathrm{d}^n \mathbf{z} \sum_{\alpha_1,\ldots,\alpha_n} \mathrm{Tr}\big[\mathbb{T}\{\mathcal{B}_{\alpha_1}(z_1)\ldots\mathcal{B}_{\alpha_n}(z_n)\varrho_E\}\big]\mathbb{T}\{\mathcal{A}_{\alpha_1}(z_1)\ldots\mathcal{A}_{\alpha_n}(z_n)\varrho(t_0)\}, \tag{4.17}$$

where again we promoted $\mathcal{A}_\alpha(s^{\pm}) := \mathcal{A}_\alpha(s)$ and $\mathcal{B}_\alpha(s^{\pm}) := \mathcal{B}_\alpha(s)$. Of course, in writing the above expression we implicitly assumed that, in the context of a contour ordering, ϱ_E should be placed as if it had t_0 as argument.

4.1.3 Including initial correlations

The hypothesis of factorized initial state is essential in order to be able to take the partial trace of Eq. (4.14). However, since we are ultimately interested in the dynamics of strongly-coupled non-Markovian systems, there is a significant desire to include initially-correlated system-environment compounds[2]. Remarkably, this can be achieved in an elegant manner using the contour idea. Similar techniques have already been employed, e.g., in many-body theory to prepare systems in thermal states before applying time evolution [44, 115, 117].

The starting point consists in writing the initial density operator of the universe in the following familiar form[3]:

$$\rho_{SE}(t_0) = \frac{e^{-\beta H^M}}{Z_0}, \qquad \beta > 0, \quad Z_0 = \mathrm{Tr}\Big[e^{-\beta H^M}\Big]. \tag{4.18}$$

Following conventions adopted in nonequilibrium Green's function theory, we will refer to H^M as the *Matsubara Hamiltonian*. The constant β has been introduced primarily for convenience, since it allows us to neatly recover thermal states as a special case: it is sufficient to take as β the inverse temperature and $H^M = H - \mu N$, with μ being the chemical potential and N being the total number operator.

[2] As we discussed in Sec. 2.2.2, a correlated initial state prohibits the emergence of a dynamical map for the system. Nevertheless, we can still expect to find a propagator for $\varrho(t)$ which depends on such initial preparation.

[3] The form (4.18) is technically strictly available only for full-rank density operators, since a matrix exponential is always non-singular. However, one can recover singular density operators by taking an appropriate limiting procedure on the eigenvalues of H^M at the end of the calculation [45].

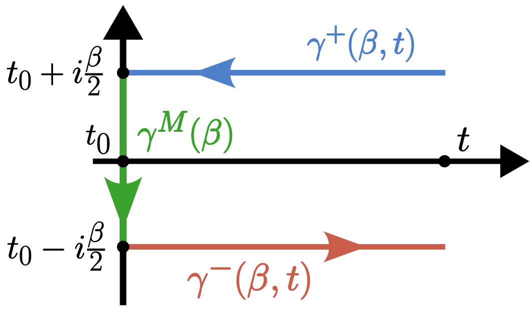

Figure 4.2: Schematic representation of the contour defined in Eq. (4.20). Starting from $t + i\beta/2$, first we have a backward branch $\gamma^+(\beta, t)$ running towards $t_0 + i\beta/2$, then there is a vertical Matsubara branch $\gamma^M(\beta)$ arriving at $t_0 - i\beta/2$, and finally we move to $t - i\beta/2$ with a forward branch $\gamma^-(\beta, t)$.

Let us now consider the time evolution of such state:

$$\begin{aligned}\rho_{SE}(t) &= U(t,t_0)\rho_{SE}(t_0)U^\dagger(t,t_0)\\ &= \frac{1}{Z_0}\mathbb{T}\exp\left[-i\int_{t_0}^{t} \mathrm{d}s\, H(s)\right]e^{-\beta H^M}\widetilde{\mathbb{T}}\exp\left[-i\int_{t}^{t_0}\mathrm{d}s\, H(s)\right] \\ &= \frac{1}{Z_0}\mathbb{T}\exp\left[-i\int_{t_0-i\beta/2}^{t-i\beta/2}\mathrm{d}z\, H(z)\right]\exp\left[-i\int_{t_0+i\beta/2}^{t_0-i\beta/2}\mathrm{d}z\, H^M\right]\widetilde{\mathbb{T}}\exp\left[-i\int_{t+i\beta/2}^{t_0+i\beta/2}\mathrm{d}z\, H(z)\right],\end{aligned} \tag{4.19}$$

where we defined $H(s \pm i\beta/2) := H(s)$ and it is intended that the time-ordering applies to the s variable. This expression can be compactly written as a single propagator on a *complex* contour as follows (see Fig. 4.2). First, we have a backward horizontal branch $\gamma^+(\beta, t)$ which runs from $t + i\beta/2$ to $t_0 + i\beta/2$. Then we move on a vertical *Matsubara branch* $\gamma^M(\beta)$ from $t_0 + i\beta/2$ to $t_0 - i\beta/2$. Finally, we go from $t_0 - i\beta/2$ to $t - i\beta/2$ with a forward horizontal branch $\gamma^-(\beta, t)$. Our new contour is

$$\gamma(\beta,t) := \gamma^+(\beta,t) * \gamma^M(\beta) * \gamma^-(\beta,t). \tag{4.20}$$

We also introduce the obvious notation $s^\pm := s \pm i\beta/2 \in \gamma^\pm(\beta, t)$. We obtain

$$\rho_{SE}(t) = \frac{1}{Z_0}\mathbb{T}\exp\left[-i\int_{\gamma(\beta,t)}\mathrm{d}z\, H(z)\right], \qquad H(z) := \begin{cases} H(s) & z = s^\pm \in \gamma^\pm(\beta,t), \\ H^M & z \in \gamma^M(\beta). \end{cases} \tag{4.21}$$

It is now convenient to introduce the following *contour propagator*:

$$W(z_2,z_1) := \begin{cases} \mathbb{T}\exp\left[-i\int_{z_1}^{z_2}\mathrm{d}z\, H(z)\right] & z_1 \preceq z_2, \\ \widetilde{\mathbb{T}}\exp\left[i\int_{z_2}^{z_1}\mathrm{d}z\, H(z)\right] & z_1 \succ z_2. \end{cases} \tag{4.22}$$

Here, $\preceq$ is the ordering relation induced by our definition of $\gamma(\beta, t)$ while $\int_{z_1}^{z_2}\mathrm{d}z$ is a line integral on $\gamma(\beta, t)$ starting at z_1 and ending at z_2. Unlike the standard physical-time propagator $U(t, t_0)$, in general $W(z_2, z_1)$ is *not* a unitary operator. However, one can easily show that the following familiar properties still hold [45]:

$$W(z,z) = \mathbb{1}, \qquad W(z_3,z_1) = W(z_3,z_2)W(z_2,z_1). \tag{4.23}$$

Moreover,

$$\frac{\mathrm{d}W(z_2,z_1)}{\mathrm{d}z_2} = \begin{cases} -iH(z_2)W(z_2,z_1) & z_1 \preceq z_2, \\ iW(z_2,z_1)H(z_1) & z_1 \succ z_2. \end{cases} \tag{4.24}$$

In terms of this object, Eq. (4.21) is simply written as

$$\rho_{SE}(t) = \frac{W(t^-,t^+)}{Z_0}. \tag{4.25}$$

Our objective now is to move to the interaction picture. To do that, we must first introduce a "free" contour propagator that generalizes $U_0(t,t_0)$. Since the Matsubara Hamiltonian is a universe operator, we can always split it as

$$H^M = H_0^M + V^M, \qquad H_0^M = H_S^M + H_E^M, \qquad V^M = \sum_\alpha A_\alpha^M \otimes B_\alpha^M, \tag{4.26}$$

where H_0^M pertains to system and environment in isolation and V^M is the interaction term. This is the same decomposition we assumed for the physical Hamiltonian, and is completely general. We can also assume that V and V^M are written using the same number of interaction indices α: this can always be ensured by padding with zero operators the decomposition with a lower number of indices. We can then clearly define

$$H_0(z) := \begin{cases} H_0(s) & z = s^\pm \in \gamma^\pm(\beta,t), \\ H_0^M & z \in \gamma^M(\beta), \end{cases} \qquad V(z) := \begin{cases} V(s) & z = s^\pm \in \gamma^\pm(\beta,t), \\ V^M & z \in \gamma^M(\beta). \end{cases} \tag{4.27}$$

Moreover, let $W_0(z_2,z_1)$ be defined through Eq. (4.22) but with $H_0(z)$ instead of $H(z)$. Then,

$$\varrho_{SE}(t) := U_0(t_0,t)\rho_{SE}(t)U_0(t,t_0) = \frac{1}{Z_0}W_0(t_0^-,t^-)W(t^-,t^+)W_0(t^+,t_0^+), \tag{4.28}$$

where we used the obvious fact that $U_0(t_2,t_1) = W_0(t_2^\pm,t_1^\pm)$.

The following lemma is needed to proceed [53], which generalizes a well-known relation concerning the transformation to interaction picture in standard physical-time quantum mechanics [1].

Lemma 4.1. *Consider three contour points $z_1, z_2, \overline{z}$ such that $z_1 \preceq z_2$ and $\overline{z} \preceq z_2$. Then,*

$$W(z_2,z_1) = W_0(z_2,\overline{z})W_I(z_2,z_1;\overline{z})W_0(\overline{z},z_1), \tag{4.29}$$

where $W_I(z_2,z_1;\overline{z})$ is defined as in Eq. (4.22) *but with $H(z)$ replaced by $W_0(\overline{z},z)V(z)W_0(z,\overline{z})$.*

Proof. It is sufficient to show that the two sides of Eq. (4.29) satisfy the same differential equation with the same initial condition. When $z_1 = z_2$, both sides are obviously equal to the identity. Also,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}z_2}[W_0(z_2,\overline{z})W_I(z_2,z_1;\overline{z})W_0(\overline{z},z_1)] &= -i[H_0(z_2)W_0(z_2,\overline{z})]W_I(z_2,z_1;\overline{z})W_0(\overline{z},z_1) \\ &\quad - iW_0(z_2,\overline{z})[W_0(\overline{z},z_2)V(z_2)W_0(z_2,\overline{z})W_I(z_2,z_1;\overline{z})]W_0(\overline{z},z_1) \\ &= -iH(z_2)W_0(z_2,\overline{z})W_I(z_2,z_1;\overline{z})W_0(\overline{z},z_1), \end{aligned} \tag{4.30}$$

which is what we wanted to prove. □

Thanks to Eq. (4.29), we can write

$$W_0(t_0^-, t^-)W(t^-, t_0) = W_I(t^-, t_0; t_0^-)W_0(t_0^-, t_0), \tag{4.31a}$$
$$W(t_0, t^+)W_0(t^+, t_0^+) = W_0(t_0, t_0^+)W_I(t_0, t^+; t_0^+), \tag{4.31b}$$

and therefore

$$\begin{aligned}\varrho_{SE}(t) &= \frac{1}{Z_0} W_0(t_0^-, t^-)W(t^-, t_0)W(t_0, t^+)W_0(t^+, t_0^+)\\ &= \frac{1}{Z_0} W_I(t^-, t_0; t_0^-)W_0(t_0^-, t_0)W_0(t_0, t_0^+)W_I(t_0, t^+; t_0^+)\\ &= \frac{1}{Z_0} W_I(t^-, t_0; t_0^-)W_0(t_0^-, t_0^+)W_I(t_0, t^+; t_0^+) = W_I(t^-, t_0; t_0^-)\frac{e^{-\beta H_0^M}}{Z_0} W_I(t_0, t^+; t_0^+).\end{aligned} \tag{4.32}$$

By the same arguments we used in Sec. 4.1.2, we immediately conclude that

$$\varrho_{SE}(t) = \mathbb{T}\left\{\exp\left[-i\int_{\gamma(\beta,t)} \mathrm{d}z\, \mathcal{V}(z)\right]\frac{e^{-\beta H_0^M}}{Z_0}\right\}, \tag{4.33}$$

where

$$\mathcal{V}(z) := \begin{cases} W_0(t_0^+, z)V(z)W_0(z, t_0^+) & z \succ t_0,\\ W_0(t_0^-, z)V(z)W_0(z, t_0^-) & z \prec t_0.\end{cases} \tag{4.34}$$

Eq. (4.33) should be compared with Eq. (4.14). While taking the partial trace over the environment in Eq. (4.14) is not achievable due to correlations in $\varrho_{SE}(t_0)$, this operation can easily be carried out in Eq. (4.33), since the factorized operator $e^{-\beta H_0^M}$ appears instead of $\varrho_{SE}(t_0)$. The price to pay is the complexification of the contour and the "splitting" of the interaction operator $\mathcal{V}(z)$ on such contour, which now assumes different expressions according to the branch. Nevertheless, we can still make the decomposition

$$\mathcal{V}(z) = \sum_\alpha \mathcal{A}_\alpha(z) \otimes \mathcal{B}_\alpha(z), \tag{4.35}$$

where

$$\mathcal{A}_\alpha(s^\pm) = U_0^\dagger(s, t_0)A_\alpha(s)U_0(s, t_0), \qquad \mathcal{B}_\alpha(s^\pm) = U_0^\dagger(s, t_0)B_\alpha(s)U_0(s, t_0), \tag{4.36a}$$
$$\mathcal{A}_\alpha(t_0 \pm i\tau) = \exp\left[\pm\left(\frac{\beta}{2} - \tau\right)H_S^M\right]A_\alpha^M \exp\left[\mp\left(\frac{\beta}{2} - \tau\right)H_S^M\right], \tag{4.36b}$$
$$\mathcal{B}_\alpha(t_0 \pm i\tau) = \exp\left[\pm\left(\frac{\beta}{2} - \tau\right)H_E^M\right]B_\alpha^M \exp\left[\mp\left(\frac{\beta}{2} - \tau\right)H_E^M\right]. \tag{4.36c}$$

Moreover,

$$\frac{e^{-\beta H_0^M}}{Z_0} = \varrho_0 \otimes \varrho_E, \qquad \varrho_0 = \frac{e^{-\beta H_S^M}}{Z_0/\mathrm{Tr}\left[e^{-\beta H_E^M}\right]}, \qquad \varrho_E = \frac{e^{-\beta H_E^M}}{\mathrm{Tr}\left[e^{-\beta H_E^M}\right]}. \tag{4.37}$$

Note that we distributed normalization constants so that ϱ_E turns out to be a valid state of the environment, for reasons that will become clear later in Sec. 4.2.2. Instead, since $e^{-\beta H_0^M}/Z_0$ is not normalized, ϱ_0 is not a normalized system state. Of course, neither ϱ_0 or ϱ_E are the true initial reduced states of system and environment.

With these definitions, taking the partial trace in Eq. (4.33) finally yields

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{\gamma(\beta,t)} \mathrm{d}^n \mathbf{z} \sum_{\alpha_1,\dots,\alpha_n} \mathrm{Tr}\big[\mathbb{T}\{\mathcal{B}_{\alpha_1}(z_1)\dots\mathcal{B}_{\alpha_n}(z_n)\varrho_E\}\big]\mathbb{T}\{\mathcal{A}_{\alpha_1}(z_1)\dots\mathcal{A}_{\alpha_n}(z_n)\varrho_0\}, \tag{4.38}$$

which is entirely analogous to Eq. (4.17) once we use the correct definitions for the quantities at play along the appropriate contour.

An interesting point concerning the above equation when compared to its counterpart for factorized initial conditions is that ϱ_0 is not recovered by setting $t = t_0$, since $\gamma(\beta, t_0) = \gamma^M(\beta)$ is still a non-trivial contour. This is of course expected, since ϱ_0 is not the initial state of the system and the Matsubara track is needed to "prepare" $\varrho(t_0)$ from ϱ_0. As in standard thermal field theory, it is possible to formulate such preparation as an imaginary-time evolution. Let $\gamma^M(\beta, \tau)$ be the vertical path running from $t_0 + i\tau$ to $t_0 - i\tau$ for $\tau \in [0, \beta/2]$, and define

$$\sigma(\tau) := \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{\gamma^M(\beta,\tau)} \mathrm{d}^n \mathbf{z} \sum_{\alpha_1,\dots,\alpha_n} \mathrm{Tr}\big[\mathbb{T}\{\mathcal{B}_{\alpha_1}(z_1)\dots\mathcal{B}_{\alpha_n}(z_n)\varrho_E\}\big]\mathbb{T}\{\mathcal{A}_{\alpha_1}(z_1)\dots\mathcal{A}_{\alpha_n}(z_n)\varrho_0\}. \tag{4.39}$$

Clearly, $\sigma(0) = \varrho_0$ and $\sigma(\beta/2) = \varrho(t_0)$, so that the evolution of $\sigma(\tau)$ can be used to represent the initial preparation of the system.

4.1.4 A compact notation

The result of this section can be summarized by saying that we are interested in further studying an expression of the form

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^n \mathbf{z}\, \mathrm{Tr}[\mathbb{T}\{B_1 \dots B_n \varrho_E\}]\mathbb{T}\{A_1 \dots A_n \varrho_0\}, \tag{4.40}$$

where we abbreviated $A_i \equiv A_{\alpha_i}(z_i)$ and $B_i \equiv B_{\alpha_i}(z_i)$. The integral symbol with a superimposed summation sign is a shorthand notation indicating that we must integrate over continuous variables and sum over discrete ones:

$$\sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^n \mathbf{z} \equiv \sum_{\alpha_1,\dots,\alpha_n} \int_{\gamma(t)} \mathrm{d}^n \mathbf{z}\,. \tag{4.41}$$

In Eq. (4.40), what we mean by the various quantities at play depends on the setting.

- For a closed system, substitute $A_i \to H(z_i)$ and $B_i \to \mathbb{1}$, and take as $\gamma(t)$ the contour in Fig. 4.1. Then $\varrho(t)$ is simply the density operator with initial condition $\varrho(t_0) = \varrho_0$.
- For an open system that is initially uncorrelated from the environment, substitute $A_i \to \mathcal{A}_{\alpha_i}(z_i)$ and $B_i \to \mathcal{B}_{\alpha_i}(z_i)$, and use again the contour $\gamma(t)$ in Fig. 4.1. Then $\varrho(t)$ is the interaction-picture system density operator with initial condition $\varrho(t_0) = \varrho_0$, and ϱ_E is the initial environment state.

- For an open system initially correlated with the environment, substitute $A_i \to \mathcal{A}_{\alpha_i}(z_i)$ and $B_i \to \mathcal{B}_{\alpha_i}(z_i)$, the operators defined in Eqs. (4.36), while ϱ_0 and ϱ_E are given in Eqs. (4.37). For the contour, we take $\gamma(t) \to \gamma(\beta, t)$ the one in Fig. 4.2 including the Matsubara track: this choice yields as $\varrho(t)$ the interaction-picture system density operator. Instead, if we take $\gamma(t) \to \gamma^M(\beta, \tau)$ we obtain the operator $\sigma(\tau)$ in Eq. (4.39) describing the initial preparation of the system.

The ability to treat all these situations using the single compact expression (4.40) is a remarkable property of the proposed contour formulation. At the end of the chapter, in Sec. 4.3, we will further sustain this encompassing character of the formalism by briefly discussing a number of completely different scenarios which nevertheless lead again to Eq. (4.40). However, in the rest of the thesis we will solely focus on the settings already described above.

4.2 Gaussian environment

Eq. (4.40) is the formal solution to the most general problem of an open quantum system, and only makes use of the von Neumann equation. In particular, all the n-point correlation functions of the environment, $\mathrm{Tr}[\mathbb{T}\{B_1 \dots B_n \varrho_E\}]$, appear in this expression, which make it hard to manipulate in practice without further knowledge about the structure of these correlations. In this section we will introduce the hypothesis of *Gaussian environment*, according to which the n-point correlation functions are uniquely and solely determined by the 1- and 2-point functions, as dictated by the celebrated *Wick's theorem* [40, 41, 118, 119].

The mathematical tractability of quadratic Hamiltonians and Gaussian states are well known in physics, and their ability to capture a wide variety of contexts in quantum optics [84], quantum information [58], and statistical mechanics [120] can hardly be overestimated. In the context of open quantum systems, the hypothesis of Gaussian environment is typically very mild and is routinely used to describe electromagnetic environments, phonon baths, metallic or superconducting leads, and more [6].

We generally assume the reader is already familiar with main concepts concerning Gaussian states. However, for the sake of clarity, we will first precisely define what we mean by Gaussian system; the reader can find in Appendix A a more detailed account of such concepts. Then we discuss a contour version of Wick's theorem, which is what we will use to simplify the correlation functions in Eq. (4.40).

4.2.1 Quadratic Hamiltonians and Gaussian states

Using the well-known language of second quantization [44], quantum Hamiltonians are often written in terms of ladder operators $\{a_i, a_i^\dagger\}_{i=1}^n$, characterized by the (anti)commutation rules

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij}, \qquad [a_i, a_j]_\zeta = [a_i^\dagger, a_j^\dagger]_\zeta = 0, \tag{4.42}$$

where

$$[X, Y]_\zeta := XY - \zeta YX \tag{4.43}$$

and $\zeta \in \{1, -1\}$ characterizes the statistical type of the system: $\zeta = 1$ stands for a *bosonic* system, where (4.43) becomes a commutator, while $\zeta = -1$ stands for a *fermionic* system, where (4.43) becomes an anticommutator.

A *quadratic Hamiltonian* is defined as a Hamiltonian which is a quadratic form in ladder operators. More precisely, in terms of the *Nambu vector* $\mathbb{a}^\dagger := (a_1^\dagger, a_1, a_2^\dagger, a_2, \ldots, a_n^\dagger, a_n)$, a quadratic Hamiltonian is of the form

$$H = \frac{1}{2}\mathbb{a}^\dagger \mathcal{H} \mathbb{a} = \frac{1}{2}\sum_{i,j=1}^{2n} \mathcal{H}_{ij} \mathbb{a}_i^\dagger \mathbb{a}_j, \tag{4.44}$$

with $\mathcal{H}$ being a Hermitian matrix of coefficients.

It is also convenient to introduce the following $2n$ Hermitian operators

$$x_j := \frac{1}{\sqrt{2}}\left(a_j^\dagger + a_j\right), \qquad p_j := \frac{i}{\sqrt{2}}\left(a_j^\dagger - a_j\right) \tag{4.45}$$

and gather them in a vector $\mathbf{r}^T := (x_1, p_1, x_2, p_2, \ldots, x_n, p_n)$. In the bosonic case, these are usually called *position* and *momentum operators*, *canonical operators*, or *quadrature operators* [40]. In the mathematical literature, $\mathbf{r}$ is also known as *Darboux basis* [121]. Instead, in the fermionic case, these are commonly called *Majorana operators* [41]. Since we aim at a description that is valid for both statistical types, we call $\mathbf{r}$ the *Darboux-Majorana vector*. The relations (4.42) are compactly written as

$$[\mathbf{r}, \mathbf{r}^T]_\zeta = \Omega, \tag{4.46}$$

where

$$\Omega \overset{(\zeta=1)}{=} i \bigoplus_{\ell=1}^{n} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \qquad \Omega \overset{(\zeta=-1)}{=} \bigoplus_{\ell=1}^{n} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbb{1}. \tag{4.47}$$

Clearly, $\Omega^T = -\zeta\Omega$ and $\Omega^{-1} = \Omega$. A quadratic Hamiltonian can also be written in this basis:

$$H = \frac{1}{2}\mathbf{r}^T h \mathbf{r} = \frac{1}{2}\sum_{i,j=1}^{2n} h_{ij} r_i r_j \tag{4.48}$$

for an appropriate coefficient matrix h. Arguably, Eq. (4.48) is often more convenient to work with if compared to Eq. (4.44), since the Darboux-Majorana basis effectively hides the difference between creation and annihilation operators.

A fundamental property of quadratic Hamiltonians is that they linearly evolve the ladder operators when viewing them as Heisenberg observables. This fact will be repeatedly used in the following pages of the thesis. More specifically, if $H = \frac{1}{2}\mathbf{r}^T h \mathbf{r}$, then a straightforward computation that makes use of Eq. (4.46) reveals that

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = i[H, \mathbf{r}] = -i\Omega h \mathbf{r} \quad \Rightarrow \quad \mathbf{r}(t) := e^{iHt}\mathbf{r}(0)\, e^{-iHt} = e^{-i\Omega h t}\mathbf{r}(0), \tag{4.49}$$

where matrix-vector multiplication is intended throughout.

A *Gaussian state* is defined through a density operator whose Matsubara Hamiltonian is quadratic, i.e., [40, 41]

$$\rho = \frac{1}{Z}\exp\left[-\frac{\beta}{2}\mathbf{r}^T h \mathbf{r}\right]. \tag{4.50}$$

If $\langle X \rangle_\rho := \operatorname{Tr} X\rho$ stands for the expectation value of the operator X with respect to the state ρ, one can find (see Appendix A) the following neat expressions for the one- and two-point correlation functions of Darboux-Majorana operators with respect to the Gaussian state (4.50):

$$\langle \mathbf{r} \rangle_\rho = 0, \qquad \langle \mathbf{r}\mathbf{r}^T \rangle_\rho = [\mathbb{1} - \zeta e^{-\beta\Omega h}]^{-1}\Omega. \tag{4.51}$$

The nice property of Gaussian states is that every correlation of the form $\langle r_{i_1} \dots r_{i_k} \rangle_\rho$ can be calculated from the knowledge of Eq. (4.51). This is the content of the celebrated *Wick's theorem*: we discuss it in the next section alongside a mild generalization of it that will be useful to us in the context of the contour formalism.

4.2.2 Contour Wick's theorem

In order to state Wick's theorem, we need an ordering operation that is somewhat different from the $\mathbb{T}$ operation we used in the previous pages. Given n operators $X_i \equiv X_i(z_i)$ with arguments on a generic contour γ and given $\zeta \in \{-1, 1\}$, we define

$$\mathbb{T}_\zeta\{X_1 \dots X_n\} := \zeta^{N(\varphi)} X_{\varphi(1)} \dots X_{\varphi(n)}, \tag{4.52}$$

where φ is a permutation of $\{1, \dots, n\}$ such that $\varphi(1) \succ \varphi(2) \succ \dots \succ \varphi(n)$ on the contour γ, and $N(\varphi)$ is the number of inversions[4] of φ. When $\zeta = 1$, there is no difference between $\mathbb{T}$ and $\mathbb{T}_\zeta$. However, when $\zeta = -1$, $\mathbb{T}_\zeta\{\dots\} = \text{sgn}(\varphi)\mathbb{T}\{\dots\}$, where $\text{sgn}(\varphi) = (-1)^{N(\varphi)}$ is the sign of the permutation φ. This means that, in the process of ordering the operators, a ζ factor must be introduced for every transposition. Of course, in contrast to $\mathbb{T}$, operators cannot be thought of as commuting inside $\mathbb{T}_\zeta$: specifically,

$$\mathbb{T}_\zeta\left\{X_{\sigma(1)} \dots X_{\sigma(n)}\right\} = \zeta^{N(\sigma)} \mathbb{T}_\zeta\{X_1 \dots X_n\}, \tag{4.53}$$

In particular, $\mathbb{T}_\zeta\{X_1 X_2\} = \zeta \mathbb{T}_\zeta\{X_2 X_1\}$. We can now state Wick's theorem [118], whose proof can be found in Appendix A.

Theorem 4.2 (Wick)**.** *Let ρ be a Gaussian state* (4.50)*. Moreover, let $\{B_i \equiv B_i(z_i)\}$ be a set of operators with arguments z_i on a generic path γ which are linear in ladder operators, meaning that $B_i = \sum_j \phi_{ij} r_j$ for some $\phi_{ij} \in \mathbb{C}$. If $\langle B_i \rangle_\rho = 0$ for every i, then*

$$\langle \mathbb{T}_\zeta\{B_1 \dots B_{2m+1}\} \rangle_\rho = 0, \tag{4.54a}$$

$$\langle \mathbb{T}_\zeta\{B_1 \dots B_{2m}\} \rangle_\rho = \frac{1}{m! 2^m} \sum_{\sigma \in \mathfrak{S}_{2m}} \zeta^{N(\sigma)} \prod_{j=1}^{m} \langle \mathbb{T}_\zeta\left\{B_{\sigma(2j-1)} B_{\sigma(2j)}\right\} \rangle_\rho, \tag{4.54b}$$

where $\mathfrak{S}_{2m}$ is the set of permutations of $\{1, \dots, 2m\}$. The right-hand side of Eq. (4.54b) *is also known as the Hafnian-Pfaffian [122, 123] of the matrix $\langle \mathbb{T}_\zeta\left\{B_i B_j\right\} \rangle_\rho$.*

Wick's theorem as formulated in Theorem 4.2 is not yet in a form that is directly useful to us, since in Eq. (4.40) we have to deal with $\text{Tr}[\mathbb{T}_\zeta\{B_1 \dots B_n \varrho_E\}]$, which is different from $\langle \mathbb{T}_\zeta\{B_1 \dots B_n\} \rangle_{\varrho_E}$. However, as the following theorem shows, the cyclicity of the trace can be exploited to link these two expressions.

[4] An *inversion* is a pair (i, j) such that $i < j$ and $\varphi(i) > \varphi(j)$.

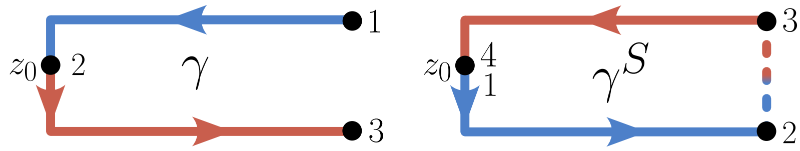

Figure 4.3: Construction of the "splitted" contour γ^S used in the proof of Theorem 4.3.

Theorem 4.3 (Contour Wick). *Consider the same setting of Theorem 4.2. In addition, suppose the contour γ is characterized by a special point z_0 at which ρ should be placed for ordering purposes. Then,*

$$\mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1 \dots B_{2m+1}\rho\}\big] = 0, \tag{4.55a}$$

$$\mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1 \dots B_{2m}\rho\}\big] = \frac{1}{m!2^m} \sum_{\sigma\in\mathfrak{S}_{2m}} \zeta^{N(\sigma)} \prod_{j=1}^{m} \mathrm{Tr}\big[\mathbb{T}_\zeta\{B_{\sigma(2j-1)}B_{\sigma(2j)}\rho\}\big]. \tag{4.55b}$$

Proof. By definition of contour ordering, we can find a permutation φ of $\{1,\dots,n\}$ and an index $k \in \{0,\dots,n\}$ such that $\varphi(1) \succ \dots \succ \varphi(n)$ and

$$\begin{aligned}\mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1 \dots B_n\rho\}\big] &= \zeta^{N(\varphi)}\zeta^{n-k}\, \mathrm{Tr}\big[B_{\varphi(1)} \dots B_{\varphi(k)}\rho B_{\varphi(k+1)} \dots B_{\varphi(n)}\big] \\ &= \zeta^{N(\varphi)}\zeta^{n-k}\, \mathrm{Tr}\big[B_{\varphi(k+1)} \dots B_{\varphi(n)}B_{\varphi(1)} \dots B_{\varphi(k)}\rho\big].\end{aligned} \tag{4.56}$$

Consider now the permutation σ of $\{1,\dots,n\}$ such that

$$B_{\varphi(k+1)} \dots B_{\varphi(n)}B_{\varphi(1)} \dots B_{\varphi(k)} = B_{\sigma(1)} \dots B_{\sigma(n)}. \tag{4.57}$$

It is easy to see that σ can be obtained from φ with $k(n-k)$ transpositions, hence we can write $\zeta^{N(\varphi)} = \zeta^{N(\sigma)}\zeta^{k(n-k)}$. Using the fact that $k(k+1)$ is always even,

$$\mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1 \dots B_n\rho\}\big] = \zeta^{N(\sigma)}\zeta^{n(k+1)}\, \mathrm{Tr}\big[B_{\sigma(1)} \dots B_{\sigma(n)}\rho\big]. \tag{4.58}$$

Now we define a "splitted" version γ^S of the contour γ as follows (see Fig. 4.3). Starting from z_0, we follow the contour up to its final point; then we suddenly fall back to its initial point and we follow again the contour up to z_0. It is clear that by construction $B_{\sigma(1)} \dots B_{\sigma(n)}$ is ordered along γ^S, hence

$$\mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1 \dots B_n\rho\}\big] = \zeta^{n(k+1)}\langle\mathbb{T}^S_\zeta\{B_1 \dots B_n\}\rangle_\rho, \tag{4.59}$$

where $\mathbb{T}^S_\zeta$ is the analogue of $\mathbb{T}_\zeta$ but following the ordering imposed by γ^S. At this point we simply apply Theorem 4.2 using γ^S instead of γ. The fact that $\langle\mathbb{T}^S_\zeta\{B_iB_j\}\rangle_\rho = \mathrm{Tr}\big[\mathbb{T}_\zeta\{B_iB_j\rho\}\big]$ is clearly a consequence of Eq. (4.59). □

4.2.3 Open dynamics with Gaussian environment

Let us now go back to the context of open quantum systems. We say that the setting under consideration has a *Gaussian environment* when the following two conditions are met:

- The environment state ϱ_E appearing in Eq. (4.40) is a Gaussian state. For factorized initial conditions, this simply means that the initial environment state is Gaussian; for correlated initial conditions, this means that H_E^M is quadratic.

- The operators B_i appearing in Eq. (4.40) are linear. For factorized initial conditions, it is sufficient that the environment's interaction operators B_α are linear and that H_E is quadratic, so that linearity is maintained when moving to the interaction picture. For correlated initial conditions, we should additionally require the operators B_α^M and H_E^M to be respectively linear and quadratic as well.

With this set of assumptions, the contour Wick's theorem 4.3 can be applied to simplify Eq. (4.40). First of all, it is important to realize that the permutation that orders $B_1 \dots B_n \varrho_E$ is the same that orders $A_1 \dots A_n \varrho_0$, hence no additional sign is introduced by writing instead

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \oint_{\gamma(t)} \mathrm{d}^n \mathbf{z} \, \mathrm{Tr}[\mathbb{T}_\zeta\{B_1 \dots B_n \varrho_E\}] \mathbb{T}_\zeta\{A_1 \dots A_n \varrho_0\}, \tag{4.60}$$

where $\zeta \in \{-1, 1\}$ is determined by the statistical type of the environment, as described in Sec. 4.2.1. In order to apply Wick's theorem as formulated by Theorem 4.3, let us now suppose that

$$\mathrm{Tr}[B_i \varrho_E] = 0, \qquad \forall i \in \{1, \dots, n\}. \tag{4.61}$$

This is the same *stability condition* we already employed in the microscopic derivation of the Redfield equation back in Sec. 2.3. The following calculations can be generalized to situations where the stability condition does not hold: the interested reader can find such calculations in Appendix B. Now, according to Theorem 4.3, all odd correlations vanish and we are left with

$$\varrho(t) = \sum_{m=0}^{\infty} \frac{(-i)^{2m}}{(2m)!} \oint_{\gamma(t)} \mathrm{d}^{2m} \mathbf{z} \, \frac{1}{m! 2^m} \sum_{\sigma \in \mathfrak{S}_{2m}} \zeta^{N(\sigma)} \prod_{j=1}^{m} C_{\sigma(2j-1), \sigma(2j)} \mathbb{T}_\zeta\{A_1 \dots A_{2m} \varrho_0\}, \tag{4.62}$$

where we introduced the two-point *contour correlation function*

$$C_{ij} \coloneqq \mathrm{Tr}\big[\mathbb{T}_\zeta\big\{B_i B_j \varrho_E\big\}\big] \equiv \mathrm{Tr}\big[\mathbb{T}_\zeta\big\{B_{\alpha_i}(z_i) B_{\alpha_j}(z_j) \varrho_E\big\}\big] =: C_{\alpha_i \alpha_j}(z_i, z_j). \tag{4.63}$$

With an appropriate change of variables,

$$\varrho(t) = \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!} \frac{1}{m! 2^m} \sum_{\sigma \in \mathfrak{S}_{2m}} \zeta^{N(\sigma)} \oint_{\gamma(t)} \mathrm{d}^{2m} \mathbf{z} \prod_{j=1}^{m} C_{2j-1, 2j} \mathbb{T}_\zeta\big\{A_{\sigma^{-1}(1)} \dots A_{\sigma^{-1}(2m)} \varrho_0\big\}. \tag{4.64}$$

However,

$$\mathbb{T}_\zeta\big\{A_{\sigma^{-1}(1)} \dots A_{\sigma^{-1}(2m)} \varrho_0\big\} = \zeta^{N(\sigma^{-1})} \mathbb{T}_\zeta\{A_1 \dots A_{2m} \varrho_0\}. \tag{4.65}$$

The factor $\zeta^{N(\sigma^{-1})}$ cancels out the factor $\zeta^{N(\sigma)}$, since taking the inverse of a permutation flips its sign. In the remaining expression, nothing depends on σ anymore and the sum over σ translates in a multiplication by $(2m)!$, yielding

$$\varrho(t) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! 2^m} \oint_{\gamma(t)} \mathrm{d}^{2m} \mathbf{z} \, C_{1,2} \dots C_{2m-1, 2m} \mathbb{T}_\zeta\{A_1 \dots A_{2m} \varrho_0\}. \tag{4.66}$$

This is the final expression representing the general dynamics of an open quantum systems interacting with a Gaussian environment. With the usual conventions, it can also be written in a suggestive and compact exponential form:

$$\varrho(t) = \mathbb{T}_\zeta\left\{\exp\left[-\frac{1}{2} \oint_{\gamma(t)} \mathrm{d}^2 \mathbf{z} \, C_{1,2} A_1 A_2\right] \varrho_0\right\}. \tag{4.67}$$

Reintroducing the full notation, we explicitly have

$$\varrho(t) = \mathbb{T}_\zeta\left\{\exp\left[-\frac{1}{2}\sum_{\alpha,\beta}\int_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, A_\alpha(z_1)C_{\alpha\beta}(z_1,z_2)A_\beta(z_2)\right]\varrho_0\right\}. \tag{4.68}$$

It is worth mentioning that an expression for the dynamics of an open system interacting with a Gaussian environment was already obtained by Feynman and Vernon in their seminal paper [110] using a path-integral technique. Their result is nowadays known as the *Feynman-Vernon influence functional*. Albeit initially limited to factorized initial conditions and bosonic environments, their approach was later extended to correlated initial states [117] and fermionic environments [111], and other equivalent techniques employing superoperators appeared in much recent years [112, 113]. By contrast, our approach gives a purely operatorial route which unifies all the various expressions that appear in the literature. In Appendix B we show that Eq. (4.67) correctly reproduces the influence functional if we unravel the contour in its physical-time components.

4.2.4 The contour correlation function

We conclude this section by discussing several properties of the contour correlation function C introduced in Eq. (4.63), which appears in the fundamental result (4.67). We begin with some fundamental symmetry properties

Theorem 4.4. *The function* $C_{\alpha\beta}(z,w) := \mathrm{Tr}\big[\mathbb{T}_\zeta\{B_\alpha(z)B_\beta(w)\varrho_E\}\big]$ *satisfies*

(i) Exchange symmetry: $C_{\alpha\beta}(z,w) = \zeta C_{\beta\alpha}(w,z)$.

(ii) $C^*_{\alpha\beta}(z,w) = C_{\overline{\beta}\overline{\alpha}}(w^*,z^*)$, *where* z^* *indicates the point corresponding to* z *on the opposite branch. For the contour in Fig. 4.2 with the Matsubara track, this is just complex conjugation; for the contour in Fig. 4.1 with horizontal tracks only, it is a branch flip:* $z = s^\pm \Rightarrow z^* = s^\mp$.

(iii) Cycle symmetry: $C_{\alpha\beta}(s^+,w) = C_{\alpha\beta}(s^-,w)$ *when* $s^+ \prec w \prec s^-$.

Proof. The exchange symmetry is an immediate consequence of the definition, since $\mathbb{T}_\zeta$ brings out a ζ factor when two of its arguments are exchanged.

To prove (ii), we first note that, by Eqs. (4.36),

$$[B_\alpha(z)]^\dagger = B_{\overline{\alpha}}(z^*). \tag{4.69}$$

Therefore,

$$C^*_{\alpha\beta}(z,w) = \langle\mathbb{T}^S_\zeta\{B_\alpha(z)B_\beta(w)\}\rangle^*_{\varrho_E} = \langle\mathbb{T}^S_\zeta\{B_{\overline{\beta}}(w^*)B_{\overline{\alpha}}(z^*)\}\rangle_{\varrho_E} = C_{\overline{\beta}\overline{\alpha}}(w^*,z^*), \tag{4.70}$$

where in the first and third equality we used the representation of C that makes use of the splitted contour γ^S [cf. Eq. (4.59)], while in the second equality we used the fact that if $z \prec w$ according to γ^S then $z^* \succ w^*$.

Finally, the cycle symmetry follows from the cyclicity of trace since, if $s^+ \prec w \prec s^-$, then $B_\alpha(s^+)$ should be placed at the beginning while $B_\alpha(s^-)$ should be placed at the end:

$$C_{\alpha\beta}(s^+,w) = \mathrm{Tr}\big[\mathbb{T}_\zeta\{B_\beta(w)\varrho_E\}B_\alpha(s)\big] = \mathrm{Tr}\big[B_\alpha(s)\mathbb{T}_\zeta\{B_\beta(w)\varrho_E\}\big] = C_{\alpha\beta}(s^-,w), \tag{4.71}$$

where we used the fact that $B_\alpha(s^\pm) \equiv B_\alpha(s)$ once it is outside the ordering. □

When combining (ii) and (i), we obtain the important property

$$\check{C} = C, \tag{4.72}$$

where we introduced the symbol ˇ to indicate the following operation, valid for any two-point contour function $F_{\alpha\beta}(z, w)$:

$$\check{F}_{\alpha\beta}(z, w) := \zeta F^{*}_{\overline{\alpha}\overline{\beta}}(z^{*}, w^{*}). \tag{4.73}$$

We call $\check{F}$ the *conjugate* of F, and when $\check{F} = F$ we say that F satisfies *conjugation symmetry*. The contour correlation function C is our prime example of function with conjugation symmetry.

It is also important to establish a link between C and the two-point correlation functions having physical times as arguments. This is often an essential final step in calculations involving the contour formalism: once the contour has served its purpose in simplifying analytical work, one should be able to revert the abstraction to discuss physical results. In general, we will refer to this procedure as *unraveling the contour*. In nonequilibrium Green's function theory one says that the *Keldysh components* are extracted from the contour functions [45, 46].

Let $F(z, w)$ be a generic matrix-valued two-point contour function. We will establish some notation to indicate the various physical-time components of F. Let us start by restricting its arguments to the horizontal branches. We define

$$F^{>}(s_1, s_2) := F(s_1^{+}, s_2^{-}), \qquad F^{<}(s_1, s_2) := F(s_1^{-}, s_2^{+}), \tag{4.74a}$$

$$F^{T}(s_1, s_2) := F(s_1^{-}, s_2^{-}), \qquad F^{\widetilde{T}}(s_1, s_2) := F(s_1^{+}, s_2^{+}). \tag{4.74b}$$

In Keldysh theory, $F^{>}$ and $F^{<}$ are respectively called *greater* and *lesser* components, while F^{T} and $F^{\widetilde{T}}$ are respectively called *time-ordered* and *anti-time-ordered* components. In case F satisfies conjugation symmetry $\check{F} = F$, these components are not all independent. For example,

$$F^{>}_{\alpha\beta}(s_1, s_2) = F_{\alpha\beta}(s_1^{+}, s_2^{-}) = \check{F}_{\alpha\beta}(s_1^{+}, s_2^{-}) = \zeta F^{*}_{\overline{\alpha}\overline{\beta}}(s_1^{-}, s_2^{+}) = \check{F}^{<}_{\alpha\beta}(s_1, s_2), \tag{4.75}$$

where, for physical-time functions $f(s_1, s_2)$, the conjugation symbol is obviously intended to act as $\check{f}_{\alpha\beta}(s_1, s_2) = \zeta f^{*}_{\overline{\alpha}\overline{\beta}}(s_1, s_2)$. Therefore, in case $\check{F} = F$ we have

$$F^{<} = \check{F}^{>}, \qquad F^{\widetilde{T}} = \check{F}^{T}. \tag{4.76}$$

Analogous components can be defined when restricting the arguments to the Matsubara branch:

$$F^{M>}(\tau_1, \tau_2) := F(t_0 + i\tau_1, t_0 - i\tau_2), \qquad F^{M<}(\tau_1, \tau_2) := F(t_0 - i\tau_1, t_0 + i\tau_2), \tag{4.77a}$$

$$F^{MT}(\tau_1, \tau_2) := F(t_0 - i\tau_1, t_0 - i\tau_2), \qquad F^{M\widetilde{T}}(\tau_1, \tau_2) := F(t_0 + i\tau_1, t_0 + i\tau_2). \tag{4.77b}$$

Differently from standard Keldysh theory, more than one *Matsubara component* is needed in our formulation to account for the two possible signs in $t_0 \pm i\tau$. Again, if $\check{F} = F$ we have the relations

$$F^{M<} = \check{F}^{M>}, \qquad F^{M\widetilde{T}} = \check{F}^{MT}. \tag{4.78}$$

Finally, we should consider the components obtained by taking an argument on the horizontal branches and the other on the Matsubara branch. We define

$$F^{\rceil\pm}(s,\tau) := F(s^+, t_0 \pm i\tau), \qquad F^{\lceil\pm}(\tau,s) := F(t_0 \pm i\tau, s^+), \tag{4.79a}$$

$$F^{\lfloor\pm}(\tau,s) := F(t_0 \pm i\tau, s^-), \qquad F^{\rfloor\pm}(s,\tau) := F(s^-, t_0 \pm i\tau). \tag{4.79b}$$

We used the symbols $\rceil$ and $\lceil$ to differentiate between the two cases in which, respectively, the first argument is on the backward branch and the second one is on the vertical one, or the other way around. Differently from standard Keldysh theory, where these are called *right* and *left* components, we need again to distinguish with an added $\pm$ sign whether the vertical argument is to be taken as $t_0 \pm i\tau$. Symmetrically, we introduced the symbols $\rfloor$ and $\lfloor$ for when the horizontal argument lies on the forward branch instead. As before, in case $\check{F} = F$ we easily identify the symmetries

$$F^{\rceil\pm} = \check{F}^{\rfloor\mp}, \qquad F^{\lceil\pm} = \check{F}^{\lfloor\mp}. \tag{4.80}$$

Let us conclude by specifying the components of the contour correlation function C. On the horizontal branches,

$$\begin{aligned} C^{>}_{\alpha\beta}(s_1,s_2) &= \langle B_\alpha(s_1)B_\beta(s_2)\rangle_{\varrho_E}, \\ C^{<}_{\alpha\beta}(s_1,s_2) &= \zeta\langle B_\beta(s_2)B_\alpha(s_1)\rangle_{\varrho_E}, \\ C^{T}_{\alpha\beta}(s_1,s_2) &= \theta(s_1-s_2)\langle B_\alpha(s_1)B_\beta(s_2)\rangle_{\varrho_E} + \zeta\theta(s_2-s_1)\langle B_\beta(s_2)B_\alpha(s_1)\rangle_{\varrho_E}, \\ C^{\widetilde{T}}_{\alpha\beta}(s_1,s_2) &= \zeta\theta(s_1-s_2)\langle B_\beta(s_2)B_\alpha(s_1)\rangle_{\varrho_E} + \theta(s_2-s_1)\langle B_\alpha(s_1)B_\beta(s_2)\rangle_{\varrho_E}. \end{aligned} \tag{4.81}$$

Note that these are all determined by the real-time correlation function $\langle B_\alpha(s_1)B_\beta(s_2)\rangle_{\varrho_E}$. This is just what we called $c_{\alpha\beta}(s_1,s_2)$ when discussing the Redfield equation back in Chap. 2. For the Matsubara components,

$$\begin{aligned} C^{M>}_{\alpha\beta}(\tau_1,\tau_2) &= \langle B_\alpha(t_0+i\tau_1)B_\beta(t_0-i\tau_2)\rangle_{\varrho_E}, \\ C^{M<}_{\alpha\beta}(\tau_1,\tau_2) &= \zeta\langle B_\beta(t_0+i\tau_2)B_\alpha(t_0-i\tau_1)\rangle_{\varrho_E}, \\ C^{MT}_{\alpha\beta}(\tau_1,\tau_2) &= \theta(\tau_1-\tau_2)\langle B_\alpha(t_0-i\tau_1)B_\beta(t_0-i\tau_2)\rangle_{\varrho_E} + \zeta\theta(\tau_2-\tau_1)\langle B_\beta(t_0-i\tau_2)B_\alpha(t_0-i\tau_1)\rangle_{\varrho_E}, \\ C^{M\widetilde{T}}_{\alpha\beta}(\tau_1,\tau_2) &= \theta(\tau_2-\tau_1)\langle B_\alpha(t_0+i\tau_1)B_\beta(t_0+i\tau_2)\rangle_{\varrho_E} + \zeta\theta(\tau_1-\tau_2)\langle B_\beta(t_0+i\tau_2)B_\alpha(t_0+i\tau_1)\rangle_{\varrho_E}. \end{aligned} \tag{4.82}$$

These are all determined by the imaginary-time function $\langle B_\alpha(t_0+i\tau_1)B_\beta(t_0+i\tau_2)\rangle_{\varrho_E}$. Finally, for the mixed components,

$$\begin{aligned} C^{\rceil+}_{\alpha\beta}(s,\tau) = C^{\rfloor+}_{\alpha\beta}(s,\tau) &= \zeta\langle B_\beta(t_0+i\tau)B_\alpha(s)\rangle_{\varrho_E}, \\ C^{\rceil-}_{\alpha\beta}(s,\tau) = C^{\rfloor-}_{\alpha\beta}(s,\tau) &= \langle B_\alpha(s)B_\beta(t_0-i\tau)\rangle_{\varrho_E}, \\ C^{\lceil+}_{\alpha\beta}(\tau,s) = C^{\lfloor+}_{\alpha\beta}(\tau,s) &= \langle B_\alpha(t_0+i\tau)B_\beta(s)\rangle_{\varrho_E}, \\ C^{\lceil-}_{\alpha\beta}(\tau,s) = C^{\lfloor-}_{\alpha\beta}(\tau,s) &= \zeta\langle B_\beta(s)B_\alpha(t_0-i\tau)\rangle_{\varrho_E}, \end{aligned} \tag{4.83}$$

which are all determined by the function $\langle B_\alpha(s)B_\beta(t_0+i\tau)\rangle_{\varrho_E}$. The additional symmetry we observe in C by flipping $\lfloor$ and $\lceil$, or by flipping $\rfloor$ and $\rceil$, is a consequence of the cycle symmetry, which is independent from the conjugation symmetry.

4.3 Extensions of the formalism

The contour formalism developed in this chapter led us to a formula, Eq. (4.67), with remarkable expressive power. It exactly describes the dynamics of an open quantum system initially either correlated or uncorrelated with a Gaussian environment, and can also be used to represent the fictitious imaginary-time preparation of the initial state. However, its encompassing character does not end there: the contour formulation can be extended to situations that are not directly related to the time evolution of the density operator.

For example, consider the problem of "experimentally" tracking the fluctuations of a quantum observable $\Lambda(t)$. In the context of quantum thermodynamics [3], where one wants to track the fluctuations of work or heat, one chooses as $\Lambda(t)$ respectively the total Hamiltonian H or the free Hamiltonian of the environment H_E. Probably the most common way of doing that is the *two-point measurement scheme* [124]: first, at time $t = 0$, we perform a projective measurement of $\Lambda(0)$; then we let the system evolve up to time t, and at that time we perform another projective measurement of $\Lambda(t)$. Let $\Lambda(t) = \sum_n \epsilon_n^t \Pi_n^t$ be the spectral decomposition of $\Lambda(t)$, where $\{\epsilon_n^t\}$ is the set of eigenvalues and Π_n^t is the projector onto the eigenspace associated with ϵ_n^t. Then, the joint probability of obtaining ϵ_n^0 at time 0 and ϵ_m^t at time t is

$$P[\epsilon_m^t, \epsilon_n^0] = \mathrm{Tr}\left[\Pi_m^t U(t,0)\Pi_n^0 \rho_0 \Pi_n^0 U(0,t)\Pi_m^t\right], \tag{4.84}$$

where ρ is the initial state of the system under investigation and U is the unitary time propagator. Correspondingly, the probability distribution of the difference $\epsilon_m^t - \epsilon_n^0$ is

$$p_t(\epsilon) = \sum_{n,m} P[\epsilon_m^t, \epsilon_n^0]\delta[\epsilon - (\epsilon_m^t - \epsilon_n^0)]. \tag{4.85}$$

One can easily show that the characteristic function $\chi_t(\lambda) := \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, p_t(\epsilon)e^{i\lambda\epsilon}$ of such distribution is

$$\chi_t(\lambda) = \mathrm{Tr}\,\rho(\lambda,t), \qquad \rho(\lambda,t) := U(t,0)e^{-i\lambda\Lambda(0)}\widetilde{\rho}_0 U(0,t)e^{i\lambda\Lambda(t)}, \tag{4.86}$$

where $\widetilde{\rho}_0 := \sum_n \Pi_n^0 \rho_0 \Pi_n^0$ is the diagonal part of ρ_0 in the eigenbasis of $\Lambda(0)$. Since $\rho(\lambda,t)$ is defined as a left-right asymmetric propagation of $\widetilde{\rho}_0$, it is not difficult to realize that $\rho(\lambda,t)$ can actually be expressed using a single exponential along an appropriate contour. In case the system under study is open, one can develop a contour formulation to describe the evolution of $\chi_t(\lambda)$ in a manner completely analogous to what we did in this chapter. The reader can find an outline of such theory in Appendix C, where the discussion is quickly specialized to the relevant topic of quantum thermodynamics and complements recent studies involving path-integral approaches [125].

Note that here we are focusing on calculating single-time quantities like $\varrho(t)$, for which it is sufficient to have a single "special point" t_0 on the contour. However, other kinds of situations can be ascribed to a contour formulation: it should in fact be possible to account for multi-time objects by specifying more than one special point. Such a generalization would enable the study, e.g., of multi-time correlation functions [126], process tensors [68], or entropic quantities through the replica method [127]. We leave this remarkable possibility to future work.

Chapter 5

Non-Markovian Stochastic Dynamics

This chapter describes the results originally published in:

[53] V. Cavina, A. D'Abbruzzo, and V. Giovannetti, *Unifying quantum stochastic methods using Wick's theorem on the Keldysh contour*, Phys. Rev. Research **7**, 043262 (2025).

However, the transport theorem in Sec. 5.1.2 is taken from:

[54] A. D'Abbruzzo, V. Giovannetti, and V. Cavina, *Exact non-Markovian master equations: A generalized derivation for Gaussian systems*, Phys. Rev. Lett. **135**, 240401 (2025).

Even though Eq. (4.67) exactly describes the dynamics of an open system in contact with a Gaussian environment, it is not directly useful in practical situations since the explicit evaluation of an ordered exponential is generally a formidable task. This is a key reason why one typically aims at finding a master equation obeyed by $\varrho(t)$, which can then be tackled either analytically or numerically. A different approach, known as *stochastic decoupling* [128–130], involves introducing a stochastic operator $R(t)$: its evolution depends on some noise, such that $\varrho(t)$ is recovered after averaging over the noise realizations, $\varrho(t) = \mathbb{E}[R(t)]$. This method often allows for the derivation of a simple master equation obeyed by $R(t)$, which is typically easier to solve because the complex environment effect is encapsulated into a noise term that can be simulated numerically.

There are several ways to perform stochastic decoupling. In the Markovian regime, a long-standing approach involves constructing stochastic master equations by continuously measuring the environment [131]: the effect is the introduction of a noise that drives the system's evolution along stochastic trajectories. The extension of this idea to the non-Markovian setting is more subtle and has been the subject of intense debate in recent decades: some argue that no genuine non-Markovian trajectory can exist without altering the original system's dynamics [132–134], while others contend that it is possible by including delay in the measurement apparatus [135]. Furthermore, recent claims suggest that a full-fledged non-Markovian trajectory can be delineated in specific Gaussian models [136].

Here we follow a different line of approach that regards stochastic decoupling as a formal tool to derive a simplified master equation, with possibly no explicit link to any measurement procedure. In Sec. 5.1 we focus on the case of bosonic Gaussian environment and present an approach that harmonizes well with the contour formalism. This is achieved by representing the environment in terms of a single noise defined on the contour. We will show in Sec. 5.2 that known stochastic master equations, such as the stochastic von Neumann equation (SVNE) [137], the quantum state diffusion equation [138, 139], and the two-state unraveling equation [140], are all encompassed by the formalism. Crucially, the contour formulation also allows us to obtain their respective extensions to initially correlated system-environment compounds and to other settings embraced by the contour idea.

This unification power will enable us to make further observations concerning the nature of the noise terms appearing in the SVNE. Specifically, using a "partial" Wick's theorem, we will show in Sec. 5.3 that the solution of the standard SVNE can be written in terms of a single real noise with positive semidefinite correlation function. Moreover, in Sec. 5.4 we demonstrate how the SVNE is influenced by an initial measurement performed on the environment. We find that if the environment satisfies appropriate semiclassical conditions, then the SVNE noise can be interpreted in terms of the outcomes of a single heterodyne initial measurement. This provides additional insights into the open problem of determining whether non-Markovian stochastic equations generally admit a measurement interpretation.

5.1 An exact stochastic master equation

5.1.1 Stochastic decoupling with contour noise

Consider an open quantum system in contact with a bosonic Gaussian environment. Thanks to Eq. (4.67), the environment's effect on the system is completely encoded by the contour correlation function C. We will now introduce a set of zero-mean Gaussian noises $\{\xi_\alpha(z)\}$, where α is the interaction index, z is the contour variable, and

$$\mathbb{E}[\xi_\alpha(z_1)\xi_\beta(z_2)] = C_{\alpha\beta}(z_1, z_2), \tag{5.1}$$

where $\mathbb{E}[\cdot]$ indicates the expectation value over the noise realizations. Note that the correspondence (5.1) is possible thanks to the following two basic observations.

- For a bosonic environment, C is symmetric, i.e., $C_{\alpha\beta}(z, w) = C_{\beta\alpha}(w, z)$, as stated in Theorem 4.4. This is essential in order to interpret C as the product of two numbers. An extension to fermionic environments would require anticommutative Grassmann noises, and is left to future work.
- The value of $C(z_1, z_2)$ changes according to the branch on which z_1 and z_2 lie, as exemplified by the components listed in Sec. 4.2.4. A single physical-time noise would never be able to capture this kind of dependence, whereas a contour noise can. Alternatively, and in a way that is arguably more artificial, one would have to introduce multiple coexistent physical-time noises. This is the approach adopted by path-integral methods.

The statement "$\{\xi_\alpha(z)\}$ is a set of zero-mean Gaussian noises" translates in the following Wick property, which we take as the defining property of Gaussian noises (cf. Theorem 4.2):

$$\mathbb{E}[\xi_1 \dots \xi_{2m+1}] = 0, \tag{5.2a}$$

$$\mathbb{E}[\xi_1 \dots \xi_{2m}] = \frac{1}{m!2^m} \sum_{\sigma\in\mathfrak{S}_{2m}} \prod_{j=1}^{m} \mathbb{E}[\xi_{\sigma(2j-1)}\xi_{\sigma(2j)}], \tag{5.2b}$$

where we used again the abbreviation $\xi_j \equiv \xi_{\alpha_j}(z_j)$. If we consider $(\xi_1, \dots, \xi_{2m})$ as a zero-mean multivariate normal random vector, Eqs. (5.2) are also known as *Isserlis' theorem*, especially in the mathematical literature [141].

For our purposes, the interesting fact is that by substituting Eq. (5.1) into Eq. (4.67), we can reverse all the steps detailed in Sec. 4.2.3 until we arrive at the analogous expression to Eq. (4.40):

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \fint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \mathbb{E}[\xi_1 \dots \xi_n] \mathbb{T}\{A_1 \dots A_n \varrho_0\}. \tag{5.3}$$

Now, let $R(t)$ be the stochastic operator defined by

$$R(t) := \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \fint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \xi_1 \dots \xi_n \mathbb{T}\{A_1 \dots A_n \varrho_0\}. \tag{5.4}$$

Clearly, $\mathbb{E}[R(t)] = \varrho(t)$. Furthermore, we recognize the definition of ordered exponential:

$$R(t) = \mathbb{T}\left\{\exp\left[-i \sum_{\alpha} \int_{\gamma(t)} \mathrm{d}z\, \xi_\alpha(z) A_\alpha(z)\right] \varrho_0\right\}. \tag{5.5}$$

Thanks to stochastic decoupling, we managed to write an equation pertaining only to the system, which, however, has the same form of the density operator of the whole universe [cf. Eq. (4.7)]. We can thus expect to be able to write a simple differential equation for $R(t)$, similar to the von Neumann equation. It is not *exactly* a von Neumann equation because the operator $\xi_\alpha(z) A_\alpha(z)$ differs depending on the branch on which z lives.

A possible way forward is to fix the contour, decompose it into its branches, and find a differential equation obeyed by $R(t)$ by inspecting the result. This is, in fact, the route that was originally taken in our paper [53]. Here, however, we choose to follow a different path: namely, after fixing the contour, we directly take the time derivative of Eq. (5.5). The derivation turns out to be slightly cleaner and requires us to develop a tool that will also be essential in the next chapter.

5.1.2 Transport theorem

In order to directly take the time derivative of $R(t)$ in Eq. (5.5), we need to be able to calculate the derivative of multidimensional integrals on $\gamma(t)$. Essentially, we need a "fundamental theorem of calculus", but formulated on $\gamma(t)$. This kind of problem is a subject of the *calculus of moving surfaces*, and the *Reynolds transport theorem*, extensively used in fluid dynamics, provides a general answer [142]. However, here we do not need the full power of the Reynolds theorem, and we will construct a tailored special case by hand.

Let $\gamma(t)$ be the contour in Fig. 4.2, which was introduced to describe the dynamics of an open quantum system initially correlated with its environment. The dependence on β is not explicitly indicated for notational simplicity, since it will turn out to be irrelevant. Obviously, the case with factorized initial conditions can be recovered by taking $\beta \to 0$ to obtain the contour in Fig. 4.1. We have the following.

Theorem 5.1 (Transport)**.** *Let $f(\mathbf{z}) \equiv f(z_1, \dots, z_n)$ be a contour function that is smooth on each branch of $\gamma(t)$. Moreover, given a vector $\mathbf{z} = (z_1, \dots, z_n)$ and given $i, j \in \{1, \dots, n\}$ with $i \le j$, define the notation $\mathbf{z}_i^j := (z_i, \dots, z_j)$. Then,*

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, f(\mathbf{z}) = \sum_{k=1}^{n} \int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w} \left[f(\mathbf{w}_1^{k-1}, t^-, \mathbf{w}_k^{n-1}) - f(\mathbf{w}_1^{k-1}, t^+, \mathbf{w}_k^{n-1})\right]. \tag{5.6}$$

Proof. We proceed by induction on n. For $n = 1$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}z\, f(z) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{t_0}^{t} \mathrm{d}s\, \big[f(s^-) - f(s^+)\big] = f(t^-) - f(t^+), \tag{5.7}$$

where we used the fact that the vertical track, if present, does not depend on t and can be omitted. Suppose now the statement to be true for $n-1$ and use the Leibniz integral rule to write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, f(\mathbf{z}) &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}z_n \int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}, z_n)\\ &= \int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, \big[f(\mathbf{w}, t^-) - f(\mathbf{w}, t^+)\big] + \int_{\gamma(t)} \mathrm{d}z_n \frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}, z_n).\end{aligned} \tag{5.8}$$

By the induction hypothesis,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}, z_n) = \sum_{k=1}^{n-1}\int_{\gamma(t)} \mathrm{d}^{n-2}\mathbf{y}\, \big[f(\mathbf{y}_1^{k-1}, t^-, \mathbf{y}_k^{n-2}, z_n) - f(\mathbf{y}_1^{k-1}, t^+, \mathbf{y}_k^{n-2}, z_n)\big]. \tag{5.9}$$

Hence, using the change of variables $(\mathbf{y}, z_n) \mapsto \mathbf{w}$,

$$\int_{\gamma(t)} \mathrm{d}z_n \frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}, z_n) = \sum_{k=1}^{n-1}\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, \big[f(\mathbf{w}_1^{k-1}, t^-, \mathbf{w}_k^{n-1}) - f(\mathbf{w}_1^{k-1}, t^+, \mathbf{w}_k^{n-1})\big]. \tag{5.10}$$

The conclusion follows by substituting Eq. (5.10) into Eq. (5.8). □

The right-hand side of Eq. (5.6) can be reduced to a single term in case f satisfies some symmetry property. Such simplification will arise frequently in the following pages, hence we state it here once and for all.

Corollary 5.2. *In case*

$$\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}_1^{k-1}, t^\pm, \mathbf{w}_k^{n-1}) = \int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, f(t^\pm, \mathbf{w}) \tag{5.11}$$

holds for every $k \in \{1, \ldots, n\}$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, f(\mathbf{z}) = n\int_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{w}\, \big[f(t^-, \mathbf{w}) - f(t^+, \mathbf{w})\big]. \tag{5.12}$$

As we discussed back in Sec. 4.1.3, the preparation of the system's initial state is an important part of the problem when discussing the case of initially correlated system-environment settings. To describe this preparation, one must use a contour $\gamma^M(\tau)$ that extends vertically with an imaginary-time track that runs from $t_0 + i\tau$ to $t_0 - i\tau$. A transport theorem can be formulated in this case too.

Theorem 5.3 (Imaginary transport)**.** *Let $f(\mathbf{z})$ be a smooth contour function on $\gamma^M(\tau)$. Then,*

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\int_{\gamma^M(\tau)} \mathrm{d}^n\mathbf{z}\, f(\mathbf{z}) = i\sum_{k=1}^{n}\int_{\gamma^M(\tau)} \mathrm{d}^{n-1}\mathbf{w}\, \big[f(\mathbf{w}_1^{k-1}, t_0 - i\tau, \mathbf{w}_k^{n-1}) - f(\mathbf{w}_1^{k-1}, t_0 + i\tau, \mathbf{w}_k^{n-1})\big]. \tag{5.13}$$

In case f satisfies the symmetry

$$\int_{\gamma^M(\tau)} \mathrm{d}^{n-1}\mathbf{w}\, f(\mathbf{w}_1^{k-1}, t_0 \pm i\tau, \mathbf{w}_k^{n-1}) = \int_{\gamma^M(\tau)} \mathrm{d}^{n-1}\mathbf{w}\, f(t_0 \pm i\tau, \mathbf{w}) \tag{5.14}$$

for every $k \in \{1, \dots, n\}$ then

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \int_{\gamma^M(\tau)} \mathrm{d}^n\mathbf{z}\, f(\mathbf{z}) = in \int_{\gamma^M(\tau)} \mathrm{d}^{n-1}\mathbf{w} \left[f(t_0 - i\tau, \mathbf{w}) - f(t_0 + i\tau, \mathbf{w}) \right]. \tag{5.15}$$

Proof. It is sufficient to closely follow the proof of Theorem 5.1. The only relevant modification concerns the base step of the induction, which modifies as

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \int_{\gamma^M(\tau)} \mathrm{d}z\, f(z) = i \int_{\tau}^{-\tau} \mathrm{d}\lambda\, f(t_0 + i\lambda) = i\left[f(t_0 - i\tau) - f(t_0 + i\tau) \right], \tag{5.16}$$

where in the first equality we used the change of variable $z = t_0 + i\lambda$. □

5.1.3 Closing the differential equation

We will now discuss how the transport theorem 5.1 enables us to obtain a relatively simple stochastic master equations for $R(t)$. Let us start by writing Eq. (5.5) as

$$R(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} M_n(t), \qquad M_n(t) := \oint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \xi_1 \dots \xi_n \mathbb{T}\{A_1 \dots A_n \varrho_0\}, \tag{5.17}$$

and let us focus on the time derivative of $M_n(t)$. The function f of Theorem 5.1 is here

$$f(\mathbf{z}) = \sum_{\alpha_1, \dots, \alpha_n} \xi_1 \dots \xi_n \mathbb{T}\{A_1 \dots A_n \varrho_0\}. \tag{5.18}$$

Assuming sufficient regularity of the contour noise, this function satisfies the smoothness hypothesis of the transport theorem. Moreover, since operators commute inside $\mathbb{T}$, f is completely symmetric in all of its arguments, so that the condition (5.11) is trivially satisfied. Corollary 5.2 then yields

$$\begin{aligned} \frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = n \sum_{\alpha} \oint_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{z} \big[&\xi_\alpha(t^-)\xi_1 \dots \xi_{n-1} \mathbb{T}\{A_\alpha(t^-) A_1 \dots A_{n-1}\varrho_0\} \\ &- \xi_\alpha(t^+)\xi_1 \dots \xi_{n-1} \mathbb{T}\{A_\alpha(t^+) A_1 \dots A_{n-1}\varrho_0\} \big]. \end{aligned} \tag{5.19}$$

But since t^- is at the end of the contour and t^+ is at the beginning (cf. Fig. 4.2),

$$\mathbb{T}\{A_\alpha(t^-) A_1 \dots A_{n-1}\varrho_0\} = A_\alpha(t) \mathbb{T}\{A_1 \dots A_{n-1}\varrho_0\}, \tag{5.20a}$$

$$\mathbb{T}\{A_\alpha(t^+) A_1 \dots A_{n-1}\varrho_0\} = \mathbb{T}\{A_1 \dots A_{n-1}\varrho_0\} A_\alpha(t), \tag{5.20b}$$

where we used the fact that $A_\alpha(t^\pm) = A_\alpha(t)$ once we are outside the ordering operation. It is then convenient to define the left-right superoperators $\hat{A}_\alpha^L$ and $\hat{A}_\alpha^R$ through the action

$$\hat{A}_\alpha^L(t) X := A_\alpha(t) X, \qquad \hat{A}_\alpha^R(t) X := X A_\alpha(t), \tag{5.21}$$

so that

$$\begin{aligned}\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} &= n\sum_\alpha \oint_{\gamma(t)} \mathrm{d}^{n-1}\mathbf{z}\left[\xi_\alpha(t^-)\hat{A}^L_\alpha(t) - \xi_\alpha(t^+)\hat{A}^R_\alpha(t)\right]\xi_1\ldots\xi_{n-1}\mathbb{T}\{A_1\ldots A_{n-1}\varrho_0\} \\ &= n\sum_\alpha\left[\xi_\alpha(t^-)\hat{A}^L_\alpha(t) - \xi_\alpha(t^+)\hat{A}^R_\alpha(t)\right]M_{n-1}(t) \equiv n\hat{\mathcal{S}}(t)M_{n-1}(t).\end{aligned} \tag{5.22}$$

This can be used in Eq. (5.17) to obtain

$$\frac{\mathrm{d}R(t)}{\mathrm{d}t} = \sum_{n=1}^{\infty}\frac{(-i)^n}{n!}n\hat{\mathcal{S}}(t)M_{n-1}(t) = \sum_{n=1}^{\infty}\frac{-i(-i)^{n-1}}{(n-1)!}\hat{\mathcal{S}}(t)M_{n-1}(t) = -i\hat{\mathcal{S}}(t)R(t). \tag{5.23}$$

We finally arrive at the following master equation for $R(t)$:

$$\begin{aligned}\frac{\mathrm{d}R(t)}{\mathrm{d}t} &= -i\sum_\alpha\left[\xi_\alpha(t^-)\hat{A}^L_\alpha(t) - \xi_\alpha(t^+)\hat{A}^R_\alpha(t)\right]R(t) \\ &= -i\sum_\alpha \xi_\alpha(t^-)A_\alpha(t)R(t) + i\sum_\alpha\xi_\alpha(t^+)R(t)A_\alpha(t).\end{aligned} \tag{5.24}$$

What about the initial condition to which such a differential equation should be subjected? In case of factorized initial system-environment compound, there is no Matsubara track and $\gamma(t_0) = \{t_0\}$ reduces to a point: as a consequence, the definition of $R(t)$ in Eq. (5.5) tells us that $R(t_0) = \varrho_0$, which is the physical initial state of the system. An issue arises in case of correlated initial system-environment compound, since $\gamma(t_0)$ equals the Matsubara track and $R(t_0)$ is obtained from ϱ_0 with an imaginary-time preparation. Remarkably, we can derive a simple stochastic master equation for such preparation too. We should focus on the quantity

$$S(\tau) := \mathbb{T}\left\{\exp\left[-i\sum_\alpha\int_{\gamma^M(\tau)}\mathrm{d}z\,\xi_\alpha(z)A_\alpha(z)\right]\varrho_0\right\}, \tag{5.25}$$

where $\gamma^M(\tau)$ is the vertical path running from $t_0 + i\tau$ to $t_0 - i\tau$, so that $S(0) = \varrho_0$ and $S(\beta/2) = R(t_0)$. The derivative of $S(\tau)$ with respect to τ can be taken using the imaginary transport theorem 5.3. An additional i factor must be introduced, and we should keep in mind that $A_\alpha(t_0 - i\tau) \neq A_\alpha(t_0 + i\tau)$, as can be seen from Eqs. (4.36). The result is

$$\frac{\mathrm{d}S(\tau)}{\mathrm{d}\tau} = \sum_\alpha\xi_\alpha(t_0 - i\tau)A_\alpha(t_0 - i\tau)S(\tau) - \sum_\alpha\xi_\alpha(t_0 + i\tau)S(\tau)A_\alpha(t_0 + i\tau), \tag{5.26}$$

with initial condition $S(0) = \varrho_0$.

Summarizing, one starts from $\varrho_0 = S(0)$, which is uniquely determined by the initial universe state by Eq. (4.37), and uses Eq. (5.26) to stochastically evolve $S(\tau)$ up to imaginary time $\beta/2$, where we know that $S(\beta/2) = R(t_0)$. This will give us the initial condition to Eq. (5.24), which can then be used to evolve R up to the desired physical time t.

5.2 Recovering known approaches

5.2.1 Stochastic von Neumann equation

Other useful non-Markovian stochastic master equations can be obtained from Eqs. (5.24) and (5.26) through further manipulation. For example, in case of factorized initial conditions, where we can just focus on Eq. (5.24), if $R(t_0) = \varrho_0 = |\psi_0\rangle\langle\psi_0|$ is a pure state, then

$R(t) = |\psi_-(t)\rangle\langle\psi_+(t)|$, where

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi_-(t)\rangle = -i\sum_\alpha \xi_\alpha(t^-)A_\alpha(t)\,|\psi_-(t)\rangle\,, \tag{5.27a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\psi_+(t)| = i\sum_\alpha \xi_\alpha(t^+)\,\langle\psi_+(t)|\,A_\alpha(t) \tag{5.27b}$$

and $|\psi_\pm(t_0)\rangle = |\psi_0\rangle$. The master equation decouples into a pair of independent pure-state stochastic equations, a fact already known in the literature as *two-state unraveling technique* [139, 140]. In case of correlated initial conditions, we can generalize the technique to the initial preparation $S(\tau)$ by noticing that if $\varrho_0 = |\psi_0\rangle\langle\psi_0|$ then $S(\tau) = |\phi_-(\tau)\rangle\langle\phi_+(\tau)|$, with

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\,|\phi_-(\tau)\rangle = \sum_\alpha \xi_\alpha(t_0 - i\tau)A_\alpha(t_0 - i\tau)\,|\phi_-(\tau)\rangle\,, \tag{5.28a}$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\,\langle\phi_+(\tau)| = -\sum_\alpha \xi_\alpha(t_0 + i\tau)\,\langle\phi_+(\tau)|\,A_\alpha(t_0 + i\tau), \tag{5.28b}$$

with $|\phi_\pm(0)\rangle = |\psi_0\rangle$. Once the imaginary time $\beta/2$ is reached, we can apply again Eqs. (5.27) to find $R(t)$ but with initial conditions $|\psi_\pm(t_0)\rangle = |\phi_\pm(\beta/2)\rangle$.

In the more general case of mixed ϱ_0, it is more instructive to rewrite Eq. (5.24) in terms of

$$\nu_\alpha(t) := \frac{\xi_\alpha(t^-) + \xi_\alpha(t^+)}{2}, \qquad \eta_\alpha(t) := \frac{\xi_\alpha(t^-) - \xi_\alpha(t^+)}{2}, \tag{5.29}$$

that is,

$$\frac{\mathrm{d}R(t)}{\mathrm{d}t} = -i\sum_\alpha \nu_\alpha(t)[A_\alpha(t), R(t)] - i\sum_\alpha \eta_\alpha(t)\{A_\alpha(t), R(t)\}. \tag{5.30}$$

Eq. (5.30) is known in the literature as *stochastic von Neumann equation* (SVNE) [137, 143–146], because it resembles a standard von Neumann equation, but with an additional anticommutator term.

Even though the SVNE was already obtained by other means, specifically through path-integral techniques [143], several observations can be made in consequence of how the noises $\nu_\alpha(t)$ and $\eta_\alpha(t)$ are brought about by the contour formalism. First, they both derive from a single contour noise $\xi_\alpha(z)$. The structure of Eq. (5.29) resembles the so-called *Keldysh rotation*, a well-known technique in nonequilibrium many-body theory that is used to achieve remarkable simplifications in the Green's functions structure [46]. This connection can be explored further if we realize that $\nu_\alpha(t)$ and $\eta_\alpha(t)$ are zero-mean Gaussian noises with correlation functions that can be calculated from Eqs. (5.29) and (5.1), and the components of C discussed in Sec. 4.2.4. We find

$$\mathbb{E}[\nu_\alpha(t)\nu_\beta(s)] = \frac{1}{2}\Big[C^>_{\alpha\beta}(t,s) + C^<_{\alpha\beta}(t,s)\Big] = \frac{1}{2}\langle\{B_\alpha(t), B_\beta(s)\}\rangle_{\varrho_E}, \tag{5.31a}$$

$$\mathbb{E}[\nu_\alpha(t)\eta_\beta(s)] = \frac{1}{2}\theta(t-s)\Big[C^>_{\alpha\beta}(t,s) - C^<_{\alpha\beta}(t,s)\Big] = \frac{1}{2}\theta(t-s)\langle[B_\alpha(t), B_\beta(s)]\rangle_{\varrho_E}, \tag{5.31b}$$

$$\mathbb{E}[\eta_\alpha(t)\eta_\beta(s)] = 0. \tag{5.31c}$$

The right-hand sides of Eqs. (5.31a) and (5.31b) are respectively known as *Keldysh component* and *retarded component* of the Green's function. In case $B_\alpha(t)$ is Hermitian, one also easily verifies that $\mathbb{E}[\nu_\alpha(t)\nu_\beta(s)] = \operatorname{Re} c_{\alpha\beta}(t,s)$ and $\mathbb{E}[\nu_\alpha(t)\eta_\beta(s)] = i\theta(t-s)\operatorname{Im} c_{\alpha\beta}(t,s)$, with $c_{\alpha\beta}(t,s) = \langle B_\alpha(t)B_\beta(s)\rangle_{\varrho_E}$. The advantage of the Keldysh rotation emerges from Eq. (5.31c), which tells us that $\eta_\alpha(t)$ has zero auto-correlation. We will explore the consequences further in Sec. 5.3.

Eq. (5.31a) is also sometimes called *noise kernel*, whereas Eq. (5.31b) is called *dissipation kernel*. The noise kernel is positive semidefinite, meaning that, for any function $f_\alpha(s)$,

$$\begin{aligned}
\sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}^2\mathbf{s}\, f_\alpha(s_1)\mathbb{E}[\nu_\alpha(s_1)\nu_\beta(s_2)]f_\beta(s_2) &= \frac{1}{2}\sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}^2\mathbf{s}\, f_\alpha(s_1)\langle\{B_\alpha(s_1), B_\beta(s_2)\}\rangle_{\varrho_E} f_\beta(s_2)\\
= \sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}^2\mathbf{s}\, f_\alpha(s_1)\langle B_\alpha(s_1)B_\beta(s)\rangle_{\varrho_E} f_\beta(s_2) &= \langle F^2\rangle_{\varrho_E} \geq 0,
\end{aligned} \tag{5.32}$$

with $F := \sum_\alpha \int_{t_0}^{t} \mathrm{d}s\, f_\alpha(s)B_\alpha(s)$. Furthermore, the dissipation kernel, encoded in the cross-correlation between $\nu_\alpha(t)$ and $\eta_\beta(s)$, does not depend on the environment's state ϱ_E, since $[B_\alpha(t), B_\beta(s)]$ is a c-number due to the Gaussian environment assumption.

Finally, it is worth noticing that our version of the SVNE is also valid for initially correlated system-environment settings. The only thing to keep in mind is that the SVNE noises are also coupled to the Matsubara components of the contour noise $\xi_\alpha(z)$ appearing in the preparation equation (5.26). Specifically, using the components of C we find

$$\mathbb{E}[\nu_\alpha(t)\xi_\beta(t_0 \pm i\tau)] = C^{\rceil\pm}_{\alpha\beta}(t,\tau) = \begin{cases}\langle B_\beta(t_0 + i\tau)B_\alpha(t)\rangle_{\varrho_E},\\ \langle B_\alpha(t)B_\beta(t_0 - i\tau)\rangle_{\varrho_E},\end{cases} \tag{5.33a}$$

$$\mathbb{E}[\eta_\alpha(t)\xi_\beta(t_0 \pm i\tau)] = 0. \tag{5.33b}$$

Remarkably, the noise $\eta_\alpha(t)$ is also decoupled from the initial preparation.

We point out that an extension of the stochastic von Neumann equation to initially correlated settings was already proposed in Refs. [145, 146] through a path-integration technique, albeit the result is limited to specific Hamiltonians and to thermal initial states. Our streamlined derivation based on the contour formalism is instead valid for any Gaussian environment and for any initial state that can be written in exponential Gaussian form.

5.2.2 Non-Markovian state diffusion

There is also another interesting way with which we can manipulate our stochastic master equation. Following an idea that was proposed in Ref. [130], let us write

$$\xi_\alpha(t^-) = Z_\alpha(t) + \chi^-_\alpha(t), \qquad \xi_\alpha(t^+) = Z^*_\alpha(t) + \chi^+_\alpha(t), \tag{5.34}$$

where $Z_\alpha(t)$ and $\chi^\pm_\alpha(t)$ are zero-mean Gaussian noises satisfying

$$\mathbb{E}[Z_\alpha(t)Z_\beta(s)] = \mathbb{E}[Z_\alpha(t)\chi^\pm_\beta(s)] = \mathbb{E}[\chi^\pm_\alpha(t)\chi^\mp_\beta(s)] = 0, \tag{5.35a}$$

$$\mathbb{E}[Z_\alpha(t)Z^*_\beta(s)] = C^<_{\alpha\beta}(t,s), \tag{5.35b}$$

$$\mathbb{E}[\chi^-_\alpha(t)\chi^-_\beta(s)] = C^T_{\alpha\beta}(t,s), \qquad \mathbb{E}[\chi^+_\alpha(t)\chi^+_\beta(s)] = C^{\widetilde{T}}_{\alpha\beta}(t,s). \tag{5.35c}$$

With Eq. (5.35a) we are assuming that these noises are all uncorrelated between each other, while Eqs. (5.35b) and (5.35c) are consequently necessary in order to guarantee the validity of Eq. (5.1). Additionally, in case of initial system-environment correlations, we require

$$\mathbb{E}[\chi^-_\alpha(t)\xi_\beta(t_0 \pm i\tau)] = \mathbb{E}[\chi^+_\alpha(t)\xi_\beta(t_0 \pm i\tau)] = 0, \tag{5.36a}$$

$$\mathbb{E}[Z_\alpha(t)\xi_\beta(t_0 \pm i\tau)] = C^{\rceil\pm}_{\alpha\beta}(t, \tau), \tag{5.36b}$$

so that the memory of the initial preparation is solely kept by $Z_\alpha(t)$. Now, the idea is to average the master equation (5.24) only with respect to the χ noises, so that we are left with the single complex-valued colored noise $Z_\alpha(t)$.

After taking the expectation value, Eq. (5.24) writes

$$\begin{aligned}\mathbb{E}\left[\frac{\mathrm{d}R(t)}{\mathrm{d}t}\right] =& - i \sum_\alpha A_\alpha(t)\big\{\mathbb{E}[Z_\alpha(t)R(t)] + \mathbb{E}[\chi^-_\alpha(t)R(t)]\big\} \\ &+ i \sum_\alpha \big\{\mathbb{E}[Z^*_\alpha(t)R(t)] + \mathbb{E}[\chi^+_\alpha(t)R(t)]\big\}A_\alpha(t).\end{aligned} \tag{5.37}$$

Since $\chi^\pm_\alpha(t)$ is only correlated with itself (possibly with a different interaction index), we can apply the *Furutsu-Novikov theorem* [147] to write

$$\mathbb{E}[\chi^\pm_\alpha(t)R(t)] = \sum_\beta \int_{t_0}^t \mathrm{d}s\, \mathbb{E}[\chi^\pm_\alpha(t)\chi^\pm_\beta(s)]\mathbb{E}\left[\frac{\delta R(t)}{\delta\chi^\pm_\beta(s)}\right], \tag{5.38}$$

with $\delta/\delta f(s)$ being the functional derivative with respect to a function $f(s)$. Since $R(t)$ depends on the noises only through the combinations $\xi_\alpha(t^-)$ and $\xi_\alpha(t^+)$, it is easy to realize that

$$\frac{\delta R(t)}{\delta\chi^-_\beta(s)} = \frac{\delta R(t)}{\delta Z_\beta(s)}, \qquad \frac{\delta R(t)}{\delta\chi^+_\beta(s)} = \frac{\delta R(t)}{\delta Z^*_\beta(s)}, \tag{5.39}$$

and therefore

$$\begin{aligned}\mathbb{E}\left[\frac{\mathrm{d}R(t)}{\mathrm{d}t}\right] =& - i \sum_\alpha A_\alpha(t)\left\{\mathbb{E}[Z_\alpha(t)R(t)] + \sum_\beta \int_{t_0}^t \mathrm{d}s\, \mathbb{E}[\chi^-_\alpha(t)\chi^-_\beta(s)]\mathbb{E}\left[\frac{\delta R(t)}{\delta Z_\beta(s)}\right]\right\} \\ &+ i \sum_\alpha \left\{\mathbb{E}[Z^*_\alpha(t)R(t)] + \sum_\beta \int_{t_0}^t \mathrm{d}s\, \mathbb{E}[\chi^+_\alpha(t)\chi^+_\beta(s)]\mathbb{E}\left[\frac{\delta R(t)}{\delta Z^*_\beta(s)}\right]\right\}A_\alpha(t).\end{aligned} \tag{5.40}$$

At this point, we define the stochastic operator $r(t) := \mathbb{E}_\chi[R(t)]$ obtained from $R(t)$ by taking the expectation value only with respect to the noises $\chi^\pm_\alpha(t)$. Using Eq. (5.35c) and recalling the expressions in Eqs. (4.81) for the time-ordered and anti-time-ordered components of the contour correlation function,

$$\begin{aligned}\frac{\mathrm{d}r(t)}{\mathrm{d}t} =& - i \sum_\alpha A_\alpha(t)\left\{Z_\alpha(t)r(t) + \sum_\beta \int_{t_0}^t \mathrm{d}s\, C^>_{\alpha\beta}(t,s)\frac{\delta r(t)}{\delta Z_\beta(s)}\right\} \\ &+ i \sum_\alpha \left\{Z^*_\alpha(t)r(t) + \sum_\beta \int_{t_0}^t \mathrm{d}s\, C^<_{\alpha\beta}(t,s)\frac{\delta r(t)}{\delta Z^*_\beta(s)}\right\}A_\alpha(t).\end{aligned} \tag{5.41}$$

We arrived at a generalized form of the so-called *non-Markovian quantum state diffusion equation* [138]. Differently from the SVNE, the dynamics is described by a single complex-valued Gaussian noise, at the price of introducing a possibly complicated functional derivative. Note that the version proposed here does not rely on the usual assumption of factorized initial preparation: in case of initial correlations it is sufficient to generate the noise $Z_\alpha(t)$ while keeping its coupling to the Matsubara component of the contour noise in Eq. (5.36b).

5.3 Reduction to single positive noise

The passage from Eq. (5.30) to Eq. (5.41) showed that there is more than one way to stochastically represent the environment's effect on the system. In this section, we show, using the insight offered by the contour formulation, that the solution of the SVNE can actually be represented in terms of $\nu_\alpha(t)$ alone[1], while the influence of $\eta_\alpha(t)$ only appears through its correlation function with $\nu_\alpha(t)$. As we will discuss, this is a consequence of the fact that $\mathbb{E}[\eta_\alpha(t)\eta_\beta(s)] = 0$, which is the striking simplification introduced by the Keldysh rotation (5.29). This reduction is remarkable because $\nu_\alpha(t)$ has a positive semidefinite covariance, contrary to the arguably more complicated complex colored noise $Z_\alpha(t)$ of Eq. (5.41). However, this will come at a cost, since after the elimination of $\eta_\alpha(t)$ it will not be immediately obvious how to express the result as the solution of a time-local differential equation.

The formal solution to the SVNE (5.30) can be written as

$$R(t) = \mathbb{T}\exp\left[-i\sum_\alpha \int_{t_0}^t \mathrm{d}s\, \left[\nu_\alpha(s)\hat{A}^-_\alpha(s) + \eta_\alpha(s)\hat{A}^+_\alpha(s)\right]\right]\varrho_0, \tag{5.42}$$

where $\hat{A}^\pm_\alpha(s) := \hat{A}^L_\alpha(s) \pm \hat{A}^R_\alpha(s)$. We need now to expand this two-term exponential.

Consider two generic collections of indexed operators $\{X_i\}$ and $\{Y_i\}$, and let us ask about the ordered product of sums $\mathbb{T}\{(X_1+Y_1)\dots(X_n+Y_n)\}$: how can we write it as a sum of ordered products? Since operators commute inside the $\mathbb{T}$ sign, we will have a sum of terms of the form $\mathbb{T}\{X_{\sigma(1)}\dots X_{\sigma(k)}Y_{\sigma(k+1)}\dots Y_{\sigma(n)}\}$, with $k \in \{0,\dots,n\}$ and $\sigma \in \mathfrak{S}_n$ being a permutation of $\{1,\dots,n\}$. However, for fixed k, we should not distinguish terms where $X_{\sigma(1)}\dots X_{\sigma(k)}$ are simply arranged in different order, and similarly for $Y_{\sigma(k+1)}\dots Y_{\sigma(n)}$. We conclude that

$$\mathbb{T}\{(X_1+Y_1)\dots(X_n+Y_n)\} = \sum_{k=0}^n \frac{1}{k!(n-k)!}\sum_{\sigma\in\mathfrak{S}_n}\mathbb{T}\{X_{\sigma(1)}\dots X_{\sigma(k)}Y_{\sigma(k+1)}\dots Y_{\sigma(n)}\}. \tag{5.43}$$

In our case, $X_i \mapsto \nu_\alpha(s)\hat{A}^-_\alpha(s)$ and $Y_i \mapsto \eta_\alpha(s)\hat{A}^+_\alpha(s)$, hence

$$R(t) = \sum_{n=0}^\infty \frac{(-i)^n}{n!}\sum_{k=0}^n \binom{n}{k} \sum\!\!\!\!\!\!\int_{t_0}^t \mathrm{d}^n\mathbf{s}\, \nu_1\dots\nu_k\eta_{k+1}\dots\eta_n \mathbb{T}\{\hat{A}^-_1\dots\hat{A}^-_k\hat{A}^+_{k+1}\dots\hat{A}^+_n\}\varrho_0, \tag{5.44}$$

where we exploited the fact that operators commute inside $\mathbb{T}$ and thus all permutations contribute equally under the integration sign. As usual, we also introduced the abbreviations $\nu_i \equiv \nu_{\alpha_i}(s_i)$, $\eta_i \equiv \eta_{\alpha_i}(s_i)$, and $\hat{A}^\pm_i \equiv \hat{A}^\pm_{\alpha_i}(s_i)$.

[1]Remember that, in case of initial system-environment correlations, the noise $\nu_\alpha(t)$ is still statistically coupled to the noises $\xi_\alpha(t_0 \pm i\tau)$ coming from the initial preparation.

Now we remember that $R(t)$ can be arbitrarily modified, as long as we preserve the property $\mathbb{E}[R(t)] = \varrho(t)$. Let us then take the expectation value of the above equation, which only affects the string of noises. Since $\mathbb{E}[\eta_i\eta_j] = 0$, Isserlis' theorem (5.2) yields the following expression:

$$\begin{aligned}\mathbb{E}[\nu_1 \dots \nu_k \eta_{k+1} \dots \eta_{2m}] = \frac{\theta(k-m)}{(k-m)!2^{k-m}} \sum_{\sigma \in \mathfrak{S}_k} \mathbb{E}[\nu_{\sigma(1)}\eta_{k+1}] \dots \mathbb{E}[\nu_{\sigma(2m-k)}\eta_{2m}] \\ \times \mathbb{E}[\nu_{\sigma(2m-k+1)}\nu_{\sigma(2m-k+2)}] \dots \mathbb{E}[\nu_{\sigma(k-1)}\nu_{\sigma(k)}].\end{aligned} \tag{5.45}$$

This structure is enforced by the fact that we must limit to those permutations that pair each η_i with a ν_j. Note that this is possible only when $k \geq m$, which justifies the appearance of $\theta(k-m)$. When substituted in Eq. (5.44), it is immediate to see that each permutation contributes equally, hence, for the purpose of calculating $\mathbb{E}[R(t)]$, we can make the effective substitution

$$\begin{aligned}\mathbb{E}[\nu_1 \dots \nu_k \eta_{k+1} \dots \nu_{2m}] \mapsto \frac{\theta(k-m)k!}{(k-m)!2^{k-m}} \mathbb{E}[\nu_1\eta_{k+1}] \dots \mathbb{E}[\nu_{2m-k}\eta_{2m}] \\ \times \mathbb{E}[\nu_{2m-k+1}\nu_{2m-k+2}] \dots \mathbb{E}[\nu_{k-1}\nu_k].\end{aligned} \tag{5.46}$$

Isserlis' theorem can now be used again in the reversed direction to regroup the expectation values involving only ν noises. Specifically, using again that permutations contribute equally to the integrals in $R(t)$,

$$\begin{aligned}\mathbb{E}[\nu_{2m-k+1}\nu_{2m-k+2}] \dots \mathbb{E}[\nu_{k-1}\nu_k] &\mapsto \sum_{\pi \in \mathfrak{S}^k_{2m-k+1}} \mathbb{E}[\nu_{\pi(2m-k+1)}\nu_{\pi(2m-k+2)}] \dots \mathbb{E}[\nu_{\pi(k-1)}\nu_{\pi(k)}] \\ &= \frac{(k-m)!2^{k-m}}{(2k-2m)!} \mathbb{E}[\nu_{2m-k+1} \dots \nu_k],\end{aligned} \tag{5.47}$$

where $\mathfrak{S}^b_a$ is the set of permutations of $\{a, \dots, b\}$, for $a \leq b$. We conclude that

$$\mathbb{E}[\nu_1 \dots \nu_k \eta_{k+1} \dots \eta_{2m}] \mapsto \frac{\theta(k-m)k!}{(2k-2m)!} \mathbb{E}[\nu_1\eta_{k+1}] \dots \mathbb{E}[\nu_{2m-k}\eta_{2m}]\mathbb{E}[\nu_{2m-k+1} \dots \nu_k], \tag{5.48}$$

a statement that we called *partial scalar Wick's theorem* in Ref. [53]. After rearranging the multiplicative factors, Eq. (5.44) becomes

$$\begin{aligned}\mathbb{E}[R(t)] = \sum_{m=0}^{\infty} \sum_{k=m}^{2m} \frac{(-i)^k}{k!} \binom{k}{2m-k} \fint_{t_0}^{t} \mathrm{d}^{2m}\mathbf{s}\, G_{1,k+1} \dots G_{2m-k,2m} \mathbb{E}[\nu_{2m-k+1} \dots \nu_k] \\ \times \mathbb{T}\{\hat{A}^-_1 \dots \hat{A}^-_k \hat{A}^+_{k+1} \dots \hat{A}^+_n\}\varrho_0,\end{aligned} \tag{5.49}$$

where

$$G_{i,j} \coloneqq -i\mathbb{E}[\nu_i\eta_j]. \tag{5.50}$$

We can now define a new stochastic operator $R'(t)$ that is obtained by removing the expectation value around the product of ν noises:

$$\begin{aligned}R'(t) \coloneqq \sum_{m=0}^{\infty} \sum_{k=m}^{2m} \frac{(-i)^k}{k!} \binom{k}{2m-k} \fint_{t_0}^{t} \mathrm{d}^{2m}\mathbf{s}\, G_{1,k+1} \dots G_{2m-k,2m} \nu_{2m-k+1} \dots \nu_k \\ \times \mathbb{T}\{\hat{A}^-_1 \dots \hat{A}^-_k \hat{A}^+_{k+1} \dots \hat{A}^+_n\}\varrho_0.\end{aligned} \tag{5.51}$$

Clearly, $\mathbb{E}[R'(t)] = \mathbb{E}[R(t)] = \varrho(t)$ by construction, and the dynamics is equivalently described using $R'(t)$ instead of $R(t)$. As we anticipated at the beginning of the subsection, the important point is that Eq. (5.51) does not explicitly depend on the noise $\eta_\alpha(t)$ and that the noise $\nu_\alpha(t)$ has a positive semidefinite covariance.

An interesting question is whether it is possible to find a differential equation that describes the evolution of $R'(t)$. Such an equation would be an exact non-Markovian stochastic equation that is written in terms of a single Gaussian noise with positive semidefinite covariance, in contrast to the state diffusion equation (5.41). We leave this remarkable possibility to future work.

5.4 Measurement interpretation

The noises $\nu_\alpha(t)$ and $\eta_\alpha(t)$ appearing in the SVNE are generally complex-valued. However, in Sec. 5.3 we saw there is a stochastic representation of the dynamics in which $\eta_\alpha(t)$ can be "eliminated" in favor of a single noise $\nu_\alpha(t)$ with positive semidefinite covariance. Unfortunately, $\nu_\alpha(t)$ cannot be interpreted *a priori* as the outcome of a continuous measurement process performed on the environment because of the general non-Markovian character of the dynamics [133]. This contrasts with what occurs in other *Markovian* stochastic descriptions [131].

In this last section we will analyze how a one-shot measurement of the environment performed at the beginning of the dynamics affects the original SVNE noises. Consequently, we will focus on finding a measurement protocol and a physical regime in which the measurement records $\mathbf{y}$ will give us some scalar stochastic estimate $b_\alpha^{(\mathbf{y})}(t)$ of the operator $B_\alpha(t)$ with the same covariance as the noise $\nu_\alpha(t)$:

$$\mathbb{E}_\nu\left[\nu_\alpha(t)\nu_\beta(s)\right] = \mathbb{E}_y[b_\alpha^{(\mathbf{y})}(t)b_\beta^{(\mathbf{y})}(s)]. \tag{5.52}$$

Here, the symbol $\mathbb{E}_\nu$ stands for an average with respect to the noises ν_α, while $\mathbb{E}_y$ stands for an average over the measurement outcomes $\mathbf{y}$. Additionally, to ensure that the dynamics after the measurement remains consistent with the one without it, we will require that averaging over $\mathbf{y}$ will eventually restore the original density operator. In other words, the system dynamics should not be altered by the measurement process. These conditions grant that, in some cases, $\nu_\alpha(t)$ can be interpreted as a "classical noise" emerging from a measurement scheme.

5.4.1 Effect of an initial measurement

Suppose the environment is initially in a Gaussian state[2] Ω, and that we perform an arbitrary finite number n of measurements on it at the initial time. In correspondence to a measurement record $\mathbf{y} = (y_1, \dots, y_n)$, the state Ω is replaced by the post-measurement state [56]

$$\Omega_\mathbf{y} = \frac{M_\mathbf{y}\Omega M_\mathbf{y}^\dagger}{\mathbb{P}(\mathbf{y})}, \qquad \mathbb{P}(\mathbf{y}) = \mathrm{Tr}\left[M_\mathbf{y}\Omega M_\mathbf{y}^\dagger\right], \tag{5.53}$$

where $M_\mathbf{y} := M_{y_n}\dots M_{y_1}$, with $\{M_{y_i}\}$ being the measurement operators and $\mathbb{P}(\mathbf{y})$ being the probability of obtaining the record $\mathbf{y}$.

[2] For factorized initial conditions, $\Omega = \varrho_E$ but this is not the case for correlated initial conditions.

In case $\Omega_{\mathbf{y}}$ is still a Gaussian state, we can apply all the machinery developed in this chapter, with an important caveat regarding the stability condition. Even if $\mathrm{Tr}[B_\alpha(t)\Omega] = 0$ is satisfied, it is not necessarily the case that the same happens after the substitution $\Omega \mapsto \Omega_{\mathbf{y}}$. This means that we should take into consideration a possibly non-vanishing average

$$E_\alpha^{(\mathbf{y})}(t) := \mathrm{Tr}\big[B_\alpha(t)\Omega_{\mathbf{y}}\big] \neq 0. \tag{5.54}$$

Correspondingly, the correlation function $c_{\alpha\beta}(t,s) = \mathrm{Tr}\big[B_\alpha(t)B_\beta(s)\Omega\big]$ gets replaced by

$$c_{\alpha\beta}^{(\mathbf{y})}(t,s) := \mathrm{Tr}\big[B_\alpha(t)B_\beta(s)\Omega_{\mathbf{y}}\big] - E_\alpha^{(\mathbf{y})}(t)E_\beta^{(\mathbf{y})}(s). \tag{5.55}$$

Luckily, the machinery we developed in the previous pages, starting from Sec. 4.2.3 with the introduction of the Gaussian environment assumption, can be generalized to a scenario where the stability condition does not hold: the interested reader can find such generalization laid out in Appendix B. In the context of this section, all we need to know is that the SVNE continues to be valid, provided we shift the ν noise precisely by the average in Eq. (5.54). Specifically,

$$\frac{\mathrm{d}R_{\mathbf{y}}(t)}{\mathrm{d}t} = -i\sum_\alpha \Big(\nu_\alpha^{(\mathbf{y})}(t) + E_\alpha^{(\mathbf{y})}(t)\Big)[A_\alpha(t), R_{\mathbf{y}}(t)] - i\sum_\alpha \eta_\alpha^{(\mathbf{y})}(t)\{A_\alpha(t), R_{\mathbf{y}}(t)\}, \tag{5.56}$$

where $R_{\mathbf{y}}(t)$ is the system's stochastic operator associated with this modified evolution and where $\nu_\alpha^{(\mathbf{y})}(t)$ and $\eta_\alpha^{(\mathbf{y})}(t)$ are zero-mean Gaussian noises with correlation functions

$$\mathbb{E}\Big[\nu_\alpha^{(\mathbf{y})}(t)\nu_\beta^{(\mathbf{y})}(s)\Big] = \frac{1}{2}\Big[c_{\alpha\beta}^{(\mathbf{y})}(t,s) + c_{\beta\alpha}^{(\mathbf{y})}(s,t)\Big], \tag{5.57a}$$

$$\mathbb{E}\Big[\nu_\alpha^{(\mathbf{y})}(t)\eta_\beta^{(\mathbf{y})}(s)\Big] = \frac{1}{2}\theta(t-s)\big[c_{\alpha\beta}(t,s) - c_{\beta\alpha}(s,t)\big], \tag{5.57b}$$

$$\mathbb{E}\Big[\eta_\alpha^{(\mathbf{y})}(t)\eta_\beta^{(\mathbf{y})}(s)\Big] = 0. \tag{5.57c}$$

Note that there are two sources of stochasticity at play: first, the fluctuation of the measurement record $\mathbf{y}$, and second, the fluctuation of the noises $\nu_\alpha^{(\mathbf{y})}(t)$ and $\eta_\alpha^{(\mathbf{y})}(t)$ at fixed $\mathbf{y}$, derived from the stochastic decoupling. The averages appearing in Eqs. (5.57) are intended with respect to this second source only. The stochasticity of $\mathbf{y}$ influences both the second moment of $\nu_\alpha^{(\mathbf{y})}(t)$ and the bias $E_\alpha^{(\mathbf{y})}(t)$. Note instead how the correlation function between $\eta_\alpha^{(\mathbf{y})}(t)$ and $\eta_\beta^{(\mathbf{y})}(s)$ does not actually depend on $\mathbf{y}$, since dissipation kernels are not influenced by the environment's state, as discussed in Sec. 5.2.1.

5.4.2 Semiclassical conditions

To find the conditions under which a generic quantum measurement scheme yields Eq. (5.52), we will narrow our field of analysis by making some assumptions. First, we take $B_\alpha \equiv X_\alpha$, where α can be thought of as a label running over the modes of the environment, and X_α is the position operator associated with mode α. We will also assume that each mode can be described as a bosonic harmonic oscillator of frequency ω_α and mass m_α.

In addition, two hypotheses on the measurement protocol will be made. In order to preserve Gaussianity, we need Gaussian post-measurement states; therefore, we will consider only measurements described by

$$M_{Y,y} := \frac{1}{(2\pi\sigma_Y^2)^{1/4}} \exp\left[-\frac{(y-Y)^2}{4\sigma_Y^2}\right]. \tag{5.58}$$

Specifically, $M_{Y,y}$ is the measurement operator associated with a measurement of the observable Y with obtained outcome y. The quantity σ_Y^{-1} can be interpreted as the precision with which such a measurement is carried out.

Secondly, we adopt a heterodyne scheme [84] in which position and momentum of each environmental mode is measured at the initial time, resulting in

$$\Omega_{\mathbf{x},\mathbf{p}} = \frac{M_{\mathbf{X},\mathbf{x}} M_{\mathbf{P},\mathbf{p}} \Omega M_{\mathbf{P},\mathbf{p}}^\dagger M_{\mathbf{X},\mathbf{x}}^\dagger}{\mathbb{P}(\mathbf{x},\mathbf{p})}, \tag{5.59}$$

where $M_{\mathbf{X},\mathbf{x}} := \prod_\alpha M_{X_\alpha,x_\alpha}$ (the ordering of the factors is irrelevant for our purposes), $M_{\mathbf{P},\mathbf{p}} := \prod_\alpha M_{P_\alpha,p_\alpha}$, with P_α being the momentum operator associated with mode α, and $\mathbb{P}(\mathbf{x},\mathbf{p})$ is the probability of obtaining the strings of outcomes $\mathbf{x}$ for the position and $\mathbf{p}$ for the momentum. For simplicity, we will indicate $\mathbf{y} = (\mathbf{x},\mathbf{p})$ and $y_\alpha = (x_\alpha, p_\alpha)$.

Finally, let us assume without much loss of generality that $\mathrm{Tr}[X_\alpha\Omega] = \mathrm{Tr}[P_\alpha\Omega] = 0$. Since Ω is a Gaussian state, it is completely characterized by the variances

$$\Delta_{X_\alpha}^2 := \mathrm{Tr}\left[X_\alpha^2\Omega\right], \qquad \Delta_{P_\alpha}^2 := \mathrm{Tr}\left[P_\alpha^2\Omega\right]. \tag{5.60}$$

As we show in Appendix D using the *Wigner function formalism* [84, 148], if the following conditions hold,

$$\sigma_{X_\alpha} \ll \Delta_{X_\alpha}, \qquad \sigma_{P_\alpha} \ll \Delta_{P_\alpha}, \qquad \sigma_{X_\alpha}\sigma_{P_\alpha} \gg 1, \tag{5.61}$$

then

$$E_\alpha^{(\mathbf{y})}(t) \simeq x_\alpha \cos[\omega_\alpha(t-t_0)] + \frac{p_\alpha}{m_\alpha\omega_\alpha}\sin[\omega_\alpha(t-t_0)], \tag{5.62a}$$

$$\mathbb{E}_y\left[E_\alpha^{(\mathbf{y})}(t)E_\beta^{(\mathbf{y})}(s)\right] \simeq \mathbb{E}_\nu\left[\nu_\alpha(t)\nu_\beta(s)\right]. \tag{5.62b}$$

By comparison with Eq. (5.52), note that $b_\alpha^{(\mathbf{y})}(t) \mapsto E_\alpha^{(\mathbf{y})}(t)$. Also, $\nu_\alpha(t)$ is the noise we had without performing the initial measurement.

Let us briefly discuss the physical interpretation behind Eqs. (5.61) and (5.62). Combining those conditions together,

$$\Delta_{X_\alpha}\Delta_{P_\alpha} \gg 1. \tag{5.63}$$

The variances associated with the initial preparation Ω are characterized by position and momentum scales that are so large that we can neglect any quantum effect. Under these assumptions, the initial Wigner function associated with Ω can be thought as a classical phase-space probability distribution. By choosing the precision properly, the distribution of outcomes coincides with the probability distribution representing the initial state. Then, Eq. (5.62a) follows from $E_\alpha^{(\mathbf{y})}(t_0) = x_\alpha$ and Eq. (5.62b) arises from the phase-space statistics of the initial state matching the statistics of the measurement outcomes.

We conclude by mentioning what happens to the master equation (5.56) in the regime identified by the conditions (5.61). The measurement is very precise, so that the post-measured state $\Omega_{\mathbf{y}}$ has very small position and momentum variances—respectively given, for any assigned mode α, by $\sigma^2_{X_\alpha}$ and $\sigma^2_{P_\alpha}$. These are much smaller than the variances associated with the original state preparation, that are now determining the fluctuations of $E^{(\mathbf{y})}_\alpha(t)$. Thus, the fluctuations of $\nu^{(\mathbf{y})}_\alpha(t)$ are very small if compared to the ones of $E^{(\mathbf{y})}_\alpha(t)$ and the fluctuations of the Hamiltonian part are totally controlled by the latter. Hence, we identified a regime where the correlation function of the ν noise can be interpreted as stemming from the stochasticity of outcomes of an appropriately chosen measurement of the environment.

Chapter 6

The Gaussian Master Equation

This chapter describes a slightly generalized version of the results originally published in:

[54] A. D'Abbruzzo, V. Giovannetti, and V. Cavina, *Exact non-Markovian master equations: A generalized derivation for Gaussian systems*, Phys. Rev. Lett. **135**, 240401 (2025).

In the previous chapter, we focused on generic open quantum systems coupled to Gaussian environments, employing stochastic equations. The question we now address is: can we derive an *exact* and *deterministic* master equation for our system? Such a tool would offer a direct representation of the dynamics, free from fictitious stochastic trajectories—a concept often tricky to grasp in the non-Markovian setting. Unfortunately, obtaining an exact master equation proves difficult without introducing further assumptions about the system.

The situation improves if we restrict our attention to *Gaussian systems* that are linearly coupled to Gaussian environments. Due to the important simplifications introduced by this assumption, several studies exist on this topic [149–153], but they are typically limited to excitation-preserving interactions. Notable specific exceptions nevertheless exist, such as the famous Hu-Paz-Zhang equation [149]. When this is the result of a rotating-wave approximation, it is however known that inaccuracies can emerge when attempting to capture energy shifts and non-Markovian effects [81–83]. A master equation free of this assumption was derived in Ref. [153], generalizing Ref. [149], but with a few caveats. First, it is only valid for bosonic particles; an extension to fermionic systems is required to study, e.g., systems with superconducting pairing [154–156] or spin-fermion Hamiltonians [83]. Second, it demands system and environment to be uncorrelated at the initial time, a condition that might not be experimentally feasible in the strong-coupling regime [117, 145, 157].

In this chapter, building upon the contour formalism developed in Chap. 4, we derive a master equation—the *Gaussian Master Equation* (GME)—that is uniformly valid for all Gaussian systems, without the need for further assumptions [54]. Our approach is applicable to both bosonic and fermionic cases[1], accommodates arbitrary forms of the system-environment coupling, and remains valid even in the presence of initial correlations. The GME exhibits a remarkably simple and compact structure, being formally identical to the Redfield equation. Naturally, its kernel is not the bare environment correlation function, but a dressed one that incorporates all virtual system-environment interactions. This formal correspondence

[1] We should point out that the master equation does not apply to hybrid quadratic models in which fermions are linearly coupled to bosons. However, these models are not Gaussian, as higher-order correlators cannot be expressed in terms of two-point ones—see, for instance, the Jaynes-Cummings model [6].

has an enormous impact on the task of solving the GME in practice. This feature differentiates it from other important approaches where the proposed equation's dependence on microscopic parameters is arguably more involved.

An attentive reader could, however, make the following observation: if the entire system-environment compound is Gaussian, why not solve the dynamics of the whole universe and then simply extract the system sector? Unfortunately, while this approach is certainly feasible for finite-size settings, the problem becomes increasingly more demanding for large environment sizes, which is arguably the most interesting regime for the vast majority of questions in the field of open quantum systems. Moreover, it is extremely wasteful to precisely evolve an environment that is intended to be an effective model: we are simply not interested in its internal evolution, and a lot of unnecessary information would be produced. For these reasons, it remains highly valuable to find an effective description of open Gaussian system.

The chapter is structured as follows. We begin in Sec. 6.1 with a brief description of the most important preexisting approaches used to construct exact master equations for open Gaussian systems. The new material we propose is discussed in Sec. 6.2, which contains a detailed derivation of the GME. Sec. 6.3 focuses on unraveling the contour notation to arrive at a physical-time description suitable for numerical approaches. Here, the GME is also put to the test with a simple example involving a fermionic system with superconductive pairing—a case not addressable by previous approaches. Finally, in Sec. 6.4 we translate the GME into a differential equation for the system's covariance matrix, which is a natural object to observe when discussing Gaussian systems.

6.1 Open Gaussian systems

6.1.1 Heisenberg-Langevin equation

The simplification arising from Gaussianity can be directly identified as the *linearity* of the Heisenberg equations of motion for the ladder operators (cf. Appendix A). In the context of open systems, one can therefore write two linearly coupled differential equations: one for the system's ladder operators and one for the environment's ladder operators. Subsequently, one formally solves the environment equation and substitutes the result back into the system equation. The result is known as *Heisenberg-Langevin (HL) equation* [158, 159], due to its resemblance to the standard Langevin equation found in dissipative classical physics [67].

In the literature, this calculation is typically carried out starting from a Hamiltonian structure of the form

$$H_S = \sum_{i,j} \varepsilon_{ij} a_i^\dagger a_j, \qquad H_E = \sum_{\mu,\nu} \omega_{\mu\nu} c_\mu^\dagger c_\nu, \qquad V = \sum_{i,\mu} \left(g_{i\mu} a_i^\dagger c_\mu + g_{i\mu}^* c_\mu^\dagger a_i \right), \tag{6.1}$$

which we will refer to as *excitation-preserving* setting. In this case, creation and annihilation operators can be considered separately. In terms of the vector $\mathbf{a}^T = (a_1, \dots, a_n)$ of annihilation operators, the HL equation turns out to be

$$\frac{\mathrm{d}\mathbf{a}(t)}{\mathrm{d}t} = -i\varepsilon\mathbf{a}(t) - i\mathbf{B}(t) - \int_0^t \mathrm{d}\tau\, \Sigma(t-\tau)\mathbf{a}(\tau), \tag{6.2}$$

where $\mathbf{B}(t) := g e^{-i\omega t}\mathbf{c}(0)$ is the evolved interaction operator associated with the environment and $\Sigma(t) := ge^{-i\omega t}g^{\dagger}$ is a memory kernel known as *embedding self-energy* [45], which is basically the Fourier transform of the environment's spectral density [158].

The HL equation (6.2) is a potentially complicated integro-differential equation. In principle, it could be approached with the Laplace transform technique [159], but in practice this can be carried out explicitly only for a very limited class of self-energies. Much easier is the task of studying the steady-state solution at $t \to \infty$, where one can instead rely on a simpler Fourier transform [158].

Note that the excitation-preserving setting does not exhaust all the possible structures one can have for an open Gaussian system: terms that violate excitation number conservation can appear in both the isolated Hamiltonians H_S, H_E and the coupling V. This is particularly important when trying to model superconductive systems [154, 156], Brownian motion with momentum coupling [160], or quantum optics beyond the rotating-wave approximation [81–83]. This general setting is instead captured by formulating the problem using the Darboux-Majorana basis introduced in Sec. 4.2.1, as we highlight in Appendix A, where we also provide a more general derivation of the HL equation.

6.1.2 Influence functional technique

While useful and straightforward, the HL equation (6.2) does not give us the full picture for what concerns the evolution of the system's density operator $\rho(t)$. More advanced techniques typically involve the nonequilibrium Green's function theory [45] or the Feynman-Vernon influence functional technique [110]. While the former is not so easily applicable outside the wide-band limit, which is arguably what we are interested in for a fully non-Markovian regime, the latter has been successfully applied to derive a number of important results.

In Refs. [150–152], the authors show that, in the excitation-preserving scenario (6.1), an exact time-local master equation for $\rho(t)$ can be found:

$$\begin{aligned}\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} &= -i[\widetilde{H}(t), \rho(t)] + \sum_{i,j}\left[\zeta\widetilde{\gamma}_{ij}(t) + 2\gamma_{ij}(t)\right]\left[a_j\rho(t)a_i^{\dagger} - \frac{1}{2}\{a_i^{\dagger}a_j, \rho(t)\}\right] \\ &+ \sum_{i,j}\widetilde{\gamma}_{ij}(t)\left[a_i^{\dagger}\rho(t)a_j - \frac{1}{2}\{a_j a_i^{\dagger}, \rho(t)\}\right], \qquad \widetilde{H}(t) = \sum_{i,j}\widetilde{\varepsilon}_{ij}(t)a_i^{\dagger}a_j.\end{aligned} \tag{6.3}$$

The coefficients, which are time-dependent in order to capture the non-Markovian features of the dynamics, are determined by the relations

$$\gamma = -\frac{1}{2}\left[\dot{u}u^{-1} + \mathrm{H.c.}\right], \qquad \widetilde{\gamma} = \dot{v} - \left[\dot{u}u^{-1}v + \mathrm{H.c.}\right], \qquad \widetilde{\varepsilon} = \frac{i}{2}\left[\dot{u}u^{-1} - \mathrm{H.c.}\right], \tag{6.4}$$

where $u(t)$ is the solution to the following homogeneous version of the HL equation:

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = -i\varepsilon u(t) - \int_0^t \mathrm{d}\tau\, \Sigma(t-\tau)u(\tau). \tag{6.5}$$

The matrix v can instead be found as

$$v(t) = \int_0^t \mathrm{d}^2\boldsymbol{\tau}\, u(\tau_1)\widetilde{\Sigma}(\tau_2 - \tau_1)u^{\dagger}(\tau_2), \tag{6.6}$$

where $\widetilde{\Sigma}(t)$ is a modified version of $\Sigma(t)$ which depends on the initial state of the environment. We refer to Ref. [151] for more detailed expressions.

Eq. (6.3) is valid for both bosonic and fermionic scenarios with excitation-preserving[2] interaction. While this approach was initially developed for factorized initial conditions, it has also been shown that initial system-environment correlations can be incorporated into the description [152].

It is important to notice that the coefficients of Eq. (6.3) are defined through a quantity, $u(t)$, which is the solution of another possibly complicated integro-differential equation that shares the Heisenberg-Langevin structure. As with Eq. (6.2), its feasibility strongly depends on the spectral characteristics of the environment. Furthermore, the size of the matrix u grows linearly with the dimension of the system, which can become demanding when studying the dynamics of many-body systems. With the GME, we will instead show that the complexity of the dynamics actually scales with the size of the subsystem that is physically coupled to the environment. This scaling is much more forgiving and intuitive for practical applications.

6.1.3 An alternative direct approach

An alternative, more direct approach to formulating a closed master equation, one that avoids auxiliary integro-differential equations, was proposed by Ferialdi in Ref. [153]. The core idea is to directly take the time derivative of the density operator, as expressed via the time-ordered exponential, and then use Wick's theorem to recompactify the resulting expression. Crucially, thanks to the overarching generality of Wick's theorem in the Gaussian setting, this method does not need to make assumptions about the coupling and simply works even outside the excitation-preserving scenario. Unfortunately, in the form described in Ref. [153], the formulas are restricted to the bosonic scenario. The result is

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\sum_{\alpha,\beta}\int_0^t \mathrm{d}s \left(\mathcal{A}_{\alpha\beta}(t,s)[A_\alpha(t),[A_\beta(s),\rho(t)]] + i\mathcal{B}_{\alpha\beta}(t,s)[A_\alpha(t),\{A_\beta(s),\rho(t)\}]\right), \quad (6.7)$$

with the time-dependent coefficients being given by

$$\mathcal{A}(t,s) := \mathrm{Re}\, c(t,s) + \sum_{n=1}^{\infty}\mathcal{R}_n(t,s), \qquad \mathcal{B}(t,s) := \mathrm{Im}\, c(t,s) + \sum_{n=1}^{\infty}\mathcal{S}_n(t,s), \quad (6.8)$$

where $\mathcal{R}_n(t,s)$ and $\mathcal{S}_n(t,s)$ are recursively defined in terms of $c(t,s)$. The precise expressions are rather involved and we refer the interested reader to consult Ref. [153] directly.

There are some evident drawbacks in the description provided by Eq. (6.7). First, it is limited to bosonic scenarios. Second, it requires a factorized initial state and it is not clear how to eventually extend it to correlated ones. Third, most importantly, the coefficients of the master equation have an involved dependence on microscopic parameters, a fact which hinders the practical application of Eq. (6.7). While there is no need to solve an integro-differential equation to even write the master equation, as for Eq. (6.3), it is still considerably difficult to express the recursion (6.8) in an intuitive manner.

The contour formalism developed in Chap. 4 allows us to solve all of the above problems [54]. We also employ direct differentiation of the density operator and Wick's theorem,

[2]Using the approach of Appendix A, where we provide the Heisenberg-Langevin equation for generic interaction by moving to the Darboux-Majorana basis, it could be possible to generalize the derivation of Ref. [151] beyond the excitation-preserving scenario.

thus retaining complete generality in the coupling structure. However, the abstraction provided by the contour is what enables us to treat in an unified fashion the *most general Gaussian context*: bosonic and fermionic scenarios are both allowed, and the inclusion of a Matsubara track paves the way to the description of correlated initial Gaussian states. Most importantly, the final result is much simpler than Eq. (6.7), and it reads[3]

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\sum_{\alpha,\beta}\int_0^t \mathrm{d}s\, \mathcal{G}^{>}_{\alpha\beta}(t,s)[A_\alpha(t), A_\beta(s)\rho(t)] + \mathrm{H.c.} \tag{6.9}$$

Remarkably, this has the shape of a Redfield equation (2.106), but where the usual environment correlation function $c(t,s)$ gets replaced by a kernel $\mathcal{G}^{>}(t,s)$ that can be found by solving a *contour Dyson equation* [45]:

$$\mathcal{G} = C + \mathcal{G} * \Sigma * C. \tag{6.10}$$

The symbol $*$ indicates convolution in contour variables, C is the contour correlation function, and Σ is a system *self-energy* contribution[4]. The precise meaning of Eq. (6.10) will be explained below in Sec. 6.2. Here, we just want to point out the main message: Eq. (6.9) is much easier to solve than Eq. (6.3) from both a structural and dimensional point of view. Furthermore, it is directly interpretable as a generalization of the Redfield equation, unlike the convoluted structure of Eq. (6.7).

Since Eq. (6.9) is capable of accounting for *any* open Gaussian system, we call it the *Gaussian Master Equation (GME)*. In the next section we provide an in-depth discussion of its derivation.

6.2 Derivation of the GME

We will now present in this section a detailed derivation of the Gaussian Master Equation. As usual, we start from the assumption that our system of interest is coupled to a Gaussian environment. Using the contour formalism, this means we start from Eq. (4.67) for the system's reduced density operator. The derivation proceeds through the following steps. In Sec. 6.2.1, we first directly take the time derivative of Eq. (4.67) using the *transport theorem* developed in the previous chapter (cf. Sec. 5.1.2). As an *intermezzo*, in Sec. 6.2.2, we show that applying a Markov-like approximation to the obtained expression is enough to recover a "contour generalization" of the Redfield equation. Moving back to the exact scenario, in Sec. 6.2.3 we introduce the Gaussian system assumption and prove a *reduction lemma* that allows us to finally close the master equation in Sec. 6.2.4.

6.2.1 Taking the time derivative

Let us start our discussion from the expression

$$\varrho(t) = \mathbb{T}_\zeta\left\{\exp\left[-\frac{1}{2}\oint_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, C_{1,2}A_1A_2\right]\varrho_0\right\}, \tag{6.11}$$

[3] In case of initial system-environment correlations, an additional term must be included: see Eq. (6.69) below for the full expression.

[4] The Σ appearing in the Dyson equation has nothing to do with the embedding self-energy of the HL equation!

which was obtained in Chap. 4 as a description of the dynamics of an open quantum system interacting with a Gaussian environment. Equivalently, if we expand the exponential,

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} M_n(t), \qquad M_n(t) := \sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{1,2} \dots C_{2n-1,2n} \mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\}. \tag{6.12}$$

The first thing we have to do is to take the derivative with respect to t. Luckily, we already know how: it is sufficient to use the transport theorem 5.1. But first, let us show that the integrand in $M_n(t)$ satisfies the condition (5.11), so that the simplified version of the theorem given by Corollary 5.2 can be used.

Lemma 6.1. *Let f be the contour function*

$$f(\mathbf{z}) = \sum_{\alpha_1,\dots,\alpha_{2n}} C_{1,2} \dots C_{2n-1,2n} \mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\}. \tag{6.13}$$

Then, the condition

$$\int_{\gamma(t)} \mathrm{d}^{2n-1}\mathbf{w}\, f(\mathbf{w}_1^{k-1}, t^\pm, \mathbf{w}_k^{2n-1}) = \int_{\gamma(t)} \mathrm{d}^{2n-1}\mathbf{w}\, f(t^\pm, \mathbf{w}) \tag{6.14}$$

is satisfied for every $k \in \{1, \dots, 2n\}$.

Proof. Suppose first that k is odd. Then the left-hand side of Eq. (6.14) can be written as

$$\begin{aligned}\sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w \sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{1,2} \dots C_{k-2,k-1} C_{\alpha\beta}(t^\pm, w) C_{k,k+1} \dots C_{2n-3,2n-2} \\ \times \mathbb{T}_\zeta\big\{A_1 \dots A_{k-1} A_\alpha(t^\pm) A_\beta(w) A_k \dots A_{2n-2}\varrho_0\big\},\end{aligned} \tag{6.15}$$

where, for clarity, we reintroduced the full notation for occurrences of $t^\pm$ and for the contour variable w that is paired with it by C. Now, with $k-1$ transpositions we can bring $A_\alpha(t^\pm)$ at the beginning of the string of ordered operators, and with subsequent $k-1$ transpositions we can bring $A_\beta(w)$ immediately to the right of $A_\alpha(t^\pm)$. Since $2(k-1)$ is even, no additional sign factor appears after this operation:

$$\sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w \sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{\alpha\beta}(t^\pm, w) C_{1,2} \dots C_{2n-3,2n-2} \mathbb{T}_\zeta\big\{A_\alpha(t^\pm) A_\beta(w) A_1 \dots A_{2n-2}\varrho_0\big\}. \tag{6.16}$$

This is precisely the right-hand side of Eq. (6.14).

We can proceed similarly in case k is even. This time, the left-hand side of Eq. (6.14) writes

$$\begin{aligned}\sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w \sum\!\!\!\!\!\!\int_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{1,2} \dots C_{k-3,k-2} C_{\beta\alpha}(w, t^\pm) C_{k-1,k} \dots C_{2n-3,2n-2} \\ \times \mathbb{T}_\zeta\big\{A_1 \dots A_{k-2} A_\beta(w) A_\alpha(t^\pm) A_{k-1} \dots A_{2n-2}\varrho_0\big\}.\end{aligned} \tag{6.17}$$

With $k-1$ transpositions we can again bring $A_\alpha(t^\pm)$ at the beginning of the string of ordered operators, and then with $k-2$ transpositions we can bring $A_\beta(w)$ immediately to the right of $A_\alpha(t^\pm)$. Since we performed a total of $2k-3$ transpositions, which is odd, a factor ζ appears. However, $C_{\beta\alpha}(w, t^\pm) = \zeta C_{\alpha\beta}(t^\pm, w)$ and the additional ζ factor absorbs the one introduced by the ordering. The result is again (6.14). □

According to Corollary 5.2, we conclude that

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\int_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, f(\mathbf{z}) = 2n\int_{\gamma(t)} \mathrm{d}^{2n-1}\mathbf{w}\,\big[f(t^-,\mathbf{w}) - f(t^+,\mathbf{w})\big], \tag{6.18}$$

with f being the contour function in Eq. (6.13). Expanding it,

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = 2n\sum_{\alpha,\beta}\int_{\gamma(t)} \mathrm{d}w \, \not{\int}_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{1,2}\dots C_{2n-3,2n-2} \tag{6.19}$$
$$\times\big[C_{\alpha\beta}(t^-,w)\mathbb{T}_\zeta\big\{A_\alpha(t^-)A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\} - C_{\alpha\beta}(t^+,w)\mathbb{T}_\zeta\big\{A_\alpha(t^+)A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\}\big].$$

Since t^+ and t^- are, respectively, the starting and ending points of $\gamma(t)$,

$$\mathbb{T}_\zeta\big\{A_\alpha(t^-)A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\} = A_\alpha(t)\mathbb{T}\big\{A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\}, \tag{6.20a}$$
$$\mathbb{T}_\zeta\big\{A_\alpha(t^+)A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\} = \mathbb{T}_\zeta\big\{A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\}A_\alpha(t), \tag{6.20b}$$

where we used the fact that $A_\alpha(t^\pm) = A_\alpha(t)$ once it is placed outside the ordering. As we did in Chap. 5, it is convenient to introduce the superoperators

$$\hat{A}^L_\alpha(t)X \coloneqq A_\alpha(t)X, \qquad \hat{A}^R_\alpha(t)X \coloneqq XA_\alpha(t), \qquad \hat{A}^\delta_\alpha(t) \coloneqq \hat{A}^L_\alpha(t) - \hat{A}^R_\alpha(t), \tag{6.21}$$

so that

$$\begin{aligned}\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = 2n\sum_{\alpha,\beta}\int_{\gamma(t)} \mathrm{d}w \, \not{\int}_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{1,2}\dots C_{2n-3,2n-2}\\ \times C_{\alpha\beta}(t^+,w)\hat{A}^\delta_\alpha(t)\mathbb{T}_\zeta\big\{A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\},\end{aligned} \tag{6.22}$$

where we also used the fact that $C_{\alpha\beta}(t^+,w) = C_{\alpha\beta}(t^-,w)$ by Theorem 4.4.

Unfortunately, it is difficult to go further without making any assumption about the system. In order to arrive at a time-local master equation we would like to make $M_m(t)$ appear again on the right-hand side, possibly with $m \neq n$. But on the right-hand side of Eq. (6.22) we see that the ordered string $\mathbb{T}_\zeta\big\{A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\}$ contains an odd number of A operators: this is never matched by an operator like $M_m(t)$, which instead is characterized by an *even* number of A operators. We need some way of "reducing" the number of A operators contained in $\mathbb{T}_\zeta$.

6.2.2 Intermezzo: contour Redfield equation

Before showing how such reduction can be achieved, we present an interesting way of obtaining a contour generalization of the Redfield equation from Eq. (6.22). In the Markov approximation, the environment correlation function decays much faster than the other timescales of the problem (cf. Sec. 2.3.3): as a consequence, $C_{\alpha\beta}(t^+,s^\pm)$ is significantly different from zero only if s is sufficiently close to t. Let us then see what happens if we make the substitution

$$\mathbb{T}_\zeta\big\{A_\beta(w)A_1\dots A_{2n-2}\varrho_0\big\} \mapsto \begin{cases} A_\beta(w)\mathbb{T}_\zeta\{A_1\dots A_{2n-2}\varrho_0\} & w \succ t_0, \\ \zeta\mathbb{T}_\zeta\{A_1\dots A_{2n-2}\varrho_0\}A_\beta(w) & w \prec t_0. \end{cases} \tag{6.23}$$

Note that in the second case a ζ factor appears because $2n-1$ transpositions are required to bring $A_\beta(w)$ to the end of the string. If we define the superoperator

$$\hat{A}^\gamma_\beta(w) := \begin{cases} \hat{A}^L_\beta(w) & w \succ t_0, \\ \zeta \hat{A}^R_\beta(w) & w \prec t_0, \end{cases} \tag{6.24}$$

we end up with

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} \simeq 2n \sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w\, C_{\alpha\beta}(t^+, w) \hat{A}^\delta_\alpha(t) \hat{A}^\gamma_\beta(w) M_{n-1}(t) \equiv -2n \hat{\mathcal{R}}(t) M_{n-1}(t), \tag{6.25}$$

where

$$\hat{\mathcal{R}}(t) := -\sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w\, C_{\alpha\beta}(t^+, w) \hat{A}^\delta_\alpha(t) \hat{A}^\gamma_\beta(w). \tag{6.26}$$

If we substitute back into Eq. (6.12), we immediately obtain a master equation for $\varrho(t)$:

$$\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n n!} \frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = \sum_{n=1}^{\infty} \frac{(-1)^n(-2n)}{2^n n!} \hat{\mathcal{R}}(t) M_{n-1}(t) = \hat{\mathcal{R}}(t)\varrho(t). \tag{6.27}$$

We argue that $\hat{\mathcal{R}}(t)$ is the generator of the time-dependent Redfield equation (2.106), augmented to include eventual initial system-environment correlations. In fact, if we decompose the contour in its branches,

$$\begin{aligned} \hat{\mathcal{R}}(t)\varrho = &-\sum_{\alpha,\beta} \int_{t_0}^{t} \mathrm{d}s \left\{ C_{\alpha\beta}(t^+, s^-)[A_\alpha(t), A_\beta(s)\varrho] - C_{\alpha\beta}(t^+, s^+)[A_\alpha(t), \zeta\varrho A_\beta(s)] \right\} \\ &+ i \sum_{\alpha,\beta} \int_0^b \mathrm{d}\tau \left\{ C_{\alpha\beta}(t^+, t_0 - i\tau)[A_\alpha(t), A_\beta(t_0 - i\tau)\varrho] + C_{\alpha\beta}(t^+, t_0 + i\tau)[A_\alpha(t), \zeta\varrho A_\beta(t_0 + i\tau)] \right\}, \end{aligned} \tag{6.28}$$

where we made the substitution $\beta \mapsto 2b$ in the definition (4.18) of the initial state to avoid notation clash with the already present interaction index β. But we know that

$$C_{\alpha\beta}(t^+, s^-) = c_{\alpha\beta}(t,s), \tag{6.29a}$$

$$C_{\alpha\beta}(t^+, s^+) = \zeta C^*_{\overline{\alpha}\overline{\beta}}(t^-, s^-) = \zeta C^*_{\overline{\alpha}\overline{\beta}}(t^+, s^-) = \zeta c_{\overline{\alpha}\overline{\beta}}(t,s), \tag{6.29b}$$

$$C_{\alpha\beta}(t^+, t_0 - i\tau) = c_{\alpha\beta}(t, t_0 - i\tau), \tag{6.29c}$$

$$C_{\alpha\beta}(t^+, t_0 + i\tau) = \zeta C^*_{\overline{\alpha}\overline{\beta}}(t^-, t_0 - i\tau) = \zeta C^*_{\overline{\alpha}\overline{\beta}}(t^+, t_0 - i\tau) = \zeta c_{\overline{\alpha}\overline{\beta}}(t, t_0 - i\tau). \tag{6.29d}$$

As a consequence,

$$\begin{aligned} \hat{\mathcal{R}}(t)\varrho = &-\sum_{\alpha,\beta} \int_{t_0}^{t} \mathrm{d}s\, c_{\alpha\beta}(t,s)[A_\alpha(t), A_\beta(s)\varrho] \\ &+ i \sum_{\alpha,\beta} \int_0^b \mathrm{d}\tau\, c_{\alpha\beta}(t, t_0 - i\tau)[A_\alpha(t), A_\beta(t_0 - i\tau)\varrho] + \text{H.c.} \end{aligned} \tag{6.30}$$

The first term is precisely the Redfield generator in Eq. (2.106), while the second one is the additional contribution coming from initial system-environment correlations, which was neglected during the development in Chap. 2.

6.2.3 The reduction lemma

Let us consider again the general case in Eq. (6.22). A way to perform the reduction takes inspiration from Sec. 6.2.2 and can be easily achieved if we assume for a moment that the A operators (anti)commute between each other.

Lemma 6.2. *Let $A_\beta \equiv A_\beta(w)$. If $[A_i, A_j]_\zeta = 0$ for any choice of i and j, then*

$$\mathbb{T}_\zeta\big\{A_\beta A_1 \dots A_{2n}\varrho_0\big\} = \hat{A}^\gamma_\beta \mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\}, \tag{6.31}$$

where $\hat{A}^\gamma_\beta$ is the superoperator defined in Eq. (6.24).

Proof. By definition of contour ordering, we can find a permutation σ of $\{1, \dots, 2n\}$ and an index $k \in \{0, \dots, 2n\}$ such that

$$\mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\} = \zeta^{N(\sigma)}\zeta^{2n-k}A_{\sigma(1)} \dots A_{\sigma(k)}\varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(2n)}. \tag{6.32}$$

Suppose now that $w > t_0$. Then there exists an index $q \in \{0, \dots, k\}$ such that

$$\mathbb{T}_\zeta\big\{A_\beta A_1 \dots A_{2n}\varrho_0\big\} = \zeta^{N(\sigma)}\zeta^{2n-k+q}A_{\sigma(1)} \dots A_{\sigma(q)}A_\beta A_{\sigma(q+1)} \dots A_{\sigma(k)}\varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(2n)}. \tag{6.33}$$

Using the relation $A_{\sigma(i)}A_\beta = \zeta A_\beta A_{\sigma(i)}$, we can move A_β at the beginning of the string of operators inserting a ζ factor at each transpositions. Since q transpositions are required, we obtain a factor of ζ^q, which cancels the one that was already there:

$$\mathbb{T}_\zeta\big\{A_\beta A_1 \dots A_{2n}\varrho_0\big\} = A_\beta \mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\}. \tag{6.34}$$

Similarly, if $w < t_0$ there exists an index $q \in \{k, \dots, 2n\}$ such that

$$\mathbb{T}_\zeta\big\{A_\beta A_1 \dots A_{2n}\varrho_0\big\} = \zeta^{N(\sigma)}\zeta^{2n-k+q+1}A_{\sigma(1)} \dots A_{\sigma(k)}\varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(q)}A_\beta A_{\sigma(q+1)} \dots A_{\sigma(2n)}. \tag{6.35}$$

Using the relation $A_\beta A_{\sigma(i)} = \zeta A_{\sigma(i)}A_\beta$, we can move A_β at the end of the string of operators. Since $2n - q$ transpositions are required, we obtain a factor $\zeta^{2n-q} = \zeta^q$, which again cancels the one that was already there. Therefore,

$$\mathbb{T}_\zeta\big\{A_\beta A_1 \dots A_{2n}\varrho_0\big\} = \zeta \mathbb{T}_\zeta\{A_1 \dots A_{2n}\varrho_0\}A_\beta, \tag{6.36}$$

which is what we wanted to prove. □

What this lemma is telling us is that if $[A_i, A_j]_\zeta = 0$ then the contour Redfield equation (6.30) holds *exactly*, without invoking the Markov approximation. The reason is rooted in the fact that, with (anti)commuting A operators, we are allowed to ignore the relative positions between them. The only thing that matters is whether they should be put to the left or to the right of ϱ_0: as we discussed in Sec. 6.2.2, this has the same effect as the Markov approximation for the purpose of writing the master equation.

Unfortunately, the condition $[A_i, A_j]_\zeta = 0$ rarely holds in practice. Nevertheless, such observation inspires us to consider its easiest relaxation:

$$[A_i, A_j]_\zeta = \ell_{ij}\mathbb{1}, \qquad \ell_{ij} \in \mathbb{C}. \tag{6.37}$$

This is what happens under a *Gaussian system assumption*. If the system Hamiltonian H_S (and H_S^M in case of correlated initial state) is quadratic and the interaction operators A_α (and A_α^M)

are linear, then A_i and A_j are also linear and their (anti)commutator must be a c-number. As we did in Chap. 4, we refer to Appendix A for a more detailed discussion about quadratic Hamiltonians and Gaussian states.

As a preliminary step, we introduce a "graded" derivative symbol ∂, which acts as follows on a string of operators [119]:

$$\partial_{\mu_j}\left[X_{\mu_1}\dots X_{\mu_j}\dots X_{\mu_n}\right] := \zeta^{j-1}X_{\mu_1}\dots X_{\mu_{j-1}}X_{\mu_{j+1}}\dots X_{\mu_n}. \tag{6.38}$$

This can be interpreted as follows: we imagine to bring X_{μ_j} at the beginning of the string of operators introducing a ζ factor for each transposition; then we eliminate X_{μ_j} by acting with the derivative on it. The following lemma clarifies that this derivative commutes with the ordering operation.

Lemma 6.3. *For any string of operators $X_1,\dots,X_n$ and any $j\in\{1,\dots,n\}$ one has*

$$\partial_j\mathbb{T}_\zeta\{X_1\dots X_n\} = \zeta^{j-1}\mathbb{T}_\zeta\left\{X_1\dots X_{j-1}X_{j+1}\dots X_n\right\}. \tag{6.39}$$

Proof. Let σ be the permutation that orders the string $X_1,\dots,X_n$. Such ordering can alternatively be achieved in the following way: first, move X_j at the beginning of the string with $j-1$ transpositions; then, order the remaining operators $X_1\dots X_{j-1}X_{j+1}\dots X_n$, calling ϕ the permutation that does that; finally, bring X_j back into position with $\sigma^{-1}(j)-1$ transpositions. This observation allows us to say that

$$\zeta^{N(\sigma)} = \zeta^{j-1}\zeta^{N(\phi)}\zeta^{p-1}, \qquad p := \sigma^{-1}(j). \tag{6.40}$$

Since $\mathbb{T}_\zeta\{X_1\dots X_n\} = \zeta^{N(\sigma)}X_{\sigma(1)}\dots X_{\sigma(n)}$, by applying ∂_j we remove X_j, appearing at position p, and we introduce an additional factor ζ^{p-1}. Using the previous relation, and the fact that the remaining operators are already ordered:

$$\begin{aligned}&\partial_j\mathbb{T}_\zeta\{X_1\dots X_n\} = \zeta^{N(\sigma)}\zeta^{p-1}X_{\sigma(1)}\dots X_{\sigma(p-1)}X_{\sigma(p+1)}\dots X_{\sigma(n)}\\ &= \zeta^{N(\phi)}\zeta^{j-1}X_{\sigma(1)}\dots X_{\sigma(p-1)}X_{\sigma(p+1)}\dots X_{\sigma(n)} = \zeta^{j-1}\mathbb{T}_\zeta\left\{X_1\dots X_{j-1}X_{j+1}\dots X_n\right\},\end{aligned} \tag{6.41}$$

which is what we wanted to prove. □

We are now ready to prove an appropriate generalization of Lemma 6.2.

Lemma 6.4 (Reduction). *If $[A_i, A_j]_\zeta$ is a c-number for any choice of i and j, then*

$$\mathbb{T}_\zeta\left\{A_\beta A_1\dots A_{2n}\varrho_0\right\} = \hat{A}^\gamma_\beta\mathbb{T}_\zeta\{A_1\dots A_{2n}\varrho_0\} - \sum_{j=1}^{2n}\zeta^{j-1}\Sigma_{\beta,j}\mathbb{T}_\zeta\left\{A_1\dots A_{j-1}A_{j+1}\dots A_{2n}\varrho_0\right\}, \tag{6.42}$$

where

$$\Sigma_{\beta,j} := \begin{cases}\theta(z_j,w)[A_\beta,A_j]_\zeta & w\succ t_0,\\ -\theta(w,z_j)[A_\beta,A_j]_\zeta & w\prec t_0.\end{cases} \tag{6.43}$$

Here, $\theta(z,w)$ is a Heaviside step function on the contour, which equals 1 when $z\succ w$ and 0 otherwise.

Proof. We proceed as in Lemma 6.2. Suppose first that $w \succ t_0$: then, in Eq. (6.33) we can move A_β at the beginning of the string thanks to $A_{\sigma(i)}A_\beta = \zeta A_\beta A_{\sigma(i)} - \zeta[A_\beta, A_{\sigma(i)}]_\zeta$:

$$
\begin{aligned}
A_{\sigma(1)} \dots A_{\sigma(q)} A_\beta &= \zeta A_{\sigma(1)} \dots A_{\sigma(q-1)} A_\beta A_{\sigma(q)} - \zeta [A_\beta, A_{\sigma(q)}]_\zeta A_{\sigma(1)} \dots A_{\sigma(q-1)} \\
&= \zeta^q A_\beta A_{\sigma(1)} \dots A_{\sigma(q)} - \sum_{i=0}^{q-1} \zeta^{i+1} [A_\beta, A_{\sigma(q-i)}]_\zeta A_{\sigma(1)} \dots A_{\sigma(q-i-1)} A_{\sigma(q-i+1)} \dots A_{\sigma(q)}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\mathbb{T}_\zeta \left\{ A_\beta A_1 \dots A_{2n} \varrho_0 \right\} = \zeta^{N(\sigma)} \zeta^{2n-k} A_\beta A_{\sigma(1)} \dots A_{\sigma(k)} \varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(2n)} \\
&- \zeta^{N(\sigma)} \zeta^{2n-k+q} \sum_{i=0}^{q-1} \zeta^{i+1} [A_\beta, A_{\sigma(q-i)}]_\zeta A_{\sigma(1)} \dots A_{\sigma(q-i-1)} A_{\sigma(q-i+1)} \dots A_{\sigma(k)} \varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(2n)} \\
&= A_\beta \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \} - \sum_{i=0}^{q-1} [A_\beta, A_{\sigma(q-i)}]_\zeta \partial_{\sigma(q-i)} \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \}.
\end{aligned}
\tag{6.44}
$$

The sum can however be extended to all indices provided we remember to keep a non-zero contribution only from those indices that are later than w on the contour:

$$
\mathbb{T}_\zeta \left\{ A_\beta A_1 \dots A_{2n} \varrho_0 \right\} = A_\beta \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \} - \sum_{j=1}^{2n} \theta(z_j, w) [A_\beta, A_j]_\zeta \partial_j \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \}. \tag{6.45}
$$

The statement (6.42) is now a consequence of Lemma 6.3.

We can similarly treat the case where $w \prec t_0$. We start from Eq. (6.35) and we use the relation $A_\beta A_{\sigma(i)} = [A_\beta, A_{\sigma(i)}]_\zeta + \zeta A_{\sigma(i)} A_\beta$ to bring A_β at the end of the string:

$$
\begin{aligned}
A_\beta A_{\sigma(q+1)} \dots A_{\sigma(2n)} &= \zeta A_{\sigma(q+1)} A_\beta A_{\sigma(q+2)} \dots A_{\sigma(2n)} + [A_\beta, A_{\sigma(q+1)}]_\zeta A_{\sigma(q+2)} \dots A_{\sigma(2n)} \\
&= \zeta^{2n-q} A_{\sigma(q+1)} \dots A_{\sigma(2n)} A_\beta + \sum_{i=1}^{2n-q} \zeta^{i+1} [A_\beta, A_{\sigma(q+i)}]_\zeta A_{\sigma(q+1)} \dots A_{\sigma(q+i-1)} A_{\sigma(q+i+1)} \dots A_{\sigma(2n)}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\mathbb{T}_\zeta \left\{ A_\beta A_1 \dots A_{2n} \varrho_0 \right\} = \zeta^{N(\sigma)} \zeta^{2n-k+1} A_{\sigma(1)} \dots A_{\sigma(k)} \varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(2n)} A_\beta \\
&+ \zeta^{N(\sigma)} \zeta^{2n-k+q+1} \sum_{i=1}^{2n-q} \zeta^{i+1} [A_\beta, A_{\sigma(q+i)}]_\zeta A_{\sigma(1)} \dots A_{\sigma(k)} \varrho_0 A_{\sigma(k+1)} \dots A_{\sigma(q+i-1)} A_{\sigma(q+i+1)} \dots A_{\sigma(2n)} \\
&= \zeta \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \} A_\beta + \sum_{i=1}^{2n-q} [A_\beta, A_{\sigma(q+i)}]_\zeta \partial_{\sigma(q+i)} \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \}.
\end{aligned}
\tag{6.46}
$$

The sum can be extended to all indices provided we remember to keep a non-zero contribution only from those indices that are earlier than w on the contour:

$$
\mathbb{T}_\zeta \left\{ A_\beta A_1 \dots A_{2n} \varrho_0 \right\} = \zeta \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \} A_\beta + \sum_{j=1}^{2n} \theta(w, z_j) [A_\beta, A_j]_\zeta \partial_j \mathbb{T}_\zeta \{ A_1 \dots A_{2n} \varrho_0 \}, \tag{6.47}
$$

and the statement (6.42) is now a consequence of Lemma 6.3. □

If $[A_i, A_j]_\zeta$ is not a c-number, i.e., for non-Gaussian systems, the procedure described in the reduction lemma does not work and a more sophisticated approach is probably required: we leave the study of this highly non-trivial problem to future research effort.

6.2.4 Closing the differential equation

If we apply the reduction lemma 6.4 to Eq. (6.22), we obtain

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = 2n \sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}w \fint_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}' C_{1,2} \dots C_{2n-3,2n-2} C_{\alpha\beta}(t^+, w) \hat{A}^\delta_\alpha(t)$$
$$\times \left[\hat{A}^\gamma_\beta(w) \mathbb{T}_\zeta\{A_1 \dots A_{2n-2}\varrho_0\} - \sum_{j=1}^{2n-2} \zeta^{j-1} \Sigma_{\beta,j} \mathbb{T}_\zeta\big\{A_1 \dots A_{j-1}A_{j+1} \dots A_{2n-2}\varrho_0\big\} \right], \tag{6.48}$$

where the dependence of $\Sigma_{\beta,j}$ on w is understood. In the first term, we recognize the appearance of $M_{n-1}(t)$, as for the contour Redfield equation. For what concerns the second term, we can actually show that the sum over j is trivial to perform, since all terms of such sum are all equal to each other under the integral sign.

Lemma 6.5. *Consider the quantity*

$$F(j) := \zeta^{j-1} \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{1,2} \dots C_{2n-1,2n} \Sigma_{\beta,j} \mathbb{T}_\zeta\big\{A_1 \dots A_{j-1}A_{j+1} \dots A_{2n}\varrho_0\big\}. \tag{6.49}$$

Then, $F(j) = F(1)$ for all $j \in \{1, \dots, 2n\}$.

Proof. Suppose first that j is even, so that

$$\begin{aligned} F(j) &= \zeta \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{1,2} \dots C_{j-1,j} \dots C_{2n-1,2n} \Sigma_{\beta,j} \mathbb{T}_\zeta\big\{A_1 \dots A_{j-1}A_{j+1} \dots A_{2n}\varrho_0\big\} \\ &= \zeta \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{j,j-1} \dots C_{2,1} \dots C_{2n-1,2n} \Sigma_{\beta,1} \mathbb{T}_\zeta\big\{A_j A_{j-1} A_3 \dots A_{j-2} A_2 A_{j+1} \dots A_{2n}\varrho_0\big\}, \end{aligned} \tag{6.50}$$

where we performed the change of variables $1 \leftrightarrow j$ and $2 \leftrightarrow j-1$. Inside the ordering, we can now exchange A_{j-1} and A_2, and we can then move A_j back into position (i.e., to the immediate right of A_{j-1}) using $j-2$ transpositions. In total, since $j-1$ is odd, an additional ζ factor is produced. Moreover, using that $C_{j,j-1}C_{2,1} = C_{j-1,j}C_{1,2}$,

$$F(j) = \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{1,2} \dots C_{2n-1,2n} \Sigma_{\beta,1} \mathbb{T}_\zeta\{A_2 \dots A_{2n}\varrho_0\} = F(1). \tag{6.51}$$

We can proceed similarly in case j is odd. This time,

$$\begin{aligned} F(j) &= \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{1,2} \dots C_{j,j+1} \dots C_{2n-1,2n} \Sigma_{\beta,j} \mathbb{T}_\zeta\big\{A_1 \dots A_{j-1}A_{j+1} \dots A_{2n}\varrho_0\big\} \\ &= \fint_{\gamma(t)} \mathrm{d}^{2n}\mathbf{z}\, C_{j,j+1} \dots C_{1,2} \dots C_{2n-1,2n} \Sigma_{\beta,1} \mathbb{T}_\zeta\big\{A_j A_{j+1} A_3 \dots A_{j-1} A_2 A_{j+2} \dots A_{2n}\varrho_0\big\}, \end{aligned} \tag{6.52}$$

where we performed the change of variables $1 \leftrightarrow j$ and $2 \leftrightarrow j+1$. Now, exchange A_2 with A_{j+1} and bring back A_j into position with $j-2$ transpositions: since $j-1$ is now even, no additional ζ factor is produced and we straightforwardly obtain again $F(1)$. □

We conclude that

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = 2n\sum_{\alpha,\beta}\int_{\gamma(t)} \mathrm{d}w\, C_{\alpha\beta}(t^+,w)\hat{A}^{\delta}_{\alpha}(t)\hat{A}^{\gamma}_{\beta}(w)M_{n-1}(t) - 2n(2n-2)\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w \times \fint_{\gamma(t)} \mathrm{d}^{2n-2}\mathbf{w}'\, C_{1,2}\dots C_{2n-3,2n-2}\Sigma_{\beta,1}C_{\alpha\beta}(t^+,w)\hat{A}^{\delta}_{\alpha}(t)\mathbb{T}_{\zeta}\{A_2\dots A_{2n-2}\varrho_0\}. \tag{6.53}$$

The second term can be written in a more convenient way by regrouping indices and integration variables. Specifically, apart from the coefficient $-2n(2n-2)$,

$$\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w \fint_{\gamma(t)} \mathrm{d}^{2n-4}\mathbf{w}'\, C_{1,2}\dots C_{2n-5,2n-4}[C*\Sigma*C]_{\alpha\beta}(t^+,w)\hat{A}^{\delta}_{\alpha}(t)\mathbb{T}_{\zeta}\big\{A_\beta(w)A_1\dots A_{2n-4}\varrho_0\big\},$$

where we defined the double convolution

$$[C*\Sigma*C]\,(z,w) := \int_{\gamma(t)} \mathrm{d}^2\mathbf{y}\, C(z,y_1)\Sigma(y_1,y_2)C(y_2,w) \tag{6.54}$$

and matrix multiplication in interaction indices is understood. If we recall Eq. (6.22), we recognize $\mathrm{d}M_{n-1}(t)/\mathrm{d}t$, but where the coefficient $C_{\alpha\beta}(t^+,w)$ is replaced by $[C*\Sigma*C]_{\alpha\beta}(t^+,w)$. Let us then define a formal operation Ψ as follows:

$$\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w\, C_{\alpha\beta}(z,w)F_\beta(w) \overset{\Psi}{\mapsto} \sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w\,[C*\Sigma*C]_{\alpha\beta}(z,w)F_\beta(w), \tag{6.55}$$

for a generic (super)operator $F_\beta(w)$. We also extend Ψ by linearity to linear combinations of quantities of the form in Eq. (6.55), in the obvious way. Then,

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = 2n\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w\, C_{\alpha\beta}(t^+,w)\hat{A}^{\delta}_{\alpha}(t)\hat{A}^{\gamma}_{\beta}(w)M_{n-1}(t) - 2n\Psi\left[\frac{\mathrm{d}M_{n-1}(t)}{\mathrm{d}t}\right]. \tag{6.56}$$

Together with the boundary condition $\mathrm{d}M_0(t)/\mathrm{d}t = 0$, this constitutes a recursive definition of $\mathrm{d}M_n(t)/\mathrm{d}t$ in terms of $M_m(t)$ with $m < n$. This recursion can be solved explicitly, as the following lemma shows.

Lemma 6.6. *The recursion* (6.56) *is solved by*

$$\frac{\mathrm{d}M_n(t)}{\mathrm{d}t} = \sum_{k=1}^{n}\frac{(-1)^k(2n)!!}{(2n-2k)!!}\hat{\mathcal{L}}_k(t)M_{n-k}(t), \tag{6.57}$$

where $\hat{\mathcal{L}}_1(t) = \hat{\mathcal{R}}(t)$*, the contour Redfield generator in Eq.* (6.26)*, and* $\hat{\mathcal{L}}_{k+1} = \Psi[\hat{\mathcal{L}}_k]$.

Proof. We proceed by induction on n. The base case for $n = 0$ is obviously true; suppose then that the result holds for $n-1$. The recursion (6.56) and the induction hypothesis yield

$$\frac{\mathrm{d}M_n}{\mathrm{d}t} = -2n\hat{\mathcal{L}}_1M_{n-1} - 2n\sum_{k=1}^{n-1}\frac{(-1)^k(2n-2)!!}{(2n-2-2k)!!}\Psi\big[\hat{\mathcal{L}}_kM_{n-1-k}\big]. \tag{6.58}$$

It is clear that $\Psi[\hat{\mathcal{L}}_k M_{n-1-k}] = \Psi[\hat{\mathcal{L}}_k]M_{n-1-k} = \hat{\mathcal{L}}_{k+1}M_{n-1-k}$. After performing the change of variable $k \mapsto k+1$,

$$\frac{\mathrm{d}M_n}{\mathrm{d}t} = -2n\hat{\mathcal{L}}_1 M_{n-1} - 2n\sum_{k=2}^{n}\frac{(-1)^{k-1}(2n-2)!!}{(2n-2k)!!}\hat{\mathcal{L}}_k M_{n-k} = \sum_{k=1}^{n}\frac{(-1)^k(2n)!!}{(2n-2k)!!}\hat{\mathcal{L}}_k M_{n-k}, \quad (6.59)$$

which is what we wanted to prove. □

Eq. (6.57) leads almost immediately to the master equation we are looking for. In fact, using Eq. (6.12) and the fact that $(2n)!! = 2^n n!$,

$$\frac{\mathrm{d}\varrho}{\mathrm{d}t} = \sum_{n=1}^{\infty}\frac{(-1)^n}{n!2^n}\frac{\mathrm{d}M_n}{\mathrm{d}t} = \sum_{n=1}^{\infty}\sum_{k=1}^{n}\frac{(-1)^{n-k}}{(n-k)!2^{n-k}}\hat{\mathcal{L}}_k M_{n-k} = \sum_{k=1}^{\infty}\hat{\mathcal{L}}_k\varrho \equiv \hat{\mathcal{L}}\varrho, \quad (6.60)$$

where in the third equality we recognized the definition of Cauchy product of two series.

Let us make a few comments on the structure of this master equation. The term $\hat{\mathcal{L}}_1(t)$ is identical to the generator of the contour Redfield equation (6.26) and is of second order in the coupling, $\hat{\mathcal{L}}_1(t) = \mathcal{O}(\lambda^2)$. According to Eq. (6.55), each subsequent application of Ψ introduces another C: as a consequence, $\hat{\mathcal{L}}_k(t) = \mathcal{O}(\lambda^{2k})$. Therefore, we understand that the contour Redfield equation is recovered from Eq. (6.60) by truncating the series at the lowest order in λ. The fact that there is such a well-defined and clean way to recover the Redfield equation in the weak-coupling limit from an exact master equation is arguably not shared by previously known master equations.

Let us also note that

$$\hat{\mathcal{L}}_k(t) = -\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w\, \mathcal{G}^{(k)}_{\alpha\beta}(t^+, w)\hat{A}^{\delta}_{\alpha}(t)\hat{A}^{\gamma}_{\beta}(w), \quad (6.61)$$

where

$$\mathcal{G}^{(1)} = C, \qquad \mathcal{G}^{(k+1)} = \mathcal{G}^{(k)} * \Sigma * C. \quad (6.62)$$

If we sum over k,

$$\hat{\mathcal{L}}(t) = -\sum_{\alpha,\beta}\int_{\gamma(t)}\mathrm{d}w\, \mathcal{G}_{\alpha\beta}(t^+, w)\hat{A}^{\delta}_{\alpha}(t)\hat{A}^{\gamma}_{\beta}(w), \quad (6.63)$$

with $\mathcal{G} = \sum_{k=1}^{\infty}\mathcal{G}^{(k)}$. This is the most general form of the GME's generator, which is remarkably equivalent to the Redfield one (6.26) upon making the substitution $C \mapsto \mathcal{G}$. By summing over k in the recursive definition of $\mathcal{G}^{(k)}$, we realize that $\mathcal{G}$ can also be implicitly defined through the equation

$$\mathcal{G} = C + \mathcal{G} * \Sigma * C, \quad (6.64)$$

as we anticipated in Sec. 6.1.3. The structure of Eq. (6.64) is well-known in physics: it is called *Dyson equation* and appears in many contexts. In particular, in nonequilibrium Green's function theory it is the equation that arises when a non-interacting Green's function C is "dressed" by an interaction mediated by a *self-energy* Σ [45]. In our context, C is the function that is needed to describe the dynamics when $[A_i, A_j]_\zeta = 0$—i.e., when the Redfield equation is exact. Instead, $\mathcal{G}$ describes the "dressing" of C due to a non-trivial (anti)commutator $[A_i, A_j]_\zeta$—an information that is contained in Σ. It is also worth emphasizing that powerful numerical approaches exist to efficiently tackle Eq. (6.64), even in the most challenging settings [161, 162].

A well-known result in nonequilibrium Green's function theory is that Dyson equations similar to (6.64) can also be formulated for systems featuring non-quadratic inter-particle interactions [45]. The key difference is that the self-energy Σ becomes dependent on C, which makes the Dyson equation non-linear. This complexity is then typically managed using diagrammatic perturbation schemes. It is natural to consider whether our framework could be extended to non-Gaussian systems by employing similar techniques; however, we defer this possibility to future work.

6.3 Unraveling the contour

The generator $\hat{\mathcal{L}}(t)$ of the GME is written in terms of an integral over the contour $\gamma(t)$. To solve the master equation in practice, it is essential to "unravel" the contour into its branches and express everything in terms of real physical times (or imaginary times when considering the initial preparation). In Sec. 6.3.1 below, we show that by unraveling the contour in Eq. (6.63), we obtain the same shape as the generalized Redfield equation (6.30) after replacing the correlation function $c_{\alpha\beta}(t,s)$ with the appropriate components of $\mathcal{G}$. In Sec. 6.3.2 we proceed by unraveling the Dyson equation (6.64) too, showing how it can be approached from a numerical standpoint.

6.3.1 From contour to physical time

As we did in Sec. 6.2.2, let us start by decomposing the contour $\gamma(t)$ into its branches:

$$\hat{\mathcal{L}}(t)\varrho = -\sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}s\, \Big\{\mathcal{G}_{\alpha\beta}(t^+,s^-)[A_\alpha(t), A_\beta(s)\varrho] - \mathcal{G}_{\alpha\beta}(t^+,s^+)[A_\alpha(t),\zeta\varrho A_\beta(s)]\Big\} \tag{6.65}$$

$$+\, i\sum_{\alpha,\beta}\int_{0}^{b} \mathrm{d}\tau\, \Big\{\mathcal{G}_{\alpha\beta}(t^+,t_0-i\tau)[A_\alpha(t), A_\beta(t_0-i\tau)\varrho] + \mathcal{G}_{\alpha\beta}(t^+,t_0+i\tau)[A_\alpha(t),\zeta\varrho A_\beta(t_0+i\tau)]\Big\}.$$

Now, we need some properties that $\mathcal{G}$ inherits from C thanks to Theorem 4.4. Recall the conjugation operation $\check{}$ that was defined in Sec. 4.2.4.

Theorem 6.7. *The contour function $\mathcal{G}_{\alpha\beta}(z,w)$ satisfies the following properties:*

- *Conjugation symmetry: $\check{\mathcal{G}} = \mathcal{G}$.*
- *Cycle symmetry: $\mathcal{G}_{\alpha\beta}(s^+,w) = \mathcal{G}_{\alpha\beta}(s^-,w)$ when $s^+ \prec w \prec s^-$.*

Proof. It is sufficient to prove that the above properties are satisfied by $\mathcal{G}^{(k)}$ for every k. We can do that by induction on k. Since $\mathcal{G}^{(1)} = C$, the base case is guaranteed by Theorem 4.4. For the inductive step, the cycle symmetry can be immediately verified. To prove the conjugation symmetry, we first show that a similar property is obeyed by the self-energy. Assume first that $z \succ t_0$ and write

$$\begin{aligned}\Sigma^*_{\alpha\beta}(z,w) &= \theta(w,z)[A_\alpha(z), A_\beta(w)]^*_\zeta = -\zeta\theta(w,z)[A_{\overline{\alpha}}(z^*), A_{\overline{\beta}}(w^*)]_\zeta \\ &= -\zeta\theta(z^*,w^*)[A_{\overline{\alpha}}(z^*), A_{\overline{\beta}}(w^*)]_\zeta = \zeta\Sigma_{\overline{\alpha}\overline{\beta}}(z^*,w^*).\end{aligned} \tag{6.66}$$

A similar calculation can be carried out in case $z \prec t_0$. Therefore,

$$\begin{aligned}\left[\mathcal{G}^{(k)}_{\alpha\beta}(z,w)\right]^* &= \zeta\sum_{\mu,\sigma}\int_{\gamma(t)} \mathrm{d}^2\mathbf{y}\,\mathcal{G}^{(k-1)}_{\overline{\alpha\mu}}(z^*,y_1^*)\Sigma_{\overline{\mu\sigma}}(y_1^*,y_2^*)C_{\overline{\sigma\beta}}(y_2^*,w^*)\\ &= \zeta\sum_{\mu,\sigma}\int_{\gamma(t)} \mathrm{d}^2\mathbf{y}\,\mathcal{G}^{(k-1)}_{\overline{\alpha}\mu}(z^*,y_1)\Sigma_{\mu\sigma}(y_1,y_2)C_{\sigma\overline{\beta}}(y_2,w^*) = \zeta\mathcal{G}^{(k)}_{\overline{\alpha\beta}}(z^*,w^*),\end{aligned} \tag{6.67}$$

where in the second equality we made some harmless changes of variables. □

Thanks to Theorem 6.7, and the fact that $s \le t$ in Eq. (6.65), we can write

$$\mathcal{G}_{\alpha\beta}(t^+,s^+) = \zeta\mathcal{G}^*_{\overline{\alpha\beta}}(t^-,s^-) = \zeta\mathcal{G}^*_{\overline{\alpha\beta}}(t^+,s^-), \tag{6.68a}$$

$$\mathcal{G}_{\alpha\beta}(t^+,t_0+i\tau) = \zeta\mathcal{G}^*_{\overline{\alpha\beta}}(t^-,t_0-i\tau) = \zeta\mathcal{G}_{\alpha\beta}(t^+,t_0-i\tau). \tag{6.68b}$$

This allows us to arrive at the final shape of the GME:

$$\begin{aligned}\hat{\mathcal{L}}(t)\varrho = &-\sum_{\alpha,\beta}\int_{t_0}^{t}\mathrm{d}s\,\mathcal{G}^{>}_{\alpha\beta}(t,s)[A_\alpha(t),A_\beta(s)\varrho]\\ &+ i\sum_{\alpha,\beta}\int_0^b \mathrm{d}\tau\,\mathcal{G}^{\rceil-}_{\alpha\beta}(t,\tau)[A_\alpha(t),A_\beta(t_0-i\tau)\varrho] + \text{H.c.},\end{aligned} \tag{6.69}$$

where we used the component notation developed in Sec. 4.2.4. This is equivalent to the Redfield equation (6.30) if we perform $c_{\alpha\beta}(t,s) \mapsto \mathcal{G}^{>}_{\alpha\beta}(t,s)$ and $c_{\alpha\beta}(t,t_0-i\tau) \mapsto \mathcal{G}^{\rceil-}_{\alpha\beta}(t,\tau)$. Note that only two components of $\mathcal{G}$ are needed to determine the master equation.

6.3.2 Components of the Dyson equation

The unraveled GME (6.69) is fully determined once we specify how the Dyson equation (6.64) must be solved to find $\mathcal{G}^{>}$ and $\mathcal{G}^{\rceil-}$. To do that, we must unravel the double convolution on the contour, so that we can express the Dyson equation in its physical components. In nonequilibrium Green's function theory, the well-known *Langreth rules* are routinely used to perform such decompositions [45]. However, due to the differences between our contour and the standard Schwinger-Keldysh contour, we prefer to develop our own translation scheme.

Before approaching Eq. (6.64), let us study the components of $\Sigma(z,w)$, defined in Eq. (6.43). Because of the presence of the θ function, the majority of its components actually nullify. Specifically, in case $z \succ t_0$, we must have $w \succ z$, while if $z \prec t_0$ we must have $w \prec z$. As a consequence, one easily verifies that

$$\Sigma^{>} = \Sigma^{<} = \Sigma^{M>} = \Sigma^{M<} = \Sigma^{\lfloor+} = \Sigma^{\lceil-} = \Sigma^{\rceil\pm} = \Sigma^{\rfloor\pm} = 0. \tag{6.70}$$

This means that we can just focus on three independent components Σ^{T}, Σ^{MT}, and $\Sigma^{\lfloor-}$. The remaining components can be found thanks to the conjugation symmetry $\check{\Sigma} = \Sigma$ proved in Theorem 6.7:

$$\Sigma^{\widetilde{T}} = \check{\Sigma}^{T}, \qquad \Sigma^{M\widetilde{T}} = \check{\Sigma}^{MT}, \qquad \Sigma^{\lceil+} = \check{\Sigma}^{\lfloor-}. \tag{6.71}$$

Let us now consider the Dyson equation (6.64). For ease of discussion, we first decompose the double convolution onto the various contour branches:

$$\mathcal{G} * \Sigma * C \equiv \mathcal{D}_{KK} + \mathcal{D}_{MM} + \mathcal{D}_{MK}, \tag{6.72}$$

where $\mathcal{D}_{KK}$ contains the contribution from just the horizontal branches, $\mathcal{D}_{MM}$ concerns just the Matsubara track, and $\mathcal{D}_{MK}$ contains the mixed contributions. Now, we decompose each term by keeping in mind the enormous simplifications introduced by Eq. (6.70), and the fact that we only need the $^{>}$ and $^{\rceil-}$ components of $\mathcal{G}$.

Let us start with $\mathcal{D}_{KK}$:

$$\mathcal{D}^{>}_{KK} = \mathcal{G}^{>} \cdot \Sigma^{T} \cdot C^{T} + \mathcal{G}^{\widetilde{T}} \cdot \Sigma^{\widetilde{T}} \cdot C^{>}, \tag{6.73a}$$

$$\mathcal{D}^{\rceil-}_{KK} = \mathcal{G}^{>} \cdot \Sigma^{T} \cdot C^{\rfloor-} + \mathcal{G}^{\widetilde{T}} \cdot \Sigma^{\widetilde{T}} \cdot C^{\rceil-}, \tag{6.73b}$$

where the convolution symbol $\cdot$ for components is

$$(f \cdot g)(t_1, t_2) := \int_{t_0}^{t} \mathrm{d}s\, f(t_1, s) g(s, t_2). \tag{6.74}$$

We see the appearance of the additional component $\mathcal{G}^{\widetilde{T}}$. However, because of cycle symmetry,

$$\mathcal{G}^{\widetilde{T}}_{\alpha\beta}(t,s) = \mathcal{G}_{\alpha\beta}(t^+, s^+) = \check{\mathcal{G}}_{\alpha\beta}(t^+, s^+) = \zeta \mathcal{G}^{*}_{\overline{\alpha}\overline{\beta}}(t^-, s^-) = \zeta \mathcal{G}^{*}_{\overline{\alpha}\overline{\beta}}(t^+, s^-) = \check{\mathcal{G}}^{>}_{\alpha\beta}(t,s). \tag{6.75}$$

For the purpose of decomposing the Dyson equation, we can then just make the identification $\mathcal{G}^{\widetilde{T}} \equiv \check{\mathcal{G}}^{>}$. The cycle symmetry applied to C also allows us to write $C^{\rfloor-} = C^{\rceil-}$. Therefore,

$$\mathcal{D}^{>}_{KK} = \mathcal{G}^{>} \cdot \Sigma^{T} \cdot C^{T} + \check{\mathcal{G}}^{>} \cdot \check{\Sigma}^{T} \cdot C^{>}, \tag{6.76a}$$

$$\mathcal{D}^{\rceil-}_{KK} = \mathcal{G}^{>} \cdot \Sigma^{T} \cdot C^{\rceil-} + \check{\mathcal{G}}^{>} \cdot \check{\Sigma}^{T} \cdot C^{\rceil-}. \tag{6.76b}$$

We can proceed similarly with $\mathcal{D}_{MM}$, finding at first

$$\mathcal{D}^{>}_{MM} = \mathcal{G}^{\rceil-} \star \Sigma^{MT} \star C^{\lfloor-} + \mathcal{G}^{\rceil+} \star \Sigma^{M\widetilde{T}} \star C^{\lfloor+}, \tag{6.77a}$$

$$\mathcal{D}^{\rceil-}_{MM} = \mathcal{G}^{\rceil-} \star \Sigma^{MT} \star C^{MT} + \mathcal{G}^{\rceil+} \star \Sigma^{M\widetilde{T}} \star C^{M>}, \tag{6.77b}$$

where

$$(f \star g)(t_1, t_2) := -i \int_{0}^{\beta/2} \mathrm{d}\tau\, f(t_1, \tau) g(\tau, t_2). \tag{6.78}$$

The cycle symmetry of $\mathcal{G}$ allows us to make the identification $\mathcal{G}^{\rceil+} = \check{\mathcal{G}}^{\rceil-}$. Moreover, cycle symmetry of C together with conjugation symmetry yields $C^{\lfloor+} = C^{\lceil+} = \check{C}^{\lfloor-}$, so that

$$\mathcal{D}^{>}_{MM} = \mathcal{G}^{\rceil-} \star \Sigma^{MT} \star C^{\lfloor-} + \check{\mathcal{G}}^{\rceil-} \star \check{\Sigma}^{MT} \star \check{C}^{\lfloor-}, \tag{6.79a}$$

$$\mathcal{D}^{\rceil-}_{MM} = \mathcal{G}^{\rceil-} \star \Sigma^{MT} \star C^{MT} + \check{\mathcal{G}}^{\rceil-} \star \check{\Sigma}^{MT} \star C^{M>}. \tag{6.79b}$$

Finally, for what concerns $\mathcal{D}_{MK}$, one finds

$$\mathcal{D}^{>}_{MK} = \mathcal{G}^{\rceil-} \star \Sigma^{\lfloor-} \cdot C^{T} - \check{\mathcal{G}}^{\rceil-} \star \check{\Sigma}^{\lfloor-} \cdot C^{>}, \tag{6.80a}$$

$$\mathcal{D}^{\rceil-}_{MK} = \mathcal{G}^{\rceil-} \star \Sigma^{\lfloor-} \cdot C^{\rceil-} - \check{\mathcal{G}}^{\rceil-} \star \check{\Sigma}^{\lfloor-} \cdot C^{\rceil-}. \tag{6.80b}$$

Gathering Eqs. (6.76), (6.79), and (6.80), and putting them back into Eq. (6.72), we arrive at the following final result. The contour Dyson equation for $\mathcal{G}$ decomposes into two coupled physical-time Dyson equations for $\mathcal{G}^>$ and $\mathcal{G}^{\rceil-}$, given by

$$\begin{aligned}\mathcal{G}^> &= C^> + \mathcal{G}^> \cdot \Sigma^T \cdot C^T + \check{\mathcal{G}}^> \cdot \check{\Sigma}^T \cdot C^> \\ &\quad + \mathcal{G}^{\rceil-} \star \left(\Sigma^{MT} \star C^{\lfloor-} + \Sigma^{\lfloor-} \cdot C^T\right) + \check{\mathcal{G}}^{\rceil-} \star \left(\check{\Sigma}^{MT} \star \check{C}^{\lfloor-} - \check{\Sigma}^{\lfloor-} \cdot C^>\right), \end{aligned} \tag{6.81a}$$

$$\begin{aligned}\mathcal{G}^{\rceil-} &= C^{\rceil-} + \mathcal{G}^> \cdot \Sigma^T \cdot C^{\rceil-} + \check{\mathcal{G}}^> \cdot \check{\Sigma}^T \cdot C^{\rceil-} \\ &\quad + \mathcal{G}^{\rceil-} \star \left(\Sigma^{MT} \star C^{MT} + \Sigma^{\lfloor-} \cdot C^{\rceil-}\right) + \check{\mathcal{G}}^{\rceil-} \star \left(\check{\Sigma}^{MT} \star C^{M>} - \check{\Sigma}^{\lfloor-} \cdot C^{\rceil-}\right). \end{aligned} \tag{6.81b}$$

While these equations may appear complex at first, they can be straightforwardly approached from a numerical standpoint with an iterative procedure, once the components of C and Σ are established.

In the special case when there is no initial system-environment correlation, Eqs. (6.81) greatly simplify. In fact, if we ignore all components related to the Matsubara track, all we need is $\mathcal{G}^>$, for which we end up with the relatively simple formula

$$\mathcal{G}^> = C^> + \mathcal{G}^> \cdot \Sigma^T \cdot C^T + \check{\mathcal{G}}^> \cdot \check{\Sigma}^T \cdot C^>. \tag{6.82}$$

6.3.3 A simple example

We now discuss a simple example that cannot be addressed using the previously known exact master equations discussed in Sec. 6.1, but that is well within the scope of the GME. The purpose here is to showcase the simplicity with which the GME can be approached from a numerical point of view: more physically relevant applications will surely be the subject of future research effort.

Consider as a system the following two-mode fermionic Hamiltonian:

$$H_S = \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 + \delta\left(a_1^\dagger a_2^\dagger - a_1 a_2\right). \tag{6.83}$$

We couple both modes to a fermionic reservoir through standard tunneling:

$$H_E = \sum_p \varepsilon_p c_p^\dagger c_p, \qquad V = \sum_p g_p c_p \left(a_1^\dagger + a_2^\dagger\right) + \text{H.c.} \tag{6.84}$$

In order to keep things simple, we assume Lorentzian spectral density, zero temperature, large negative chemical potential[5], and initial decoupling from the system, so that the environment correlation function can be taken as the one we already employed back in Chap. 3:

$$c(t) = \frac{\gamma\lambda}{2} e^{-\lambda|t|}, \qquad \gamma, \lambda > 0. \tag{6.85}$$

Because of the fermionic statistics, this setup cannot be treated using the Ferialdi's master equation (6.7). Additionally, because of the pairing term δ, the system violates the conservation of the number of excitations, meaning that it cannot be treated either with the master

[5] Linear coupling to a Gaussian thermal fermionic bath as in Eq. (6.84) gives rise to the two correlation functions $c^+(t) = \int_{-\infty}^{\infty} \mathrm{d}\omega\, J(\omega) f(\omega) e^{i\omega t}$ and $c^-(t) = \int_{-\infty}^{\infty} \mathrm{d}\omega\, J(\omega)[1 - f(\omega)] e^{-i\omega t}$, where $J(\omega)$ is the spectral density and $f(\omega) := [1 + e^{(\omega-\mu)/T}]^{-1}$ is the Fermi-Dirac distribution function (see, e.g., Ref. [113]). Assuming zero temperature and large negative chemical potential translates in the simplification $f(\omega) \simeq 0$ for the purpose of calculating $c^\pm(t)$, which then become $c^+(t) \simeq 0$ and $c^-(t) \simeq \int_{-\infty}^{\infty} \mathrm{d}\omega\, J(\omega) e^{-i\omega t}$. The latter coincides with Eq. (6.85) if we take as $J(\omega)$ the Lorentzian function $J(\omega) = \frac{\gamma\lambda}{2\pi} \frac{\lambda}{\omega^2 + \lambda^2}$.

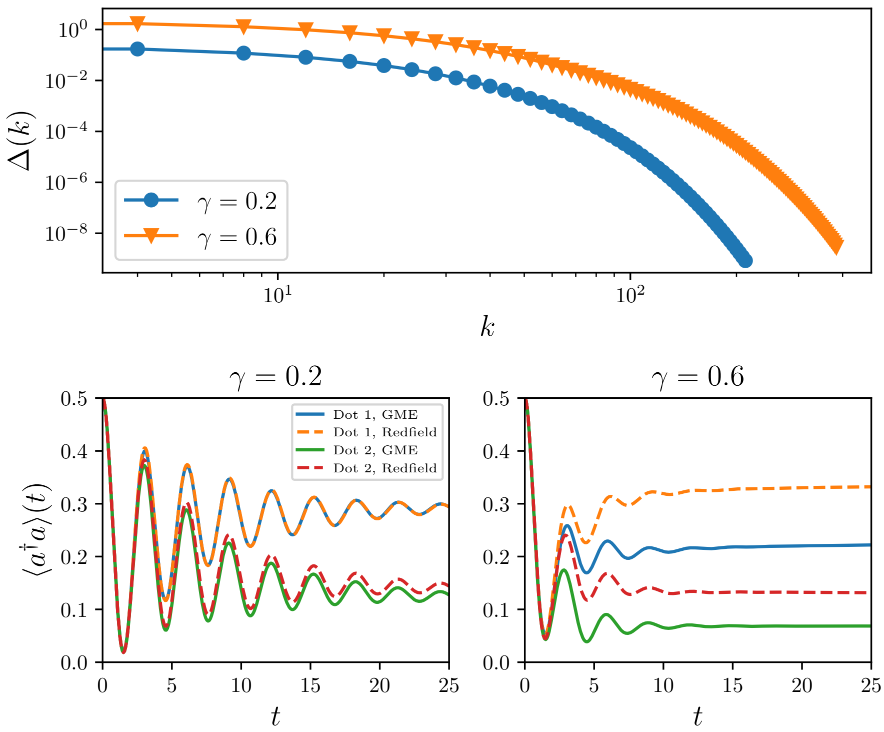

Figure 6.1: (Top) Correction to the solution of the Dyson equation at kth order, meaning $\Delta(k) := \max \|\mathcal{G}^{(k+1)}\|$, maximized over the time grid, for two different values of the coupling γ. (Bottom) Evolution of the dots' populations, with $\epsilon_1 = 0.5$, $\epsilon_2 = 1$, $\delta = 0.7$, and $\lambda = 1.5$. The Dyson equation is solved up to the higher order shown in the top plot.

equation (6.3) obtained from the influence functional. Instead, the GME does not have any problem in treating this scenario. From a physical standpoint, note that H_S can be used as a toy model for two quantum dots coupled to a p-wave superconductor, which induces the pairing δ by proximity effect [154]. With appropriate extensions, this example could serve as a starting point for studying, e.g., the exact dynamics of a p-wave Cooper pair splitter [163, 164].

We approach the problem numerically using the following steps. First, we solve the unraveled Dyson equation (6.82) iteratively on a discrete time grid, obtaining $\mathcal{G}$ up to a certain order in the coupling. As shown in Fig. 6.1, we find that the convergence rate depends on γ: the stronger the coupling the higher the order one should stop at to achieve a fixed target accuracy.

After that, we are able to solve the GME with a standard Runge-Kutta integrator, similarly to what we did in Chap. 3 for the Redfield equation and its regularizations. In Fig. 6.1 we report the resulting evolution of the dots' populations $\langle a_i^\dagger a_i \rangle(t)$ after having initialized the system in the pure state $(|00\rangle + |11\rangle)/\sqrt{2}$, for two different values of γ. The competition between dissipation and pairing causes damped oscillations that eventually settle on a steady-state value. We also plot the results predicted by the time-dependent Redfield equation: as expected, relevant deviations from the GME are found at strong coupling.

6.4 Lyapunov equation for the covariance matrix

As we extensively argued in the previous pages, the GME is able to completely capture the exact dynamics of an open Gaussian systems. Since the overall universe Hamiltonian is quadratic, if the universe starts out in a Gaussian state, the Gaussianity property must be preserved by the evolution (see Appendix A). Similarly, in case $\varrho(t_0)$ is a Gaussian state, we expect the solution of the GME, $\varrho(t)$, to remain a Gaussian state for all times $t \geq t_0$. In this section, we prove that this is indeed the case and we formulate the GME as an evolution equation for the covariance matrix of the system.

The first step is to write the *adjoint* GME, which describes the evolution of observables in Heisenberg picture, rather than density operators in Schrödinger picture. If $\dot{\varrho}(t) = \hat{\mathcal{L}}(t)\varrho(t)$, then for observables we have $\dot{X}(t) = \hat{\mathcal{L}}^\dagger(t)X(t)$, where the adjoint generator $\hat{\mathcal{L}}^\dagger(t)$ is defined by relation [6]

$$\mathrm{Tr}\big[X(t)\hat{\mathcal{L}}(t)\varrho(t)\big] = \mathrm{Tr}\big[\varrho(t)\hat{\mathcal{L}}^\dagger(t)X(t)\big]. \tag{6.86}$$

A simple computation reveals that if $\hat{\mathcal{L}}(t)$ is the GME generator (6.69), then

$$\begin{aligned}\hat{\mathcal{L}}^\dagger(t)X = &-\sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}s\, \mathcal{G}^{>}_{\alpha\beta}(t,s)[X, A_\alpha(t)]A_\beta(s) \\ &+ i\sum_{\alpha,\beta}\int_0^b \mathrm{d}\tau\, \mathcal{G}^{\rceil -}_{\alpha\beta}(t,\tau)[X, A_\alpha(t)]A_\beta(t_0 - i\tau) + \mathrm{H.c.}\end{aligned} \tag{6.87}$$

The Gaussian system assumption ensures the existence of a linear relationship

$$A_\alpha(z) = \sum_j \mathbb{A}_{\alpha j}(z) r_j \tag{6.88}$$

for appropriate coefficients $\mathbb{A}_{\alpha j}(z) \in \mathbb{C}$, where $\mathbf{r}$ is the Darboux-Majorana vector defined back in Sec. 4.2.1. Thanks to this,

$$\hat{\mathcal{L}}(t)X = \sum_{i,j} M_{ij}(t)[X, r_i]r_j + \mathrm{H.c.}, \tag{6.89}$$

where

$$M(t) := -\int_{t_0}^{t} \mathrm{d}s\, \mathbb{A}^T(t)\mathcal{G}^{>}(t,s)\mathbb{A}(s) + i\int_0^b \mathrm{d}\tau\, \mathbb{A}^T(t)\mathcal{G}^{\rceil -}(t,\tau)\mathbb{A}(t_0 - i\tau). \tag{6.90}$$

We are now interested in the case where X represents the covariance matrix of the system. We refer to Appendix A for a more detailed discussion about covariance matrices for Gaussian systems; here we will only briefly provide the most common definition, which is [40, 41, 165]

$$\Gamma_{ij} := \mathrm{Tr}\big[(r_i r_j + \zeta r_j r_i)\varrho\big] = 2\,\mathrm{Tr}\big[r_i r_j \varrho\big] - \Omega_{ij}, \qquad \Gamma^T = \Gamma^* = \zeta\Gamma. \tag{6.91}$$

In the bosonic case ($\zeta = 1$) this is a real, symmetric, positive definite matrix with eigenvalues in the interval $[1, \infty)$. Instead, in the fermionic case ($\zeta = -1$) this is a pure imaginary, skew-symmetric matrix with eigenvalues in the interval $[-1, 1]$.

Let us now specialize Eq. (6.89) to $X \mapsto \hat{\Gamma}_{kq} := 2r_k r_q - \Omega_{kq}\mathbb{1}$, so that $\Gamma_{kq} = \mathrm{Tr}\,[\hat{\Gamma}_{kq}\varrho]$. After a long but straightforward calculation, one arrives at

$$\frac{\mathrm{d}\hat{\Gamma}_{kq}}{\mathrm{d}t} = \sum_{i,j} M_{ij}(t)\Big(\Omega_{qi}\hat{\Gamma}_{kj} + \zeta\Omega_{ki}\hat{\Gamma}_{qj} + \Omega_{qi}\Omega_{kj}\mathbb{1} + \zeta\Omega_{ki}\Omega_{qj}\mathbb{1}\Big) + \mathrm{H.c.} \tag{6.92}$$

Once we take the expectation value, this turns into a matrix differential equation:

$$\begin{aligned}\frac{\mathrm{d}\Gamma}{\mathrm{d}t} &= \Gamma(\Omega M)^T + \zeta(\Omega M)\Gamma^T + \Omega M^T\Omega^T + \zeta\Omega M\Omega^T + \mathrm{H.c.}\\ &= \Gamma(\Omega M)^T + (\Omega M)\Gamma - \Omega(M + \zeta M^T)\Omega + \mathrm{H.c.}\\ &= 2\,\mathrm{Re}[\Omega M]\Gamma + 2\Gamma\,\mathrm{Re}[\Omega M]^T - \Omega(M + \zeta M^T + M^\dagger + \zeta M^*)\Omega.\end{aligned} \tag{6.93}$$

We arrived at the following *continuous Lyapunov differential equation*:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}t} = X\Gamma + \Gamma X^T + Y, \tag{6.94a}$$

$$X := 2\,\mathrm{Re}[\Omega M], \qquad Y := -\Omega(M + \zeta M^T + M^\dagger + \zeta M^*)\Omega. \tag{6.94b}$$

This type of equation has been extensively studied in the mathematical literature, and its associated stability analysis and solution algorithms are well known [166]. In the context of open quantum systems, the occurrence of the Lyapunov equation has been discussed in Refs. [165, 167, 168]. Here we just point out that Eq. (6.94) proves the claim made at the beginning of the section: if the system starts in a Gaussian state, it remains Gaussian at all subsequent times, with its covariance matrix determined by Eq. (6.94). Note also that a differential equation for the covariance matrix is characterized by a complexity that scales linearly with the dimension of the system, unlike any differential equation for the density operator, which exhibits exponential scaling.

Chapter 7

Conclusions

As we argued in the Introduction, microscopic derivations of master equations occupy a central role in the theory of open quantum systems, as they provide the main route towards the exploration of the effects originated by the system-environment coupling. This research area is characterized by many technical, unsolved questions. In this thesis, we illustrated some steps forward we were able to make in this context, in the weak- as well as strong-coupling regimes. Let us now draw our conclusions by summarizing key findings, weak points, and possible next steps.

- Chapter 3: **Regularization Techniques**
  We proposed two new state-of-the-art numerical techniques to regularize master equations that violate positivity. These proposals were shown to outperform existing methods in mimicking the exact dynamics and can be applied beyond the standard setting of the Redfield equation.
  - The main limitation of both methods lies in computational complexity, which limits their application to many-body systems. Inspired by the vast literature on quantum tomography [94], it could be possible to devise some optimization that eases the burden of computing projections in high-dimensional spaces.
  - Unfortunately, the projection idea—which is central for both techniques—has not been clearly linked to some physical argument. It is still an open problem to understand the implications of the regularization, e.g., on the thermodynamics of the system and the steady-state manifold structure.

- Chapter 4: **Contour Formulation**
  We established a fruitful link between the theory of open quantum systems, as formulated with density operators and master equations, and the Schwinger-Keldysh contour employed in many-body physics. In doing that, we avoided the typical complexities of field theories while still providing a compact and useful framework to discuss quantum dynamics.
  - Given the generality of the contour construction, it is worth exploring how to extend the contour formulation to other scenarios, such as non-Hermitian physics [116], counting statistics for quantum thermodynamics [124], multi-time correlation functions [126], process tensors [68], and entropic quantities through the replica method [127].

- Chapter 5: **Non-Markovian Stochastic Dynamics**
  We employed the contour formalism to unify stochastic approaches for the description of systems coupled to Gaussian environments. Specifically, we provided a common intersection point between them in the form of a stochastic decoupling with single contour noise.
  - Again, given the generality of the contour formulation, it is worth exploring how to formulate non-Markovian stochastic equations in different contexts. Can we use it to perform counting statistics? Can we formulate a stochastic theory for fermionic variables?
  - We showed how the double-noise structure of typical non-Markovian stochastic equations derives from a Keldysh rotation applied to a single contour noise: is it plausible that such insight can lead to advantages during numerical simulations? We also showed how one of the noises can be "eliminated" from the solution, at least in certain cases: is it possible to come up with an alternative stochastic master equation that reflects this property?
  - Another fundamental question is: can we provide a continuous measurement interpretation for non-Markovian stochastic equations [136]? Does our one-shot interpretation give some insight in this direction? Are semiclassical conditions necessary or not?
- Chapter 6: **The Gaussian Master Equation**
  We microscopically derived the exact master equation that describes the dynamics of all Gaussian systems linearly coupled to Gaussian environments, the GME. Thanks to the contour formulation, the result is compact and intuitive: the Redfield kernel is dressed by a system self-energy, yielding the well-known structure of a Dyson equation. This is in contrast with previous more limited and complicated approaches.
  - It is worth dedicating serious resources to the creation of optimized code to numerically solve the GME in practice. Preliminary tests hint that the task is approachable, and that there is strong potential for the discovery of possibly new non-Markovian effects in Gaussian systems.
  - Of course the GME is not directly suitable to mixed statistics, like the spin-boson model [8, 160], or non-linear interactions. Nevertheless, the appearance of a Dyson equation suggests the possibility of performing perturbation theory in terms of more sophisticated self-energy terms: see, e.g., the recursive techniques of Refs. [169, 170] or the self-consistent mean-field approaches illustrated in Refs. [45, 171].

In summary, we believe we have put forward ideas capable of slightly advancing the broad field of open quantum systems with both numerical and analytical techniques, and we showed how such techniques can effectively lead to interesting results. We hope these methods can find a role in the long-term research effort of increasing our understanding of realistic quantum systems.

Appendix A

Review on Gaussian Systems

Starting from Sec. 4.2.1, the thesis makes extensive use of the concept of *Gaussian system* as a simplified yet powerful setting where analytical calculations are feasible. Gaussian systems are a well-known topic in both classical and quantum physics, but in order to make the thesis as self-contained as possible, the present Appendix offers a review of the most important facts concerning quantum Gaussian systems.

We begin in Sec. A.1 with the definition and basic properties of *quadratic Hamiltonians*. Next, in Sec. A.2, we discuss (bosonic and fermionic) *Gaussian states* and provide a compact proof of the celebrated *Wick's theorem*. The presented material up to this point is sufficient for understanding the content of Chaps. 4 and 5. Finally, in Sec. A.3 we apply the developed tools to briefly discuss *open* Gaussian systems, as a prerequisite for a confident approach to the content of Chap. 6.

A.1 Quadratic Hamiltonians

Using the well-known language of second quantization [44], quantum Hamiltonians are often written in terms of *creation and annihilation operators*, $\{a_i, a_i^\dagger\}_{i=1}^n$, also known as *ladder operators*. Such operators are characterized by the (anti)commutation rules

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij}, \qquad [a_i, a_j]_\zeta = [a_i^\dagger, a_j^\dagger]_\zeta = 0, \tag{A.1}$$

where

$$[X, Y]_\zeta \coloneqq XY - \zeta YX \tag{A.2}$$

and $\zeta \in \{1, -1\}$ characterizes the statistical type of the system: $\zeta = 1$ stands for a *bosonic* system, where (A.2) becomes a commutator, whereas $\zeta = -1$ stands for a *fermionic* system, where (A.2) becomes an anticommutator.

A *quadratic Hamiltonian* is simply a Hamiltonian which can be expressed as a quadratic form in creation and annihilation operators. More precisely, if we introduce the so-called *Nambu vector* $\mathbb{a}^\dagger \coloneqq (a_1^\dagger, a_1, a_2^\dagger, a_2, \ldots, a_n^\dagger, a_n)$, a quadratic Hamiltonian is of the form [172]

$$H = \frac{1}{2}\mathbb{a}^\dagger \mathcal{H} \mathbb{a} = \frac{1}{2}\sum_{i,j=1}^{2n} \mathcal{H}_{ij} \mathbb{a}_i^\dagger \mathbb{a}_j, \tag{A.3}$$

with $\mathcal{H}$ being a Hermitian matrix of coefficients. In the bosonic case, it is also customary to require $\mathcal{H}$ to be positive definite[1]. In conventional treatments, it is customary to call *quadratic* also Hamiltonians that include a *linear* term, i.e., $H = \frac{1}{2}\mathbb{a}^\dagger\mathcal{H}\mathbb{a} + \xi^\dagger\mathbb{a}$. In the bosonic case, since $\mathcal{H}$ is invertible, the shift can however be reabsorbed by noticing that $H = \frac{1}{2}\mathbb{c}^\dagger\mathcal{H}\mathbb{c} + \alpha$ with $\mathbb{c} := \mathbb{a} + \mathcal{H}^{-1}\xi$ and α an irrelevant constant. Instead, in the fermionic case one can show that no physical Gaussian state can be generated from H with $\xi \neq 0$, as a consequence of superselection rules [41]. For these reasons, we will restrict to Eq. (A.3) without much loss of generality. In this Appendix we will also assume $\mathcal{H}$ to be time-independent, even though all the subsequent expressions can be straightforwardly generalized to the time-dependent case.

It is often convenient to introduce the following $2n$ Hermitian operators

$$x_j := \frac{1}{\sqrt{2}}\left(a_j^\dagger + a_j\right), \qquad p_j := \frac{i}{\sqrt{2}}\left(a_j^\dagger - a_j\right) \tag{A.4}$$

and gather them in a vector $\mathbf{r}^T := (x_1, p_1, x_2, p_2, \ldots, x_n, p_n)$. In the bosonic case, these are usually called *position* and *momentum operators*, *canonical operators*, or *quadrature operators* [40]. In the mathematical literature, $\mathbf{r}$ is also known as *Darboux basis* [121]. Instead, in the fermionic case, these are commonly called *Majorana operators* [41]. Since we aim at a description that is valid for both statistical types, we call $\mathbf{r}$ the *Darboux-Majorana vector*. In matrix form,

$$\mathbf{r} = F\mathbb{a}, \qquad F = \frac{1}{\sqrt{2}}\bigoplus_{\ell=1}^{n}\begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}, \tag{A.5}$$

and it is easy to realize that F is a unitary transformation. Moreover,

$$[\mathbf{r}, \mathbf{r}^T]_\zeta = \Omega, \tag{A.6}$$

where

$$\Omega \overset{(\zeta=1)}{=} i\bigoplus_{\ell=1}^{n}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \qquad \Omega \overset{(\zeta=-1)}{=} \bigoplus_{\ell=1}^{n}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbb{1}. \tag{A.7}$$

Clearly, $\Omega^T = -\zeta\Omega$ and $\Omega^{-1} = \Omega$. If we define $h := F\mathcal{H}F^\dagger = h^\dagger$, the quadratic Hamiltonian (A.3) can also be written as

$$H = \frac{1}{2}\mathbf{r}^T h\mathbf{r} = \frac{1}{2}\sum_{i,j=1}^{2n} h_{ij} r_i r_j. \tag{A.8}$$

Eq. (A.8) is often more convenient to work with if compared with Eq. (A.3), since the Darboux-Majorana basis effectively hides the difference between creation and annihilation operators. Importantly, the coefficient matrix h can always be chosen such that $h^T = \zeta h$. In fact,

$$\frac{1}{2}\mathbf{r}^T(h - \zeta h^T)\mathbf{r} = \frac{1}{2}\sum_{i,j=1}^{2n}\left[h_{ij}r_ir_j - \zeta h_{ij}r_jr_i\right] = \frac{1}{2}\sum_{i,j=1}^{2n} h_{ij}\Omega_{ij} \tag{A.9}$$

[1]The condition $\mathcal{H} > 0$ is usually justified by saying that the spectrum of $\mathcal{H}$ must be bounded from below in order to guarantee the existence of a ground state. In the fermionic case this problem does not appear because each mode can only contribute with a single energy quantum.

is a constant that can be ignored.

Consider now a linear transformation $\mathbf{s} := M\mathbf{r}$. In case we want $\mathbf{s}$ to be a valid Darboux-Majorana vector, meaning that $[\mathbf{s}, \mathbf{s}^T]_\zeta = \Omega$, it is easy to see that

$$M\Omega M^T = \Omega. \tag{A.10}$$

In the bosonic case, this corresponds to the requirement that M must be a symplectic matrix, while in the fermionic case it means that M is an orthogonal matrix. Under this change of basis,

$$H = \frac{1}{2}\mathbf{s}^T\widetilde{h}\mathbf{s}, \qquad h = M^T\widetilde{h}M. \tag{A.11}$$

Let us look again at the property $h = h^\dagger = \zeta h^T$. In the bosonic case, this means that h is real and symmetric (and positive definite); in the fermionic case, this means that h is imaginary and skew-symmetric. Well-known results in linear algebra can then be invoked to say the following: M can be chosen such that Eq. (A.10) is satisfied and[2]

$$\widetilde{h} \stackrel{(\zeta=1)}{=} \bigoplus_{\ell=1}^{n} \begin{bmatrix} \varepsilon_\ell & 0 \\ 0 & \varepsilon_\ell \end{bmatrix}, \qquad \widetilde{h} \stackrel{(\zeta=-1)}{=} \bigoplus_{\ell=1}^{n} \begin{bmatrix} 0 & i\varepsilon_\ell \\ -i\varepsilon_\ell & 0 \end{bmatrix}, \tag{A.12}$$

for appropriate[3] real numbers $\varepsilon_\ell \geq 0$ determined by the condition that $\pm\varepsilon_\ell$ are the eigenvalues of Ωh. For $\zeta = 1$, this result is usually known as *Williamson's theorem* and the numbers ε_ℓ are referred to as *symplectic eigenvalues* of h [40]. For $\zeta = -1$ this is a well-known normal decomposition of imaginary skew-symmetric matrices [41].

The advantage of choosing $\widetilde{h}$ as in Eq. (A.12) is that

$$F^\dagger\widetilde{h}F = \bigoplus_{\ell=1}^{n} \begin{bmatrix} \varepsilon_\ell & 0 \\ 0 & \zeta\varepsilon_\ell \end{bmatrix}, \tag{A.13}$$

which means that, if we introduce the Nambu vector $\mathbb{b}^\dagger = (b_1^\dagger, b_1, b_2^\dagger, b_2, \ldots, b_n^\dagger, b_n)$ associated with the new basis $\mathbf{s} = F\mathbb{b}$, we obtain a *diagonalized* form of the Hamiltonian that does not mixes different modes between each other:

$$H = \frac{1}{2}\mathbb{b}^\dagger F^\dagger\widetilde{h}F\mathbb{b} = \frac{1}{2}\sum_{\ell=1}^{n} \varepsilon_\ell\left(b_\ell^\dagger b_\ell + \zeta b_\ell b_\ell^\dagger\right) = \sum_{\ell=1}^{n} \varepsilon_\ell b_\ell^\dagger b_\ell + \text{const.} \tag{A.14}$$

Finally, a fundamental property of quadratic Hamiltonians is that they linearly evolve the ladder operators when viewing them as Heisenberg observables. More specifically, if $H = \frac{1}{2}\mathbf{r}^T h\mathbf{r}$, then a straightforward computation that makes use of Eq. (A.6) reveals that

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = i[H, \mathbf{r}] = -i\Omega h\mathbf{r} \quad \Rightarrow \quad \mathbf{r}(t) := e^{iHt}\mathbf{r}(0)e^{-iHt} = e^{-i\Omega ht}\mathbf{r}(0), \tag{A.15}$$

where matrix-vector multiplication is intended throughout.

[2]Any imaginary skew-symmetric h can be put in form (A.12) by an orthogonal M, while not every real symmetric h can be put in form (A.12) by a symplectic M. It is the condition $h > 0$ which allows the diagonalization to exist in the bosonic case.

[3]In the bosonic case, we actually have $\varepsilon_\ell > 0$, as a consequence of $h > 0$.

A.2 Gaussian states

A *Gaussian state* is defined through a density operator whose Matsubara Hamiltonian is quadratic, i.e., [40, 41]

$$\rho = \frac{1}{Z}\exp\left[-\frac{\beta}{2}\mathbf{r}^T h\mathbf{r}\right], \qquad Z = \mathrm{Tr}\exp\left[-\frac{\beta}{2}\mathbf{r}^T h\mathbf{r}\right], \quad \beta > 0. \tag{A.16}$$

Note that, according to this definition, Gaussian density operator are full-rank mixed states. *Pure Gaussian states* can also be defined using appropriate limiting procedures. For instance, the ground state of the Matsubara Hamiltonian, obtained in the limit $\beta \to \infty$, is customarily also referred to as a Gaussian state. Alternatively, other pure states that can reasonably be called Gaussian can be obtained by sending specific eigenvalues of h to infinity [45]. For the sake of simplicity, in this thesis we will restrict to the form provided by Eq. (A.16).

We call *Gaussian system* a system described by a quadratic Hamiltonian $H = \frac{1}{2}\mathbf{r}^T h\mathbf{r}$ and whose state is Gaussian, $\rho \propto \exp[-\frac{\beta}{2}\mathbf{r}^T h_\rho \mathbf{r}]$. Such state remains Gaussian at all subsequent times, since

$$\begin{aligned}
\rho(t) &= \frac{1}{Z}e^{-iHt}\exp\left[-\frac{\beta}{2}\mathbf{r}^T h_\rho\mathbf{r}\right]e^{iHt} = \frac{1}{Z}\sum_{n=0}^{\infty}\frac{(-\beta)^n}{2^n n!}\left(e^{-iHt}\mathbf{r}^T h_\rho \mathbf{r} e^{iHt}\right)^n \\
&= \frac{1}{Z}\sum_{n=0}^{\infty}\frac{(-\beta)^n}{2^n n!}\left(\mathbf{r}^T e^{-i\Omega ht}h_\rho e^{i\Omega ht}\mathbf{r}\right)^n \\
&= \frac{1}{Z}\exp\left[-\frac{\beta}{2}\mathbf{r}^T h_\rho(t)\mathbf{r}\right], \qquad h_\rho(t) := e^{-i\Omega ht}h_\rho e^{i\Omega ht}.
\end{aligned} \tag{A.17}$$

Let us now explore what are the correlation functions associated with a Gaussian state. As usual, we will write $\langle X\rangle_\rho := \mathrm{Tr}\big[X\rho\big]$ for the expectation value of the operator X with respect to the state ρ.

Theorem A.1. *If ρ is the Gaussian state $\rho \propto \exp[-\frac{\beta}{2}\mathbf{r}^T h\mathbf{r}]$, then*

$$\langle \mathbf{r}\rangle_\rho = 0, \qquad \langle \mathbf{r}\mathbf{r}^T\rangle_\rho = [\mathbb{1} - \zeta e^{-\beta\Omega h}]^{-1}\Omega. \tag{A.18}$$

Proof. Let us consider the normal form of h in Eq. (A.12). The following is a well-known property of creation and annihilation operators when dealing with a diagonal Hamiltonian [6, 44]:

$$\langle \mathbb{b}\rangle_\rho = 0, \qquad \langle \mathbb{b}\mathbb{b}^\dagger\rangle_\rho = \bigoplus_{\ell=1}^{n}\begin{bmatrix} 1+\zeta f(\varepsilon_\ell) & 0 \\ 0 & f(\varepsilon_\ell)\end{bmatrix}, \tag{A.19}$$

where

$$f(\varepsilon) = \frac{1}{e^{\beta\varepsilon} - \zeta} \tag{A.20}$$

is the Bose-Einstein (Fermi-Dirac) function for $\zeta = 1$ ($\zeta = -1$). Moving to the Darboux-Majorana basis, one finds

$$\langle \mathbf{s}\mathbf{s}^T\rangle_\rho\Omega = F\langle \mathbb{b}\mathbb{b}^\dagger\rangle_\rho F^\dagger\Omega = \frac{1}{2}\bigoplus_{\ell=1}^{n}\begin{bmatrix} 1 & i[1+2\zeta f(\varepsilon_\ell)] \\ -i[1+2\zeta f(\varepsilon_\ell)] & 1\end{bmatrix}. \tag{A.21}$$

Moreover, we can write

$$\Omega h = \Omega M^T \widetilde{h} M = M^{-1}\Omega\widetilde{h}M = M^{-1}\bigoplus_{\ell=1}^{n}\begin{bmatrix} 0 & i\varepsilon_\ell \\ -i\varepsilon_\ell & 0 \end{bmatrix} M = M^{-1}F\bigoplus_{\ell=1}^{n}\begin{bmatrix} \varepsilon_\ell & 0 \\ 0 & -\varepsilon_\ell \end{bmatrix} F^\dagger M. \tag{A.22}$$

Since $M^{-1}F$ is the inverse of $F^\dagger M$, we can apply a matrix function to Ωh as follows:

$$\begin{aligned}[\mathbb{1} - \zeta e^{-\beta\Omega h}]^{-1} &= M^{-1}F\bigoplus_{\ell=1}^{n}\begin{bmatrix} (1-\zeta e^{-\beta\varepsilon_\ell})^{-1} & 0 \\ 0 & (1-\zeta e^{\beta\varepsilon_\ell})^{-1} \end{bmatrix} F^\dagger M \\ &= M^{-1}\langle \mathbf{s}\mathbf{s}^T\rangle_\rho \Omega M = M^{-1}\langle \mathbf{s}\mathbf{s}^T\rangle_\rho M^{-T}\Omega = \langle \mathbf{r}\mathbf{r}^T\rangle_\rho\Omega,\end{aligned} \tag{A.23}$$

which yields the desired result. In the second equality we used the easily verifiable relations

$$\frac{1}{1-\zeta e^{-\beta\epsilon}} + \frac{1}{1-\zeta e^{\beta\epsilon}} = 1, \qquad \frac{1}{1-\zeta e^{-\beta\epsilon}} - \frac{1}{1-\zeta e^{\beta\epsilon}} = 1 + 2\zeta f(\varepsilon_\ell). \tag{A.24}$$

□

The Gaussian state (A.16) is therefore completely determined by the value of $\langle \mathbf{r}\mathbf{r}^T\rangle_\rho$. It is common to "factor out" the contribution of the (anti)commutation relation (A.6) as

$$\langle \mathbf{r}\mathbf{r}^T\rangle_\rho \equiv \frac{\Omega+\Gamma}{2}, \qquad \Gamma_{ij} := \langle r_i r_j + \zeta r_j r_i\rangle_\rho, \tag{A.25}$$

where Γ is called *covariance matrix*. Using Eq. (A.18), one finds

$$\Gamma = \begin{cases} \coth\left(\frac{\beta\Omega h}{2}\right)\Omega & \zeta = 1, \\ \tanh\left(\frac{\beta h}{2}\right) & \zeta = -1. \end{cases} \tag{A.26}$$

In the bosonic case ($\zeta = 1$) this is a real, symmetric, and positive definite matrix with eigenvalues in the interval $[1, \infty)$. Instead, in the fermionic case ($\zeta = -1$), it is a pure imaginary, skew-symmetric matrix with eigenvalues in the interval $[-1, 1]$. Further details can be found, e.g., in Refs. [40, 41, 165].

The nice thing about Gaussian states is that every correlation of the form $\langle r_{i_1} \dots r_{i_k}\rangle_\rho$ can be calculated from the knowledge of $\langle \mathbf{r}\rangle_\rho$ and $\langle \mathbf{r}\mathbf{r}^T\rangle_\rho$: this is the content of the celebrated *Wick's theorem*, which we will now discuss.

Let B_i be an arbitrary *linear* combination of ladder operators. In Darboux-Majorana basis, this amounts to the existence of a relationship $B_i = \sum_j \phi_{ij} r_j$, $\phi_{ij} \in \mathbb{C}$, which can be conveniently expressed in vector form as $\mathbf{B} = \phi\mathbf{r}$. Suppose also that the index i takes value in an arbitrary ordered set, so that it makes sense to consider the ζ-graded ordering operation $\mathbb{T}_\zeta$ of a product of B_i operators. Wick's theorem can then be expressed as follows [118].

Theorem A.2 (Wick). *If $\rho \propto \exp\left[-\frac{\beta}{2}\mathbf{r}^T h\mathbf{r}\right]$ is a Gaussian state and $\mathbf{B} = \phi\mathbf{r}$, then, for any $m \in \mathbb{N}$,*

$$\langle \mathbb{T}_\zeta\{B_1 \dots B_{2m+1}\}\rangle_\rho = 0, \qquad \langle \mathbb{T}_\zeta\{B_1 \dots B_{2m}\}\rangle_\rho = \mathrm{Hpf}_\zeta(S), \tag{A.27}$$

where $\mathrm{Hpf}_\zeta(S)$ is the Hafnian-Pfaffian[122, 123] of the matrix $S_{ij} := \langle \mathbb{T}_\zeta\{B_i B_j\}\rangle_\rho = \zeta S_{ji}$, given by

$$\mathrm{Hpf}_\zeta(S) := \frac{1}{m!2^m}\sum_{\sigma\in\mathfrak{S}_{2m}} \zeta^{N(\sigma)}\prod_{j=1}^{m} S_{\sigma(2j-1),\sigma(2j)}. \tag{A.28}$$

Proof. By definition of $\mathbb{T}_\zeta$, there is a permutation φ of $\{1, \ldots, n\}$ such that $\varphi(1) \succ \ldots \succ \varphi(n)$ and

$$\langle \mathbb{T}_\zeta\{B_1 \ldots B_n\}\rangle_\rho = \zeta^{N(\varphi)}\langle B_{\varphi(1)} \ldots B_{\varphi(n)}\rangle_\rho = \zeta^{N(\varphi)}\Big(\phi\langle \mathbf{r}B_{\varphi(2)} \ldots B_{\varphi(n)}\rangle_\rho\Big)_{\varphi(1)}, \tag{A.29}$$

where in the second equality we used the linearity hypothesis on $B_{\varphi(1)}$. Let us then focus on the vector $\langle \mathbf{r}B_{\varphi(2)} \ldots B_{\varphi(n)}\rangle_\rho$. We can repeatedly apply the relation $\mathbf{r}B_i = [\mathbf{r}, B_i]_\zeta + \zeta B_i\mathbf{r}$ until we manage to bring $\mathbf{r}$ at the end of the string of operators:

$$\langle \mathbf{r}B_{\varphi(2)} \ldots B_{\varphi(n)}\rangle_\rho = \sum_{j=2}^{n} \zeta^j[\mathbf{r}, B_{\varphi(j)}]_\zeta\langle B_{\varphi(2)} \ldots B_{\varphi(j-1)}B_{\varphi(j+1)} \ldots B_{\varphi(n)}\rangle_\rho + \zeta^{n+1}\langle B_{\varphi(2)} \ldots B_{\varphi(n)}\mathbf{r}\rangle_\rho, \tag{A.30}$$

where we used the fact that $[\mathbf{r}, \mathbf{B}^T]_\zeta = \Omega\phi^T$ is a matrix of coefficients. However, thanks to Eq. (A.15), we know that $\mathbf{r}\rho = e^{-\beta\Omega h}\rho\mathbf{r}$, and therefore, by the cyclic property of the trace,

$$[\mathbb{1} - \zeta^{n+1}e^{-\beta\Omega h}]\langle \mathbf{r}B_{\varphi(2)} \ldots B_{\varphi(n)}\rangle_\rho = \sum_{j=2}^{n} \zeta^j[\mathbf{r}, B_{\varphi(j)}]_\zeta\langle B_{\varphi(2)} \ldots B_{\varphi(j-1)}B_{\varphi(j+1)} \ldots B_{\varphi(n)}\rangle_\rho. \tag{A.31}$$

Applying $[\mathbb{1} - \zeta^{n+1}e^{-\beta\Omega h}]^{-1}$ on both sides, writing $[\mathbf{r}, \mathbf{B}^T]_\zeta = \Omega\phi^T$ and substituting above, we can see that

$$\begin{aligned}\langle \mathbb{T}_\zeta\{B_1 \ldots B_n\}\rangle_\rho = \zeta^{N(\varphi)} \sum_{j=2}^{n} \zeta^j \Big(\phi[\mathbb{1} - \zeta^{n+1}e^{-\beta\Omega h}]^{-1}\Omega\phi^T\Big)_{\varphi(1),\varphi(j)} \\ \times \langle B_{\varphi(2)} \ldots B_{\varphi(j-1)}B_{\varphi(j+1)} \ldots B_{\varphi(n)}\rangle_\rho.\end{aligned} \tag{A.32}$$

We know that $\langle \mathbf{B}\rangle_\rho = \phi\langle \mathbf{r}\rangle_\rho = 0$. A straightforward induction argument is then able to conclude that $\langle B_{\varphi(1)} \ldots B_{\varphi(n)}\rangle_\rho = 0$ for every odd n; using Eq. (A.32) we immediately conclude that in this case $\langle \mathbb{T}_\zeta\{B_1 \ldots B_n\}\rangle_\rho = 0$ as well. Suppose then that $n = 2m$ is an even number. Thanks to Eq. (A.18),

$$\langle \mathbf{B}\mathbf{B}^T\rangle_\rho = \phi\langle \mathbf{r}\mathbf{r}^T\rangle_\rho\phi^T = \phi[\mathbb{1} - \zeta e^{-\beta\Omega h}]^{-1}\Omega\phi^T, \tag{A.33}$$

and we recognize its appearance in Eq. (A.32):

$$\langle \mathbb{T}_\zeta\{B_1 \ldots B_{2m}\}\rangle_\rho = \zeta^{N(\varphi)} \sum_{j=2}^{2m} \zeta^j\langle B_{\varphi(1)}B_{\varphi(j)}\rangle_\rho\langle B_{\varphi(2)} \ldots B_{\varphi(j-1)}B_{\varphi(j+1)} \ldots B_{\varphi(2m)}\rangle_\rho. \tag{A.34}$$

The B operators appearing on the right-hand side are all correctly ordered. This means that we can put them inside $\mathbb{T}_\zeta$ without introducing any sign:

$$\langle \mathbb{T}_\zeta\{B_1 \ldots B_{2m}\}\rangle_\rho = \zeta^{N(\varphi)} \sum_{j=2}^{2m} \zeta^j\langle \mathbb{T}_\zeta\big\{B_{\varphi(1)}B_{\varphi(j)}\big\}\rangle_\rho\langle \mathbb{T}_\zeta\big\{B_{\varphi(2)} \ldots B_{\varphi(j-1)}B_{\varphi(j+1)} \ldots B_{\varphi(2m)}\big\}\rangle_\rho. \tag{A.35}$$

This is precisely the recursive definition of the Hafnian-Pfaffian associated with the matrix $\langle \mathbb{T}_\zeta\big\{B_{\varphi(i)}B_{\varphi(j)}\big\}\rangle_\rho$ [122, 123], so that

$$\langle \mathbb{T}_\zeta\{B_1 \ldots B_{2m}\}\rangle_\rho = \frac{\zeta^{N(\varphi)}}{m!2^m} \sum_{\sigma\in\mathfrak{S}_{2m}} \zeta^{N(\sigma)} \prod_{j=1}^{m}\langle \mathbb{T}_\zeta\big\{B_{\varphi(\sigma(2j-1))}B_{\varphi(\sigma(2j))}\big\}\rangle_\rho. \tag{A.36}$$

Employing the change of variable $\varphi \circ \sigma \mapsto \sigma$, we finally arrive at

$$\langle \mathbb{T}_\zeta\{B_1 \dots B_{2m}\}\rangle_\rho = \frac{1}{m!2^m} \sum_{\sigma\in\mathfrak{S}_{2m}} \zeta^{N(\sigma)} \prod_{j=1}^{m} \langle \mathbb{T}_\zeta\big\{B_{\sigma(2j-1)}B_{\sigma(2j)}\big\}\rangle_\rho, \tag{A.37}$$

which is what we wanted to prove. □

A.3 Open Gaussian systems

Suppose now our Gaussian system is partitioned into a subsystem S of interest, which we will simply call *open Gaussian system*, and an environment E. Let $\mathbf{r}$ denote the Darboux-Majorana vector of the system, and let $\mathbf{s}$ denote the Darboux-Majorana vector of the environment. The (anti)commutation relation (A.6) for the global setup translates in the rules

$$[\mathbf{r}, \mathbf{r}^T]_\zeta = \Omega_S, \qquad [\mathbf{s}, \mathbf{s}^T]_\zeta = \Omega_E, \qquad [\mathbf{r}, \mathbf{s}^T]_\zeta = 0, \tag{A.38}$$

where Ω_S and Ω_E represent the restrictions of Ω to the indices associated, respectively, with system and environment. Furthermore, in the ordered basis $(\mathbf{r}, \mathbf{s})$, the total Hamiltonian matrix h inherits the block partition

$$h = \begin{pmatrix} h_S & v \\ v^\dagger & h_E \end{pmatrix}, \qquad v^* = \zeta v, \tag{A.39}$$

where h_S and h_E are the isolated Hamiltonians of system and environment, whereas v is the interaction part. The property $v^* = \zeta v$ must be satisfied if we arrange h such that $h^T = \zeta h$. Corresponding to the structure (A.39), we get the split $H = H_S + H_E + V$ for the Hamiltonian operator, where

$$H_S = \frac{1}{2}\mathbf{r}^T h_S \mathbf{r}, \qquad H_E = \frac{1}{2}\mathbf{s}^T h_E \mathbf{s}, \qquad V = \mathbf{r}^T v \mathbf{s}. \tag{A.40}$$

The study of the dynamics of the system S is precisely the subject of Chap. 6. Here, we will just discuss how Eq. (A.15) is generalized to the open setting, yielding the so-called *Heisenberg-Langevin (HL) equation* [158, 159]. It is worth noticing that usual derivations of the HL equation are carried out using ladder operators with excitation-preserving interaction, which decouples the equation for a_i from the equation for $a_i^\dagger$. Our present approach shows that such simplification is unnecessary: it is sufficient to frame the problem using the Darboux-Majorana basis and a streamlined derivation of the HL equation follows in the same way.

The Heisenberg equations of motion for the Darboux-Majorana vectors are found to be

$$\frac{d\mathbf{r}}{dt} = i[H, \mathbf{r}] = -i\Omega_S(h_S\mathbf{r} + v\mathbf{s}), \qquad \frac{d\mathbf{s}}{dt} = i[H, \mathbf{s}] = -i\Omega_E(h_E\mathbf{s} + v^\dagger\mathbf{r}). \tag{A.41}$$

The equation for $\mathbf{s}$ is formally solved by

$$\mathbf{s}(t) = e^{-i\Omega_E h_E t}\mathbf{s}(0) - i\int_0^t d\tau\, e^{-i\Omega_E h_E (t-\tau)}\Omega_E v^\dagger \mathbf{r}(\tau). \tag{A.42}$$

Substituting into the equation for $\mathbf{r}$, we directly obtain the HL equation [cf. Eq. (6.2)]

$$\frac{d\mathbf{r}(t)}{dt} = -i\Omega_S\left[h_S\mathbf{r}(t) + \mathbf{B}(t) - i\int_0^t d\tau\, \Sigma(t-\tau)\mathbf{r}(\tau)\right], \tag{A.43}$$

where

$$\mathbf{B}(t) := v e^{-i\Omega_E h_E t}\mathbf{s}(0), \qquad \Sigma(t) := v e^{-i\Omega_E h_E t}\Omega_E v^\dagger. \tag{A.44}$$

The vector $\mathbf{B}(t)$ is precisely the environment's interaction operator we used throughout the thesis, since $V = \mathbf{r}^T\mathbf{B}$ with $\mathbf{B} = v\mathbf{s}$, which turns into $\mathbf{B}(t)$ when moving to the interaction picture. Instead, $\Sigma(t)$ is a memory kernel known as *embedding self-energy*, especially in the community around many-body physics [45]. In the language of open quantum systems, it is basically the Fourier transform of the environment's spectral density [158]. To see this, let us assume for simplicity that h_E is already in the normal form (A.12), so that

$$\Omega_E h_E = F_E D_E F_E^\dagger, \qquad D_E = \bigoplus_\ell \begin{bmatrix} \varepsilon_\ell & 0 \\ 0 & -\varepsilon_\ell \end{bmatrix}, \tag{A.45}$$

and F_E is the restriction of F to the environment indices. Moreover, we know that $v = F_S \mathcal{V} F_E^\dagger$, where F_S is the restriction of F to the system indices and $\mathcal{V}$ is the coefficient matrix of the interaction in the basis of ladder operators. Then,

$$\begin{aligned} \Sigma(t) &= v F_E e^{-iD_E t} F_E^\dagger \Omega_E v^\dagger = F_S \mathcal{V} e^{-iD_E t} F_E^\dagger \Omega_E F_E \mathcal{V}^\dagger F_S^\dagger \\ &= F_S \mathcal{V} \left[\bigoplus_\ell \begin{pmatrix} e^{-i\varepsilon_\ell t} & 0 \\ 0 & -\zeta e^{i\varepsilon_\ell t} \end{pmatrix} \right] \mathcal{V}^\dagger F_S^\dagger = \int_{-\infty}^{\infty} \mathrm{d}x\, F_S \mathcal{J}(x) F_S^\dagger e^{-ixt}, \end{aligned} \tag{A.46}$$

where

$$\mathcal{J}(x) := \mathcal{V} \left[\bigoplus_\ell \begin{pmatrix} \delta(x-\varepsilon_\ell) & 0 \\ 0 & -\zeta\delta(x+\varepsilon_\ell) \end{pmatrix} \right] \mathcal{V}^\dagger \tag{A.47}$$

is a spectral density matrix. The additional presence of F_S simply accounts for the transformation to the Darboux-Majorana basis.

Appendix B

Gaussian Environment Propagator

In Chap. 4, we derived the most general form for the density operator of an open system linearly coupled to a Gaussian environment satisfying the stability condition $\mathrm{Tr}[B_\alpha(z)\varrho_E] = 0$. We obtained Eq. (4.67), repeated here for convenience:

$$\varrho(t) = \mathbb{T}_\zeta \left\{ \exp\left[-\frac{1}{2} \sum_{\alpha,\beta} \int_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, C_{\alpha\beta}(z_1, z_2) A_\alpha(z_1) A_\beta(z_2) \right] \varrho(t_0) \right\}. \tag{B.1}$$

This Appendix is dedicated to additional discussions around Eq. (B.1).

First, in Sec. B.1 we unravel the contour and we show that Eq. (B.1) is equivalent to the Feynman-Vernon influence functional [110], which was previously derived in the literature using superoperators or path-integral techniques. Then, in Sec. B.2 we restrict to the bosonic scenario and discuss how Eq. (B.1) can be generalized to the case where the stability condition does not hold. This result is then used in Sec. B.3 to derive the corresponding generalization of the stochastic von Neumann equation, which is utilized in the main text for the discussion on the measurement interpretation (cf. Sec. 5.4).

B.1 Recovering the influence functional

Let us discuss how the Feynman-Vernon influence functional expression [110, 112] can be recovered from Eq. (B.1) after an unraveling of the contour. For simplicity, we will here assume factorized initial state, so that the contour $\gamma(t)$ is solely composed of horizontal branches (cf. Fig. 4.1): this is enough to recover the standard form of the influence functional. The calculation can of course be generalized to correlated initial states by including the Matsubara track.

The contour unraveling yields the following for the exponent in Eq. (B.1):

$$\begin{aligned} -\frac{1}{2} \sum_{\alpha,\beta} \int_{t_0}^{t} \mathrm{d}^2\mathbf{s} \Big\{ & C^{T}_{\alpha\beta}(s_1, s_2) A_\alpha(s_1^-) A_\beta(s_2^-) - C^{>}_{\alpha\beta}(s_1, s_2) A_\alpha(s_1^+) A_\beta(s_2^-) \\ & - C^{<}_{\alpha\beta}(s_1, s_2) A_\alpha(s_1^-) A_\beta(s_2^+) + C^{\widetilde{T}}_{\alpha\beta}(s_1, s_2) A_\alpha(s_1^+) A_\beta(s_2^+) \Big\}, \end{aligned} \tag{B.2}$$

where we employed the notations concerning the components of two-point contour functions, as established in Sec. 4.2.4. Now we recall the relations

$$C^{T}(s_1, s_2) = \theta(s_1 - s_2)C^{>}(s_1, s_2) + \theta(s_2 - s_1)C^{<}(s_1, s_2), \tag{B.3}$$

$$C^{\widetilde{T}}(s_1, s_2) = \theta(s_1 - s_2)C^{<}(s_1, s_2) + \theta(s_2 - s_1)C^{>}(s_1, s_2), \tag{B.4}$$

which allow us to rewrite Eq. (B.2) as

$$\begin{aligned}
-\frac{1}{2}\sum_{\alpha,\beta}\int_{t_0}^{t} \mathrm{d}^2\mathbf{s}\Big\{\theta(s_1 - s_2)\Big[&C^{>}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^-)A_\beta(s_2^-) - A_\alpha(s_1^+)A_\beta(s_2^-)\big) \\
&+ C^{<}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^+)A_\beta(s_2^+) - A_\alpha(s_1^-)A_\beta(s_2^+)\big)\Big] \\
+ \theta(s_2 - s_1)\Big[&C^{>}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^+)A_\beta(s_2^+) - A_\alpha(s_1^+)A_\beta(s_2^-)\big) \\
&+ C^{<}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^-)A_\beta(s_2^-) - A_\alpha(s_1^-)A_\beta(s_2^+)\big)\Big]\Big\}.
\end{aligned}$$

Let us perform a harmless change of variables $s_1 \leftrightarrow s_2$ and $\alpha \leftrightarrow \beta$ for the term containing $\theta(s_2 - s_1)$. Since we have everything inside a $\mathbb{T}_\zeta$ operation, we can freely commute operators provided we add a ζ factor for each transposition. For example, $A_\alpha(s_1^+)A_\beta(s_2^-) \mapsto A_\beta(s_2^+)A_\alpha(s_1^-) \mapsto \zeta A_\alpha(s_1^-)A_\beta(s_2^+)$. Thanks also to the property $C^{>}_{\beta\alpha}(s_2, s_1) = \zeta C^{<}_{\alpha\beta}(s_1, s_2)$, we conclude that the term multiplying $\theta(s_2 - s_1)$ is equal to the one multiplying $\theta(s_1 - s_2)$, for the purpose of calculating Eq. (B.1). We can then focus on

$$\begin{aligned}
-\sum_{\alpha,\beta}\int_{t_0}^{t}\mathrm{d}s_1\int_{t_0}^{s_1}\mathrm{d}s_2\,\Big[&C^{>}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^-)A_\beta(s_2^-) - A_\alpha(s_1^+)A_\beta(s_2^-)\big) \\
&+ C^{<}_{\alpha\beta}(s_1, s_2)\big(A_\alpha(s_1^+)A_\beta(s_2^+) - A_\alpha(s_1^-)A_\beta(s_2^+)\big)\Big].
\end{aligned} \tag{B.5}$$

At this point, we introduce the so-called *dissipation kernel* $C^K_{\alpha\beta}(t, s)$ and *noise kernel* $C^R_{\alpha\beta}(t, s)$:

$$C^{K}_{\alpha\beta}(t, s) := \frac{1}{2}\Big[C^{>}_{\alpha\beta}(t, s) + C^{<}_{\alpha\beta}(t, s)\Big], \tag{B.6}$$

$$C^{R}_{\alpha\beta}(t, s) := \frac{1}{2}\theta(t - s)\Big[C^{>}_{\alpha\beta}(t, s) - C^{<}_{\alpha\beta}(t, s)\Big]. \tag{B.7}$$

These are nothing more than, respectively, the Keldysh and retarded components of C [46], which also appeared when discussing the stochastic master equations in Sec. 5.2.1. In terms of them, Eq. (B.5) assumes the form

$$\begin{aligned}
-\sum_{\alpha,\beta}\int_{t_0}^{t}\mathrm{d}s_1\int_{t_0}^{s_1}\mathrm{d}s_2\,\Big\{&C^{K}_{\alpha\beta}(s_1, s_2)\big[A_\alpha(s_1^-) - A_\alpha(s_1^+)\big]\big[A_\beta(s_2^-) + A_\beta(s_2^+)\big] \\
&+ C^{R}_{\alpha\beta}(s_1, s_2)\big[A_\alpha(s_1^-) - A_\alpha(s_1^+)\big]\big[A_\beta(s_2^-) - A_\beta(s_2^+)\big]\Big\}.
\end{aligned} \tag{B.8}$$

This is the exponent that should be placed in Eq. (B.1). In order to fully unravel the contour description, the last step consists in translating the contour-ordering operation $\mathbb{T}_\zeta$ into a standard time-ordering one, with $\varrho(t_0)$ being placed outside of it. To do that, we must prescribe how the $A_\alpha(z)$ operators should be placed with respect to $\varrho(t_0)$: it is natural to accomplish this using the left-right superoperators $\hat{A}^L_\alpha(t)$ and $\hat{A}^R_\alpha(t)$. Specifically, given the shape of the contour, $A_\alpha(s^-) \mapsto \hat{A}^L_\alpha(s)$ and $A_\alpha(s^+) \mapsto \hat{A}^R_\alpha(s)$. If we also introduce the commutator and anti-commutator superoperators $\hat{A}^c := \hat{A}^L - \hat{A}^R$ and $\hat{A}^a := \hat{A}^L + \hat{A}^R$, we end up with

$$\varrho(t) = \mathbb{T}_\zeta \exp\Big[-\hat{\mathcal{F}}(t, t_0)\Big]\varrho(t_0), \tag{B.9}$$

where $\hat{\mathcal{F}}(t, t_0)$ is precisely the influence functional [6, 110, 112]:

$$\hat{\mathcal{F}}(t, t_0) = \sum_{\alpha,\beta} \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2 \left[C^K_{\alpha\beta}(s_1, s_2)\hat{A}^c_\alpha(s_1)\hat{A}^a_\beta(s_2) + C^R_{\alpha\beta}(s_1, s_2)\hat{A}^c_\alpha(s_1)\hat{A}^c_\beta(s_2)\right]. \tag{B.10}$$

B.2 Relaxing the stability condition

Eq. (B.1) was obtained assuming the validity of the stability condition $\mathrm{Tr}[B_\alpha(z)\varrho_E] = 0$. In the context of Gaussian environments, such condition is satisfied provided ϱ_E is generated by a purely quadratic Hamiltonian with no linear term. As we discussed in Appendix A, while this is a natural requirement in the fermionic setting, we should be more careful when considering bosonic setups, where a linear shift can in principle be present. In this section, we therefore restrict to $\zeta = 1$ and show how Eq. (B.1) can be generalized to the case in which

$$E_i := \mathrm{Tr}[B_i \varrho_E] \neq 0. \tag{B.11}$$

Hereafter we will again employ the compact notation developed in Sec. 4.1.4.

We need to start again from the formula [cf. Eq. (4.40)]

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \fint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \mathrm{Tr}[\mathbb{T}\{B_1 \dots B_n \varrho_E\}]\mathbb{T}\{A_1 \dots A_n \varrho_0\}. \tag{B.12}$$

The trick is to introduce the *shifted* environment operators

$$\widetilde{B}_i := B_i - E_i \mathbb{1}, \tag{B.13}$$

which obviously satisfy the stability condition $\mathrm{Tr}\,[\widetilde{B}_i\varrho_E] = 0$. What we need is to expand the n-point correlation function $\mathrm{Tr}[\mathbb{T}\{B_1 \dots B_n\varrho_E\}]$ using $B_i = \widetilde{B}_i + E_i\mathbb{1}$, so that we arrive at an expression in terms of the shifted environment operators.

This can be done using the formula

$$\mathbb{T}\{(X_1 + Y_1)\dots(X_n + Y_n)\} = \sum_{k=0}^{n} \frac{1}{k!(n-k)!} \sum_{\sigma\in\mathfrak{S}_n} \mathbb{T}\big\{X_{\sigma(1)} \dots X_{\sigma(k)} Y_{\sigma(k+1)} \dots Y_{\sigma(n)}\big\}, \tag{B.14}$$

which we discussed back in Sec. 5.3. In our case, $X_i \mapsto E_i\mathbb{1}$ and $Y_i \mapsto \widetilde{B}_i$, hence

$$\varrho(t) = \sum_{n=0}^{\infty}\sum_{k=0}^{n} \frac{(-i)^n}{k!(n-k)!} \fint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, E_1 \dots E_k\, \mathrm{Tr}\Big[\mathbb{T}\{\widetilde{B}_{k+1} \dots \widetilde{B}_n \varrho_E\}\Big]\mathbb{T}\{A_1 \dots A_n \varrho_0\}, \tag{B.15}$$

where we used the fact that every permutation contributes equally to the integral, after appropriate changes of variables.

Now, if we define $q := n - k$ we can equivalently write

$$\varrho(t) = \sum_{k,q=0}^{\infty} \frac{(-i)^{k+q}}{k!q!} \oint_{\gamma(t)} \mathrm{d}^k\mathbf{w} \oint_{\gamma(t)} \mathrm{d}^q\mathbf{w}'\, E_1 \dots E_k \,\mathrm{Tr}\Big[\mathbb{T}\{\widetilde{B}'_1 \dots \widetilde{B}'_q \varrho_E\}\Big] \mathbb{T}\{A_1 \dots A_k A'_1 \dots A'_q \varrho_0\}, \tag{B.16}$$

where a prime indicates that the corresponding quantity depends on $\mathbf{w}'$ instead of $\mathbf{w}$. The contour Wick's theorem 4.3 can now be applied to the correlation function of the shifted operators, yielding

$$\varrho(t) = \sum_{k,m=0}^{\infty} \frac{(-i)^k}{k!} \frac{(-1)^m}{m!2^m} \oint_{\gamma(t)} \mathrm{d}^k\mathbf{w} \oint_{\gamma(t)} \mathrm{d}^{2m}\mathbf{w}'\, E_1 \dots E_k \widetilde{C}'_{1,2} \dots \widetilde{C}'_{2m-1,2m} \mathbb{T}\{A_1 \dots A_k A'_1 \dots A'_{2m} \varrho_0\}, \tag{B.17}$$

where the two-point contour correlation function of the shifted operators is

$$\widetilde{C}_{i,j} := \mathrm{Tr}\Big[\mathbb{T}\{\widetilde{B}_i \widetilde{B}_j \varrho_E\}\Big] = \mathrm{Tr}\big[\mathbb{T}\{B_i B_j \varrho_E\}\big] - E_i E_j = C_{i,j} - E_i E_j. \tag{B.18}$$

This is easily seen to be expressed as the following ordered exponential:

$$\varrho(t) = \mathbb{T}\bigg\{\exp\bigg[-i \oint_{\gamma(t)} \mathrm{d}z\, E_1 A_1 - \frac{1}{2} \oint_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, \widetilde{C}_{1,2} A_1 A_2\bigg] \varrho_0\bigg\}, \tag{B.19}$$

which is the desired generalization of Eq. (B.1).

B.3 Stochastic decoupling without stability condition

In Sec. 5.4 we found that it is useful to derive a stochastic master equation that does not rely on the stability condition: we will now illustrate how this can be achieved by performing stochastic decoupling from Eq. (B.19).

Unlike the standard scenario, we must introduce a set $\{\xi_\alpha(z)\}$ of contour Gaussian noises with non-vanishing average. Specifically, we require

$$\mathbb{E}[\xi_\alpha(z)] = E_\alpha(z), \qquad \mathbb{E}[\xi_\alpha(z_1)\xi_\beta(z_2)] = C_{\alpha\beta}(z_1, z_2). \tag{B.20}$$

Clearly, we can also consider the shifted noises

$$\widetilde{\xi}_\alpha(z) := \xi_\alpha(z) - E_\alpha(z), \tag{B.21}$$

which satisfy

$$\mathbb{E}[\widetilde{\xi}_\alpha(z)] = 0, \qquad \mathbb{E}[\widetilde{\xi}_\alpha(z_1)\widetilde{\xi}_\beta(z_2)] = \widetilde{C}_{\alpha\beta}(z_1, z_2). \tag{B.22}$$

Therefore, Eq. (B.19) is equivalent to

$$\varrho(t) = \mathbb{T}\bigg\{\exp\bigg[-i \oint_{\gamma(t)} \mathrm{d}z\, \mathbb{E}[\xi_1] A_1 - \frac{1}{2} \oint_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, \mathbb{E}[\widetilde{\xi}_1 \widetilde{\xi}_2] A_1 A_2\bigg] \varrho_0\bigg\}. \tag{B.23}$$

The expansion of the exponential gives

$$\begin{aligned}\varrho(t) = \sum_{k,m=0}^{\infty} \frac{(-i)^k}{k!} \frac{(-1)^m}{m!2^m} \oint_{\gamma(t)} \mathrm{d}^k\mathbf{w} \oint_{\gamma(t)} \mathrm{d}^{2m}\mathbf{w}'\, \mathbb{E}[\xi_1] \dots \mathbb{E}[\xi_k] \\ \times \mathbb{E}[\widetilde{\xi}'_1 \widetilde{\xi}'_2] \dots \mathbb{E}[\widetilde{\xi}'_{2m-1} \widetilde{\xi}'_{2m}] \mathbb{T}\big\{A_1 \dots A_k A'_1 \dots A'_{2m} \varrho_0\big\}.\end{aligned} \tag{B.24}$$

Then, we can use Isserlis' theorem (5.2) to recompactify the shifted noises:

$$\varrho(t) = \sum_{k,q=0}^{\infty} \frac{(-i)^{k+q}}{k!q!} \fint_{\gamma(t)} \mathrm{d}^k \mathbf{w} \fint_{\gamma(t)} \mathrm{d}^q \mathbf{w}' \,\mathbb{E}[\xi_1] \dots \mathbb{E}[\xi_k] \mathbb{E}[\widetilde{\xi}'_1 \dots \widetilde{\xi}'_q] \mathbb{T}\{A_1 \dots A_k A'_1 \dots A'_q \varrho_0\}. \tag{B.25}$$

Since $\widetilde{\xi}_i + \mathbb{E}[\xi_i] = \xi_i$, this is just

$$\varrho(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \fint_{\gamma(t)} \mathrm{d}^n \mathbf{z} \,\mathbb{E}[\xi_1 \dots \xi_n] \mathbb{T}\{A_1 \dots A_n \varrho_0\}, \tag{B.26}$$

which is completely equivalent to the result we obtained in Chap. 5 with the stability condition. The difference, of course, is that ξ_i no longer averages to zero. When performing the stochastic replacement $\varrho(t) = \mathbb{E}[R(t)]$, we still obtain all of the stochastic master equations we discussed in Chap. 5.

The shape of the stochastic von Neumann equation is particularly interesting in this context, because it shows how the presence of the shift contributes only to the Hamiltonian noise and not to the dissipation. Specifically, one immediately arrives at

$$\frac{\mathrm{d}R(t)}{\mathrm{d}t} = -i \sum_{\alpha} \nu_\alpha(t)[A_\alpha(t), R(t)] - i \sum_{\alpha} \eta_\alpha(t)\{A_\alpha(t), R(t)\}, \tag{B.27}$$

where

$$\nu_\alpha(t) = \frac{\xi_\alpha(t^-) + \xi_\alpha(t^+)}{2}, \qquad \eta_\alpha(t) = \frac{\xi_\alpha(t^-) - \xi_\alpha(t^+)}{2}. \tag{B.28}$$

Crucially, $\xi_\alpha(z)$ is here the noise with non-vanishing average. But since one has the decomposition $\xi_\alpha(z) = \widetilde{\xi}_\alpha(z) + E_\alpha(z)$ with $E_\alpha(t^\pm) \equiv E_\alpha(t)$,

$$\nu_\alpha(t) = \frac{\widetilde{\xi}_\alpha(t^-) + \widetilde{\xi}_\alpha(t^+)}{2} + E_\alpha(t) =: \widetilde{\nu}_\alpha(t) + E_\alpha(t), \tag{B.29}$$

$$\eta_\alpha(t) = \frac{\widetilde{\xi}_\alpha(t^-) - \widetilde{\xi}_\alpha(t^+)}{2}. \tag{B.30}$$

Because of the minus sign, the dissipation $\eta_\alpha(t)$ is not influenced by the presence of the shift, as we anticipated above. The master equation writes

$$\frac{\mathrm{d}R(t)}{\mathrm{d}t} = -i \sum_{\alpha} (\widetilde{\nu}_\alpha(t) + E_\alpha(t))[A_\alpha(t), R(t)] - i \sum_{\alpha} \eta_\alpha(t)\{A_\alpha(t), R(t)\}, \tag{B.31}$$

where the correlation functions characterizing $\widetilde{\nu}_\alpha(t)$ and $\widetilde{\eta}_\alpha(t)$ are now calculated using the shifted contour Green's function $\widetilde{\mathcal{C}}_{\alpha\beta}(t,s)$.

Appendix C

Contour for Quantum Thermodynamics

As we discussed in Chap. 4, the contour approach to quantum dynamics can be successfully applied to situations which do not directly involve the evolution of a density operator. In this Appendix, we briefly discuss a possible way of applying the contour formalism in the context of quantum thermodynamics [3].

Specifically, after a short introduction to the standard two-point measurement (TPM) scheme in Sec. C.1, we will show in Sec. C.2 how to derive a compact contour expression for the characteristic function of a TPM. Moreover, in Sec. C.3 we extend this idea to the problem of tracking heat in an open system. Remarkably, we will find that the characteristic function can be recovered from an operator that is structurally identical to the density operator but with an environment correlation function modified by the presence of a counting field. This analogy is exploited in Sec. C.4 to derive exact master equations from which the heat statistics can be efficiently extracted.

C.1 Two-point measurement scheme

Suppose we are given a quantum observable $\Lambda(t)$ in Schrödinger picture, which is possibly time dependent. A common technique to "experimentally" track the fluctuations of $\Lambda(t)$ is the *two-point measurement (TPM) scheme* [124]: first, at time $t = 0$, we perform a projective measurement of $\Lambda(0)$; then we let the system evolve up to time t, and at that time we perform another projective measurement of $\Lambda(t)$. Let $\Lambda(t) = \sum_n \epsilon_n^t \Pi_n^t$ be the spectral decomposition of $\Lambda(t)$, where $\{\epsilon_n^t\}$ is the set of eigenvalues and Π_n^t is the projector onto the eigenspace associated with ϵ_n^t. The joint probability of obtaining ϵ_n^0 at time 0 and ϵ_m^t at time t is

$$P[\epsilon_m^t, \epsilon_n^0] = \mathrm{Tr}\left[\Pi_m^t U(t,0)\Pi_n^0 \rho_0 \Pi_n^0 U(0,t)\Pi_m^t\right], \tag{C.1}$$

where ρ_0 is the initial state of the system under investigation. Correspondingly, the probability distribution of the difference $\epsilon_m^t - \epsilon_n^0$ is

$$p_t(\epsilon) = \sum_{n,m} P[\epsilon_m^t, \epsilon_n^0]\delta[\epsilon - (\epsilon_m^t - \epsilon_n^0)]. \tag{C.2}$$

It is often more convenient to describe $p_t(\epsilon)$ using the associated *characteristic function*,

$$\chi_t(\lambda) := \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, p_t(\epsilon) e^{i\lambda\epsilon} = \sum_{n,m} P[\epsilon_m^t, \epsilon_n^0] e^{i\lambda(\epsilon_m^t - \epsilon_n^0)}, \tag{C.3}$$

since all of the moments of $p_t(\epsilon)$ can be recovered by differentiation:

$$\langle \epsilon^n \rangle_t := \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \epsilon^n p_t(\epsilon) = i^n \left. \frac{\partial^n \chi_t(\lambda)}{\partial \lambda^n} \right|_{\lambda=0}. \tag{C.4}$$

Let us then focus on $\chi_t(\lambda)$. Using the fact that $e^{-i\lambda\Lambda(0)/2}\Pi_n^0 \rho_0 \Pi_n^0 e^{-i\lambda\Lambda(0)/2} = e^{-i\lambda\epsilon_n^0}\Pi_n^0\rho_0\Pi_n^0$, we can rewrite

$$\chi_t(\lambda) = \sum_m e^{i\lambda\epsilon_m^t}\, \mathrm{Tr}\big[\Pi_m^t U(t,0) e^{-i\lambda\Lambda(0)/2} \widetilde{\rho}_0 e^{-i\lambda\Lambda(0)/2} U(0,t) \Pi_m^t\big], \tag{C.5}$$

where $\widetilde{\rho}_0 := \sum_n \Pi_n^0 \rho_0 \Pi_n^0$ is the diagonal part of ρ_0 in the eigenbasis of $\Lambda(0)$. Moreover, thanks to the cyclic property of the trace and the facts that $(\Pi_m^t)^2 = \Pi_m^t$ and $[\widetilde{\rho}_0, \Lambda(0)] = 0$,

$$\chi_t(\lambda) = \sum_m e^{i\lambda\epsilon_m^t}\, \mathrm{Tr}\big[U(t,0) e^{-i\lambda\Lambda(0)} \widetilde{\rho}_0 U(0,t) \Pi_m^t\big], \tag{C.6}$$

which can also be rewritten in the compact form

$$\chi_t(\lambda) = \mathrm{Tr}\,\rho(\lambda,t), \qquad \rho(\lambda,t) := U(t,0) e^{-i\lambda\Lambda(0)} \widetilde{\rho}_0 U(0,t) e^{i\lambda\Lambda(t)}. \tag{C.7}$$

Before moving on, we mention that the two-point measurement scheme is not the only way to approach the problem of fluctuation tracking. A popular alternative is to replace the projective measurement at time 0 with a weak measurement, with the effect of turning the probability distribution (C.2) into a quasi-probability distribution. The advantage is that any coherences of the initial state in the observable's basis can be exploited to improve the amount of information gathered through the measurement process. In the literature, the *Kirkwood-Dirac quasi-probability* [173] is often considered:

$$P^{\mathrm{KD}}[\epsilon_m^t, \epsilon_n^0] = \mathrm{Tr}\big[U(t,0)\Pi_n^0 \rho_0 U(0,t) \Pi_m^t\big], \tag{C.8}$$

which can be complex. The characteristic function associated with (C.8) is immediately given by Eq. (C.7), but with ρ_0 instead of $\widetilde{\rho}_0$. It would be interesting to study the implications of such a substitution within the context of the contour formalism, but we leave such questions to future work.

C.2 Contour for the characteristic function

Since $\rho(\lambda,t)$ in Eq. (C.7) is written in terms of exponentials multiplied on the two sides of $\widetilde{\rho}_0$, it should be easy to realize how the characteristic function $\chi_t(\lambda)$ can be written in terms of a contour-ordered exponential. We write

$$U(t,0) = \mathbb{T}\exp\left[-i\int_\lambda^{t+\lambda} \mathrm{d}s\, H(s-\lambda)\right], \qquad e^{-i\lambda\Lambda(0)} = \exp\left[-i\int_0^\lambda \mathrm{d}s\, \Lambda(0)\right], \tag{C.9a}$$

$$U(0,t) = \widetilde{\mathbb{T}}\exp\left[-i\int_t^0 \mathrm{d}s\, H(s)\right], \qquad e^{i\lambda\Lambda(t)} = \exp\left[-i\int_{t+\lambda}^t \mathrm{d}s\, \Lambda(t)\right]. \tag{C.9b}$$

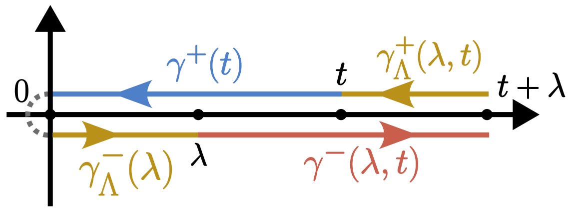

Figure C.1: Schematic representation of the contour $\gamma(\lambda, t)$ in Eq. (C.10).

This brings us to the contour depicted in Fig. C.1: we start from the point $t+\lambda$ and we go to t using $\Lambda(t)$; then we proceed towards 0 using the Hamiltonian; after that, we move to λ using $\Lambda(0)$ and, finally, we reach again $t+\lambda$ using the Hamiltonian. While the backward branch $\gamma^+(t)$ is the same as the one in Fig. 4.1, we shifted the forward branch $\gamma^-(t) \mapsto \gamma^-(\lambda, t)$ and we introduce two additional "virtual" tracks $\gamma^+_\Lambda(\lambda, t)$ and $\gamma^-_\Lambda(\lambda)$. The complete contour is

$$\gamma(\lambda, t) := \gamma^+_\Lambda(\lambda, t) * \gamma^+(t) * \gamma^-_\Lambda(\lambda) * \gamma^-(\lambda, t), \tag{C.10}$$

and

$$\rho(\lambda, t) = \mathbb{T}\left\{\exp\left[-i \int_{\gamma(\lambda,t)} \mathrm{d}z\, H(z)\right] \widetilde{\rho}_0\right\}, \tag{C.11}$$

where

$$H(z) := \begin{cases} \Lambda(t) & z \in \gamma^+_\Lambda(\lambda, t), \\ H(s) & z = s^+ \in \gamma^+(t), \\ \Lambda(0) & z \in \gamma^-_\Lambda(\lambda), \\ H(s-\lambda) & z = s^- \in \gamma^-(\lambda, t). \end{cases} \tag{C.12}$$

This has the same structure as Eq. (4.7).

C.3 Heat statistics of an open system

Suppose now our system of interest is open. Furthermore, we will assume for definiteness that $\Lambda(t) \equiv H_E$ is equal to the free Hamiltonian of the environment, taken to be time independent. In quantum thermodynamics, this choice corresponds to tracking the statistics of *heat* transferred between system and environment [124]. Other choices, such as internal energy, work, or entropy, are certainly possible and will be the subject of future research work (see also Ref. [125]).

As usual, it is convenient to move to the interaction picture. In terms of the contour propagator W [cf. Eq. (4.22)], we have

$$\rho_{SE}(\lambda, t) = W[(t+\lambda)^-, 0]\widetilde{\rho}_{SE,0} W[0, (t+\lambda)^+], \tag{C.13}$$

where we added the subscript SE to point out that the state is of the whole system-environment compound. According to Lemma 4.1,

$$W(s^-, 0) = W_0(s^-, 0) W_I(s^-, 0; 0), \qquad W(0, s^+) = W_I(0, s^+; 0) W_0(0, s^+), \tag{C.14}$$

where W_0 is the free propagator, constructed from $H_0(z)$, and W_I is the propagator constructed from $\mathcal{V}(z) = W_0(0,z)V(z)W_0(z,0)$, where

$$H_0(z) := \begin{cases} H_E & z \in \gamma_\Lambda^+(\lambda,t), \\ H_0(s) & \in z = s^+ \in \gamma^+(t), \\ H_E & z \in \gamma_\Lambda^-(\lambda), \\ H_0(s-\lambda) & z = s^- \in \gamma^-(\lambda,t), \end{cases} \qquad V(z) := \begin{cases} 0 & z \in \gamma_\Lambda^+(\lambda,t), \\ V(s) & \in z = s^+ \in \gamma^+(t), \\ 0 & z \in \gamma_\Lambda^-(\lambda), \\ V(s-\lambda) & z = s^- \in \gamma^-(\lambda,t). \end{cases} \tag{C.15}$$

Therefore,

$$\chi_t(\lambda) = \mathrm{Tr}\big\{W_0[(t+\lambda)^-,0]W_I[(t+\lambda)^-,0;0]\widetilde{\rho}_{SE,0}W_I[0,(t+\lambda)^+;0]W_0[0,(t+\lambda)^+]\big\}. \tag{C.16}$$

However,

$$W_0[0,(t+\lambda)^+]W_0[(t+\lambda)^-,0] = U_0(0,t)e^{i\lambda H_E}U_0(t,0)e^{-i\lambda H_E} = \mathbb{1}, \tag{C.17}$$

so that actually

$$\chi_t(\lambda) = \mathrm{Tr}\big\{W_I[(t+\lambda)^-,0;0]\widetilde{\rho}_{SE,0}W_I[0,(t+\lambda)^+;0]\big\}. \tag{C.18}$$

This has an immediate expression in terms of a contour-ordered exponential:

$$\chi_t(\lambda) = \mathrm{Tr}\,\varrho_{SE}(\lambda,t), \qquad \varrho_{SE}(\lambda,t) = \mathbb{T}\left\{\exp\left[-i\int_{\gamma(\lambda,t)}\mathrm{d}z\,\mathcal{V}(z)\right]\widetilde{\rho}_{SE,0}\right\}. \tag{C.19}$$

Note, however, that $\mathcal{V}(z) = 0$ when z lives on the virtual tracks $\gamma_\Lambda^+(\lambda,t)$ and $\gamma_\Lambda^-(\lambda)$. This means that the integral in Eq. (C.19) can be reduced to an integral on the standard contour $\gamma(t)$ of Fig. 4.1. Of course, the dependence on λ does not disappear: it is contained in the interaction operators. Specifically,

$$\mathcal{V}(s^+) = U_0(0,s)V(s)U_0(s,0) =: \mathcal{V}^\lambda(s^+), \tag{C.20a}$$

$$\mathcal{V}(s^-) = e^{i\lambda H_E}U_0(0,s)V(s)U_0(s,0)e^{-i\lambda H_E} =: \mathcal{V}^\lambda(s^-), \tag{C.20b}$$

so that

$$\varrho_{SE}(\lambda,t) = \mathbb{T}\left\{\exp\left[-i\int_{\gamma(t)}\mathrm{d}z\,\mathcal{V}^\lambda(z)\right]\widetilde{\rho}_{SE,0}\right\}. \tag{C.21}$$

Finally, in case $\widetilde{\rho}_{SE,0} = \widetilde{\rho}_0 \otimes \widetilde{\rho}_E$ happens to be factorized[1], one can immediately take the partial trace over the environment to find

$$\chi_t(\lambda) = \mathrm{Tr}\,\varrho(\lambda,t), \tag{C.22}$$

$$\varrho(\lambda,t) = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{\gamma(t)}\mathrm{d}^n\mathbf{z}\sum_{\alpha_1,\dots,\alpha_n}\mathrm{Tr}\big[\mathbb{T}\{\mathcal{B}_{\alpha_1}^\lambda(z_1)\dots\mathcal{B}_{\alpha_n}^\lambda(z_n)\widetilde{\rho}_E\}\big]\mathbb{T}\{\mathcal{A}_{\alpha_1}(z_1)\dots\mathcal{A}_{\alpha_n}(z_n)\widetilde{\rho}_0\},$$

where we used the decomposition $\mathcal{V}^\lambda(z) = \sum_\alpha \mathcal{A}_\alpha(z)\otimes\mathcal{B}_\alpha^\lambda(z)$. The dependence on λ solely involves the environment operators:

$$\mathcal{B}_\alpha^\lambda(s^+) = \mathcal{B}_\alpha(s), \qquad \mathcal{B}_\alpha^\lambda(s^-) = \mathcal{B}_\alpha(s+\lambda), \tag{C.23}$$

where, as usual, $\mathcal{B}_\alpha(s)$ is the physical-time interaction-picture version of the environment operator. Remarkably, Eq. (C.22) has precisely the form of Eq. (4.40).

[1] In case $\widetilde{\rho}_{SE,0}$ is not factorized, one can proceed as in Sec. 4.1.3 by adding a Matsubara track.

C.4 Master equations for the heat statistics

Using the notation established in Sec. 4.1.4, Eq. (C.22) can be more compactly expressed as

$$\varrho(\lambda, t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \oint_{\gamma(t)} \mathrm{d}^n\mathbf{z}\, \mathrm{Tr}\big[\mathbb{T}_\zeta\{B_1^\lambda \dots B_n^\lambda \varrho_E\}\big]\mathbb{T}_\zeta\{A_1 \dots A_n \varrho_0\}. \tag{C.24}$$

If we make the Gaussian environment hypothesis,

$$\varrho(\lambda, t) = \mathbb{T}_\zeta\left\{\exp\left[-\frac{1}{2}\oint_{\gamma(t)} \mathrm{d}^2\mathbf{z}\, C_{1,2}^\lambda A_1 A_2\right]\varrho_0\right\}, \tag{C.25}$$

where the environment effect is encoded by the modified contour correlation function

$$C_{i,j}^\lambda \coloneqq \mathrm{Tr}\,\mathbb{T}_\zeta\{B_i^\lambda B_j^\lambda \varrho_E\}. \tag{C.26}$$

From here one can repeat all the calculations that were performed in Chaps. 5 and 6 and obtain all kinds of exact master equations for $\varrho(\lambda, t)$.

However, it is worth pointing out that C^λ does not satisfy the same properties as C. In fact, since B_i^λ has a different expression on the two branches of the contour, one can readily verify that cycle and conjugation symmetry (cf. Theorem 4.4) do not hold for C^λ. The table of components for C^λ thus turns out definitely more complex than the one for C. For example,

$$C_{\alpha\beta}^{\lambda,T}(t,s) = C_{\alpha\beta}^{T}(t,s), \qquad C_{\alpha\beta}^{\lambda,\widetilde{T}}(t,s) = C_{\alpha\beta}^{\widetilde{T}}(t,s), \tag{C.27a}$$

$$C_{\alpha\beta}^{\lambda,>}(t,s) = C_{\alpha\beta}^{>}(t,s+\lambda), \qquad C_{\alpha\beta}^{\lambda,<}(t,s) = C_{\alpha\beta}^{<}(t+\lambda,s). \tag{C.27b}$$

It would certainly be interesting to perform a complete study of the different properties of C^λ, as this would allow a mindful extension of the content of the thesis to the quantum thermodynamics context. Here we will just point out the following striking consequence of the difference between C and C^λ. If we perform stochastic decoupling on Eq. (C.25), we can straightforwardly proceed to obtain a stochastic von Neumann equation:

$$\frac{\mathrm{d}R(\lambda,t)}{\mathrm{d}t} = -i\sum_\alpha \nu_\alpha^\lambda(t)[A_\alpha(t), R(\lambda,t)] - i\sum_\alpha \eta_\alpha^\lambda(t)\{A_\alpha(t), R(\lambda,t)\}, \tag{C.28}$$

where $\varrho(\lambda, t) = \mathbb{E}[R(\lambda, t)]$, whereas $\nu_\alpha^\lambda(t)$ and $\eta_\alpha^\lambda(t)$ are the noises that are obtained after a Keldysh rotation of the contour noise $\xi_\alpha^\lambda(z)$ obeying $\mathbb{E}[\xi_\alpha^\lambda(z)\xi_\beta^\lambda(w)] = C_{\alpha\beta}^\lambda(z,w)$. Specifically,

$$\nu_\alpha^\lambda(t) \coloneqq \frac{\xi_\alpha^\lambda(t^-) + \xi_\alpha^\lambda(t^+)}{2}, \qquad \eta_\alpha^\lambda(t) \coloneqq \frac{\xi_\alpha^\lambda(t^-) - \xi_\alpha^\lambda(t^+)}{2}. \tag{C.29}$$

However, a calculation reveals the following correlation functions:

$$\mathbb{E}[\nu_\alpha^\lambda(t)\nu_\beta^\lambda(s)] = \frac{1}{4}\Big[C_{\alpha\beta}^>(t,s) + C_{\alpha\beta}^<(t,s) + C_{\alpha\beta}^>(t,s+\lambda) + C_{\alpha\beta}^<(t+\lambda,s)\Big], \tag{C.30a}$$

$$\mathbb{E}[\nu_\alpha^\lambda(t)\eta_\beta^\lambda(s)] = \frac{1}{4}\mathrm{sign}(t-s)\Big[C_{\alpha\beta}^>(t,s) - C_{\alpha\beta}^<(t,s)\Big] + \frac{1}{4}\Big[C_{\alpha\beta}^>(t,s+\lambda) - C_{\alpha\beta}^<(t+\lambda,s)\Big], \tag{C.30b}$$

$$\mathbb{E}[\eta_\alpha^\lambda(t)\eta_\beta^\lambda(s)] = \frac{1}{4}\Big[C_{\alpha\beta}^>(t,s) + C_{\alpha\beta}^<(t,s) - C_{\alpha\beta}^>(t,s+\lambda) - C_{\alpha\beta}^<(t+\lambda,s)\Big]. \tag{C.30c}$$

Differently from Eqs. (5.31), the covariance of $\eta_\alpha^\lambda(t)$ with itself is not zero, which is an important difference that is worth exploring in future work.

Appendix D

Measurements and Wigner Function

In Sec. 5.4, we discussed sufficient semiclassical conditions, reported in Eq. (5.61), under which the stochastic von Neumann equation (5.30) can be given a certain measurement interpretation. Specifically, the noise $\nu_\alpha(t)$ was interpreted in terms of a one-shot heterodyne environment measurement performed at the beginning of the dynamics. In this Appendix, we provide the derivation of Eqs. (5.62) using the Wigner function formalism [84, 148]. The phase-space representation of quantum dynamics is one of the most effective ways to describe the evolution of bosonic systems while keeping the connection to the classical limit as clear as possible. This characteristic likely makes it the most appropriate tool for elaborating on the content of Sec. 5.4.

The Appendix is structured as follows. First, in Sec. D.1, we briefly review essential tools from the phase-space representation of quantum dynamics, such as the concept of Wigner function itself. Then, in Sec. D.2, we discuss how a weak Gaussian heterodyne measurement affects the Wigner function. The obtained result is finally manipulated in Sec. D.3 using the semiclassical conditions (5.61), thereby demonstrating that we indeed arrive at the conclusions of Sec. 5.4.

D.1 Weyl symbol and Wigner function

The starting point to formulate the phase-space representation of quantum dynamics is the establishment of a one-to-one correspondence between quantum operators and ordinary phase-space functions. There are many ways to do that, but a popular choice is the *Weyl transform* [148]. Specifically, given an operator A we define its *Weyl symbol* as

$$\mathcal{W}[A](\mathbf{x},\mathbf{p}) := \int_{-\infty}^{\infty} \mathrm{d}^n\xi \left\langle \mathbf{x} - \frac{\xi}{2} \middle| A \middle| \mathbf{x} + \frac{\xi}{2} \right\rangle \exp[i\mathbf{p}\cdot\xi]. \tag{D.1}$$

Here we are assuming to work in a $2n$-dimensional phase space with coordinates $\mathbf{x}$ and momenta $\mathbf{p}$. The *Wigner function* is simply the Weyl symbol of the density operator. By direct computation it is immediate to see that

$$\mathrm{Tr}[A] = \int_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\, \langle \mathbf{x}|A|\mathbf{x}\rangle = \frac{1}{(2\pi)^n} \iint_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\, \mathrm{d}^n\mathbf{p}\, \mathcal{W}[A](\mathbf{x},\mathbf{p}). \tag{D.2}$$

One also finds the important formula [148]

$$\mathrm{Tr}[AB] = \frac{1}{(2\pi)^n} \iint_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\, \mathrm{d}^n\mathbf{p}\, \mathcal{W}[A](\mathbf{x},\mathbf{p}) \mathcal{W}[B](\mathbf{x},\mathbf{p}), \tag{D.3}$$

which can be used to reconstruct the complete statistics of an operator from its Weyl symbol—simply take as B the density operator of the current state.

Particularly important are the Weyl symbols associated with simple functions of position and momentum operators, which we report here without proof [148].

$$\mathcal{W}[X_i](\mathbf{x},\mathbf{p}) = x_i, \qquad \mathcal{W}[P_i](\mathbf{x},\mathbf{p}) = p_i, \tag{D.4a}$$

$$\mathcal{W}[X_iX_j](\mathbf{x},\mathbf{p}) = x_ix_j, \qquad \mathcal{W}[P_iP_j](\mathbf{x},\mathbf{p}) = p_ip_j, \tag{D.4b}$$

$$\mathcal{W}[X_iP_j](\mathbf{x},\mathbf{p}) = x_ip_j + \frac{i\delta_{ij}}{2}, \qquad \mathcal{W}[P_iX_j](\mathbf{x},\mathbf{p}) = p_ix_j - \frac{i\delta_{ij}}{2}. \tag{D.4c}$$

D.2 Wigner function after heterodyne measurement

Using the tools described in the previous section, we are now ready to tackle the setting that was put forward in Sec. 5.4. Given an initial Gaussian environment state Ω, let us perform a weak Gaussian measurement of the position. We will pretend at first that the environment is composed of a single mode with position and momentum operators X and P: thanks to the independence between modes, it will be straightforward to generalize what we will say to an arbitrary number of modes. The post-measurement state conditioned on obtaining the outcome x' is $\Omega_{x'} = \widetilde{\Omega}_{x'}/\mathbb{P}(x')$, where $\mathbb{P}(x') = \operatorname{Tr}\widetilde{\Omega}_{x'}$ and

$$\widetilde{\Omega}_{x'} = M_{X,x'}\Omega M^\dagger_{X,x'}, \qquad M_{X,x'} = \frac{1}{(2\pi\sigma_X^2)^{1/4}}\exp\left[-\frac{(X-x')^2}{4\sigma_X^2}\right], \tag{D.5}$$

with σ_X^{-1} being the measurement's precision.

We can easily calculate the Weyl symbol of $\widetilde{\Omega}_{x'}$:

$$\begin{aligned}\mathcal{W}[\widetilde{\Omega}_{x'}](x,p) &= \frac{1}{\sqrt{2\pi\sigma_X^2}}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\left\langle x-\frac{\xi}{2}\middle|\Omega\middle|x+\frac{\xi}{2}\right\rangle\exp\left[ip\xi-\frac{(x-\frac{\xi}{2}-x')^2}{4\sigma_X^2}-\frac{(x+\frac{\xi}{2}-x')^2}{4\sigma_X^2}\right]\\ &= \frac{1}{\sqrt{2\pi\sigma_X^2}}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\left\langle x-\frac{\xi}{2}\middle|\Omega\middle|x+\frac{\xi}{2}\right\rangle\exp\left[ip\xi-\frac{(x-x')^2}{2\sigma_X^2}-\frac{\xi^2}{8\sigma_X^2}\right].\end{aligned} \tag{D.6}$$

After inserting the following identity:

$$1 = \int_{-\infty}^{\infty}\mathrm{d}\tau\,\delta(\tau-\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\epsilon\,e^{i(\tau-\xi)\epsilon}, \tag{D.7}$$

replacing the ξ appearing in the last exponential with τ and doing the integral in ξ, we remain with

$$\mathcal{W}[\widetilde{\Omega}_{x'}](x,p) = \frac{1}{2\pi}\frac{1}{\sqrt{2\pi\sigma_X^2}}\int_{-\infty}^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\epsilon\,\mathcal{W}[\Omega](x,p-\epsilon)\exp\left[i\tau\epsilon-\frac{\tau^2}{8\sigma_X^2}-\frac{(x-x')^2}{2\sigma_X^2}\right]. \tag{D.8}$$

Since the integral in τ gives

$$\int_{-\infty}^{\infty}\mathrm{d}\tau\exp\left[i\tau\epsilon-\frac{\tau^2}{8\sigma_X^2}\right] = \sqrt{8\pi\sigma_X^2}e^{-2\epsilon^2\sigma_X^2}, \tag{D.9}$$

we conclude that

$$\mathcal{W}[\widetilde{\Omega}_{x'}](x,p) = \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \mathcal{W}[\Omega](x, p-\epsilon) \exp\left[-\frac{(x-x')^2}{2\sigma_X^2} - 2\epsilon^2\sigma_X^2\right]. \tag{D.10}$$

The above equation tells us that the post-measurement state undergoes a momentum perturbation, whose strength varies according to the measurement precision. If the measurement is extremely imprecise, $\sigma_X \to \infty$, the post-measurement Wigner function remains unaltered, $\mathcal{W}[\Omega_{x'}] = \mathcal{W}[\Omega]$.

With a similar calculation, one can show that if we perform instead a measurement of the momentum,

$$\mathcal{W}[\widetilde{\Omega}_{p'}](x,p) = \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \mathcal{W}[\Omega](x-\epsilon, p) \exp\left[-\frac{(p-p')^2}{2\sigma_P^2} - 2\epsilon^2\sigma_P^2\right]. \tag{D.11}$$

A *heterodyne measurement* [84] is obtained by combining a measurement of the position with a measurement of the momentum. If we define $y' = (x', p')$ and if we assume the momentum measurement to be performed before the position measurement, in this case one has the post-measurement state $\Omega_{y'} = \widetilde{\Omega}_{y'}/\mathbb{P}(y')$, where $\mathbb{P}(y') = \mathrm{Tr}\,\widetilde{\Omega}_{y'}$ and $\widetilde{\Omega}_{y'} = M_{X,x'}M_{P,p'}\Omega M_{P,p'}^\dagger M_{X,x'}^\dagger$. The associated Weyl symbol is simply

$$\begin{aligned}\mathcal{W}[\widetilde{\Omega}_{y'}](x,p) = \frac{1}{\pi^2}\iint_{-\infty}^{\infty} \mathrm{d}\epsilon_1\, \mathrm{d}\epsilon_2 \mathcal{W}[\Omega](x-\epsilon_2, p-\epsilon_1) \exp\left[-2\epsilon_1^2\sigma_X^2 - 2\epsilon_2^2\sigma_P^2\right]\\ \times \exp\left[-\frac{(x-x')^2}{2\sigma_X^2} - \frac{(p-\epsilon_1-p')^2}{2\sigma_P^2}\right].\end{aligned} \tag{D.12}$$

D.3 Semiclassical conditions

Suppose now our initial state has the following Wigner function,

$$\mathcal{W}[\Omega](x,p) = \frac{1}{\Delta_X\Delta_P} \exp\left[-\frac{x^2}{2\Delta_X^2} - \frac{p^2}{2\Delta_P^2}\right], \tag{D.13}$$

and let us impose the conditions that were reported in Eq. (5.61), i.e.,

$$\sigma_X\sigma_P \gg 1, \qquad \sigma_X \ll \Delta_X, \qquad \sigma_P \ll \Delta_P. \tag{D.14}$$

Then, we must also have $\sigma_X\Delta_P \gg 1$ and $\sigma_P\Delta_X \gg 1$. As a consequence, the integrand in Eq. (D.12) is strongly peaked around $\epsilon_1 = \epsilon_2 = 0$ and we can approximate the result by removing the ϵ dependence in $\mathcal{W}[\Omega]$ and in the exponential containing p. Integrating away the remaining exponential weights, one finds

$$\mathcal{W}[\widetilde{\Omega}_{y'}](x,p) \simeq \frac{1}{2\pi\sigma_X\sigma_P}\mathcal{W}[\Omega](x,p) \exp\left[-\frac{(x-x')^2}{2\sigma_X^2} - \frac{(p-p')^2}{2\sigma_P^2}\right]. \tag{D.15}$$

Since $\sigma_X \ll \Delta_X$ and $\sigma_P \ll \Delta_P$, we can also replace the arguments of $\mathcal{W}[\Omega]$ with the measurement outcomes, as the exponential factors are strongly peaked around them. Under the conditions (D.14) it is also easy to compute the normalization factor:

$$\mathbb{P}(y') = \operatorname{Tr}\widetilde{\Omega}_{y'} = \frac{1}{2\pi}\iint_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{d}p\,\mathcal{W}[\widetilde{\Omega}_{y'}](x,p) \simeq \frac{\mathcal{W}[\Omega](x',p')}{2\pi}. \tag{D.16}$$

We conclude that the Wigner function of the post-measurement state conditioned on the outcome $y' = (x',p')$ of a Gaussian heterodyne measurement under the conditions (D.14) is

$$\mathcal{W}[\Omega_{y'}](x,p) \simeq \frac{1}{\sigma_X\sigma_P}\exp\left[-\frac{(x-x')^2}{2\sigma_X^2} - \frac{(p-p')^2}{2\sigma_P^2}\right]. \tag{D.17}$$

The variances of the post-measurement state are given by the inverse of the measurement precisions, which are much smaller than the variances of the distribution of the outcomes. Eq. (D.17) is also easily extended to the multi-mode scenario as

$$\mathcal{W}[\Omega_{\mathbf{y}'}](\mathbf{x},\mathbf{p}) \simeq \frac{1}{\prod_\alpha \sigma_{X_\alpha}\sigma_{P_\alpha}}\exp\left[-\sum_\alpha \frac{(x_\alpha-x'_\alpha)^2}{2\sigma_{X_\alpha}^2} - \sum_\alpha \frac{(p_\alpha-p'_\alpha)^2}{2\sigma_{P_\alpha}^2}\right]. \tag{D.18}$$

Let us now use Eq. (D.18) to calculate $E_\alpha^{(\mathbf{y}')}(t) = \operatorname{Tr}\left[X_\alpha(t)\Omega_{\mathbf{y}'}\right]$, showing that it returns precisely Eq. (5.62a). Since

$$X_\alpha(t) = X_\alpha\cos(\omega_\alpha t) + \frac{P_\alpha}{m_\alpha\omega_\alpha}\sin(\omega_\alpha t), \tag{D.19}$$

we immediately find the expected result:

$$\begin{aligned}
E_\alpha^{(\mathbf{y}')}(t) &= \frac{1}{(2\pi)^n}\iint_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\,\mathrm{d}^n\mathbf{p}\,\mathcal{W}[X_\alpha](\mathbf{x},\mathbf{p})\mathcal{W}[\Omega_{\mathbf{y}'}](\mathbf{x},\mathbf{p}) \\
&\simeq \frac{1}{2\pi\sigma_{X_\alpha}\sigma_{P_\alpha}}\iint_{-\infty}^{\infty} \mathrm{d}x_\alpha\,\mathrm{d}p_\alpha\left[x_\alpha\cos(\omega_\alpha t) + \frac{p_\alpha}{m_\alpha\omega_\alpha}\sin(\omega_\alpha t)\right]\exp\left[-\frac{(x_\alpha-x'_\alpha)^2}{2\sigma_{X_\alpha}^2} - \frac{(p_\alpha-p'_\alpha)^2}{2\sigma_{P_\alpha}^2}\right] \\
&= x'_\alpha\cos(\omega_\alpha t) + \frac{p'_\alpha}{m_\alpha\omega_\alpha}\sin(\omega_\alpha t) =: x'_\alpha(t),
\end{aligned}$$

where we used the fact that $\mathcal{W}[X_\alpha](\mathbf{x},\mathbf{p}) = x_\alpha$ and $\mathcal{W}[P_\alpha](\mathbf{x},\mathbf{p}) = p_\alpha$.

By direct computation, we also see that

$$\mathbb{E}_y\left[E_\alpha^{(\mathbf{y})}(t)E_\beta^{(\mathbf{y})}(s)\right] \simeq \frac{1}{(2\pi)^n}\iint_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\,\mathrm{d}^n\mathbf{p}\,\mathcal{W}[\Omega](\mathbf{x},\mathbf{p})x_\alpha(t)x_\beta(s). \tag{D.20}$$

On the other hand,

$$\begin{aligned}
\mathbb{E}_\nu\left[\nu_\alpha(t)\nu_\beta(s)\right] &= \frac{1}{2}\operatorname{Tr}\left[\{X_\alpha(t),X_\beta(s)\}\Omega\right] \\
&= \operatorname{Tr}\left[X_\alpha X_\beta\Omega\right]\cos(\omega_\alpha t)\cos\left(\omega_\beta s\right) + \operatorname{Tr}\left[P_\alpha P_\beta\Omega\right]\frac{\sin(\omega_\alpha t)\sin\left(\omega_\beta s\right)}{m_\alpha m_\beta\omega_\alpha\omega_\beta} \\
&+ \frac{1}{2}\operatorname{Tr}\left[\{X_\alpha,P_\beta\}\Omega\right]\frac{\cos(\omega_\alpha t)\sin\left(\omega_\beta s\right)}{m_\beta\omega_\beta} + \frac{1}{2}\operatorname{Tr}\left[\{P_\alpha,X_\beta\}\Omega\right]\frac{\sin(\omega_\alpha t)\cos\left(\omega_\beta s\right)}{m_\alpha\omega_\alpha}.
\end{aligned} \tag{D.21}$$

But we also know how to directly calculate the traces appearing on the right-hand side, leading to

$$\begin{aligned}\mathbb{E}_\nu\left[\nu_\alpha(t)\nu_\beta(s)\right] = \frac{1}{(2\pi)^n}\iint_{-\infty}^{\infty} \mathrm{d}^n\mathbf{x}\,\mathrm{d}^n\mathbf{p}\,\mathcal{W}[\Omega](\mathbf{x},\mathbf{p})& \\ \times\Big[x_\alpha x_\beta\cos(\omega_\alpha t)\cos(\omega_\beta s) + p_\alpha p_\beta\frac{\sin(\omega_\alpha t)\sin(\omega_\beta s)}{m_\alpha m_\beta\omega_\alpha\omega_\beta}& \\ + x_\alpha p_\beta\frac{\cos(\omega_\alpha t)\sin(\omega_\beta s)}{m_\beta\omega_\beta} + p_\alpha x_\beta\frac{\sin(\omega_\alpha t)\cos(\omega_\beta s)}{m_\alpha\omega_\alpha}\Big],&\end{aligned} \tag{D.22}$$

which is the same as the right-hand side of Eq. (D.20). This was precisely the content of Eq. (5.62b) in the main text.

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